Full wwPDB EM Validation Report ⓘ

Apr 30, 2024 – 11:39 pm BST

PDB ID	:	4AB3
EMDB ID	:	EMD-2003
Title	:	ATP-triggered molecular mechanics of the chaperonin GroEL
Authors	:	Clare, D.K.; Vasishtan, D.; Stagg, S.; Quispe, J.; Farr, G.W.; Topf, M.; Horwich, A.L.; Saibil, H.R.
Deposited on	:	2011-12-06
Resolution	:	8.50 Å(reported)
Based on initial model	:	1OEL

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

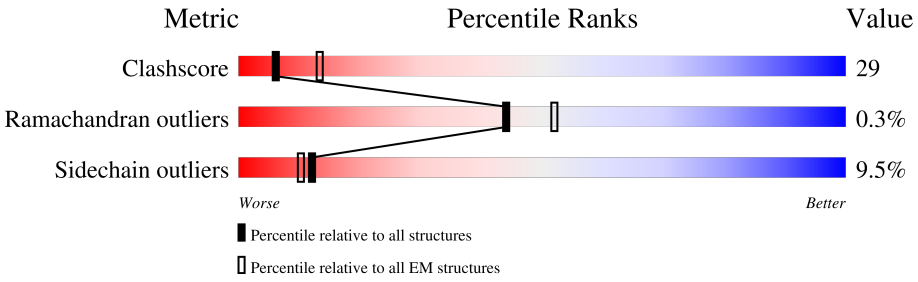
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	548	10% 57% 29% 7%
1	B	548	10% 56% 30% 7%
1	C	548	10% 56% 29% 7%
1	D	548	10% 56% 30% 7%
1	E	548	10% 57% 29% 7%
1	F	548	10% 57% 29% 7%
1	G	548	10% 57% 29% 7%
1	H	548	11% 52% 34% 9%

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Mol	Chain	Length	Quality of chain
1	I	548	11% 52% 34% 8%
1	J	548	11% 52% 34% 8%
1	K	548	11% 52% 34% 8%
1	L	548	11% 52% 34% 9%
1	M	548	11% 51% 35% 8%
1	N	548	11% 51% 34% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	1525	-	-	X	-
2	PO4	B	1525	-	-	X	-
2	PO4	C	1525	-	-	X	-
2	PO4	D	1525	-	-	X	-
2	PO4	E	1525	-	-	X	-
2	PO4	F	1525	-	-	X	-
2	PO4	G	1525	-	-	X	-
2	PO4	H	1525	-	-	X	-
2	PO4	I	1525	-	-	X	-
2	PO4	J	1525	-	-	X	-
2	PO4	K	1525	-	-	X	-
2	PO4	L	1525	-	-	X	-
2	PO4	M	1525	-	-	X	-
2	PO4	N	1525	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 54293 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 60 KDA CHAPERONIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	B	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	C	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	D	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	E	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	F	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	G	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	H	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	I	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	J	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	K	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	L	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	M	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		
1	N	524	Total	C	N	O	S	0	1
			3845	2391	664	770	20		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	engineered mutation	UNP P0A6F5
B	398	ALA	ASP	engineered mutation	UNP P0A6F5

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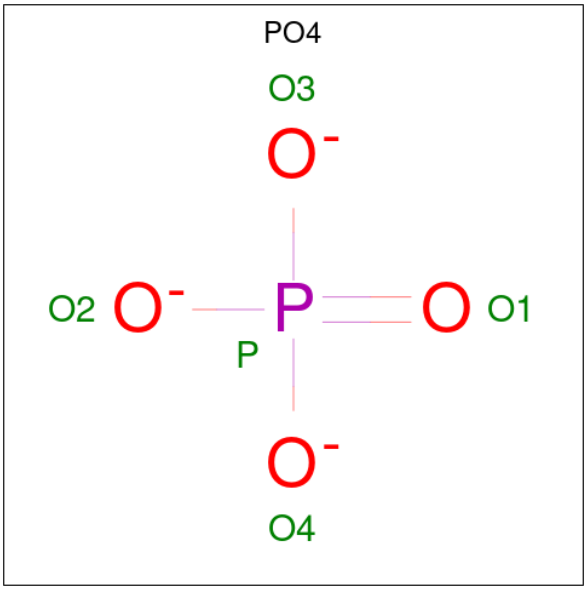
Chain	Residue	Modelled	Actual	Comment	Reference
C	398	ALA	ASP	engineered mutation	UNP P0A6F5
D	398	ALA	ASP	engineered mutation	UNP P0A6F5
E	398	ALA	ASP	engineered mutation	UNP P0A6F5
F	398	ALA	ASP	engineered mutation	UNP P0A6F5
G	398	ALA	ASP	engineered mutation	UNP P0A6F5
H	398	ALA	ASP	engineered mutation	UNP P0A6F5
I	398	ALA	ASP	engineered mutation	UNP P0A6F5
J	398	ALA	ASP	engineered mutation	UNP P0A6F5
K	398	ALA	ASP	engineered mutation	UNP P0A6F5
L	398	ALA	ASP	engineered mutation	UNP P0A6F5
M	398	ALA	ASP	engineered mutation	UNP P0A6F5
N	398	ALA	ASP	engineered mutation	UNP P0A6F5

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total P 1 1	0
2	B	1	Total P 1 1	0
2	C	1	Total P 1 1	0
2	D	1	Total P 1 1	0
2	E	1	Total P 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
2	F	1	Total P 1 1	0
2	G	1	Total P 1 1	0
2	H	1	Total P 1 1	0
2	I	1	Total P 1 1	0
2	J	1	Total P 1 1	0
2	K	1	Total P 1 1	0
2	L	1	Total P 1 1	0
2	M	1	Total P 1 1	0
2	N	1	Total P 1 1	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Mg 1 1	0
3	B	1	Total Mg 1 1	0
3	C	1	Total Mg 1 1	0
3	D	1	Total Mg 1 1	0
3	E	1	Total Mg 1 1	0
3	F	1	Total Mg 1 1	0
3	G	1	Total Mg 1 1	0
3	H	1	Total Mg 1 1	0
3	I	1	Total Mg 1 1	0
3	J	1	Total Mg 1 1	0

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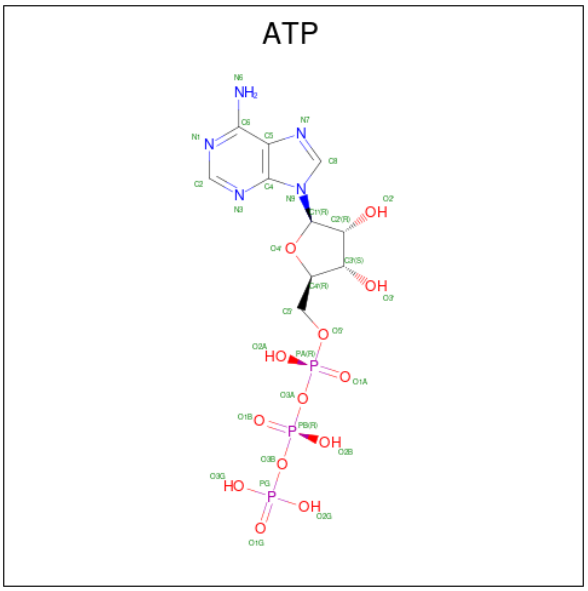
Mol	Chain	Residues	Atoms	AltConf
3	K	1	Total Mg 1 1	0
3	L	1	Total Mg 1 1	0
3	M	1	Total Mg 1 1	0
3	N	1	Total Mg 1 1	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O P 31 10 5 13 3	0
4	B	1	Total C N O P 31 10 5 13 3	0
4	C	1	Total C N O P 31 10 5 13 3	0
4	D	1	Total C N O P 31 10 5 13 3	0
4	E	1	Total C N O P 31 10 5 13 3	0
4	F	1	Total C N O P 31 10 5 13 3	0
4	G	1	Total C N O P 31 10 5 13 3	0

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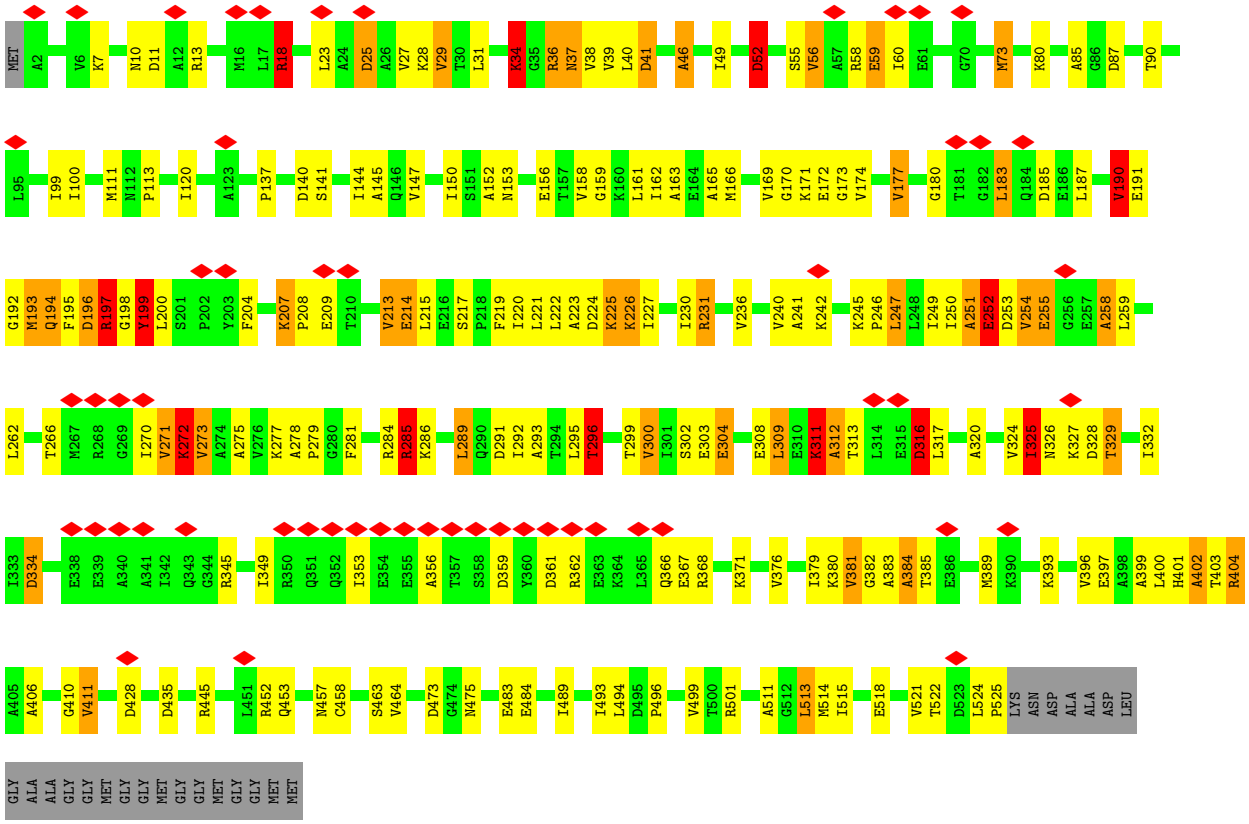
Mol	Chain	Residues	Atoms					AltConf
4	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	J	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	M	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	N	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

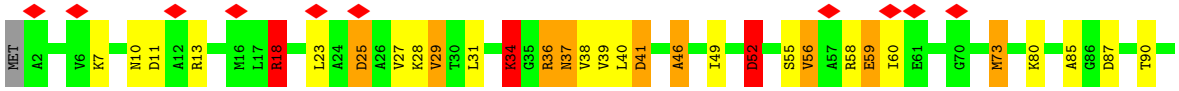
• Molecule 1: 60 KDA CHAPERONIN

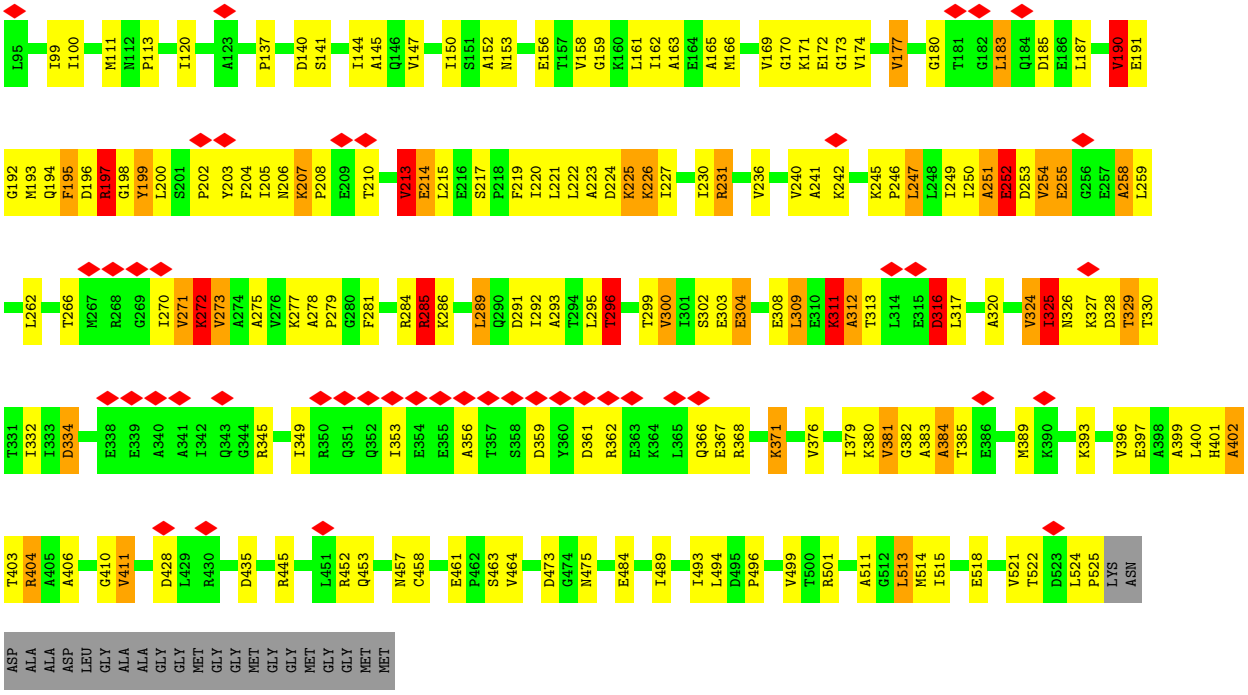
Chain A:



• Molecule 1: 60 KDA CHAPERONIN

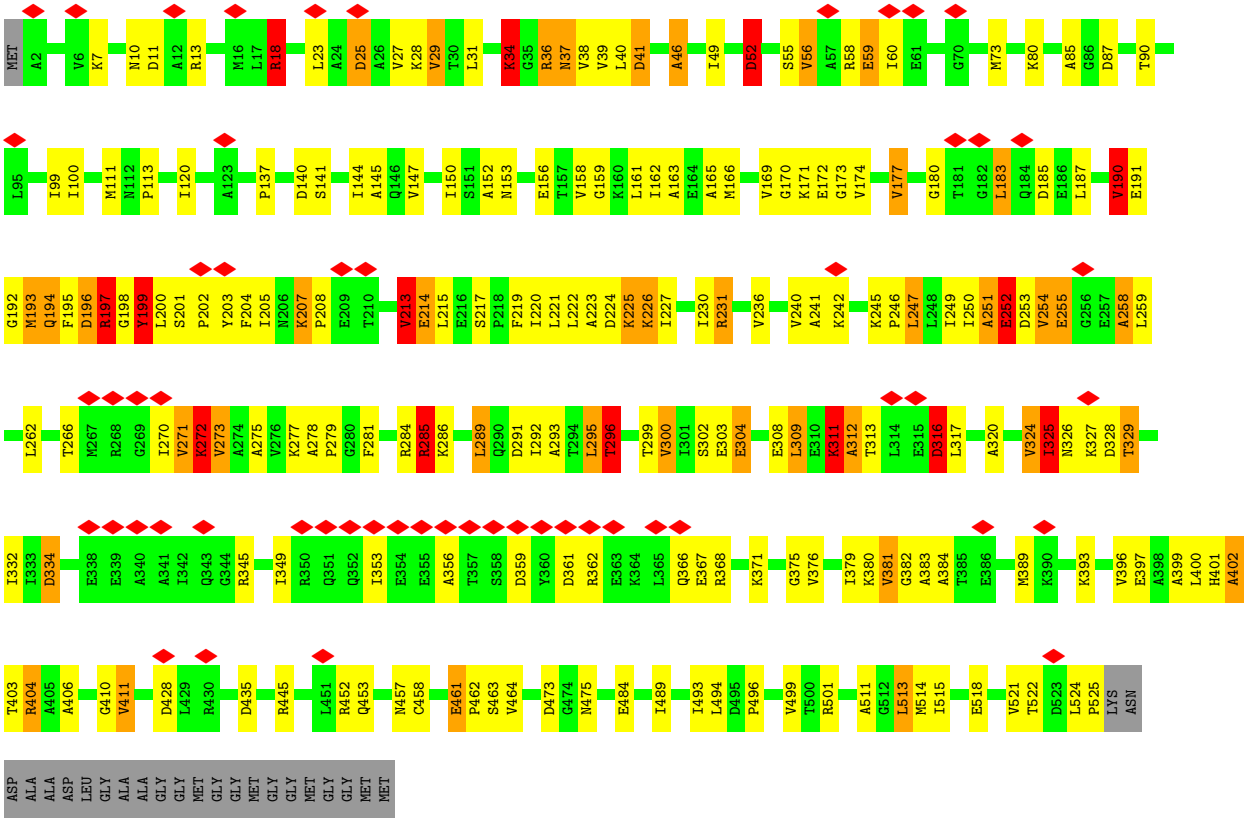
Chain B:





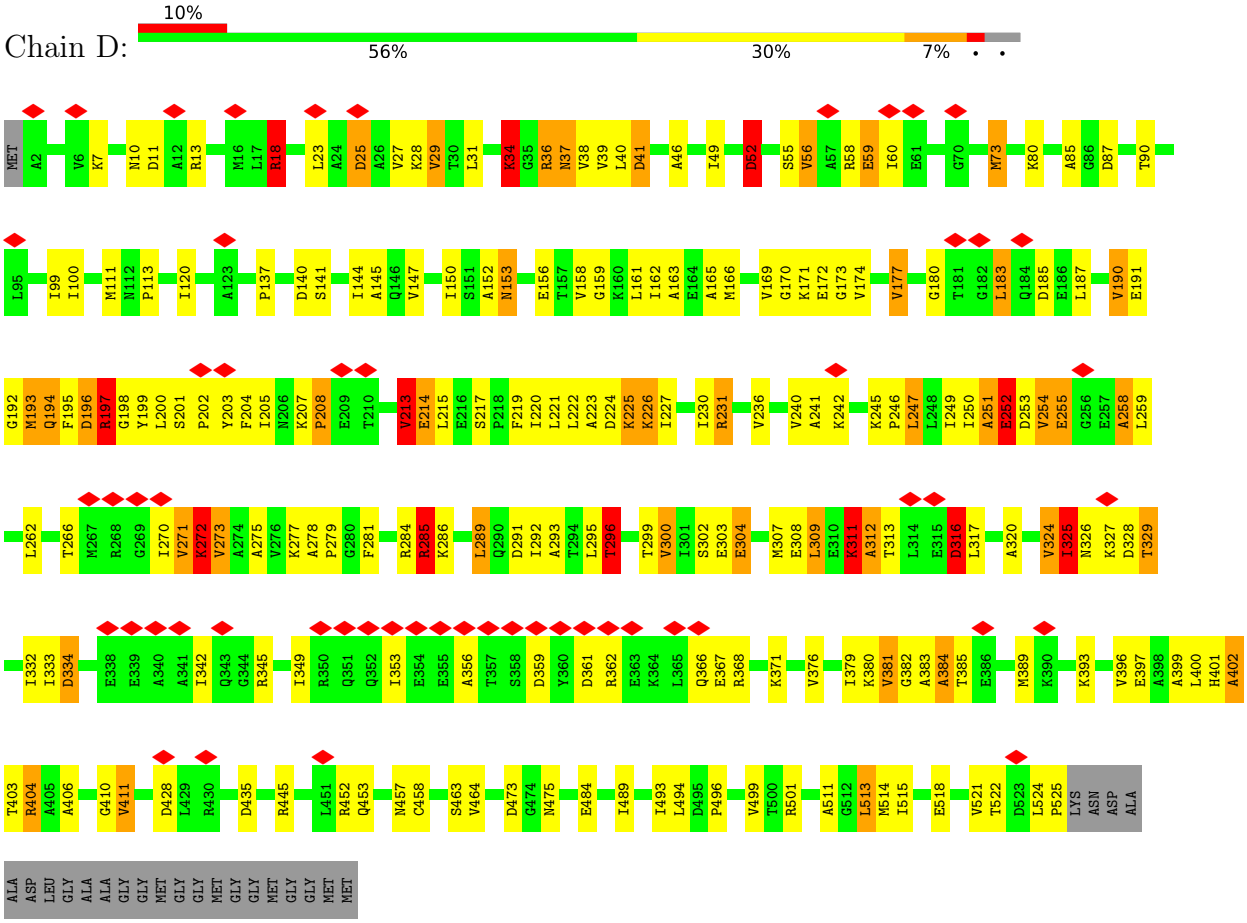
• Molecule 1: 60 KDA CHAPERONIN

Chain C:



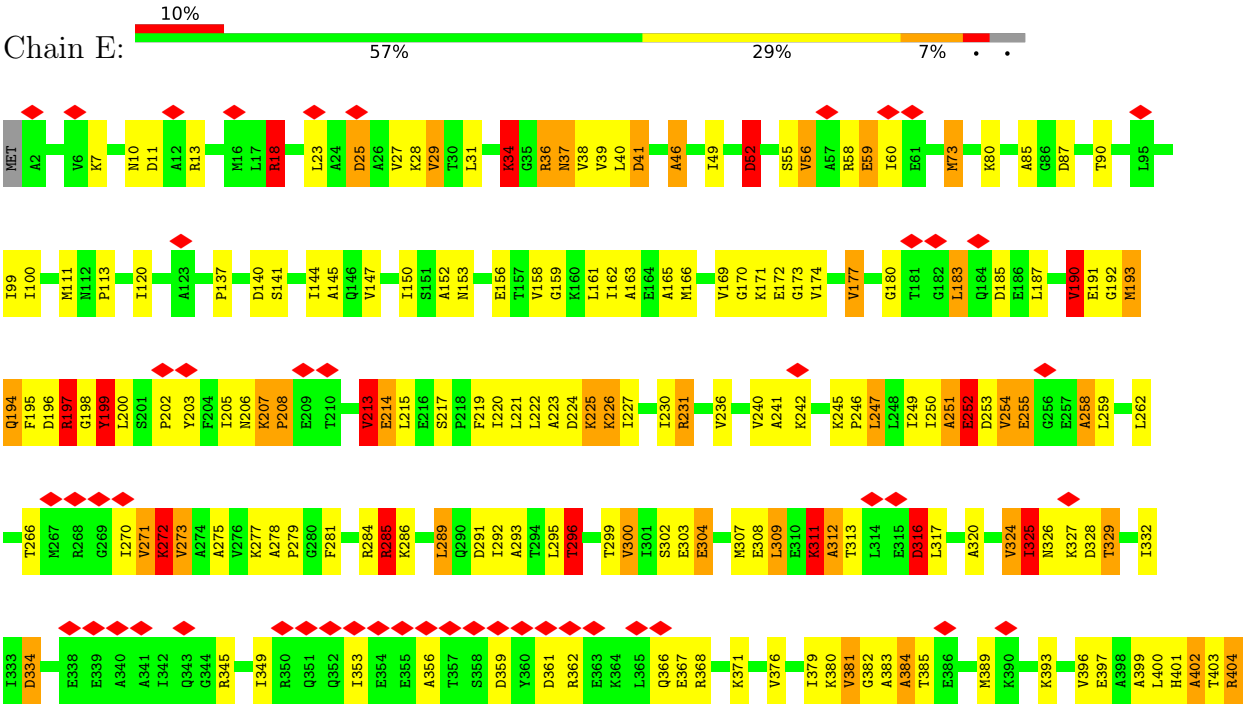
• Molecule 1: 60 KDA CHAPERONIN

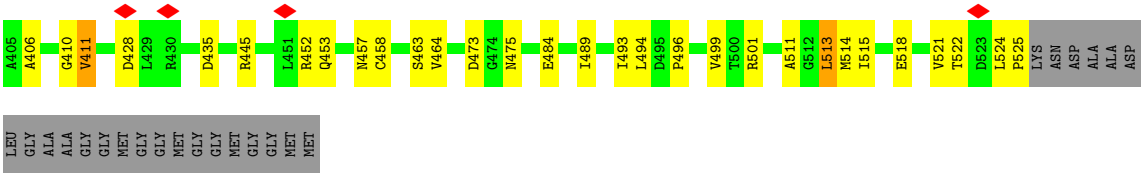
Chain D:



• Molecule 1: 60 KDA CHAPERONIN

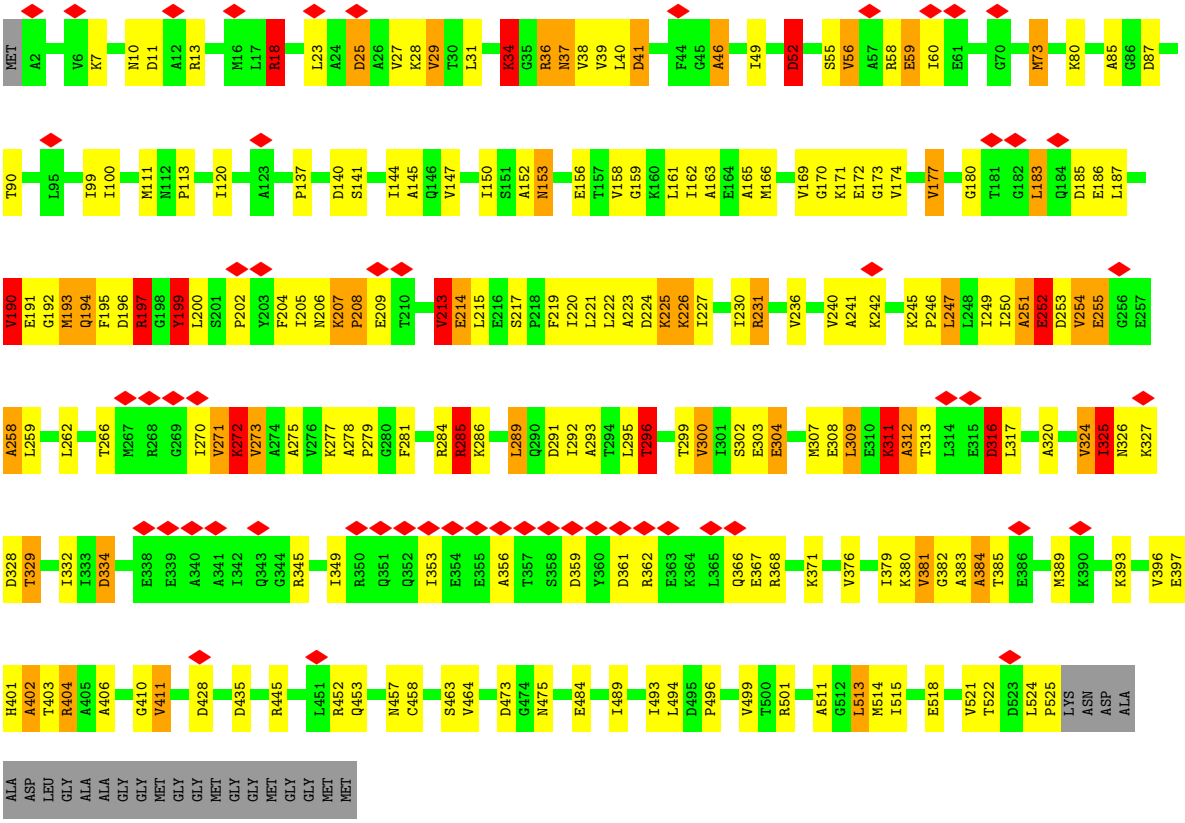
Chain E:





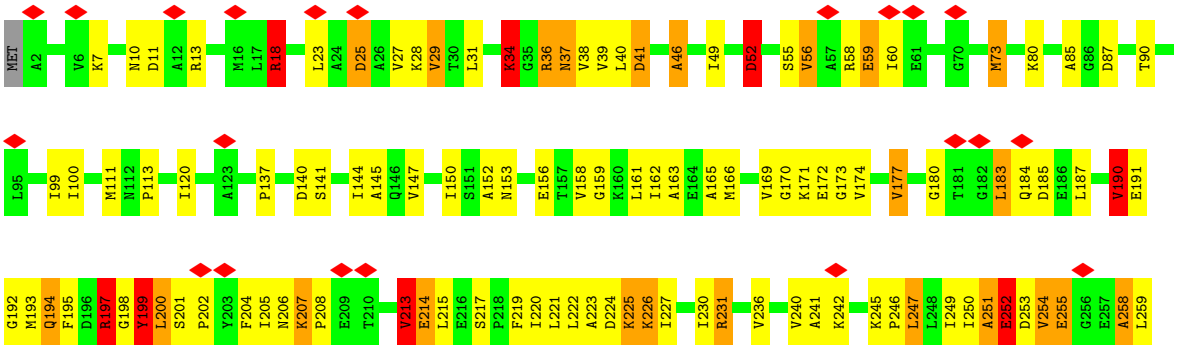
• Molecule 1: 60 KDA CHAPERONIN

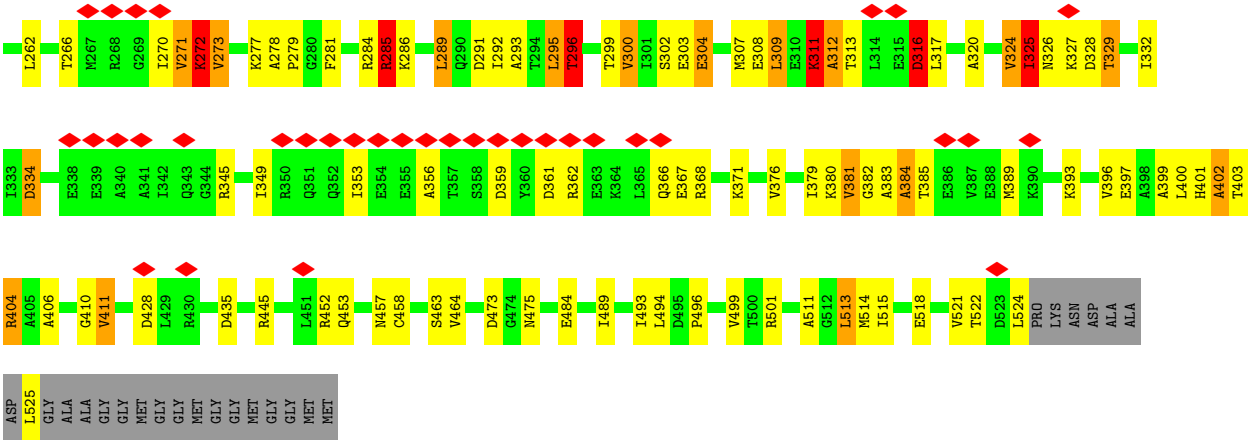
Chain F:



• Molecule 1: 60 KDA CHAPERONIN

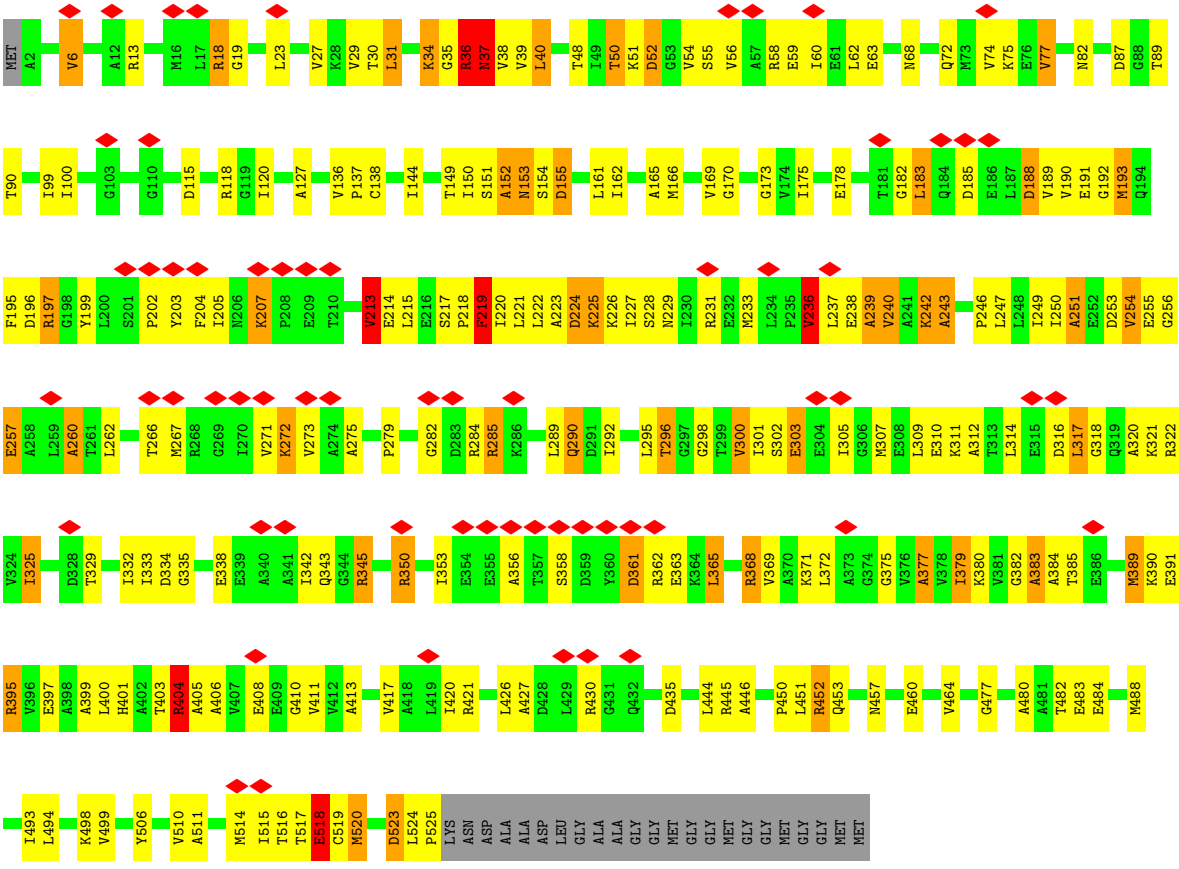
Chain G:





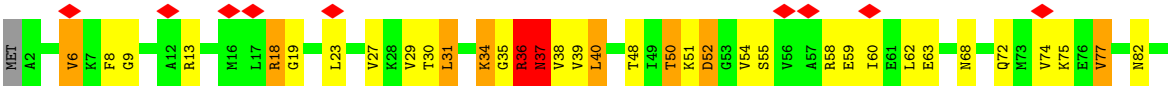
• Molecule 1: 60 KDA CHAPERONIN

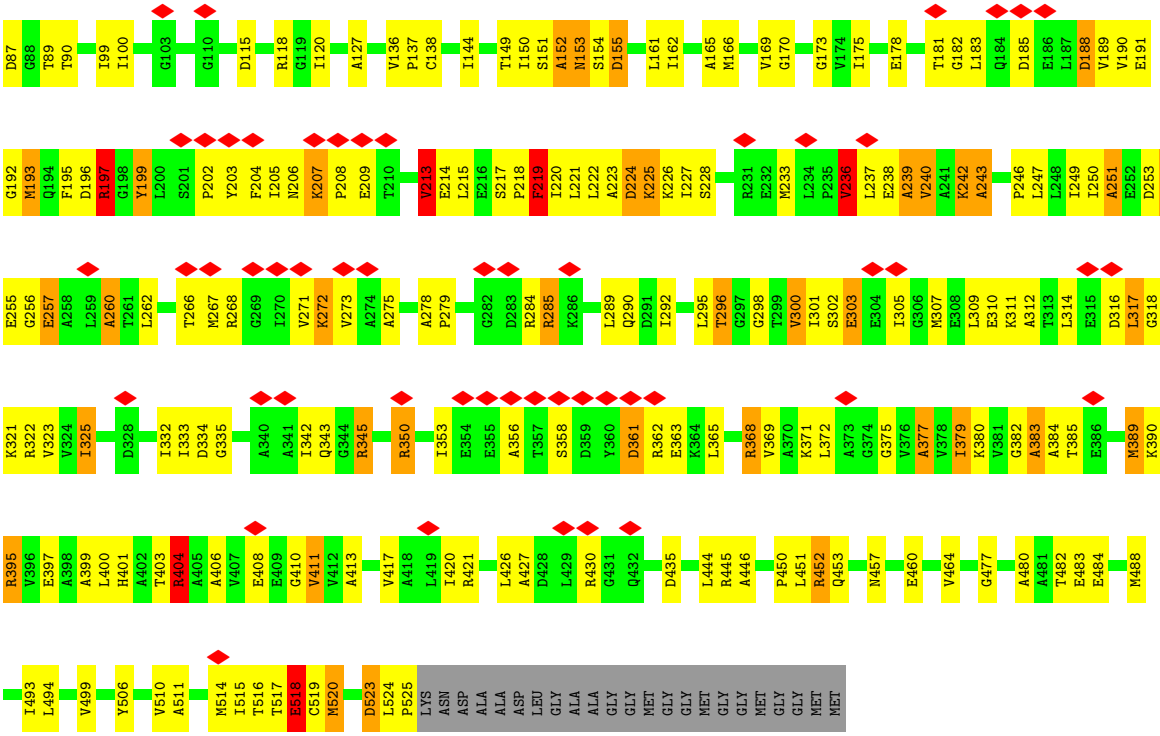
Chain H:



• Molecule 1: 60 KDA CHAPERONIN

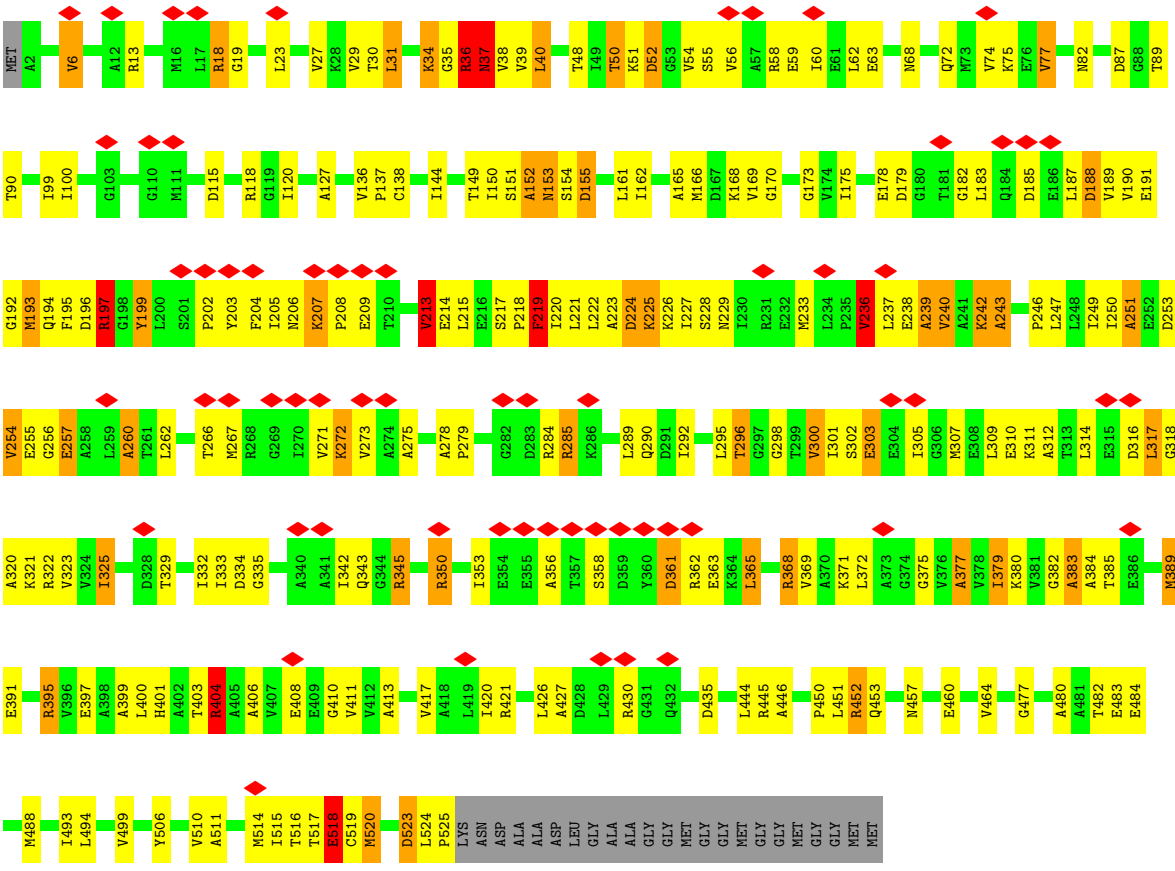
Chain I:





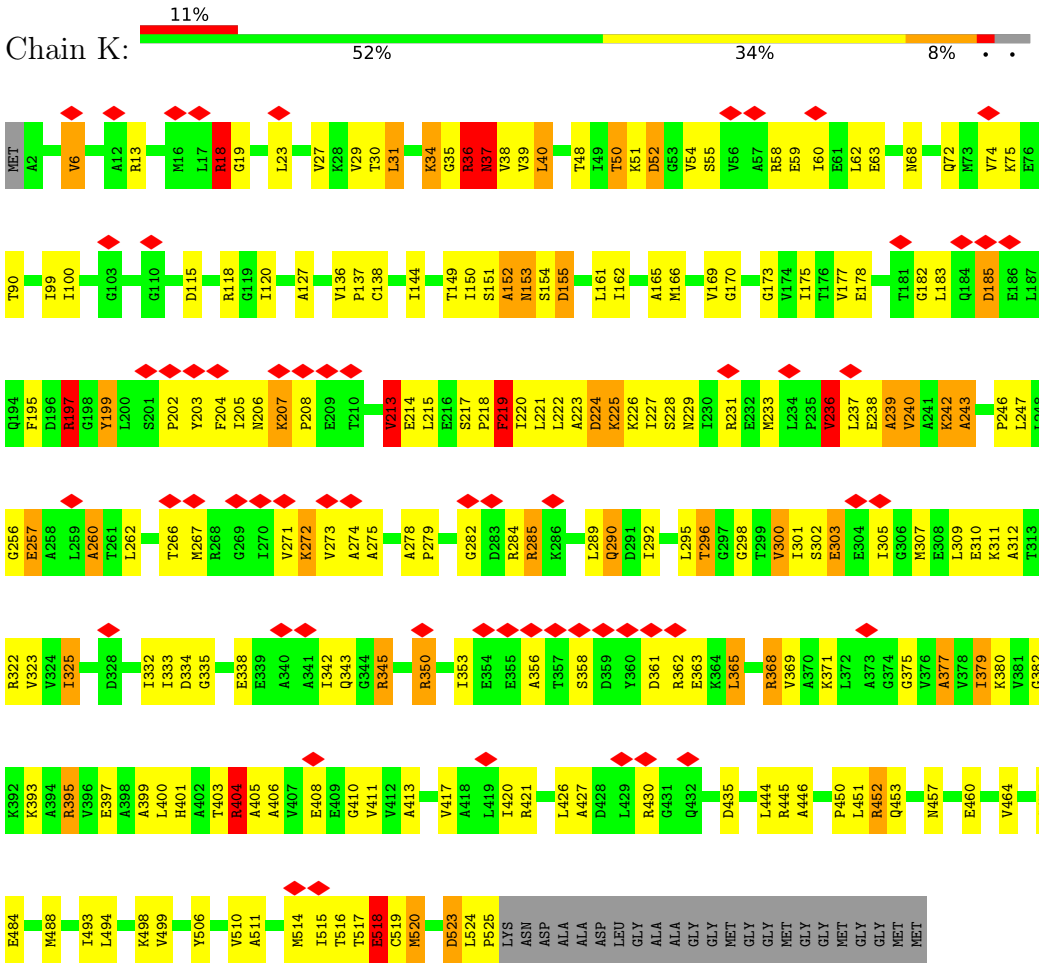
• Molecule 1: 60 KDA CHAPERONIN

Chain J:



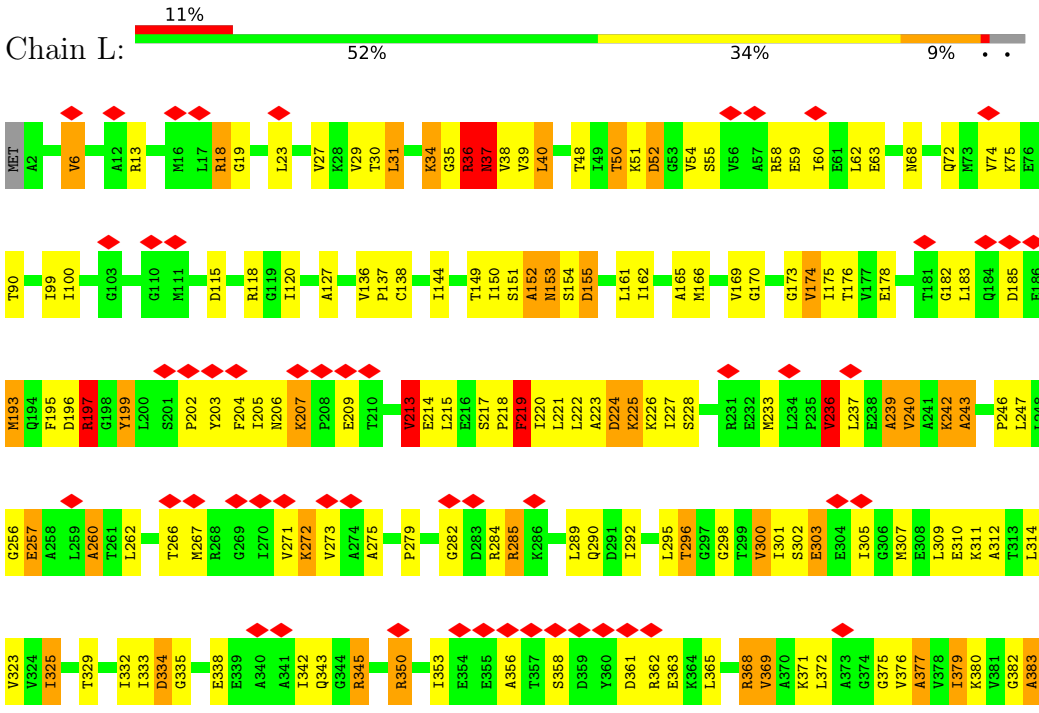
• Molecule 1: 60 KDA CHAPERONIN

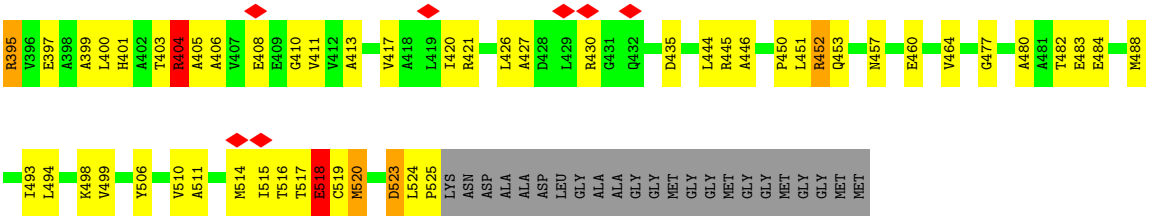
Chain K:



• Molecule 1: 60 KDA CHAPERONIN

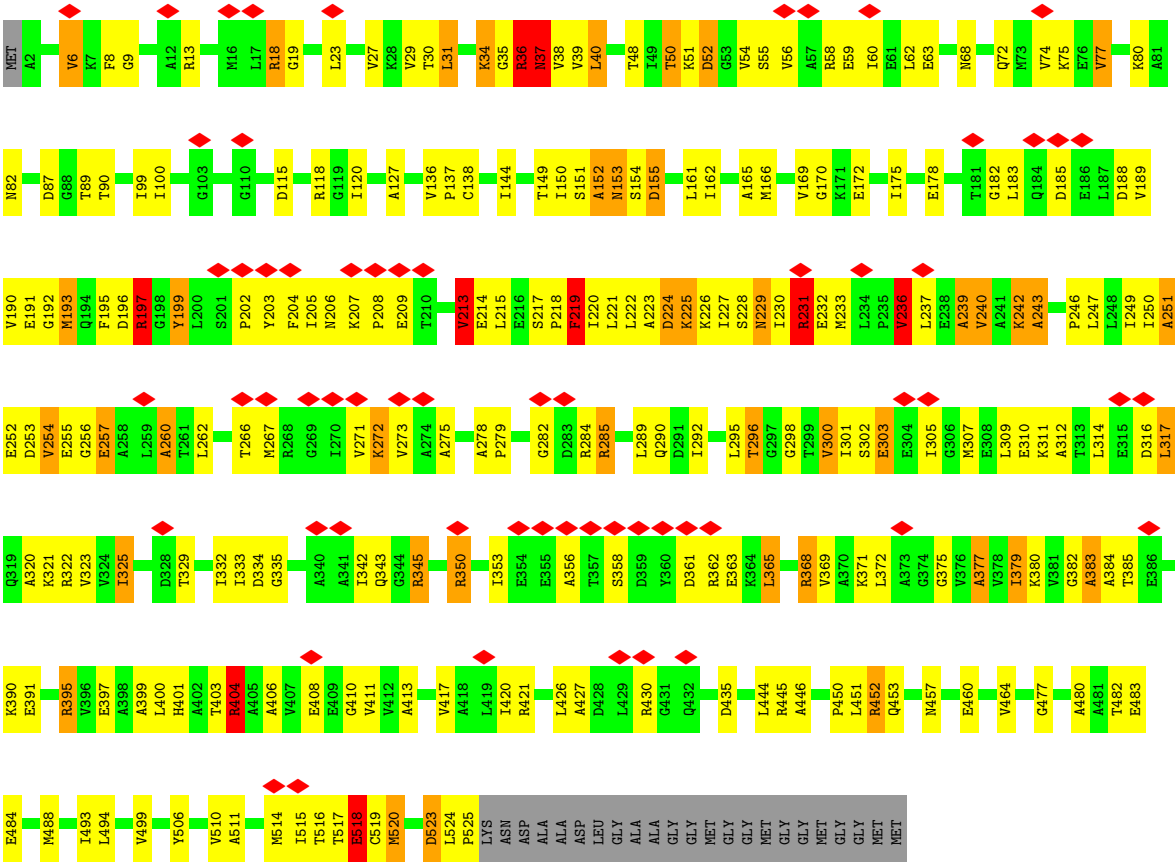
Chain L:





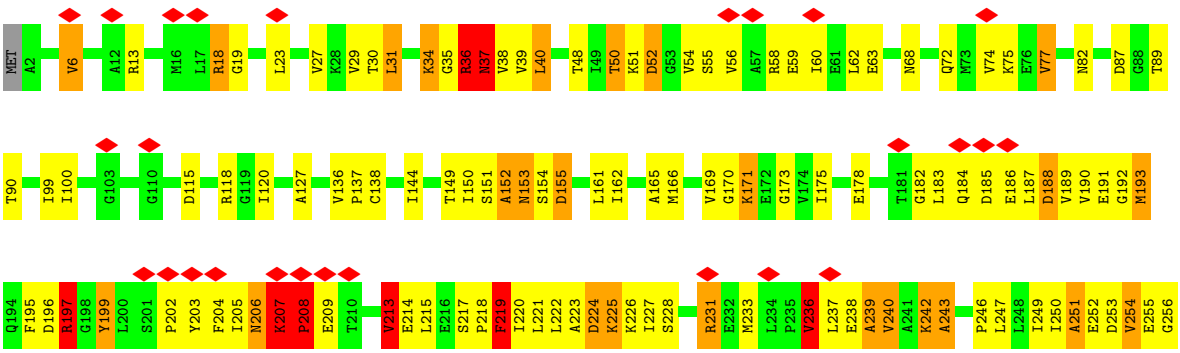
• Molecule 1: 60 KDA CHAPERONIN

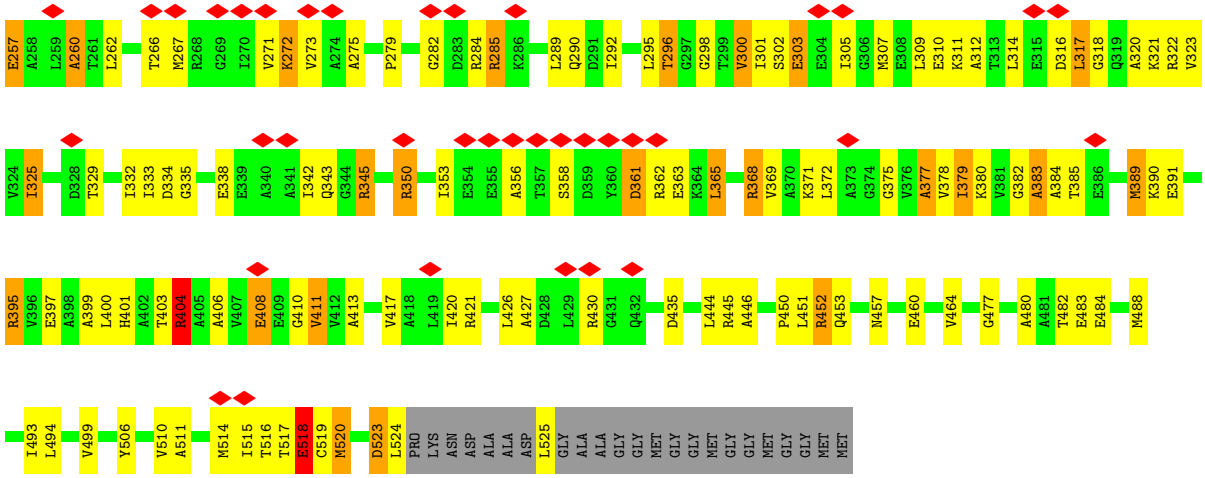
Chain M:



• Molecule 1: 60 KDA CHAPERONIN

Chain N:




E257 A258 L259 A260 T261 L262 T266 M267 R268 G269 I270 V271 K272 V273 A274 A275 P279 G282 D283 R284 R285 K286 L289 Q290 D291 I292 L295 T296 G297 G298 T299 V300 I301 S302 E303 E304 I305 G306 M307 E308 L309 E310 K311 A312 T313 L314 E315 D316 L317 G318 Q319 A320 K321 R322 V323
V324 I325 D328 T329 I332 I333 D334 G335 E338 E339 A340 A341 I342 Q343 G344 R345 R350 I353 E354 E355 A356 T357 S358 D359 Y360 D361 R362 E363 K364 L365 R368 V369 A370 K371 L372 A373 G374 G375 V376 A377 V378 I379 K380 V381 G382 A383 A384 T385 E386 M389 K390 E391
R395 V396 E397 A398 A399 L400 H401 A402 T403 R404 A405 A406 V407 E408 E409 G410 V411 V412 A413 V417 A418 L419 I420 R421 L426 A427 D428 L429 R430 G431 Q432 D435 L444 R445 A446 P450 L451 R452 Q453 M457 E460 V464 G477 A480 A481 T482 E483 E484 M488
I493 L494 V499 Y506 V510 A511 M514 I515 T516 T517 E518 C519 M520 D523 L524 PRO LYS ASN ASP ALA ALA ASP L525 GLY ALA ALA GLY GLY MET GLY GLY MET GLY GLY MET GLY GLY MET MET

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D7	Depositor
Number of particles used	15000	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE WAS PHASE FLIPPED	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	148500	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	2.147	Depositor
Minimum map value	-1.318	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	387.84, 387.84, 387.84	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.02, 2.02, 2.02	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.84	6/3873 (0.2%)	1.48	78/5229 (1.5%)
1	B	0.86	7/3872 (0.2%)	1.49	81/5227 (1.5%)
1	C	0.86	7/3872 (0.2%)	1.49	82/5227 (1.6%)
1	D	0.86	7/3872 (0.2%)	1.49	81/5227 (1.5%)
1	E	0.86	7/3872 (0.2%)	1.49	81/5227 (1.5%)
1	F	0.86	7/3872 (0.2%)	1.50	81/5227 (1.5%)
1	G	0.86	7/3872 (0.2%)	1.50	85/5227 (1.6%)
1	H	1.01	3/3872 (0.1%)	1.62	80/5227 (1.5%)
1	I	1.01	2/3872 (0.1%)	1.61	82/5227 (1.6%)
1	J	1.01	2/3872 (0.1%)	1.61	80/5227 (1.5%)
1	K	1.02	3/3872 (0.1%)	1.61	78/5227 (1.5%)
1	L	1.01	2/3872 (0.1%)	1.62	83/5227 (1.6%)
1	M	1.01	2/3872 (0.1%)	1.60	78/5227 (1.5%)
1	N	1.08	11/3872 (0.3%)	1.67	94/5227 (1.8%)
All	All	0.94	73/54209 (0.1%)	1.56	1144/73180 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	19
1	B	0	18
1	C	0	18
1	D	0	18
1	E	0	19
1	F	0	19
1	G	0	18
1	H	1	13
1	I	1	14

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	1	14
1	K	1	15
1	L	1	14
1	M	1	14
1	N	1	18
All	All	7	231

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	518	GLU	CA-CB	13.48	1.83	1.53
1	M	518	GLU	CA-CB	13.48	1.83	1.53
1	H	518	GLU	CA-CB	13.48	1.83	1.53
1	J	518	GLU	CA-CB	13.48	1.83	1.53
1	K	518	GLU	CA-CB	13.47	1.83	1.53
1	I	518	GLU	CA-CB	13.46	1.83	1.53
1	N	518	GLU	CA-CB	13.45	1.83	1.53
1	N	208	PRO	CA-C	11.95	1.76	1.52
1	C	7	LYS	C-N	-11.67	1.07	1.34
1	A	7	LYS	C-N	-11.66	1.07	1.34
1	E	7	LYS	C-N	-11.66	1.07	1.34
1	G	7	LYS	C-N	-11.66	1.07	1.34
1	B	7	LYS	C-N	-11.66	1.07	1.34
1	D	7	LYS	C-N	-11.66	1.07	1.34
1	F	7	LYS	C-N	-11.66	1.07	1.34
1	C	213	VAL	C-N	-11.26	1.08	1.34
1	D	213	VAL	C-N	-11.24	1.08	1.34
1	F	213	VAL	C-N	-11.24	1.08	1.34
1	G	213	VAL	C-N	-11.23	1.08	1.34
1	B	213	VAL	C-N	-11.23	1.08	1.34
1	E	213	VAL	C-N	-11.23	1.08	1.34
1	N	207	LYS	CE-NZ	8.36	1.70	1.49
1	N	208	PRO	C-N	8.30	1.53	1.34
1	N	207	LYS	CA-CB	7.98	1.71	1.53
1	D	11	ASP	C-N	7.91	1.52	1.34
1	G	11	ASP	C-N	7.91	1.52	1.34
1	A	11	ASP	C-N	7.90	1.52	1.34
1	B	11	ASP	C-N	7.90	1.52	1.34
1	E	11	ASP	C-N	7.90	1.52	1.34
1	F	11	ASP	C-N	7.90	1.52	1.34
1	C	11	ASP	C-N	7.89	1.52	1.34
1	N	207	LYS	CB-CG	7.55	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	243	ALA	CA-CB	7.43	1.68	1.52
1	J	243	ALA	CA-CB	7.43	1.68	1.52
1	L	243	ALA	CA-CB	7.42	1.68	1.52
1	N	243	ALA	CA-CB	7.42	1.68	1.52
1	M	243	ALA	CA-CB	7.41	1.68	1.52
1	H	243	ALA	CA-CB	7.40	1.68	1.52
1	K	243	ALA	CA-CB	7.37	1.68	1.52
1	N	207	LYS	CD-CE	7.31	1.69	1.51
1	B	52	ASP	C-N	-7.22	1.20	1.33
1	A	52	ASP	C-N	-7.18	1.20	1.33
1	E	52	ASP	C-N	-7.18	1.20	1.33
1	C	230	ILE	C-N	7.17	1.50	1.34
1	D	52	ASP	C-N	-7.17	1.20	1.33
1	F	230	ILE	C-N	7.17	1.50	1.34
1	G	230	ILE	C-N	7.17	1.50	1.34
1	D	230	ILE	C-N	7.17	1.50	1.34
1	F	52	ASP	C-N	-7.17	1.20	1.33
1	A	230	ILE	C-N	7.17	1.50	1.34
1	B	230	ILE	C-N	7.17	1.50	1.34
1	C	52	ASP	C-N	-7.17	1.20	1.33
1	E	230	ILE	C-N	7.17	1.50	1.34
1	G	52	ASP	C-N	-7.15	1.20	1.33
1	B	513	LEU	C-N	-6.61	1.18	1.34
1	E	513	LEU	C-N	-6.59	1.18	1.34
1	A	513	LEU	C-N	-6.58	1.19	1.34
1	F	513	LEU	C-N	-6.58	1.19	1.34
1	C	513	LEU	C-N	-6.58	1.19	1.34
1	G	513	LEU	C-N	-6.57	1.19	1.34
1	D	513	LEU	C-N	-6.56	1.19	1.34
1	B	518	GLU	C-N	-6.28	1.19	1.34
1	F	518	GLU	C-N	-6.25	1.19	1.34
1	C	518	GLU	C-N	-6.25	1.19	1.34
1	A	518	GLU	C-N	-6.24	1.19	1.34
1	E	518	GLU	C-N	-6.24	1.19	1.34
1	G	518	GLU	C-N	-6.24	1.19	1.34
1	D	518	GLU	C-N	-6.23	1.19	1.34
1	H	242	LYS	CA-CB	6.14	1.67	1.53
1	K	242	LYS	CA-CB	6.05	1.67	1.53
1	N	207	LYS	CG-CD	5.58	1.71	1.52
1	N	208	PRO	N-CA	5.49	1.56	1.47
1	N	207	LYS	C-N	5.29	1.44	1.34

All (1144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	243	ALA	CB-CA-C	-22.85	75.83	110.10
1	L	243	ALA	CB-CA-C	-22.84	75.83	110.10
1	N	243	ALA	CB-CA-C	-22.84	75.84	110.10
1	J	243	ALA	CB-CA-C	-22.84	75.85	110.10
1	H	243	ALA	CB-CA-C	-22.82	75.86	110.10
1	K	243	ALA	CB-CA-C	-22.80	75.90	110.10
1	M	243	ALA	CB-CA-C	-22.78	75.93	110.10
1	K	242	LYS	N-CA-CB	-22.64	69.85	110.60
1	H	242	LYS	N-CA-CB	-22.38	70.32	110.60
1	J	518	GLU	N-CA-CB	20.19	146.95	110.60
1	L	518	GLU	N-CA-CB	20.18	146.92	110.60
1	I	518	GLU	N-CA-CB	20.16	146.89	110.60
1	K	518	GLU	N-CA-CB	20.15	146.87	110.60
1	H	518	GLU	N-CA-CB	20.13	146.84	110.60
1	M	518	GLU	N-CA-CB	20.12	146.81	110.60
1	N	518	GLU	N-CA-CB	20.12	146.81	110.60
1	L	242	LYS	CB-CA-C	19.73	149.86	110.40
1	J	242	LYS	CB-CA-C	19.25	148.90	110.40
1	N	242	LYS	CB-CA-C	19.24	148.88	110.40
1	I	242	LYS	CB-CA-C	19.21	148.81	110.40
1	J	518	GLU	CB-CA-C	-18.30	73.80	110.40
1	K	518	GLU	CB-CA-C	-18.29	73.82	110.40
1	M	518	GLU	CB-CA-C	-18.29	73.83	110.40
1	L	518	GLU	CB-CA-C	-18.28	73.84	110.40
1	I	518	GLU	CB-CA-C	-18.27	73.86	110.40
1	N	518	GLU	CB-CA-C	-18.27	73.87	110.40
1	H	518	GLU	CB-CA-C	-18.25	73.89	110.40
1	N	260	ALA	N-CA-CB	18.12	135.47	110.10
1	M	242	LYS	N-CA-CB	-17.91	78.36	110.60
1	M	260	ALA	N-CA-CB	17.64	134.79	110.10
1	J	260	ALA	N-CA-CB	17.24	134.24	110.10
1	H	260	ALA	N-CA-CB	17.24	134.23	110.10
1	K	260	ALA	N-CA-CB	17.23	134.22	110.10
1	I	260	ALA	N-CA-CB	14.68	130.65	110.10
1	L	260	ALA	N-CA-CB	14.64	130.60	110.10
1	J	242	LYS	N-CA-CB	-14.60	84.31	110.60
1	I	242	LYS	N-CA-CB	-14.59	84.35	110.60
1	N	242	LYS	N-CA-CB	-14.57	84.37	110.60
1	H	242	LYS	CA-CB-CG	14.27	144.79	113.40
1	L	242	LYS	N-CA-CB	-14.21	85.02	110.60
1	K	242	LYS	CA-CB-CG	13.92	144.03	113.40
1	I	260	ALA	CB-CA-C	-13.22	90.27	110.10
1	L	260	ALA	CB-CA-C	-13.21	90.28	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	452	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	J	452	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	N	452	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	H	452	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	I	452	ARG	NE-CZ-NH1	11.57	126.09	120.30
1	K	452	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	L	452	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	N	208	PRO	N-CA-C	11.52	142.06	112.10
1	C	518	GLU	O-C-N	-11.50	104.29	122.70
1	E	518	GLU	O-C-N	-11.50	104.30	122.70
1	G	518	GLU	O-C-N	-11.49	104.31	122.70
1	F	518	GLU	O-C-N	-11.49	104.32	122.70
1	A	518	GLU	O-C-N	-11.48	104.32	122.70
1	D	518	GLU	O-C-N	-11.48	104.33	122.70
1	B	518	GLU	O-C-N	-11.45	104.37	122.70
1	N	208	PRO	CA-C-N	11.44	142.36	117.20
1	N	207	LYS	CD-CE-NZ	11.34	137.79	111.70
1	D	518	GLU	C-N-CA	11.34	150.05	121.70
1	C	518	GLU	C-N-CA	11.34	150.04	121.70
1	E	518	GLU	C-N-CA	11.34	150.04	121.70
1	F	518	GLU	C-N-CA	11.34	150.04	121.70
1	A	518	GLU	C-N-CA	11.33	150.03	121.70
1	G	518	GLU	C-N-CA	11.33	150.03	121.70
1	B	518	GLU	C-N-CA	11.32	150.00	121.70
1	J	260	ALA	CB-CA-C	-11.20	93.30	110.10
1	H	260	ALA	CB-CA-C	-11.20	93.31	110.10
1	K	260	ALA	CB-CA-C	-11.17	93.35	110.10
1	F	29	VAL	CA-C-N	-10.95	93.11	117.20
1	A	29	VAL	CA-C-N	-10.94	93.14	117.20
1	E	29	VAL	CA-C-N	-10.93	93.15	117.20
1	M	242	LYS	CB-CA-C	10.93	132.26	110.40
1	G	29	VAL	CA-C-N	-10.93	93.15	117.20
1	C	29	VAL	CA-C-N	-10.93	93.16	117.20
1	D	29	VAL	CA-C-N	-10.93	93.16	117.20
1	B	29	VAL	CA-C-N	-10.93	93.16	117.20
1	M	260	ALA	CB-CA-C	-10.90	93.74	110.10
1	N	260	ALA	CB-CA-C	-10.32	94.62	110.10
1	C	7	LYS	C-N-CA	-10.31	95.93	121.70
1	A	7	LYS	C-N-CA	-10.29	95.96	121.70
1	E	7	LYS	C-N-CA	-10.29	95.96	121.70
1	G	7	LYS	C-N-CA	-10.29	95.97	121.70
1	B	7	LYS	C-N-CA	-10.29	95.98	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	7	LYS	C-N-CA	-10.28	95.99	121.70
1	F	7	LYS	C-N-CA	-10.28	95.99	121.70
1	C	7	LYS	O-C-N	10.28	139.14	122.70
1	G	7	LYS	O-C-N	10.26	139.11	122.70
1	A	7	LYS	O-C-N	10.26	139.11	122.70
1	E	7	LYS	O-C-N	10.25	139.10	122.70
1	B	7	LYS	O-C-N	10.24	139.08	122.70
1	K	377	ALA	N-CA-CB	10.22	124.42	110.10
1	F	7	LYS	O-C-N	10.22	139.05	122.70
1	D	7	LYS	O-C-N	10.21	139.04	122.70
1	N	377	ALA	N-CA-CB	10.21	124.39	110.10
1	H	377	ALA	N-CA-CB	10.20	124.37	110.10
1	I	377	ALA	N-CA-CB	10.20	124.37	110.10
1	J	377	ALA	N-CA-CB	10.19	124.37	110.10
1	L	377	ALA	N-CA-CB	10.19	124.37	110.10
1	M	377	ALA	N-CA-CB	10.19	124.37	110.10
1	E	29	VAL	O-C-N	9.97	138.66	122.70
1	G	29	VAL	O-C-N	9.97	138.66	122.70
1	N	207	LYS	CB-CG-CD	9.97	137.51	111.60
1	A	29	VAL	O-C-N	9.96	138.63	122.70
1	F	29	VAL	O-C-N	9.96	138.63	122.70
1	C	29	VAL	O-C-N	9.95	138.63	122.70
1	B	29	VAL	O-C-N	9.95	138.62	122.70
1	D	29	VAL	O-C-N	9.95	138.62	122.70
1	E	214	GLU	CB-CA-C	-9.85	90.71	110.40
1	D	214	GLU	CB-CA-C	-9.84	90.72	110.40
1	F	214	GLU	CB-CA-C	-9.84	90.72	110.40
1	A	214	GLU	CB-CA-C	-9.84	90.73	110.40
1	B	214	GLU	CB-CA-C	-9.83	90.74	110.40
1	G	214	GLU	CB-CA-C	-9.83	90.74	110.40
1	C	214	GLU	CB-CA-C	-9.82	90.76	110.40
1	I	37	ASN	N-CA-CB	9.71	128.07	110.60
1	K	37	ASN	N-CA-CB	9.69	128.03	110.60
1	M	37	ASN	N-CA-CB	9.69	128.03	110.60
1	H	37	ASN	N-CA-CB	9.68	128.03	110.60
1	J	37	ASN	N-CA-CB	9.68	128.03	110.60
1	N	37	ASN	N-CA-CB	9.68	128.03	110.60
1	L	37	ASN	N-CA-CB	9.67	128.01	110.60
1	D	41	ASP	N-CA-CB	9.66	127.99	110.60
1	C	41	ASP	N-CA-CB	9.64	127.96	110.60
1	B	41	ASP	N-CA-CB	9.64	127.95	110.60
1	E	41	ASP	N-CA-CB	9.64	127.95	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	41	ASP	N-CA-CB	9.63	127.94	110.60
1	G	41	ASP	N-CA-CB	9.63	127.94	110.60
1	F	41	ASP	N-CA-CB	9.63	127.93	110.60
1	F	501	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	B	501	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	G	501	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	J	18	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	L	18	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	A	501	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	C	7	LYS	CA-C-N	-9.44	96.44	117.20
1	D	501	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	E	501	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	A	7	LYS	CA-C-N	-9.42	96.47	117.20
1	E	7	LYS	CA-C-N	-9.42	96.47	117.20
1	G	7	LYS	CA-C-N	-9.42	96.48	117.20
1	B	7	LYS	CA-C-N	-9.41	96.49	117.20
1	D	7	LYS	CA-C-N	-9.41	96.50	117.20
1	F	7	LYS	CA-C-N	-9.41	96.50	117.20
1	C	501	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	N	207	LYS	CA-CB-CG	9.39	134.07	113.40
1	N	219	PHE	N-CA-CB	9.39	127.50	110.60
1	M	18	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	H	18	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	N	208	PRO	C-N-CA	-9.36	98.31	121.70
1	K	219	PHE	N-CA-CB	9.35	127.42	110.60
1	N	18	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	L	219	PHE	N-CA-CB	9.29	127.31	110.60
1	I	18	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	I	219	PHE	N-CA-CB	9.28	127.30	110.60
1	M	219	PHE	N-CA-CB	9.28	127.30	110.60
1	K	242	LYS	CB-CA-C	9.27	128.95	110.40
1	J	219	PHE	N-CA-CB	9.27	127.28	110.60
1	K	18	ARG	NE-CZ-NH1	9.25	124.93	120.30
1	H	219	PHE	N-CA-CB	9.24	127.23	110.60
1	G	199	TYR	C-N-CA	-9.23	98.62	121.70
1	J	18	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	L	18	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	M	18	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	N	18	ARG	NE-CZ-NH2	-9.09	115.76	120.30
1	H	242	LYS	CB-CA-C	9.04	128.48	110.40
1	H	18	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	G	52	ASP	C-N-CA	-9.03	103.34	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	52	ASP	C-N-CA	-9.03	103.35	122.30
1	C	52	ASP	C-N-CA	-9.02	103.35	122.30
1	I	18	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	A	52	ASP	C-N-CA	-9.02	103.36	122.30
1	D	52	ASP	C-N-CA	-9.02	103.36	122.30
1	K	18	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	B	52	ASP	C-N-CA	-9.00	103.40	122.30
1	E	52	ASP	C-N-CA	-9.00	103.41	122.30
1	H	243	ALA	N-CA-CB	8.94	122.62	110.10
1	K	243	ALA	N-CA-CB	8.93	122.60	110.10
1	M	243	ALA	N-CA-CB	8.89	122.55	110.10
1	N	243	ALA	N-CA-CB	8.86	122.51	110.10
1	J	243	ALA	N-CA-CB	8.86	122.51	110.10
1	I	243	ALA	N-CA-CB	8.86	122.50	110.10
1	L	243	ALA	N-CA-CB	8.85	122.49	110.10
1	F	18	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	B	18	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	E	18	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	G	18	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	C	18	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	D	18	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	L	115	ASP	CB-CA-C	8.65	127.69	110.40
1	N	115	ASP	CB-CA-C	8.64	127.68	110.40
1	A	18	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	I	115	ASP	CB-CA-C	8.64	127.68	110.40
1	H	115	ASP	CB-CA-C	8.63	127.67	110.40
1	K	115	ASP	CB-CA-C	8.63	127.67	110.40
1	J	115	ASP	CB-CA-C	8.63	127.66	110.40
1	M	115	ASP	CB-CA-C	8.63	127.66	110.40
1	N	240	VAL	CA-CB-CG2	-8.58	98.04	110.90
1	D	225	LYS	N-CA-CB	8.54	125.97	110.60
1	M	240	VAL	CA-CB-CG2	-8.54	98.09	110.90
1	B	225	LYS	N-CA-CB	8.54	125.97	110.60
1	G	225	LYS	N-CA-CB	8.54	125.96	110.60
1	E	225	LYS	N-CA-CB	8.53	125.96	110.60
1	A	225	LYS	N-CA-CB	8.53	125.96	110.60
1	C	225	LYS	N-CA-CB	8.52	125.94	110.60
1	F	225	LYS	N-CA-CB	8.52	125.94	110.60
1	I	240	VAL	CA-CB-CG2	-8.51	98.13	110.90
1	L	240	VAL	CA-CB-CG2	-8.51	98.14	110.90
1	J	240	VAL	CA-CB-CG2	-8.49	98.17	110.90
1	G	213	VAL	O-C-N	8.48	136.27	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	240	VAL	CA-CB-CG2	-8.48	98.17	110.90
1	F	213	VAL	O-C-N	8.48	136.27	122.70
1	K	240	VAL	CA-CB-CG2	-8.48	98.19	110.90
1	E	213	VAL	O-C-N	8.47	136.26	122.70
1	C	213	VAL	O-C-N	8.47	136.26	122.70
1	B	213	VAL	O-C-N	8.47	136.25	122.70
1	D	213	VAL	O-C-N	8.44	136.20	122.70
1	L	257	GLU	N-CA-CB	-8.42	95.44	110.60
1	F	29	VAL	C-N-CA	-8.25	101.08	121.70
1	A	29	VAL	C-N-CA	-8.24	101.09	121.70
1	B	29	VAL	C-N-CA	-8.24	101.09	121.70
1	C	29	VAL	C-N-CA	-8.23	101.11	121.70
1	D	29	VAL	C-N-CA	-8.23	101.12	121.70
1	E	29	VAL	C-N-CA	-8.23	101.12	121.70
1	G	29	VAL	C-N-CA	-8.23	101.12	121.70
1	N	207	LYS	CB-CA-C	8.16	126.73	110.40
1	E	56	VAL	CB-CA-C	-8.14	95.94	111.40
1	G	56	VAL	CB-CA-C	-8.13	95.96	111.40
1	A	56	VAL	CB-CA-C	-8.12	95.97	111.40
1	D	56	VAL	CB-CA-C	-8.12	95.97	111.40
1	A	518	GLU	N-CA-CB	8.12	125.22	110.60
1	F	56	VAL	CB-CA-C	-8.12	95.98	111.40
1	C	56	VAL	CB-CA-C	-8.11	95.98	111.40
1	B	56	VAL	CB-CA-C	-8.11	95.99	111.40
1	D	518	GLU	CA-C-N	8.11	135.04	117.20
1	A	518	GLU	CA-C-N	8.10	135.03	117.20
1	C	518	GLU	CA-C-N	8.10	135.03	117.20
1	E	518	GLU	CA-C-N	8.10	135.03	117.20
1	F	518	GLU	CA-C-N	8.10	135.03	117.20
1	G	518	GLU	CA-C-N	8.10	135.02	117.20
1	B	518	GLU	CA-C-N	8.09	135.00	117.20
1	E	518	GLU	N-CA-CB	8.08	125.14	110.60
1	C	518	GLU	N-CA-CB	8.06	125.11	110.60
1	N	310	GLU	CB-CA-C	-8.06	94.28	110.40
1	J	284	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	H	310	GLU	CB-CA-C	-8.06	94.29	110.40
1	K	310	GLU	CB-CA-C	-8.05	94.30	110.40
1	N	284	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	F	518	GLU	N-CA-CB	8.04	125.07	110.60
1	G	518	GLU	N-CA-CB	8.04	125.07	110.60
1	H	284	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	D	518	GLU	N-CA-CB	8.03	125.06	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	518	GLU	N-CA-CB	8.03	125.05	110.60
1	K	284	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	I	404	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	I	395	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	M	310	GLU	CB-CA-C	-8.00	94.39	110.40
1	I	284	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	J	310	GLU	CB-CA-C	-8.00	94.40	110.40
1	L	310	GLU	CB-CA-C	-8.00	94.41	110.40
1	L	284	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	M	395	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	M	284	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	I	310	GLU	CB-CA-C	-7.95	94.50	110.40
1	N	395	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	M	404	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	K	395	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	J	404	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	N	404	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	H	395	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	L	404	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	H	404	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	K	404	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	F	213	VAL	CA-C-N	-7.86	99.92	117.20
1	G	213	VAL	CA-C-N	-7.85	99.92	117.20
1	C	213	VAL	CA-C-N	-7.85	99.92	117.20
1	D	213	VAL	CA-C-N	-7.85	99.93	117.20
1	B	213	VAL	CA-C-N	-7.85	99.94	117.20
1	E	213	VAL	CA-C-N	-7.84	99.95	117.20
1	L	395	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	J	395	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	K	213	VAL	O-C-N	-7.78	110.25	122.70
1	I	213	VAL	O-C-N	-7.76	110.28	122.70
1	N	213	VAL	O-C-N	-7.76	110.28	122.70
1	J	213	VAL	O-C-N	-7.76	110.28	122.70
1	L	213	VAL	O-C-N	-7.76	110.28	122.70
1	H	213	VAL	O-C-N	-7.74	110.32	122.70
1	M	213	VAL	O-C-N	-7.72	110.34	122.70
1	B	258	ALA	N-CA-CB	7.72	120.91	110.10
1	D	258	ALA	N-CA-CB	7.72	120.91	110.10
1	A	258	ALA	N-CA-CB	7.72	120.91	110.10
1	C	258	ALA	N-CA-CB	7.72	120.91	110.10
1	E	258	ALA	N-CA-CB	7.71	120.89	110.10
1	F	258	ALA	N-CA-CB	7.70	120.88	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	258	ALA	N-CA-CB	7.69	120.87	110.10
1	F	18	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	G	18	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	A	18	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	D	18	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	L	77	VAL	CB-CA-C	-7.61	96.94	111.40
1	N	77	VAL	CB-CA-C	-7.61	96.95	111.40
1	I	77	VAL	CB-CA-C	-7.61	96.95	111.40
1	K	77	VAL	CB-CA-C	-7.61	96.95	111.40
1	B	18	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	J	77	VAL	CB-CA-C	-7.60	96.96	111.40
1	H	77	VAL	CB-CA-C	-7.60	96.97	111.40
1	E	18	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	M	77	VAL	CB-CA-C	-7.59	96.98	111.40
1	L	224	ASP	N-CA-CB	7.58	124.25	110.60
1	N	224	ASP	N-CA-CB	7.58	124.23	110.60
1	M	224	ASP	N-CA-CB	7.57	124.23	110.60
1	N	208	PRO	O-C-N	-7.56	110.60	122.70
1	C	18	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	D	39	VAL	O-C-N	7.56	134.80	122.70
1	F	39	VAL	O-C-N	7.54	134.77	122.70
1	A	39	VAL	O-C-N	7.53	134.74	122.70
1	B	39	VAL	O-C-N	7.52	134.74	122.70
1	G	39	VAL	O-C-N	7.52	134.74	122.70
1	I	303	GLU	CB-CA-C	-7.52	95.35	110.40
1	C	39	VAL	O-C-N	7.51	134.72	122.70
1	E	39	VAL	O-C-N	7.51	134.71	122.70
1	J	303	GLU	CB-CA-C	-7.50	95.40	110.40
1	F	452	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	G	452	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	A	316	ASP	N-CA-CB	7.42	123.95	110.60
1	F	316	ASP	N-CA-CB	7.42	123.95	110.60
1	B	316	ASP	N-CA-CB	7.41	123.94	110.60
1	C	316	ASP	N-CA-CB	7.41	123.94	110.60
1	E	316	ASP	N-CA-CB	7.41	123.93	110.60
1	C	452	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	G	316	ASP	N-CA-CB	7.40	123.92	110.60
1	E	452	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	D	316	ASP	N-CA-CB	7.40	123.91	110.60
1	A	452	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	D	452	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	B	452	ARG	NE-CZ-NH2	-7.37	116.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	345	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	M	345	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	J	224	ASP	N-CA-CB	7.30	123.74	110.60
1	J	345	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	K	345	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	L	345	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	I	224	ASP	N-CA-CB	7.29	123.73	110.60
1	H	345	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	H	18	ARG	CD-NE-CZ	7.17	133.63	123.60
1	I	251	ALA	N-CA-CB	7.17	120.13	110.10
1	A	289	LEU	CB-CG-CD1	-7.15	98.84	111.00
1	I	18	ARG	CD-NE-CZ	7.15	133.61	123.60
1	J	251	ALA	N-CA-CB	7.15	120.11	110.10
1	F	289	LEU	CB-CG-CD1	-7.15	98.85	111.00
1	C	289	LEU	CB-CG-CD1	-7.14	98.86	111.00
1	B	289	LEU	CB-CG-CD1	-7.14	98.86	111.00
1	G	289	LEU	CB-CG-CD1	-7.14	98.86	111.00
1	H	251	ALA	N-CA-CB	7.14	120.10	110.10
1	E	289	LEU	CB-CG-CD1	-7.14	98.87	111.00
1	M	251	ALA	N-CA-CB	7.13	120.08	110.10
1	I	345	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	D	289	LEU	CB-CG-CD1	-7.12	98.90	111.00
1	N	18	ARG	CD-NE-CZ	7.12	133.56	123.60
1	H	303	GLU	CB-CA-C	-7.11	96.18	110.40
1	J	18	ARG	CD-NE-CZ	7.11	133.55	123.60
1	L	18	ARG	CD-NE-CZ	7.11	133.56	123.60
1	K	303	GLU	CB-CA-C	-7.11	96.18	110.40
1	M	18	ARG	CD-NE-CZ	7.11	133.55	123.60
1	N	251	ALA	N-CA-CB	7.11	120.05	110.10
1	K	251	ALA	N-CA-CB	7.10	120.04	110.10
1	K	18	ARG	CD-NE-CZ	7.08	133.52	123.60
1	L	251	ALA	N-CA-CB	7.08	120.01	110.10
1	C	59	GLU	N-CA-CB	-7.04	97.93	110.60
1	D	59	GLU	N-CA-CB	-7.04	97.93	110.60
1	E	59	GLU	N-CA-CB	-7.03	97.94	110.60
1	K	362	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	A	59	GLU	N-CA-CB	-7.03	97.95	110.60
1	G	59	GLU	N-CA-CB	-7.03	97.95	110.60
1	H	362	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	59	GLU	N-CA-CB	-7.01	97.97	110.60
1	F	59	GLU	N-CA-CB	-7.01	97.98	110.60
1	I	362	ARG	NE-CZ-NH1	7.01	123.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	362	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	N	185	ASP	CB-CA-C	6.98	124.36	110.40
1	H	185	ASP	CB-CA-C	6.98	124.36	110.40
1	I	185	ASP	CB-CA-C	6.98	124.35	110.40
1	L	185	ASP	CB-CA-C	6.97	124.35	110.40
1	L	362	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	J	185	ASP	CB-CA-C	6.97	124.34	110.40
1	M	185	ASP	CB-CA-C	6.97	124.34	110.40
1	J	362	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	K	118	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	M	362	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	H	224	ASP	N-CA-CB	6.94	123.10	110.60
1	K	224	ASP	N-CA-CB	6.93	123.07	110.60
1	F	463	SER	N-CA-CB	6.92	120.89	110.50
1	H	118	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	E	463	SER	N-CA-CB	6.89	120.83	110.50
1	N	231	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	G	463	SER	N-CA-CB	6.89	120.83	110.50
1	A	463	SER	N-CA-CB	6.89	120.83	110.50
1	C	39	VAL	N-CA-CB	6.88	126.64	111.50
1	F	39	VAL	N-CA-CB	6.88	126.63	111.50
1	A	39	VAL	N-CA-CB	6.87	126.62	111.50
1	D	463	SER	N-CA-CB	6.87	120.81	110.50
1	J	118	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	G	39	VAL	N-CA-CB	6.87	126.62	111.50
1	J	404	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	E	39	VAL	N-CA-CB	6.87	126.61	111.50
1	B	463	SER	N-CA-CB	6.87	120.80	110.50
1	D	39	VAL	N-CA-CB	6.86	126.60	111.50
1	B	39	VAL	N-CA-CB	6.86	126.59	111.50
1	L	404	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	I	118	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	C	463	SER	N-CA-CB	6.84	120.76	110.50
1	M	34	LYS	CB-CA-C	6.83	124.05	110.40
1	H	34	LYS	CB-CA-C	6.82	124.04	110.40
1	K	404	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	L	118	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	J	34	LYS	CB-CA-C	6.81	124.03	110.40
1	K	34	LYS	CB-CA-C	6.81	124.03	110.40
1	I	34	LYS	CB-CA-C	6.81	124.02	110.40
1	L	34	LYS	CB-CA-C	6.81	124.02	110.40
1	I	404	ARG	NE-CZ-NH1	6.81	123.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	34	LYS	CB-CA-C	6.81	124.02	110.40
1	M	118	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	F	247	LEU	CB-CA-C	-6.80	97.28	110.20
1	A	247	LEU	CB-CA-C	-6.80	97.28	110.20
1	D	247	LEU	CB-CA-C	-6.80	97.28	110.20
1	E	247	LEU	CB-CA-C	-6.80	97.28	110.20
1	N	404	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	B	247	LEU	CB-CA-C	-6.79	97.29	110.20
1	N	118	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	G	247	LEU	CB-CA-C	-6.79	97.30	110.20
1	C	247	LEU	CB-CA-C	-6.78	97.31	110.20
1	B	230	ILE	O-C-N	6.77	133.54	122.70
1	C	87	ASP	N-CA-CB	6.77	122.79	110.60
1	D	230	ILE	O-C-N	6.77	133.53	122.70
1	G	87	ASP	N-CA-CB	6.77	122.78	110.60
1	A	87	ASP	N-CA-CB	6.77	122.78	110.60
1	A	230	ILE	O-C-N	6.77	133.53	122.70
1	D	251	ALA	N-CA-CB	-6.76	100.63	110.10
1	D	362	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	E	87	ASP	N-CA-CB	6.76	122.77	110.60
1	I	395	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	F	230	ILE	O-C-N	6.76	133.51	122.70
1	G	230	ILE	O-C-N	6.75	133.51	122.70
1	H	404	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	E	230	ILE	O-C-N	6.75	133.51	122.70
1	A	251	ALA	N-CA-CB	-6.75	100.65	110.10
1	C	230	ILE	O-C-N	6.75	133.50	122.70
1	E	251	ALA	N-CA-CB	-6.75	100.65	110.10
1	G	251	ALA	N-CA-CB	-6.74	100.66	110.10
1	B	251	ALA	N-CA-CB	-6.73	100.67	110.10
1	C	251	ALA	N-CA-CB	-6.73	100.67	110.10
1	F	251	ALA	N-CA-CB	-6.73	100.67	110.10
1	M	404	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	N	395	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	M	395	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	K	395	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	E	362	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	L	303	GLU	CB-CA-C	-6.68	97.05	110.40
1	N	303	GLU	CB-CA-C	-6.68	97.05	110.40
1	M	303	GLU	CB-CA-C	-6.67	97.05	110.40
1	B	362	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	362	ARG	NE-CZ-NH1	6.65	123.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	395	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	362	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	J	300	VAL	CB-CA-C	-6.62	98.81	111.40
1	J	395	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	I	300	VAL	CB-CA-C	-6.62	98.83	111.40
1	G	362	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	E	213	VAL	C-N-CA	-6.61	105.17	121.70
1	F	213	VAL	C-N-CA	-6.61	105.18	121.70
1	F	362	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	J	152	ALA	CB-CA-C	6.61	120.01	110.10
1	I	383	ALA	N-CA-CB	6.60	119.34	110.10
1	L	152	ALA	CB-CA-C	6.60	120.00	110.10
1	L	383	ALA	N-CA-CB	6.60	119.34	110.10
1	B	213	VAL	C-N-CA	-6.60	105.21	121.70
1	H	383	ALA	N-CA-CB	6.60	119.33	110.10
1	G	213	VAL	C-N-CA	-6.59	105.21	121.70
1	H	152	ALA	CB-CA-C	6.59	119.99	110.10
1	I	152	ALA	CB-CA-C	6.59	119.99	110.10
1	J	383	ALA	N-CA-CB	6.59	119.33	110.10
1	M	383	ALA	N-CA-CB	6.59	119.33	110.10
1	N	383	ALA	N-CA-CB	6.59	119.33	110.10
1	K	152	ALA	CB-CA-C	6.59	119.98	110.10
1	K	383	ALA	N-CA-CB	6.59	119.32	110.10
1	C	213	VAL	C-N-CA	-6.58	105.24	121.70
1	D	213	VAL	C-N-CA	-6.58	105.24	121.70
1	N	152	ALA	CB-CA-C	6.58	119.97	110.10
1	M	152	ALA	CB-CA-C	6.57	119.96	110.10
1	L	395	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	A	253	ASP	CB-CG-OD1	6.56	124.20	118.30
1	L	300	VAL	CB-CA-C	-6.54	98.97	111.40
1	C	253	ASP	CB-CG-OD1	6.54	124.19	118.30
1	N	300	VAL	CB-CA-C	-6.54	98.97	111.40
1	B	253	ASP	CB-CG-OD1	6.54	124.18	118.30
1	I	242	LYS	CA-CB-CG	6.54	127.78	113.40
1	K	37	ASN	CB-CA-C	6.53	123.46	110.40
1	J	242	LYS	CA-CB-CG	6.53	127.76	113.40
1	K	300	VAL	CB-CA-C	-6.53	99.00	111.40
1	D	252	GLU	N-CA-CB	6.52	122.34	110.60
1	G	252	GLU	N-CA-CB	6.52	122.34	110.60
1	G	253	ASP	CB-CG-OD1	6.52	124.17	118.30
1	B	252	GLU	N-CA-CB	6.52	122.34	110.60
1	C	252	GLU	N-CA-CB	6.52	122.34	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	GLU	N-CA-CB	6.51	122.33	110.60
1	J	37	ASN	CB-CA-C	6.51	123.43	110.40
1	L	37	ASN	CB-CA-C	6.51	123.43	110.40
1	E	253	ASP	CB-CG-OD1	6.51	124.16	118.30
1	F	252	GLU	N-CA-CB	6.51	122.32	110.60
1	E	252	GLU	N-CA-CB	6.51	122.32	110.60
1	F	253	ASP	CB-CG-OD1	6.51	124.16	118.30
1	M	300	VAL	CB-CA-C	-6.51	99.03	111.40
1	N	37	ASN	CB-CA-C	6.51	123.42	110.40
1	H	37	ASN	CB-CA-C	6.50	123.41	110.40
1	H	300	VAL	CB-CA-C	-6.50	99.05	111.40
1	M	37	ASN	CB-CA-C	6.50	123.41	110.40
1	N	242	LYS	CA-CB-CG	6.50	127.71	113.40
1	I	37	ASN	CB-CA-C	6.50	123.40	110.40
1	B	367	GLU	CB-CA-C	-6.50	97.41	110.40
1	D	253	ASP	CB-CG-OD1	6.50	124.15	118.30
1	F	367	GLU	CB-CA-C	-6.49	97.42	110.40
1	D	367	GLU	CB-CA-C	-6.49	97.42	110.40
1	C	367	GLU	CB-CA-C	-6.49	97.42	110.40
1	A	367	GLU	CB-CA-C	-6.48	97.43	110.40
1	E	367	GLU	CB-CA-C	-6.47	97.45	110.40
1	G	367	GLU	CB-CA-C	-6.47	97.45	110.40
1	D	273	VAL	CB-CA-C	-6.47	99.11	111.40
1	L	242	LYS	CA-CB-CG	6.47	127.63	113.40
1	B	273	VAL	CB-CA-C	-6.46	99.13	111.40
1	F	273	VAL	CB-CA-C	-6.46	99.13	111.40
1	A	273	VAL	CB-CA-C	-6.46	99.13	111.40
1	C	273	VAL	CB-CA-C	-6.46	99.13	111.40
1	G	273	VAL	CB-CA-C	-6.46	99.13	111.40
1	E	273	VAL	CB-CA-C	-6.45	99.14	111.40
1	H	365	LEU	CB-CA-C	6.45	122.45	110.20
1	I	365	LEU	CB-CA-C	6.45	122.45	110.20
1	J	365	LEU	CB-CA-C	6.45	122.45	110.20
1	K	365	LEU	CB-CA-C	6.44	122.44	110.20
1	M	365	LEU	CB-CA-C	6.44	122.44	110.20
1	L	365	LEU	CB-CA-C	6.43	122.43	110.20
1	N	365	LEU	CB-CA-C	6.43	122.42	110.20
1	J	397	GLU	CB-CA-C	6.43	123.26	110.40
1	H	397	GLU	CB-CA-C	6.43	123.25	110.40
1	K	397	GLU	CB-CA-C	6.43	123.25	110.40
1	M	397	GLU	CB-CA-C	6.42	123.25	110.40
1	L	397	GLU	CB-CA-C	6.42	123.24	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	207	LYS	C-N-CD	-6.42	106.47	120.60
1	I	397	GLU	CB-CA-C	6.41	123.22	110.40
1	D	153	ASN	CB-CA-C	6.41	123.21	110.40
1	N	397	GLU	CB-CA-C	6.40	123.21	110.40
1	D	39	VAL	CA-C-N	-6.37	103.19	117.20
1	F	39	VAL	CA-C-N	-6.37	103.19	117.20
1	F	153	ASN	CB-CA-C	6.37	123.13	110.40
1	C	39	VAL	CA-C-N	-6.36	103.21	117.20
1	B	39	VAL	CA-C-N	-6.36	103.21	117.20
1	A	39	VAL	CA-C-N	-6.36	103.22	117.20
1	G	39	VAL	CA-C-N	-6.35	103.23	117.20
1	F	87	ASP	N-CA-CB	6.35	122.03	110.60
1	E	39	VAL	CA-C-N	-6.34	103.25	117.20
1	D	87	ASP	N-CA-CB	6.33	121.98	110.60
1	J	197	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	D	311	LYS	N-CA-CB	6.22	121.80	110.60
1	C	311	LYS	N-CA-CB	6.22	121.79	110.60
1	G	311	LYS	N-CA-CB	6.21	121.79	110.60
1	M	266	THR	N-CA-CB	6.21	122.11	110.30
1	C	34	LYS	N-CA-CB	6.21	121.78	110.60
1	A	34	LYS	N-CA-CB	6.21	121.78	110.60
1	A	311	LYS	N-CA-CB	6.21	121.78	110.60
1	N	266	THR	N-CA-CB	6.21	122.09	110.30
1	B	34	LYS	N-CA-CB	6.21	121.77	110.60
1	D	34	LYS	N-CA-CB	6.21	121.77	110.60
1	B	311	LYS	N-CA-CB	6.20	121.77	110.60
1	E	311	LYS	N-CA-CB	6.20	121.76	110.60
1	F	34	LYS	N-CA-CB	6.20	121.76	110.60
1	F	311	LYS	N-CA-CB	6.20	121.76	110.60
1	H	266	THR	N-CA-CB	6.20	122.08	110.30
1	E	34	LYS	N-CA-CB	6.19	121.75	110.60
1	G	34	LYS	N-CA-CB	6.19	121.75	110.60
1	K	266	THR	N-CA-CB	6.19	122.06	110.30
1	N	59	GLU	CB-CA-C	6.19	122.78	110.40
1	I	266	THR	N-CA-CB	6.19	122.06	110.30
1	J	59	GLU	CB-CA-C	6.19	122.77	110.40
1	K	59	GLU	CB-CA-C	6.19	122.77	110.40
1	H	59	GLU	CB-CA-C	6.18	122.76	110.40
1	L	266	THR	N-CA-CB	6.18	122.04	110.30
1	M	59	GLU	CB-CA-C	6.18	122.75	110.40
1	L	59	GLU	CB-CA-C	6.17	122.75	110.40
1	H	452	ARG	NE-CZ-NH2	-6.17	117.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	59	GLU	CB-CA-C	6.17	122.73	110.40
1	J	266	THR	N-CA-CB	6.16	122.01	110.30
1	C	153	ASN	N-CA-CB	6.14	121.66	110.60
1	A	153	ASN	N-CA-CB	6.13	121.64	110.60
1	G	153	ASN	N-CA-CB	6.13	121.64	110.60
1	E	153	ASN	N-CA-CB	6.13	121.63	110.60
1	I	197	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	M	452	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	312	ALA	CB-CA-C	6.09	119.24	110.10
1	N	452	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	312	ALA	CB-CA-C	6.08	119.22	110.10
1	E	312	ALA	CB-CA-C	6.08	119.22	110.10
1	F	312	ALA	CB-CA-C	6.08	119.21	110.10
1	A	312	ALA	CB-CA-C	6.07	119.20	110.10
1	G	312	ALA	CB-CA-C	6.07	119.20	110.10
1	D	312	ALA	CB-CA-C	6.06	119.19	110.10
1	H	482	THR	N-CA-CB	6.05	121.80	110.30
1	K	482	THR	N-CA-CB	6.05	121.80	110.30
1	M	482	THR	N-CA-CB	6.05	121.80	110.30
1	N	482	THR	N-CA-CB	6.05	121.80	110.30
1	E	231	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	J	482	THR	N-CA-CB	6.05	121.79	110.30
1	L	482	THR	N-CA-CB	6.05	121.79	110.30
1	N	197	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	F	231	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	87	ASP	N-CA-CB	6.03	121.46	110.60
1	H	197	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	I	452	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	I	482	THR	N-CA-CB	6.02	121.74	110.30
1	M	197	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	231	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	M	239	ALA	CB-CA-C	6.01	119.11	110.10
1	J	452	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	L	452	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	I	363	GLU	CB-CA-C	5.99	122.39	110.40
1	A	58	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	J	363	GLU	CB-CA-C	5.99	122.38	110.40
1	D	231	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	J	197	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	E	402	ALA	N-CA-CB	-5.98	101.73	110.10
1	I	197	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	231	ARG	NE-CZ-NH1	5.97	123.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	363	GLU	CB-CA-C	5.97	122.34	110.40
1	G	402	ALA	N-CA-CB	-5.97	101.75	110.10
1	L	363	GLU	CB-CA-C	5.97	122.33	110.40
1	B	402	ALA	N-CA-CB	-5.96	101.75	110.10
1	A	402	ALA	N-CA-CB	-5.96	101.75	110.10
1	D	402	ALA	N-CA-CB	-5.96	101.75	110.10
1	M	363	GLU	CB-CA-C	5.96	122.33	110.40
1	I	368	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	K	363	GLU	CB-CA-C	5.96	122.32	110.40
1	K	452	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	N	363	GLU	CB-CA-C	5.96	122.32	110.40
1	F	402	ALA	N-CA-CB	-5.95	101.76	110.10
1	A	371	LYS	CB-CA-C	5.95	122.30	110.40
1	C	402	ALA	N-CA-CB	-5.95	101.77	110.10
1	F	371	LYS	CB-CA-C	5.95	122.30	110.40
1	B	371	LYS	CB-CA-C	5.95	122.29	110.40
1	M	379	ILE	CB-CA-C	-5.95	99.71	111.60
1	H	379	ILE	CB-CA-C	-5.95	99.71	111.60
1	C	371	LYS	CB-CA-C	5.94	122.29	110.40
1	G	34	LYS	CB-CA-C	5.94	122.29	110.40
1	G	231	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	G	371	LYS	CB-CA-C	5.94	122.29	110.40
1	N	252	GLU	CB-CA-C	-5.94	98.51	110.40
1	E	371	LYS	CB-CA-C	5.94	122.28	110.40
1	J	379	ILE	CB-CA-C	-5.94	99.72	111.60
1	I	379	ILE	CB-CA-C	-5.94	99.72	111.60
1	F	34	LYS	CB-CA-C	5.94	122.27	110.40
1	L	252	GLU	CB-CA-C	-5.94	98.53	110.40
1	D	371	LYS	CB-CA-C	5.93	122.27	110.40
1	E	34	LYS	CB-CA-C	5.93	122.27	110.40
1	J	368	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	L	197	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	M	252	GLU	CB-CA-C	-5.93	98.53	110.40
1	A	34	LYS	CB-CA-C	5.93	122.27	110.40
1	B	231	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	D	34	LYS	CB-CA-C	5.93	122.27	110.40
1	K	379	ILE	CB-CA-C	-5.93	99.73	111.60
1	L	239	ALA	CB-CA-C	5.93	119.00	110.10
1	L	379	ILE	CB-CA-C	-5.93	99.74	111.60
1	G	58	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	N	379	ILE	CB-CA-C	-5.93	99.75	111.60
1	C	34	LYS	CB-CA-C	5.92	122.25	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	368	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	34	LYS	CB-CA-C	5.91	122.23	110.40
1	N	239	ALA	CB-CA-C	5.91	118.97	110.10
1	H	239	ALA	CB-CA-C	5.91	118.97	110.10
1	J	239	ALA	CB-CA-C	5.90	118.95	110.10
1	H	368	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	I	239	ALA	CB-CA-C	5.89	118.93	110.10
1	N	40	LEU	CB-CA-C	-5.88	99.02	110.20
1	K	40	LEU	CB-CA-C	-5.88	99.02	110.20
1	N	368	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	M	368	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	L	40	LEU	CB-CA-C	-5.88	99.04	110.20
1	H	40	LEU	CB-CA-C	-5.87	99.04	110.20
1	I	40	LEU	CB-CA-C	-5.87	99.05	110.20
1	M	40	LEU	CB-CA-C	-5.87	99.05	110.20
1	J	40	LEU	CB-CA-C	-5.87	99.05	110.20
1	K	368	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	40	LEU	CB-CA-C	-5.86	99.07	110.20
1	E	40	LEU	CB-CA-C	-5.86	99.07	110.20
1	F	11	ASP	O-C-N	-5.86	113.33	122.70
1	C	11	ASP	O-C-N	-5.85	113.33	122.70
1	B	40	LEU	CB-CA-C	-5.85	99.08	110.20
1	F	58	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	G	40	LEU	CB-CA-C	-5.85	99.08	110.20
1	N	208	PRO	N-CA-CB	-5.85	96.16	102.60
1	B	11	ASP	O-C-N	-5.85	113.34	122.70
1	C	40	LEU	CB-CA-C	-5.85	99.09	110.20
1	J	13	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	11	ASP	O-C-N	-5.84	113.35	122.70
1	D	40	LEU	CB-CA-C	-5.84	99.09	110.20
1	G	11	ASP	O-C-N	-5.84	113.35	122.70
1	D	11	ASP	O-C-N	-5.84	113.35	122.70
1	E	11	ASP	O-C-N	-5.84	113.35	122.70
1	E	58	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	F	40	LEU	CB-CA-C	-5.84	99.11	110.20
1	K	197	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	C	58	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	N	6	VAL	CB-CA-C	-5.82	100.34	111.40
1	I	6	VAL	CB-CA-C	-5.82	100.35	111.40
1	F	457	ASN	CB-CA-C	5.81	122.03	110.40
1	C	452	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	H	6	VAL	CB-CA-C	-5.81	100.36	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	457	ASN	CB-CA-C	5.81	122.02	110.40
1	L	6	VAL	CB-CA-C	-5.81	100.37	111.40
1	E	197	ARG	CB-CA-C	5.81	122.01	110.40
1	K	6	VAL	CB-CA-C	-5.80	100.37	111.40
1	M	6	VAL	CB-CA-C	-5.80	100.37	111.40
1	J	6	VAL	CB-CA-C	-5.80	100.38	111.40
1	J	401	HIS	CA-CB-CG	5.80	123.46	113.60
1	L	401	HIS	CA-CB-CG	5.80	123.46	113.60
1	H	334	ASP	CB-CA-C	5.80	122.00	110.40
1	D	197	ARG	CB-CA-C	5.80	122.00	110.40
1	G	197	ARG	CB-CA-C	5.80	122.00	110.40
1	K	334	ASP	CB-CA-C	5.80	122.00	110.40
1	A	197	ARG	CB-CA-C	5.80	122.00	110.40
1	K	401	HIS	CA-CB-CG	5.80	123.45	113.60
1	C	197	ARG	CB-CA-C	5.79	121.98	110.40
1	N	401	HIS	CA-CB-CG	5.79	123.44	113.60
1	J	334	ASP	CB-CA-C	5.79	121.98	110.40
1	M	401	HIS	CA-CB-CG	5.79	123.44	113.60
1	B	197	ARG	CB-CA-C	5.79	121.97	110.40
1	I	401	HIS	CA-CB-CG	5.79	123.44	113.60
1	F	197	ARG	CB-CA-C	5.78	121.97	110.40
1	H	401	HIS	CA-CB-CG	5.78	123.43	113.60
1	I	334	ASP	CB-CA-C	5.78	121.97	110.40
1	G	452	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	L	334	ASP	CB-CA-C	5.78	121.96	110.40
1	M	334	ASP	CB-CA-C	5.78	121.96	110.40
1	G	296	THR	CA-CB-CG2	-5.77	104.33	112.40
1	N	334	ASP	CB-CA-C	5.76	121.93	110.40
1	F	452	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	296	THR	CA-CB-CG2	-5.76	104.34	112.40
1	E	296	THR	CA-CB-CG2	-5.76	104.34	112.40
1	L	520	MET	N-CA-CB	5.76	120.96	110.60
1	M	520	MET	N-CA-CB	5.75	120.95	110.60
1	E	452	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	296	THR	CA-CB-CG2	-5.75	104.36	112.40
1	N	520	MET	N-CA-CB	5.74	120.94	110.60
1	A	452	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	H	520	MET	N-CA-CB	5.74	120.93	110.60
1	D	58	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	J	520	MET	N-CA-CB	5.74	120.92	110.60
1	D	296	THR	CA-CB-CG2	-5.73	104.38	112.40
1	I	520	MET	N-CA-CB	5.73	120.91	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	520	MET	N-CA-CB	5.73	120.91	110.60
1	C	445	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	277	LYS	CB-CA-C	-5.71	98.97	110.40
1	F	296	THR	CA-CB-CG2	-5.71	104.40	112.40
1	G	445	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	58	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	277	LYS	CB-CA-C	-5.71	98.98	110.40
1	B	296	THR	CA-CB-CG2	-5.71	104.40	112.40
1	D	452	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	E	277	LYS	CB-CA-C	-5.71	98.98	110.40
1	F	445	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	C	277	LYS	CB-CA-C	-5.71	98.98	110.40
1	G	277	LYS	CB-CA-C	-5.71	98.99	110.40
1	D	277	LYS	CB-CA-C	-5.70	99.00	110.40
1	J	87	ASP	CB-CG-OD2	5.70	123.43	118.30
1	M	197	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	F	277	LYS	CB-CA-C	-5.70	99.01	110.40
1	D	411	VAL	CB-CA-C	-5.69	100.60	111.40
1	F	80	LYS	CB-CA-C	5.68	121.77	110.40
1	F	411	VAL	CB-CA-C	-5.68	100.61	111.40
1	G	80	LYS	CB-CA-C	5.68	121.77	110.40
1	G	411	VAL	CB-CA-C	-5.68	100.60	111.40
1	J	228	SER	N-CA-CB	5.68	119.02	110.50
1	H	87	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	80	LYS	CB-CA-C	5.68	121.76	110.40
1	A	411	VAL	CB-CA-C	-5.68	100.61	111.40
1	E	80	LYS	CB-CA-C	5.68	121.76	110.40
1	B	80	LYS	CB-CA-C	5.67	121.75	110.40
1	C	80	LYS	CB-CA-C	5.67	121.75	110.40
1	E	411	VAL	CB-CA-C	-5.67	100.62	111.40
1	A	445	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	452	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	411	VAL	CB-CA-C	-5.67	100.63	111.40
1	B	445	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	445	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	G	457	ASN	CB-CA-C	5.67	121.74	110.40
1	D	80	LYS	CB-CA-C	5.67	121.74	110.40
1	C	411	VAL	CB-CA-C	-5.67	100.63	111.40
1	K	197	ARG	CB-CA-C	5.67	121.73	110.40
1	M	197	ARG	CB-CA-C	5.66	121.73	110.40
1	I	87	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	457	ASN	CB-CA-C	5.66	121.72	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	457	ASN	CB-CA-C	5.66	121.72	110.40
1	K	87	ASP	CB-CG-OD2	5.66	123.39	118.30
1	N	197	ARG	CB-CA-C	5.66	121.72	110.40
1	H	236	VAL	CA-CB-CG1	-5.66	102.42	110.90
1	E	457	ASN	CB-CA-C	5.65	121.71	110.40
1	J	236	VAL	CA-CB-CG1	-5.65	102.42	110.90
1	E	445	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	G	200	LEU	CA-CB-CG	-5.65	102.30	115.30
1	L	236	VAL	CA-CB-CG1	-5.65	102.43	110.90
1	M	236	VAL	CA-CB-CG1	-5.65	102.42	110.90
1	J	197	ARG	CB-CA-C	5.65	121.70	110.40
1	I	87	ASP	OD1-CG-OD2	-5.65	112.57	123.30
1	H	197	ARG	CB-CA-C	5.65	121.69	110.40
1	L	87	ASP	OD1-CG-OD2	-5.65	112.57	123.30
1	M	87	ASP	CB-CG-OD2	5.65	123.38	118.30
1	H	87	ASP	OD1-CG-OD2	-5.64	112.58	123.30
1	I	236	VAL	CA-CB-CG1	-5.64	102.44	110.90
1	L	87	ASP	CB-CG-OD2	5.64	123.38	118.30
1	L	197	ARG	CB-CA-C	5.64	121.68	110.40
1	K	311	LYS	CB-CA-C	5.64	121.68	110.40
1	H	368	ARG	CB-CA-C	-5.63	99.13	110.40
1	J	87	ASP	OD1-CG-OD2	-5.63	112.60	123.30
1	I	197	ARG	CB-CA-C	5.63	121.66	110.40
1	K	87	ASP	OD1-CG-OD2	-5.63	112.60	123.30
1	B	457	ASN	CB-CA-C	5.63	121.66	110.40
1	K	368	ARG	CB-CA-C	-5.63	99.14	110.40
1	M	368	ARG	CB-CA-C	-5.63	99.14	110.40
1	N	368	ARG	CB-CA-C	-5.63	99.15	110.40
1	H	311	LYS	CB-CA-C	5.62	121.65	110.40
1	I	36	ARG	N-CA-CB	5.62	120.72	110.60
1	M	87	ASP	OD1-CG-OD2	-5.62	112.61	123.30
1	L	368	ARG	CB-CA-C	-5.62	99.17	110.40
1	K	236	VAL	CA-CB-CG1	-5.62	102.48	110.90
1	H	197	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	N	87	ASP	CB-CG-OD2	5.61	123.35	118.30
1	N	87	ASP	OD1-CG-OD2	-5.61	112.64	123.30
1	K	36	ARG	N-CA-CB	5.61	120.69	110.60
1	L	13	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	N	236	VAL	CA-CB-CG1	-5.60	102.50	110.90
1	J	368	ARG	CB-CA-C	-5.60	99.20	110.40
1	J	445	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	I	368	ARG	CB-CA-C	-5.59	99.22	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	36	ARG	N-CA-CB	5.59	120.66	110.60
1	H	36	ARG	N-CA-CB	5.59	120.65	110.60
1	I	445	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	N	36	ARG	N-CA-CB	5.57	120.63	110.60
1	K	239	ALA	CB-CA-C	5.57	118.45	110.10
1	L	36	ARG	N-CA-CB	5.57	120.62	110.60
1	L	87	ASP	CB-CG-OD1	5.57	123.31	118.30
1	L	197	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	N	208	PRO	CA-C-O	-5.55	106.87	120.20
1	M	36	ARG	N-CA-CB	5.55	120.59	110.60
1	N	197	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	M	311	LYS	CB-CA-C	5.54	121.49	110.40
1	L	311	LYS	CB-CA-C	5.54	121.48	110.40
1	D	285	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	I	87	ASP	CB-CG-OD1	5.54	123.29	118.30
1	D	87	ASP	CB-CG-OD2	5.53	123.28	118.30
1	N	311	LYS	CB-CA-C	5.53	121.46	110.40
1	L	445	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	F	87	ASP	CB-CG-OD2	5.52	123.27	118.30
1	D	87	ASP	OD1-CG-OD2	-5.51	112.82	123.30
1	B	87	ASP	CB-CG-OD1	5.51	123.26	118.30
1	N	87	ASP	CB-CG-OD1	5.51	123.26	118.30
1	F	87	ASP	OD1-CG-OD2	-5.51	112.83	123.30
1	E	87	ASP	CB-CG-OD1	5.51	123.26	118.30
1	K	87	ASP	CB-CG-OD1	5.50	123.25	118.30
1	E	46	ALA	N-CA-CB	-5.50	102.40	110.10
1	B	285	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	E	87	ASP	OD1-CG-OD2	-5.50	112.85	123.30
1	D	46	ALA	N-CA-CB	-5.50	102.41	110.10
1	F	46	ALA	N-CA-CB	-5.49	102.41	110.10
1	H	87	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	46	ALA	N-CA-CB	-5.49	102.41	110.10
1	M	87	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	46	ALA	N-CA-CB	-5.49	102.42	110.10
1	J	311	LYS	CB-CA-C	5.49	121.38	110.40
1	C	46	ALA	N-CA-CB	-5.48	102.43	110.10
1	F	285	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	G	46	ALA	N-CA-CB	-5.48	102.43	110.10
1	H	228	SER	N-CA-CB	5.48	118.72	110.50
1	J	87	ASP	CB-CG-OD1	5.48	123.23	118.30
1	H	239	ALA	N-CA-CB	-5.47	102.44	110.10
1	I	311	LYS	CB-CA-C	5.47	121.35	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	156	GLU	CB-CA-C	-5.46	99.49	110.40
1	E	251	ALA	CB-CA-C	-5.46	101.92	110.10
1	A	156	GLU	CB-CA-C	-5.45	99.50	110.40
1	C	156	GLU	CB-CA-C	-5.45	99.50	110.40
1	G	251	ALA	CB-CA-C	-5.45	101.92	110.10
1	C	87	ASP	OD1-CG-OD2	-5.45	112.95	123.30
1	G	156	GLU	CB-CA-C	-5.45	99.50	110.40
1	B	87	ASP	OD1-CG-OD2	-5.45	112.95	123.30
1	G	87	ASP	OD1-CG-OD2	-5.44	112.96	123.30
1	C	251	ALA	CB-CA-C	-5.44	101.94	110.10
1	D	251	ALA	CB-CA-C	-5.44	101.94	110.10
1	G	87	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	87	ASP	OD1-CG-OD2	-5.44	112.97	123.30
1	K	13	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	87	ASP	CB-CG-OD1	5.43	123.19	118.30
1	F	156	GLU	CB-CA-C	-5.43	99.53	110.40
1	I	239	ALA	N-CA-CB	-5.43	102.50	110.10
1	F	251	ALA	CB-CA-C	-5.43	101.95	110.10
1	L	239	ALA	N-CA-CB	-5.43	102.50	110.10
1	A	251	ALA	CB-CA-C	-5.43	101.96	110.10
1	K	197	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	285	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	251	ALA	CB-CA-C	-5.42	101.96	110.10
1	D	87	ASP	CB-CG-OD1	5.42	123.18	118.30
1	G	285	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	18	ARG	CD-NE-CZ	5.42	131.19	123.60
1	E	87	ASP	CB-CG-OD2	5.42	123.18	118.30
1	F	345	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	N	445	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	18	ARG	CD-NE-CZ	5.42	131.18	123.60
1	C	285	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	D	156	GLU	CB-CA-C	-5.42	99.57	110.40
1	E	18	ARG	CD-NE-CZ	5.41	131.18	123.60
1	A	18	ARG	CD-NE-CZ	5.41	131.18	123.60
1	F	140	ASP	N-CA-CB	-5.41	100.87	110.60
1	J	239	ALA	N-CA-CB	-5.41	102.53	110.10
1	B	156	GLU	CB-CA-C	-5.41	99.59	110.40
1	F	87	ASP	CB-CG-OD1	5.41	123.17	118.30
1	M	239	ALA	N-CA-CB	-5.41	102.53	110.10
1	B	140	ASP	N-CA-CB	-5.40	100.88	110.60
1	C	140	ASP	N-CA-CB	-5.40	100.88	110.60
1	A	140	ASP	N-CA-CB	-5.40	100.88	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	499	VAL	CG1-CB-CG2	-5.40	102.26	110.90
1	A	87	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	345	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	345	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	G	18	ARG	CD-NE-CZ	5.40	131.16	123.60
1	K	228	SER	N-CA-CB	5.40	118.59	110.50
1	N	239	ALA	N-CA-CB	-5.40	102.54	110.10
1	D	18	ARG	CD-NE-CZ	5.39	131.15	123.60
1	E	140	ASP	N-CA-CB	-5.39	100.89	110.60
1	G	200	LEU	CD1-CG-CD2	5.39	126.68	110.50
1	K	499	VAL	CG1-CB-CG2	-5.39	102.27	110.90
1	M	499	VAL	CG1-CB-CG2	-5.39	102.27	110.90
1	D	140	ASP	N-CA-CB	-5.39	100.89	110.60
1	F	18	ARG	CD-NE-CZ	5.39	131.15	123.60
1	E	285	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	N	296	THR	N-CA-CB	5.39	120.54	110.30
1	B	254	VAL	CB-CA-C	-5.38	101.17	111.40
1	N	411	VAL	CB-CA-C	-5.38	101.17	111.40
1	G	140	ASP	N-CA-CB	-5.38	100.91	110.60
1	I	411	VAL	CB-CA-C	-5.38	101.18	111.40
1	L	296	THR	N-CA-CB	5.38	120.52	110.30
1	M	445	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	H	296	THR	N-CA-CB	5.38	120.52	110.30
1	J	296	THR	N-CA-CB	5.38	120.52	110.30
1	K	296	THR	N-CA-CB	5.38	120.51	110.30
1	M	296	THR	N-CA-CB	5.38	120.51	110.30
1	A	254	VAL	CB-CA-C	-5.37	101.19	111.40
1	D	401	HIS	CA-CB-CG	5.37	122.74	113.60
1	I	296	THR	N-CA-CB	5.37	120.51	110.30
1	A	87	ASP	CB-CG-OD2	5.37	123.13	118.30
1	E	254	VAL	CB-CA-C	-5.37	101.20	111.40
1	C	254	VAL	CB-CA-C	-5.37	101.20	111.40
1	L	499	VAL	CG1-CB-CG2	-5.37	102.31	110.90
1	C	87	ASP	CB-CG-OD2	5.37	123.13	118.30
1	G	254	VAL	CB-CA-C	-5.36	101.21	111.40
1	J	188	ASP	CB-CG-OD1	5.36	123.13	118.30
1	L	188	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	254	VAL	CB-CA-C	-5.36	101.21	111.40
1	F	254	VAL	CB-CA-C	-5.36	101.22	111.40
1	F	401	HIS	CA-CB-CG	5.36	122.71	113.60
1	J	499	VAL	CG1-CB-CG2	-5.36	102.33	110.90
1	H	445	ARG	NE-CZ-NH1	5.36	122.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	153	ASN	CA-CB-CG	5.36	125.18	113.40
1	B	401	HIS	CA-CB-CG	5.35	122.70	113.60
1	G	87	ASP	CB-CG-OD2	5.35	123.12	118.30
1	D	345	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	D	381	VAL	CA-CB-CG2	-5.35	102.87	110.90
1	E	401	HIS	CA-CB-CG	5.35	122.70	113.60
1	M	231	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	N	228	SER	N-CA-CB	5.35	118.53	110.50
1	I	153	ASN	CA-CB-CG	5.35	125.17	113.40
1	L	153	ASN	CA-CB-CG	5.35	125.17	113.40
1	A	401	HIS	CA-CB-CG	5.35	122.69	113.60
1	B	381	VAL	CA-CB-CG2	-5.35	102.88	110.90
1	C	381	VAL	CA-CB-CG2	-5.35	102.88	110.90
1	E	345	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	H	153	ASN	CA-CB-CG	5.35	125.16	113.40
1	A	272	LYS	N-CA-CB	-5.34	100.99	110.60
1	I	499	VAL	CG1-CB-CG2	-5.34	102.35	110.90
1	C	401	HIS	CA-CB-CG	5.34	122.67	113.60
1	J	153	ASN	CA-CB-CG	5.34	125.14	113.40
1	E	272	LYS	N-CA-CB	-5.33	101.00	110.60
1	G	401	HIS	CA-CB-CG	5.33	122.67	113.60
1	F	272	LYS	N-CA-CB	-5.33	101.00	110.60
1	G	272	LYS	N-CA-CB	-5.33	101.00	110.60
1	H	188	ASP	CB-CG-OD1	5.33	123.10	118.30
1	K	445	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	M	153	ASN	CA-CB-CG	5.33	125.13	113.40
1	D	272	LYS	N-CA-CB	-5.33	101.01	110.60
1	N	499	VAL	CG1-CB-CG2	-5.33	102.38	110.90
1	N	153	ASN	CA-CB-CG	5.33	125.12	113.40
1	A	381	VAL	CA-CB-CG2	-5.33	102.91	110.90
1	B	272	LYS	N-CA-CB	-5.33	101.02	110.60
1	E	381	VAL	CA-CB-CG2	-5.33	102.91	110.90
1	G	345	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	I	188	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	345	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	272	LYS	N-CA-CB	-5.32	101.03	110.60
1	K	188	ASP	CB-CG-OD1	5.32	123.09	118.30
1	N	188	ASP	CB-CG-OD1	5.32	123.08	118.30
1	F	381	VAL	CA-CB-CG2	-5.31	102.93	110.90
1	G	381	VAL	CA-CB-CG2	-5.31	102.93	110.90
1	I	228	SER	N-CA-CB	5.31	118.46	110.50
1	H	310	GLU	CA-CB-CG	5.30	125.06	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	13	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	K	310	GLU	CA-CB-CG	5.30	125.06	113.40
1	G	473	ASP	N-CA-CB	5.30	120.14	110.60
1	C	359	ASP	CA-CB-CG	-5.30	101.75	113.40
1	G	359	ASP	CA-CB-CG	-5.30	101.75	113.40
1	K	239	ALA	N-CA-CB	-5.29	102.69	110.10
1	A	473	ASP	N-CA-CB	5.29	120.12	110.60
1	F	359	ASP	CA-CB-CG	-5.29	101.77	113.40
1	F	473	ASP	N-CA-CB	5.29	120.11	110.60
1	L	254	VAL	CG1-CB-CG2	-5.29	102.44	110.90
1	A	359	ASP	CA-CB-CG	-5.28	101.78	113.40
1	B	473	ASP	N-CA-CB	5.28	120.11	110.60
1	D	359	ASP	CA-CB-CG	-5.28	101.78	113.40
1	E	359	ASP	CA-CB-CG	-5.28	101.78	113.40
1	N	52	ASP	CA-CB-CG	-5.28	101.78	113.40
1	B	359	ASP	CA-CB-CG	-5.28	101.78	113.40
1	D	473	ASP	N-CA-CB	5.28	120.10	110.60
1	H	317	LEU	CB-CA-C	-5.28	100.17	110.20
1	K	52	ASP	CA-CB-CG	-5.28	101.78	113.40
1	M	52	ASP	CA-CB-CG	-5.28	101.78	113.40
1	J	317	LEU	CB-CA-C	-5.28	100.17	110.20
1	C	473	ASP	N-CA-CB	5.28	120.10	110.60
1	H	52	ASP	CA-CB-CG	-5.28	101.79	113.40
1	E	473	ASP	N-CA-CB	5.28	120.10	110.60
1	G	199	TYR	O-C-N	-5.27	114.27	122.70
1	L	52	ASP	CA-CB-CG	-5.27	101.81	113.40
1	J	52	ASP	CA-CB-CG	-5.26	101.82	113.40
1	N	310	GLU	CA-CB-CG	5.26	124.97	113.40
1	G	73	MET	CB-CA-C	-5.26	99.88	110.40
1	I	52	ASP	CA-CB-CG	-5.26	101.83	113.40
1	M	390	LYS	CB-CA-C	5.26	120.92	110.40
1	N	254	VAL	CG1-CB-CG2	-5.26	102.49	110.90
1	I	390	LYS	CB-CA-C	5.26	120.91	110.40
1	D	73	MET	CB-CA-C	-5.25	99.89	110.40
1	A	73	MET	CB-CA-C	-5.25	99.90	110.40
1	J	390	LYS	CB-CA-C	5.25	120.90	110.40
1	H	254	VAL	CG1-CB-CG2	-5.25	102.50	110.90
1	I	317	LEU	CB-CA-C	-5.25	100.23	110.20
1	H	390	LYS	CB-CA-C	5.24	120.89	110.40
1	M	254	VAL	CG1-CB-CG2	-5.24	102.51	110.90
1	K	317	LEU	CB-CA-C	-5.24	100.24	110.20
1	B	73	MET	CB-CA-C	-5.24	99.92	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	73	MET	CB-CA-C	-5.24	99.92	110.40
1	L	390	LYS	CB-CA-C	5.24	120.88	110.40
1	N	390	LYS	CB-CA-C	5.24	120.88	110.40
1	C	73	MET	CB-CA-C	-5.24	99.92	110.40
1	H	371	LYS	N-CA-CB	-5.24	101.17	110.60
1	K	254	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	F	73	MET	CB-CA-C	-5.24	99.93	110.40
1	K	390	LYS	CB-CA-C	5.24	120.87	110.40
1	M	317	LEU	CB-CA-C	-5.24	100.25	110.20
1	K	371	LYS	N-CA-CB	-5.23	101.18	110.60
1	M	371	LYS	N-CA-CB	-5.23	101.18	110.60
1	M	310	GLU	CA-CB-CG	5.23	124.91	113.40
1	J	371	LYS	N-CA-CB	-5.23	101.19	110.60
1	H	13	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	G	277	LYS	CA-CB-CG	5.22	124.89	113.40
1	B	230	ILE	CA-C-N	-5.22	105.72	117.20
1	L	317	LEU	CB-CA-C	-5.22	100.28	110.20
1	D	230	ILE	CA-C-N	-5.22	105.72	117.20
1	N	371	LYS	N-CA-CB	-5.22	101.21	110.60
1	L	371	LYS	N-CA-CB	-5.21	101.21	110.60
1	B	277	LYS	CA-CB-CG	5.21	124.87	113.40
1	C	277	LYS	CA-CB-CG	5.21	124.87	113.40
1	A	230	ILE	CA-C-N	-5.21	105.73	117.20
1	G	230	ILE	CA-C-N	-5.21	105.73	117.20
1	F	230	ILE	CA-C-N	-5.21	105.74	117.20
1	D	277	LYS	CA-CB-CG	5.21	124.86	113.40
1	I	254	VAL	CG1-CB-CG2	-5.21	102.56	110.90
1	A	277	LYS	CA-CB-CG	5.21	124.85	113.40
1	E	230	ILE	CA-C-N	-5.21	105.74	117.20
1	F	277	LYS	CA-CB-CG	5.21	124.86	113.40
1	I	371	LYS	N-CA-CB	-5.21	101.23	110.60
1	C	230	ILE	CA-C-N	-5.20	105.76	117.20
1	N	13	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	E	277	LYS	CA-CB-CG	5.20	124.83	113.40
1	A	194	GLN	N-CA-CB	-5.20	101.25	110.60
1	E	194	GLN	N-CA-CB	-5.20	101.25	110.60
1	G	194	GLN	N-CA-CB	-5.19	101.25	110.60
1	D	194	GLN	N-CA-CB	-5.19	101.26	110.60
1	J	310	GLU	CA-CB-CG	5.19	124.81	113.40
1	L	255	GLU	N-CA-CB	5.19	119.94	110.60
1	L	310	GLU	CA-CB-CG	5.19	124.81	113.40
1	B	87	ASP	CB-CG-OD2	5.18	122.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	194	GLN	N-CA-CB	-5.18	101.27	110.60
1	F	194	GLN	N-CA-CB	-5.18	101.27	110.60
1	J	254	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	I	389	MET	CB-CA-C	5.18	120.76	110.40
1	N	389	MET	CB-CA-C	5.17	120.75	110.40
1	J	389	MET	CB-CA-C	5.17	120.74	110.40
1	L	389	MET	CB-CA-C	5.17	120.74	110.40
1	K	389	MET	CB-CA-C	5.17	120.73	110.40
1	M	389	MET	CB-CA-C	5.17	120.73	110.40
1	H	389	MET	CB-CA-C	5.16	120.73	110.40
1	I	310	GLU	CA-CB-CG	5.16	124.76	113.40
1	B	153	ASN	N-CA-CB	5.15	119.88	110.60
1	F	324	VAL	N-CA-CB	-5.13	100.20	111.50
1	G	324	VAL	N-CA-CB	-5.13	100.21	111.50
1	E	324	VAL	N-CA-CB	-5.13	100.22	111.50
1	A	324	VAL	N-CA-CB	-5.12	100.23	111.50
1	C	304	GLU	CB-CA-C	-5.12	100.16	110.40
1	C	324	VAL	N-CA-CB	-5.12	100.23	111.50
1	D	324	VAL	N-CA-CB	-5.12	100.23	111.50
1	L	228	SER	N-CA-CB	5.12	118.18	110.50
1	B	324	VAL	N-CA-CB	-5.12	100.24	111.50
1	G	304	GLU	CB-CA-C	-5.12	100.17	110.40
1	I	268	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	304	GLU	CB-CA-C	-5.11	100.17	110.40
1	E	304	GLU	CB-CA-C	-5.11	100.17	110.40
1	A	304	GLU	CB-CA-C	-5.10	100.20	110.40
1	D	36	ARG	C-N-CA	5.10	134.45	121.70
1	B	304	GLU	CB-CA-C	-5.10	100.20	110.40
1	F	304	GLU	CB-CA-C	-5.10	100.21	110.40
1	F	36	ARG	C-N-CA	5.09	134.43	121.70
1	B	36	ARG	C-N-CA	5.09	134.43	121.70
1	N	317	LEU	CB-CA-C	-5.09	100.53	110.20
1	C	36	ARG	C-N-CA	5.09	134.42	121.70
1	E	36	ARG	C-N-CA	5.09	134.42	121.70
1	M	13	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	J	523	ASP	N-CA-CB	5.08	119.74	110.60
1	A	36	ARG	C-N-CA	5.07	134.39	121.70
1	I	523	ASP	N-CA-CB	5.07	119.72	110.60
1	L	523	ASP	N-CA-CB	5.07	119.72	110.60
1	G	36	ARG	C-N-CA	5.06	134.36	121.70
1	N	523	ASP	N-CA-CB	5.06	119.71	110.60
1	M	523	ASP	N-CA-CB	5.06	119.71	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	523	ASP	N-CA-CB	5.05	119.70	110.60
1	H	523	ASP	N-CA-CB	5.05	119.68	110.60
1	C	461	GLU	CB-CA-C	5.03	120.46	110.40
1	B	461	GLU	CB-CA-C	5.02	120.44	110.40
1	J	361	ASP	CB-CA-C	5.02	120.44	110.40
1	I	361	ASP	CB-CA-C	5.01	120.43	110.40
1	H	361	ASP	CB-CA-C	5.01	120.41	110.40
1	L	369	VAL	N-CA-CB	5.00	122.50	111.50
1	N	361	ASP	CB-CA-C	5.00	120.40	110.40

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	37	ASN	CA
1	I	37	ASN	CA
1	J	37	ASN	CA
1	K	37	ASN	CA
1	L	37	ASN	CA
1	M	37	ASN	CA
1	N	37	ASN	CA

All (231) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Sidechain
1	A	18	ARG	Sidechain
1	A	190	VAL	Peptide
1	A	193	MET	Mainchain
1	A	196	ASP	Peptide
1	A	197	ARG	Mainchain,Peptide
1	A	231	ARG	Sidechain
1	A	255	GLU	Peptide
1	A	281	PHE	Peptide
1	A	284	ARG	Sidechain
1	A	285	ARG	Sidechain
1	A	29	VAL	Mainchain
1	A	296	THR	Peptide
1	A	325	ILE	Peptide
1	A	329	THR	Peptide
1	A	368	ARG	Sidechain
1	A	404	ARG	Sidechain
1	A	52	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	B	13	ARG	Sidechain
1	B	18	ARG	Sidechain
1	B	190	VAL	Peptide
1	B	196	ASP	Peptide
1	B	197	ARG	Mainchain,Peptide
1	B	231	ARG	Sidechain
1	B	255	GLU	Peptide
1	B	281	PHE	Peptide
1	B	284	ARG	Sidechain
1	B	285	ARG	Sidechain
1	B	29	VAL	Mainchain
1	B	296	THR	Peptide
1	B	325	ILE	Peptide
1	B	329	THR	Peptide
1	B	368	ARG	Sidechain
1	B	404	ARG	Sidechain
1	B	52	ASP	Mainchain
1	C	13	ARG	Sidechain
1	C	18	ARG	Sidechain
1	C	190	VAL	Peptide
1	C	196	ASP	Peptide
1	C	197	ARG	Mainchain,Peptide
1	C	231	ARG	Sidechain
1	C	255	GLU	Peptide
1	C	281	PHE	Peptide
1	C	284	ARG	Sidechain
1	C	285	ARG	Sidechain
1	C	29	VAL	Mainchain
1	C	296	THR	Peptide
1	C	325	ILE	Peptide
1	C	329	THR	Peptide
1	C	368	ARG	Sidechain
1	C	404	ARG	Sidechain
1	C	52	ASP	Mainchain
1	D	13	ARG	Sidechain
1	D	18	ARG	Sidechain
1	D	193	MET	Mainchain
1	D	196	ASP	Peptide
1	D	197	ARG	Mainchain,Peptide
1	D	231	ARG	Sidechain
1	D	255	GLU	Peptide
1	D	281	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	D	284	ARG	Sidechain
1	D	285	ARG	Sidechain
1	D	29	VAL	Mainchain
1	D	296	THR	Peptide
1	D	325	ILE	Peptide
1	D	329	THR	Peptide
1	D	368	ARG	Sidechain
1	D	404	ARG	Sidechain
1	D	52	ASP	Mainchain
1	E	13	ARG	Sidechain
1	E	18	ARG	Sidechain
1	E	190	VAL	Peptide
1	E	193	MET	Mainchain
1	E	196	ASP	Peptide
1	E	197	ARG	Mainchain,Peptide
1	E	231	ARG	Sidechain
1	E	255	GLU	Peptide
1	E	281	PHE	Peptide
1	E	284	ARG	Sidechain
1	E	285	ARG	Sidechain
1	E	29	VAL	Mainchain
1	E	296	THR	Peptide
1	E	325	ILE	Peptide
1	E	329	THR	Peptide
1	E	368	ARG	Sidechain
1	E	404	ARG	Sidechain
1	E	52	ASP	Mainchain
1	F	13	ARG	Sidechain
1	F	18	ARG	Sidechain
1	F	190	VAL	Peptide
1	F	193	MET	Mainchain
1	F	196	ASP	Peptide
1	F	197	ARG	Mainchain,Peptide
1	F	231	ARG	Sidechain
1	F	255	GLU	Peptide
1	F	281	PHE	Peptide
1	F	284	ARG	Sidechain
1	F	285	ARG	Sidechain
1	F	29	VAL	Mainchain
1	F	296	THR	Peptide
1	F	325	ILE	Peptide
1	F	329	THR	Peptide

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Mol	Chain	Res	Type	Group
1	F	368	ARG	Sidechain
1	F	404	ARG	Sidechain
1	F	52	ASP	Mainchain
1	G	13	ARG	Sidechain
1	G	18	ARG	Sidechain
1	G	190	VAL	Peptide
1	G	197	ARG	Mainchain,Peptide
1	G	199	TYR	Mainchain
1	G	231	ARG	Sidechain
1	G	255	GLU	Peptide
1	G	281	PHE	Peptide
1	G	284	ARG	Sidechain
1	G	285	ARG	Sidechain
1	G	29	VAL	Mainchain
1	G	296	THR	Peptide
1	G	325	ILE	Peptide
1	G	329	THR	Peptide
1	G	368	ARG	Sidechain
1	G	404	ARG	Sidechain
1	G	52	ASP	Mainchain
1	H	213	VAL	Mainchain
1	H	219	PHE	Sidechain
1	H	285	ARG	Sidechain
1	H	345	ARG	Sidechain
1	H	350	ARG	Sidechain
1	H	368	ARG	Sidechain
1	H	395	ARG	Sidechain
1	H	404	ARG	Sidechain
1	H	421	ARG	Sidechain
1	H	452	ARG	Sidechain
1	H	50	THR	Peptide
1	H	506	TYR	Sidechain
1	H	58	ARG	Sidechain
1	I	197	ARG	Mainchain
1	I	213	VAL	Mainchain
1	I	219	PHE	Sidechain
1	I	285	ARG	Sidechain
1	I	345	ARG	Sidechain
1	I	350	ARG	Sidechain
1	I	368	ARG	Sidechain
1	I	395	ARG	Sidechain
1	I	404	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	I	421	ARG	Sidechain
1	I	452	ARG	Sidechain
1	I	50	THR	Peptide
1	I	506	TYR	Sidechain
1	I	58	ARG	Sidechain
1	J	197	ARG	Mainchain
1	J	213	VAL	Mainchain
1	J	219	PHE	Sidechain
1	J	285	ARG	Sidechain
1	J	345	ARG	Sidechain
1	J	350	ARG	Sidechain
1	J	368	ARG	Sidechain
1	J	395	ARG	Sidechain
1	J	404	ARG	Sidechain
1	J	421	ARG	Sidechain
1	J	452	ARG	Sidechain
1	J	50	THR	Peptide
1	J	506	TYR	Sidechain
1	J	58	ARG	Sidechain
1	K	18	ARG	Sidechain
1	K	197	ARG	Mainchain
1	K	213	VAL	Mainchain
1	K	219	PHE	Sidechain
1	K	285	ARG	Sidechain
1	K	345	ARG	Sidechain
1	K	350	ARG	Sidechain
1	K	368	ARG	Sidechain
1	K	395	ARG	Sidechain
1	K	404	ARG	Sidechain
1	K	421	ARG	Sidechain
1	K	452	ARG	Sidechain
1	K	50	THR	Peptide
1	K	506	TYR	Sidechain
1	K	58	ARG	Sidechain
1	L	197	ARG	Mainchain
1	L	213	VAL	Mainchain
1	L	219	PHE	Sidechain
1	L	285	ARG	Sidechain
1	L	345	ARG	Sidechain
1	L	350	ARG	Sidechain
1	L	368	ARG	Sidechain
1	L	395	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	L	404	ARG	Sidechain
1	L	421	ARG	Sidechain
1	L	452	ARG	Sidechain
1	L	50	THR	Peptide
1	L	506	TYR	Sidechain
1	L	58	ARG	Sidechain
1	M	197	ARG	Mainchain
1	M	213	VAL	Mainchain
1	M	219	PHE	Sidechain
1	M	285	ARG	Sidechain
1	M	345	ARG	Sidechain
1	M	350	ARG	Sidechain
1	M	368	ARG	Sidechain
1	M	395	ARG	Sidechain
1	M	404	ARG	Sidechain
1	M	421	ARG	Sidechain
1	M	452	ARG	Sidechain
1	M	50	THR	Peptide
1	M	506	TYR	Sidechain
1	M	58	ARG	Sidechain
1	N	197	ARG	Mainchain,Peptide
1	N	206	ASN	Peptide
1	N	207	LYS	Peptide
1	N	208	PRO	Peptide
1	N	213	VAL	Mainchain
1	N	219	PHE	Sidechain
1	N	285	ARG	Sidechain
1	N	345	ARG	Sidechain
1	N	350	ARG	Sidechain
1	N	368	ARG	Sidechain
1	N	395	ARG	Sidechain
1	N	404	ARG	Sidechain
1	N	421	ARG	Sidechain
1	N	452	ARG	Sidechain
1	N	50	THR	Peptide
1	N	506	TYR	Sidechain
1	N	58	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3846	0	3967	219	0
1	B	3845	0	3962	231	0
1	C	3845	0	3962	229	0
1	D	3845	0	3962	233	0
1	E	3845	0	3962	222	0
1	F	3845	0	3962	232	0
1	G	3845	0	3962	228	0
1	H	3845	0	3965	254	0
1	I	3845	0	3965	251	0
1	J	3845	0	3965	259	0
1	K	3845	0	3965	264	0
1	L	3845	0	3965	262	0
1	M	3845	0	3965	258	0
1	N	3845	0	3965	272	0
2	A	1	0	0	3	0
2	B	1	0	0	3	0
2	C	1	0	0	4	0
2	D	1	0	0	3	0
2	E	1	0	0	4	0
2	F	1	0	0	3	0
2	G	1	0	0	3	0
2	H	1	0	0	5	0
2	I	1	0	0	5	0
2	J	1	0	0	5	0
2	K	1	0	0	5	0
2	L	1	0	0	5	0
2	M	1	0	0	5	0
2	N	1	0	0	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	1	0	0	0	0
4	A	31	0	12	2	0
4	B	31	0	12	2	0
4	C	31	0	12	3	0
4	D	31	0	12	2	0
4	E	31	0	12	3	0
4	F	31	0	12	2	0
4	G	31	0	12	2	0
4	H	31	0	12	4	0
4	I	31	0	12	4	0
4	J	31	0	12	5	0
4	K	31	0	12	4	0
4	L	31	0	12	5	0
4	M	31	0	12	5	0
4	N	31	0	12	5	0
All	All	54293	0	55662	3207	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (3207) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:ILE:HD12	1:D:262:LEU:CD1	1.30	1.62
1:C:249:ILE:HD12	1:C:262:LEU:CD1	1.30	1.61
1:E:249:ILE:HD12	1:E:262:LEU:CD1	1.30	1.60
1:B:249:ILE:HD12	1:B:262:LEU:CD1	1.30	1.59
1:A:249:ILE:HD12	1:A:262:LEU:CD1	1.29	1.57
1:M:518:GLU:CA	1:M:518:GLU:CB	1.83	1.57
1:F:249:ILE:HD12	1:F:262:LEU:CD1	1.30	1.57
1:H:518:GLU:CA	1:H:518:GLU:CB	1.83	1.56
1:N:518:GLU:CA	1:N:518:GLU:CB	1.83	1.56
1:G:249:ILE:HD12	1:G:262:LEU:CD1	1.30	1.55
1:I:518:GLU:CB	1:I:518:GLU:CA	1.83	1.55
1:L:518:GLU:CB	1:L:518:GLU:CA	1.83	1.54
1:N:207:LYS:NZ	1:N:207:LYS:CE	1.70	1.53
1:N:208:PRO:CA	1:N:208:PRO:C	1.76	1.51
1:K:518:GLU:CA	1:K:518:GLU:CB	1.83	1.51
1:J:518:GLU:CA	1:J:518:GLU:CB	1.83	1.51
1:F:200:LEU:HD21	1:F:254:VAL:CG2	1.12	1.46
1:D:200:LEU:HD21	1:D:254:VAL:CG2	1.12	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:LEU:HD21	1:E:254:VAL:CG2	1.12	1.45
1:A:200:LEU:HD21	1:A:254:VAL:CG2	1.12	1.44
1:C:200:LEU:HD21	1:C:254:VAL:CG2	1.12	1.42
1:B:200:LEU:HD21	1:B:254:VAL:CG2	1.12	1.42
1:A:200:LEU:CD2	1:A:254:VAL:CG2	1.87	1.41
1:C:200:LEU:CD2	1:C:254:VAL:HG21	1.32	1.40
1:D:200:LEU:CD2	1:D:254:VAL:HG21	1.32	1.39
1:B:200:LEU:CD2	1:B:254:VAL:HG21	1.32	1.39
1:A:200:LEU:CD2	1:A:254:VAL:HG21	1.32	1.37
1:E:200:LEU:CD2	1:E:254:VAL:HG21	1.32	1.36
1:F:200:LEU:CD2	1:F:254:VAL:HG21	1.32	1.35
1:M:23:LEU:CD1	1:M:60:ILE:HD12	1.58	1.34
1:C:249:ILE:CD1	1:C:262:LEU:HD11	1.59	1.33
1:B:249:ILE:CD1	1:B:262:LEU:HD11	1.59	1.33
1:D:249:ILE:CD1	1:D:262:LEU:HD11	1.59	1.33
1:K:23:LEU:CD1	1:K:60:ILE:HD12	1.58	1.32
1:N:23:LEU:CD1	1:N:60:ILE:HD12	1.58	1.32
1:H:23:LEU:CD1	1:H:60:ILE:HD12	1.58	1.32
1:L:23:LEU:CD1	1:L:60:ILE:HD12	1.58	1.32
1:I:233:MET:CE	1:I:249:ILE:HD13	1.60	1.32
1:J:23:LEU:CD1	1:J:60:ILE:HD12	1.58	1.32
1:A:249:ILE:CD1	1:A:262:LEU:HD11	1.58	1.31
1:E:249:ILE:CD1	1:E:262:LEU:HD11	1.59	1.31
1:I:23:LEU:CD1	1:I:60:ILE:HD12	1.58	1.31
1:J:233:MET:CE	1:J:249:ILE:HD13	1.60	1.30
1:F:249:ILE:CD1	1:F:262:LEU:HD11	1.58	1.29
1:G:249:ILE:CD1	1:G:262:LEU:HD11	1.59	1.29
1:D:200:LEU:CD2	1:D:254:VAL:CG2	1.87	1.29
1:M:518:GLU:CB	1:M:518:GLU:C	2.01	1.29
1:L:518:GLU:CB	1:L:518:GLU:C	2.01	1.28
1:K:233:MET:CE	1:K:249:ILE:HD13	1.62	1.28
1:N:233:MET:CE	1:N:249:ILE:HD13	1.63	1.28
1:N:518:GLU:CB	1:N:518:GLU:C	2.01	1.28
1:H:233:MET:CE	1:H:249:ILE:HD13	1.63	1.27
1:I:518:GLU:CB	1:I:518:GLU:C	2.01	1.27
1:L:233:MET:CE	1:L:249:ILE:HD13	1.65	1.27
1:J:518:GLU:CB	1:J:518:GLU:C	2.01	1.26
1:H:518:GLU:CB	1:H:518:GLU:C	2.02	1.26
1:K:518:GLU:CB	1:K:518:GLU:C	2.01	1.25
1:M:233:MET:CE	1:M:249:ILE:HD13	1.66	1.25
1:C:200:LEU:CD2	1:C:254:VAL:CG2	1.87	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:301:ILE:CD1	1:K:312:ALA:HB2	1.69	1.23
1:L:301:ILE:CD1	1:L:312:ALA:HB2	1.69	1.23
1:J:301:ILE:CD1	1:J:312:ALA:HB2	1.69	1.23
1:M:301:ILE:CD1	1:M:312:ALA:HB2	1.69	1.23
1:I:301:ILE:CD1	1:I:312:ALA:HB2	1.69	1.22
1:N:301:ILE:CD1	1:N:312:ALA:HB2	1.68	1.21
1:B:200:LEU:CD2	1:B:254:VAL:CG2	1.87	1.21
1:H:23:LEU:HD12	1:H:60:ILE:CD1	1.71	1.21
1:I:23:LEU:HD12	1:I:60:ILE:CD1	1.71	1.21
1:J:23:LEU:HD12	1:J:60:ILE:CD1	1.71	1.20
1:H:301:ILE:CD1	1:H:312:ALA:HB2	1.69	1.20
1:N:23:LEU:HD12	1:N:60:ILE:CD1	1.71	1.20
1:K:23:LEU:HD12	1:K:60:ILE:CD1	1.71	1.20
1:L:23:LEU:HD12	1:L:60:ILE:CD1	1.71	1.19
1:M:23:LEU:HD12	1:M:60:ILE:CD1	1.71	1.19
1:G:23:LEU:HG	1:G:60:ILE:HD12	1.21	1.18
1:F:23:LEU:HG	1:F:60:ILE:HD12	1.21	1.18
1:C:193:MET:HG2	1:C:295:LEU:HG	1.23	1.18
1:C:249:ILE:HD11	1:C:262:LEU:HD21	1.22	1.17
1:G:249:ILE:HD11	1:G:262:LEU:HD21	1.23	1.17
1:L:37:ASN:N	1:M:518:GLU:HA	1.60	1.17
1:D:249:ILE:HD11	1:D:262:LEU:HD21	1.22	1.17
1:J:37:ASN:N	1:K:518:GLU:HA	1.59	1.17
1:B:249:ILE:HD11	1:B:262:LEU:HD21	1.23	1.16
1:E:249:ILE:CD1	1:E:262:LEU:CD1	2.20	1.16
1:A:249:ILE:HD11	1:A:262:LEU:HD21	1.22	1.16
1:I:37:ASN:N	1:J:518:GLU:HA	1.59	1.16
1:K:37:ASN:N	1:L:518:GLU:HA	1.59	1.15
1:M:37:ASN:N	1:N:518:GLU:HA	1.59	1.15
1:A:23:LEU:HG	1:A:60:ILE:HD12	1.21	1.15
1:E:249:ILE:HD11	1:E:262:LEU:HD21	1.23	1.15
1:A:249:ILE:CD1	1:A:262:LEU:CD1	2.20	1.15
1:J:233:MET:HE2	1:J:249:ILE:HD13	1.30	1.14
1:B:249:ILE:CD1	1:B:262:LEU:CD1	2.21	1.14
1:I:233:MET:HE2	1:I:249:ILE:HD13	1.29	1.14
1:E:200:LEU:CD2	1:E:254:VAL:CG2	1.87	1.14
1:F:249:ILE:HD11	1:F:262:LEU:HD21	1.22	1.14
1:A:193:MET:HE3	1:A:332:ILE:HD12	1.28	1.14
1:G:249:ILE:CD1	1:G:262:LEU:CD1	2.21	1.13
1:E:23:LEU:HG	1:E:60:ILE:HD12	1.21	1.13
1:D:193:MET:HE3	1:D:332:ILE:HD12	1.27	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LEU:HG	1:B:60:ILE:HD12	1.21	1.12
1:D:249:ILE:CD1	1:D:262:LEU:CD1	2.20	1.12
1:E:193:MET:HE3	1:E:332:ILE:HD12	1.30	1.11
1:L:301:ILE:HD13	1:L:312:ALA:HB2	1.29	1.11
1:F:200:LEU:CD2	1:F:254:VAL:CG2	1.87	1.11
1:H:301:ILE:HD13	1:H:312:ALA:HB2	1.28	1.11
1:F:193:MET:HE3	1:F:332:ILE:HD12	1.28	1.10
1:H:518:GLU:HA	1:N:37:ASN:N	1.59	1.10
1:I:301:ILE:HD13	1:I:312:ALA:HB2	1.29	1.10
1:H:37:ASN:N	1:I:518:GLU:HA	1.59	1.10
1:M:38:VAL:HA	1:N:519:CYS:H	1.11	1.10
1:B:193:MET:HE3	1:B:332:ILE:HD12	1.31	1.10
1:H:38:VAL:HA	1:I:519:CYS:H	1.11	1.10
1:B:199:TYR:HB3	1:B:325:ILE:HD11	1.33	1.10
1:C:199:TYR:HB3	1:C:325:ILE:HD11	1.33	1.10
1:E:249:ILE:HD11	1:E:262:LEU:CD2	1.82	1.10
1:I:38:VAL:HA	1:J:519:CYS:H	1.11	1.10
1:C:23:LEU:HG	1:C:60:ILE:HD12	1.21	1.09
1:F:249:ILE:HD11	1:F:262:LEU:CD2	1.82	1.09
1:K:38:VAL:HA	1:L:519:CYS:H	1.11	1.09
1:D:249:ILE:HD11	1:D:262:LEU:CD2	1.82	1.09
1:G:200:LEU:HD11	1:G:254:VAL:HG21	1.34	1.09
1:A:150:ILE:CD1	1:A:493:ILE:HA	1.83	1.09
1:I:301:ILE:CD1	1:I:312:ALA:CB	2.31	1.09
1:J:301:ILE:CD1	1:J:312:ALA:CB	2.31	1.09
1:F:249:ILE:CD1	1:F:262:LEU:CD1	2.20	1.09
1:K:301:ILE:HD13	1:K:312:ALA:HB2	1.29	1.09
1:C:150:ILE:CD1	1:C:493:ILE:HA	1.83	1.08
1:D:23:LEU:HG	1:D:60:ILE:HD12	1.21	1.08
1:G:150:ILE:CD1	1:G:493:ILE:HA	1.83	1.08
1:H:301:ILE:CD1	1:H:312:ALA:CB	2.31	1.08
1:G:249:ILE:HD11	1:G:262:LEU:CD2	1.82	1.08
1:H:233:MET:HE2	1:H:249:ILE:HD13	1.29	1.08
1:H:519:CYS:H	1:N:38:VAL:HA	1.11	1.08
1:L:38:VAL:HA	1:M:519:CYS:H	1.11	1.08
1:N:301:ILE:CD1	1:N:312:ALA:CB	2.31	1.08
1:A:249:ILE:HD11	1:A:262:LEU:CD2	1.82	1.08
1:K:301:ILE:CD1	1:K:312:ALA:CB	2.31	1.08
1:M:301:ILE:CD1	1:M:312:ALA:CB	2.31	1.08
1:A:199:TYR:HB3	1:A:325:ILE:HD11	1.33	1.07
1:J:301:ILE:HD13	1:J:312:ALA:HB2	1.28	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:301:ILE:HD13	1:N:312:ALA:HB2	1.29	1.07
1:B:150:ILE:CD1	1:B:493:ILE:HA	1.84	1.07
1:C:249:ILE:HD11	1:C:262:LEU:CD2	1.82	1.07
1:E:150:ILE:CD1	1:E:493:ILE:HA	1.83	1.07
1:B:249:ILE:HD11	1:B:262:LEU:CD2	1.82	1.07
1:L:233:MET:HE1	1:L:249:ILE:HD13	1.32	1.07
1:J:38:VAL:HA	1:K:519:CYS:H	1.11	1.07
1:L:301:ILE:CD1	1:L:312:ALA:CB	2.31	1.07
1:M:233:MET:HE2	1:M:249:ILE:HD13	1.31	1.07
1:N:208:PRO:C	1:N:208:PRO:HA	1.63	1.07
1:C:249:ILE:CD1	1:C:262:LEU:CD1	2.20	1.06
1:D:150:ILE:CD1	1:D:493:ILE:HA	1.84	1.06
1:F:150:ILE:CD1	1:F:493:ILE:HA	1.84	1.06
1:D:199:TYR:HB3	1:D:325:ILE:HD11	1.30	1.05
1:F:199:TYR:HB3	1:F:325:ILE:HD11	1.33	1.05
1:E:199:TYR:HB3	1:E:325:ILE:HD11	1.33	1.05
1:G:199:TYR:HB3	1:G:325:ILE:HD11	1.33	1.04
1:K:233:MET:HE2	1:K:249:ILE:HD13	1.35	1.04
1:K:233:MET:HE1	1:K:249:ILE:HD13	1.37	1.04
1:M:301:ILE:HD13	1:M:312:ALA:HB2	1.29	1.04
1:J:203:TYR:CG	1:J:267:MET:SD	2.52	1.03
1:C:249:ILE:HD12	1:C:262:LEU:HD13	1.38	1.03
1:I:203:TYR:CG	1:I:267:MET:SD	2.52	1.03
1:K:203:TYR:CG	1:K:267:MET:SD	2.52	1.03
1:M:203:TYR:CG	1:M:267:MET:SD	2.51	1.03
1:N:233:MET:HE2	1:N:249:ILE:HD13	1.33	1.03
1:H:203:TYR:CG	1:H:267:MET:SD	2.52	1.02
1:L:203:TYR:CG	1:L:267:MET:SD	2.51	1.02
1:N:203:TYR:CG	1:N:267:MET:SD	2.51	1.02
1:A:249:ILE:HD12	1:A:262:LEU:HD13	1.38	1.02
1:N:182:GLY:HA3	1:N:383:ALA:H	1.24	1.02
1:J:233:MET:HE1	1:J:249:ILE:HD13	1.41	1.01
1:J:233:MET:CE	1:J:249:ILE:CD1	2.37	1.01
1:H:233:MET:HE2	1:H:249:ILE:CD1	1.90	1.01
1:F:249:ILE:HD12	1:F:262:LEU:HD13	1.38	1.01
1:I:233:MET:CE	1:I:249:ILE:CD1	2.37	1.00
1:M:233:MET:HE2	1:M:249:ILE:CD1	1.90	1.00
1:H:233:MET:CE	1:H:249:ILE:CD1	2.39	1.00
1:L:182:GLY:HA3	1:L:383:ALA:H	1.24	1.00
1:N:233:MET:CE	1:N:249:ILE:CD1	2.40	1.00
1:N:233:MET:HE1	1:N:249:ILE:HD13	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ILE:HD12	1:B:262:LEU:HD13	1.38	1.00
1:G:249:ILE:HD12	1:G:262:LEU:HD13	1.39	1.00
1:L:233:MET:HE2	1:L:249:ILE:HD13	1.44	1.00
1:E:249:ILE:HD12	1:E:262:LEU:HD13	1.38	1.00
1:N:233:MET:HE2	1:N:249:ILE:CD1	1.92	1.00
1:G:200:LEU:HD22	1:G:259:LEU:HD22	1.45	0.99
1:I:233:MET:HE2	1:I:249:ILE:CD1	1.91	0.99
1:J:182:GLY:HA3	1:J:383:ALA:H	1.24	0.99
1:K:233:MET:CE	1:K:249:ILE:CD1	2.39	0.99
1:D:249:ILE:CD1	1:D:262:LEU:HD21	1.93	0.99
1:J:223:ALA:HB2	1:J:309:LEU:HD21	1.44	0.99
1:J:233:MET:HE2	1:J:249:ILE:CD1	1.91	0.99
1:K:223:ALA:HB2	1:K:309:LEU:HD21	1.44	0.99
1:D:249:ILE:HD12	1:D:262:LEU:HD13	1.38	0.99
1:G:200:LEU:CD1	1:G:254:VAL:HG11	1.93	0.98
1:K:518:GLU:C	1:K:518:GLU:HB3	1.83	0.98
1:I:223:ALA:HB2	1:I:309:LEU:HD21	1.45	0.98
1:I:233:MET:HE1	1:I:249:ILE:HD13	1.42	0.98
1:F:249:ILE:CD1	1:F:262:LEU:HD21	1.93	0.98
1:N:518:GLU:C	1:N:518:GLU:HB3	1.83	0.98
1:I:182:GLY:HA3	1:I:383:ALA:H	1.24	0.98
1:M:223:ALA:HB2	1:M:309:LEU:HD21	1.43	0.98
1:A:249:ILE:CD1	1:A:262:LEU:HD21	1.93	0.98
1:H:223:ALA:HB2	1:H:309:LEU:HD21	1.44	0.98
1:H:227:ILE:HD13	1:H:233:MET:SD	2.05	0.97
1:M:182:GLY:HA3	1:M:383:ALA:H	1.24	0.97
1:C:249:ILE:CD1	1:C:262:LEU:HD21	1.93	0.97
1:I:518:GLU:C	1:I:518:GLU:HB3	1.83	0.97
1:L:223:ALA:HB2	1:L:309:LEU:HD21	1.43	0.97
1:E:249:ILE:CD1	1:E:262:LEU:HD21	1.93	0.97
1:J:227:ILE:HD13	1:J:233:MET:SD	2.04	0.97
1:L:233:MET:CE	1:L:249:ILE:CD1	2.42	0.97
1:M:233:MET:CE	1:M:249:ILE:CD1	2.43	0.97
1:J:518:GLU:C	1:J:518:GLU:HB3	1.83	0.97
1:K:227:ILE:HD13	1:K:233:MET:SD	2.05	0.97
1:M:233:MET:HE1	1:M:249:ILE:HD13	1.46	0.97
1:G:200:LEU:HD11	1:G:254:VAL:CG2	1.94	0.97
1:H:233:MET:HE1	1:H:249:ILE:HD13	1.44	0.97
1:K:233:MET:HE2	1:K:249:ILE:CD1	1.93	0.97
1:B:249:ILE:CD1	1:B:262:LEU:HD21	1.93	0.97
1:G:249:ILE:CD1	1:G:262:LEU:HD21	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:227:ILE:HD13	1:I:233:MET:SD	2.05	0.97
1:N:223:ALA:HB2	1:N:309:LEU:HD21	1.42	0.97
1:H:182:GLY:HA3	1:H:383:ALA:H	1.27	0.97
1:A:249:ILE:HD12	1:A:262:LEU:HD11	0.97	0.97
1:E:249:ILE:HD12	1:E:262:LEU:HD11	0.97	0.96
1:F:249:ILE:HD12	1:F:262:LEU:HD11	0.97	0.96
1:K:182:GLY:HA3	1:K:383:ALA:H	1.24	0.96
1:A:249:ILE:CD1	1:A:262:LEU:CD2	2.44	0.96
1:B:249:ILE:CD1	1:B:262:LEU:CD2	2.44	0.96
1:M:227:ILE:HD13	1:M:233:MET:SD	2.06	0.96
1:L:227:ILE:HD13	1:L:233:MET:SD	2.06	0.95
1:C:249:ILE:CD1	1:C:262:LEU:CD2	2.44	0.95
1:G:249:ILE:CD1	1:G:262:LEU:CD2	2.44	0.95
1:G:249:ILE:HD12	1:G:262:LEU:HD11	0.97	0.95
1:M:518:GLU:C	1:M:518:GLU:HB3	1.83	0.95
1:C:249:ILE:HD12	1:C:262:LEU:HD11	0.97	0.95
1:N:227:ILE:HD13	1:N:233:MET:SD	2.05	0.95
1:B:249:ILE:HD12	1:B:262:LEU:HD11	0.97	0.94
1:L:518:GLU:C	1:L:518:GLU:HB3	1.83	0.94
1:H:518:GLU:C	1:H:518:GLU:HB3	1.83	0.94
1:L:233:MET:HE2	1:L:249:ILE:CD1	1.97	0.94
1:D:249:ILE:HD12	1:D:262:LEU:HD11	0.97	0.94
1:D:249:ILE:CD1	1:D:262:LEU:CD2	2.44	0.94
1:E:249:ILE:CD1	1:E:262:LEU:CD2	2.44	0.94
1:C:200:LEU:HD23	1:C:254:VAL:HG21	1.49	0.93
1:B:200:LEU:HD23	1:B:254:VAL:HG21	1.49	0.93
1:F:249:ILE:CD1	1:F:262:LEU:CD2	2.44	0.93
1:F:220:ILE:HD13	1:F:332:ILE:HD13	1.49	0.93
1:G:220:ILE:HD13	1:G:332:ILE:HD13	1.49	0.93
1:L:242:LYS:CA	1:M:257:GLU:HA	1.99	0.93
1:M:242:LYS:CA	1:N:257:GLU:HA	1.99	0.93
1:F:200:LEU:HD23	1:F:254:VAL:HG21	1.49	0.93
1:J:203:TYR:CD2	1:J:267:MET:SD	2.62	0.93
1:N:203:TYR:CD2	1:N:267:MET:SD	2.62	0.93
1:D:23:LEU:HG	1:D:60:ILE:CD1	1.99	0.93
1:K:203:TYR:CD2	1:K:267:MET:SD	2.62	0.93
1:C:23:LEU:HG	1:C:60:ILE:CD1	1.99	0.93
1:J:242:LYS:CA	1:K:257:GLU:HA	1.99	0.93
1:L:203:TYR:CD2	1:L:267:MET:SD	2.62	0.92
1:A:200:LEU:HD23	1:A:254:VAL:HG21	1.49	0.92
1:A:220:ILE:HD13	1:A:332:ILE:HD13	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:242:LYS:CA	1:I:257:GLU:HA	1.99	0.92
1:H:257:GLU:HA	1:N:242:LYS:CA	1.99	0.92
1:M:203:TYR:CD2	1:M:267:MET:SD	2.62	0.92
1:D:200:LEU:HD23	1:D:254:VAL:HG21	1.49	0.92
1:I:203:TYR:CD2	1:I:267:MET:SD	2.62	0.92
1:E:23:LEU:HG	1:E:60:ILE:CD1	1.99	0.92
1:H:203:TYR:CD2	1:H:267:MET:SD	2.62	0.92
1:G:23:LEU:HG	1:G:60:ILE:CD1	1.98	0.92
1:B:23:LEU:HG	1:B:60:ILE:CD1	1.98	0.92
1:B:220:ILE:HD13	1:B:332:ILE:HD13	1.49	0.92
1:E:220:ILE:HD13	1:E:332:ILE:HD13	1.49	0.91
1:I:242:LYS:CA	1:J:257:GLU:HA	1.99	0.91
1:A:23:LEU:HG	1:A:60:ILE:CD1	1.98	0.91
1:C:23:LEU:HA	1:C:60:ILE:HD13	1.52	0.91
1:D:23:LEU:HA	1:D:60:ILE:HD13	1.52	0.91
1:F:23:LEU:HG	1:F:60:ILE:CD1	1.99	0.91
1:C:213:VAL:CG1	1:C:325:ILE:HG12	2.01	0.91
1:B:23:LEU:HA	1:B:60:ILE:HD13	1.52	0.91
1:E:213:VAL:CG1	1:E:325:ILE:HG12	2.01	0.91
1:C:220:ILE:HD13	1:C:332:ILE:HD13	1.49	0.90
1:E:23:LEU:HA	1:E:60:ILE:HD13	1.52	0.90
1:F:213:VAL:CG1	1:F:325:ILE:HG12	2.01	0.90
1:D:220:ILE:HD13	1:D:332:ILE:HD13	1.49	0.90
1:D:213:VAL:CG1	1:D:325:ILE:HG12	2.01	0.90
1:G:213:VAL:CG1	1:G:325:ILE:HG12	2.01	0.90
1:E:200:LEU:HD23	1:E:254:VAL:HG21	1.49	0.90
1:K:242:LYS:CA	1:L:257:GLU:HA	2.01	0.90
1:A:23:LEU:HA	1:A:60:ILE:HD13	1.52	0.90
1:B:213:VAL:CG1	1:B:325:ILE:HG12	2.01	0.90
1:F:23:LEU:HA	1:F:60:ILE:HD13	1.52	0.90
1:J:23:LEU:HD12	1:J:60:ILE:HD12	0.89	0.89
1:K:223:ALA:HB3	1:K:251:ALA:HB2	1.53	0.89
1:K:23:LEU:HD12	1:K:60:ILE:HD12	0.89	0.89
1:K:193:MET:SD	1:K:292:ILE:HA	2.12	0.89
1:G:23:LEU:HA	1:G:60:ILE:HD13	1.52	0.89
1:L:223:ALA:HB3	1:L:251:ALA:HB2	1.54	0.89
1:M:23:LEU:HD12	1:M:60:ILE:HD12	0.89	0.89
1:I:23:LEU:HD12	1:I:60:ILE:HD12	0.90	0.89
1:L:23:LEU:HD12	1:L:60:ILE:HD12	0.89	0.89
1:N:223:ALA:HB3	1:N:251:ALA:HB2	1.54	0.89
1:N:206:ASN:HA	1:N:207:LYS:HG2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:206:ASN:HA	1:N:207:LYS:CG	2.04	0.88
1:I:223:ALA:HB3	1:I:251:ALA:HB2	1.52	0.88
1:H:23:LEU:HD12	1:H:60:ILE:HD12	0.89	0.88
1:J:223:ALA:HB3	1:J:251:ALA:HB2	1.52	0.88
1:C:193:MET:HE3	1:C:292:ILE:HG23	1.56	0.88
1:H:223:ALA:HB3	1:H:251:ALA:HB2	1.53	0.87
1:M:223:ALA:HB3	1:M:251:ALA:HB2	1.54	0.87
1:N:23:LEU:HD12	1:N:60:ILE:HD12	0.89	0.87
1:C:193:MET:HE3	1:C:332:ILE:HD12	1.57	0.87
1:A:249:ILE:HD12	1:A:262:LEU:CG	2.05	0.87
1:F:150:ILE:HD12	1:F:493:ILE:HA	1.57	0.86
1:G:200:LEU:N	1:G:200:LEU:HD12	1.88	0.86
1:G:249:ILE:HD12	1:G:262:LEU:CG	2.05	0.86
1:H:242:LYS:C	1:I:257:GLU:HA	1.96	0.86
1:M:242:LYS:C	1:N:257:GLU:HA	1.96	0.86
1:B:249:ILE:HD12	1:B:262:LEU:CG	2.05	0.86
1:N:204:PHE:HA	1:N:207:LYS:NZ	1.89	0.86
1:H:219:PHE:HB2	1:H:240:VAL:HG13	1.57	0.85
1:K:219:PHE:HB2	1:K:240:VAL:HG13	1.57	0.85
1:L:242:LYS:C	1:M:257:GLU:HA	1.97	0.85
1:B:150:ILE:HD12	1:B:493:ILE:HA	1.57	0.85
1:F:249:ILE:HD12	1:F:262:LEU:CG	2.05	0.85
1:J:219:PHE:HB2	1:J:240:VAL:HG13	1.57	0.85
1:N:219:PHE:HB2	1:N:240:VAL:HG13	1.57	0.85
1:E:249:ILE:HD12	1:E:262:LEU:CG	2.05	0.85
1:I:219:PHE:HB2	1:I:240:VAL:HG13	1.57	0.85
1:M:301:ILE:HD12	1:M:312:ALA:CB	2.07	0.85
1:C:249:ILE:HD12	1:C:262:LEU:CG	2.05	0.85
1:L:219:PHE:HB2	1:L:240:VAL:HG13	1.57	0.85
1:D:150:ILE:HD12	1:D:493:ILE:HA	1.58	0.85
1:D:249:ILE:HD12	1:D:262:LEU:CG	2.05	0.85
1:L:301:ILE:HD12	1:L:312:ALA:CB	2.07	0.84
1:N:208:PRO:HA	1:N:208:PRO:O	1.76	0.84
1:H:257:GLU:HA	1:N:242:LYS:C	1.98	0.84
1:K:37:ASN:N	1:L:518:GLU:CA	2.36	0.84
1:K:199:TYR:HB3	1:K:325:ILE:HD11	1.58	0.84
1:J:301:ILE:HD12	1:J:312:ALA:CB	2.07	0.83
1:M:219:PHE:HB2	1:M:240:VAL:HG13	1.57	0.83
1:E:150:ILE:HD12	1:E:493:ILE:HA	1.60	0.83
1:I:301:ILE:HD12	1:I:312:ALA:CB	2.07	0.83
1:H:301:ILE:HD12	1:H:312:ALA:CB	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:242:LYS:C	1:J:257:GLU:HA	1.98	0.83
1:C:150:ILE:HD12	1:C:493:ILE:HA	1.60	0.83
1:K:301:ILE:HD12	1:K:312:ALA:CB	2.07	0.83
1:J:242:LYS:C	1:K:257:GLU:HA	1.98	0.83
1:L:207:LYS:HE2	1:L:207:LYS:HA	1.61	0.83
1:K:242:LYS:C	1:L:257:GLU:HA	1.98	0.83
1:N:301:ILE:HD12	1:N:312:ALA:CB	2.07	0.82
1:M:37:ASN:N	1:N:518:GLU:CA	2.36	0.82
1:C:223:ALA:O	1:C:251:ALA:HA	1.80	0.82
1:A:223:ALA:O	1:A:251:ALA:HA	1.80	0.82
1:N:138:CYS:N	1:N:410:GLY:HA2	1.95	0.82
1:H:138:CYS:N	1:H:410:GLY:HA2	1.95	0.82
1:L:150:ILE:HD11	1:L:493:ILE:HA	1.62	0.82
1:M:138:CYS:N	1:M:410:GLY:HA2	1.95	0.82
1:C:192:GLY:HA2	1:C:332:ILE:O	1.80	0.82
1:F:249:ILE:HD13	1:F:262:LEU:HD11	1.62	0.82
1:K:150:ILE:HD11	1:K:493:ILE:HA	1.62	0.82
1:L:38:VAL:HA	1:M:519:CYS:N	1.95	0.82
1:M:38:VAL:HA	1:N:519:CYS:N	1.94	0.82
1:G:150:ILE:HD12	1:G:493:ILE:HA	1.60	0.81
1:G:200:LEU:CD2	1:G:254:VAL:HG11	2.10	0.81
1:A:150:ILE:HD12	1:A:493:ILE:HA	1.60	0.81
1:K:38:VAL:HA	1:L:519:CYS:N	1.95	0.81
1:L:162:ILE:HD13	1:L:400:LEU:HA	1.62	0.81
1:C:193:MET:CE	1:C:292:ILE:HG23	2.11	0.81
1:I:138:CYS:N	1:I:410:GLY:HA2	1.95	0.81
1:L:138:CYS:N	1:L:410:GLY:HA2	1.95	0.81
1:L:183:LEU:HD23	1:L:183:LEU:H	1.45	0.81
1:M:150:ILE:HD11	1:M:493:ILE:HA	1.61	0.81
1:I:38:VAL:HA	1:J:519:CYS:N	1.95	0.81
1:K:162:ILE:HD13	1:K:400:LEU:HA	1.62	0.81
1:M:36:ARG:C	1:N:518:GLU:HA	2.01	0.81
1:H:38:VAL:HA	1:I:519:CYS:N	1.95	0.81
1:J:150:ILE:HD11	1:J:493:ILE:HA	1.62	0.81
1:M:162:ILE:HD13	1:M:400:LEU:HA	1.62	0.81
1:J:38:VAL:HA	1:K:519:CYS:N	1.95	0.81
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.63	0.81
1:F:223:ALA:O	1:F:251:ALA:HA	1.80	0.81
1:J:162:ILE:HD13	1:J:400:LEU:HA	1.62	0.81
1:N:208:PRO:HB2	1:N:209:GLU:OE2	1.80	0.81
1:E:223:ALA:O	1:E:251:ALA:HA	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:162:ILE:HD13	1:I:400:LEU:HA	1.62	0.80
1:H:150:ILE:HD11	1:H:493:ILE:HA	1.61	0.80
1:N:162:ILE:HD13	1:N:400:LEU:HA	1.62	0.80
1:J:36:ARG:C	1:K:518:GLU:HA	2.01	0.80
1:J:138:CYS:N	1:J:410:GLY:HA2	1.95	0.80
1:K:36:ARG:C	1:L:518:GLU:HA	2.01	0.80
1:K:138:CYS:N	1:K:410:GLY:HA2	1.95	0.80
1:L:36:ARG:C	1:M:518:GLU:HA	2.01	0.80
1:H:162:ILE:HD13	1:H:400:LEU:HA	1.62	0.80
1:I:150:ILE:HD11	1:I:493:ILE:HA	1.62	0.80
1:L:38:VAL:CA	1:M:519:CYS:H	1.94	0.80
1:D:137:PRO:HA	1:D:410:GLY:HA2	1.63	0.80
1:G:223:ALA:O	1:G:251:ALA:HA	1.80	0.80
1:B:223:ALA:O	1:B:251:ALA:HA	1.80	0.80
1:D:223:ALA:O	1:D:251:ALA:HA	1.80	0.80
1:D:193:MET:HE3	1:D:332:ILE:CD1	2.09	0.79
1:G:137:PRO:HA	1:G:410:GLY:CA	2.12	0.79
1:B:137:PRO:HA	1:B:410:GLY:CA	2.12	0.79
1:B:249:ILE:HD13	1:B:262:LEU:HD11	1.62	0.79
1:D:137:PRO:HA	1:D:410:GLY:CA	2.12	0.79
1:E:137:PRO:HA	1:E:410:GLY:HA2	1.63	0.79
1:E:199:TYR:HB3	1:E:325:ILE:CD1	2.12	0.79
1:H:518:GLU:CA	1:N:37:ASN:N	2.36	0.79
1:N:150:ILE:HD11	1:N:493:ILE:HA	1.62	0.79
1:N:206:ASN:HA	1:N:207:LYS:CB	2.11	0.79
1:A:137:PRO:HA	1:A:410:GLY:CA	2.12	0.79
1:H:36:ARG:C	1:I:518:GLU:HA	2.01	0.79
1:H:38:VAL:CA	1:I:519:CYS:H	1.94	0.79
1:H:519:CYS:N	1:N:38:VAL:HA	1.94	0.79
1:N:204:PHE:HD1	1:N:207:LYS:HZ1	1.29	0.79
1:F:137:PRO:HA	1:F:410:GLY:CA	2.12	0.79
1:I:199:TYR:HB3	1:I:325:ILE:HD11	1.65	0.79
1:C:199:TYR:HB3	1:C:325:ILE:CD1	2.12	0.79
1:C:137:PRO:HA	1:C:410:GLY:CA	2.12	0.79
1:C:137:PRO:HA	1:C:410:GLY:HA2	1.63	0.79
1:H:518:GLU:HA	1:N:36:ARG:C	2.01	0.79
1:I:36:ARG:C	1:J:518:GLU:HA	2.01	0.79
1:C:249:ILE:HD13	1:C:262:LEU:HD11	1.62	0.79
1:E:137:PRO:HA	1:E:410:GLY:CA	2.12	0.79
1:M:199:TYR:HB3	1:M:325:ILE:HD11	1.65	0.79
1:N:199:TYR:HB3	1:N:325:ILE:HD11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LYS:HE3	1:C:207:LYS:H	1.47	0.78
1:F:137:PRO:HA	1:F:410:GLY:HA2	1.63	0.78
1:I:38:VAL:CA	1:J:519:CYS:H	1.94	0.78
1:A:193:MET:HE3	1:A:332:ILE:CD1	2.10	0.78
1:I:301:ILE:HD12	1:I:312:ALA:HB2	1.65	0.78
1:J:199:TYR:HB3	1:J:325:ILE:HD11	1.65	0.78
1:A:137:PRO:HA	1:A:410:GLY:HA2	1.63	0.78
1:G:137:PRO:HA	1:G:410:GLY:HA2	1.63	0.78
1:L:199:TYR:HB3	1:L:325:ILE:HD11	1.65	0.78
1:B:199:TYR:HB3	1:B:325:ILE:CD1	2.12	0.78
1:H:519:CYS:H	1:N:38:VAL:CA	1.94	0.78
1:I:30:THR:O	1:I:35:GLY:HA3	1.84	0.78
1:K:30:THR:O	1:K:35:GLY:HA3	1.84	0.78
1:D:300:VAL:HG23	1:D:312:ALA:HB2	1.66	0.78
1:F:193:MET:HE3	1:F:332:ILE:CD1	2.10	0.78
1:J:37:ASN:N	1:K:518:GLU:CA	2.36	0.78
1:E:200:LEU:HB2	1:E:259:LEU:HD13	1.66	0.78
1:C:300:VAL:HG23	1:C:312:ALA:HB2	1.66	0.78
1:F:200:LEU:HB2	1:F:259:LEU:HD13	1.66	0.77
1:F:300:VAL:HG23	1:F:312:ALA:HB2	1.66	0.77
1:G:300:VAL:HG23	1:G:312:ALA:HB2	1.66	0.77
1:A:249:ILE:HD13	1:A:262:LEU:HD11	1.62	0.77
1:B:137:PRO:HA	1:B:410:GLY:HA2	1.63	0.77
1:F:199:TYR:HB3	1:F:325:ILE:CD1	2.12	0.77
1:G:23:LEU:CG	1:G:60:ILE:HD12	2.11	0.77
1:M:30:THR:O	1:M:35:GLY:HA3	1.84	0.77
1:M:295:LEU:HA	1:M:342:ILE:HD11	1.66	0.77
1:E:249:ILE:HD13	1:E:262:LEU:HD11	1.62	0.77
1:E:300:VAL:HG23	1:E:312:ALA:HB2	1.66	0.77
1:A:200:LEU:HB2	1:A:259:LEU:HD13	1.66	0.77
1:C:200:LEU:HD12	1:C:275:ALA:HB3	1.66	0.77
1:D:23:LEU:CG	1:D:60:ILE:HD12	2.11	0.77
1:J:38:VAL:CA	1:K:519:CYS:H	1.94	0.77
1:N:295:LEU:HA	1:N:342:ILE:HD11	1.66	0.77
1:A:200:LEU:HD12	1:A:275:ALA:HB3	1.66	0.77
1:F:192:GLY:HA2	1:F:332:ILE:O	1.85	0.77
1:H:38:VAL:HA	1:I:519:CYS:O	1.85	0.77
1:H:295:LEU:HA	1:H:342:ILE:HD11	1.66	0.77
1:K:38:VAL:CA	1:L:519:CYS:H	1.94	0.77
1:L:30:THR:O	1:L:35:GLY:HA3	1.84	0.77
1:C:150:ILE:HD13	1:C:493:ILE:HG23	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:LEU:HD12	1:D:275:ALA:HB3	1.66	0.77
1:K:182:GLY:CA	1:K:383:ALA:H	1.98	0.77
1:A:300:VAL:HG23	1:A:312:ALA:HB2	1.66	0.77
1:A:199:TYR:HB3	1:A:325:ILE:CD1	2.12	0.77
1:B:300:VAL:HG23	1:B:312:ALA:HB2	1.66	0.77
1:D:200:LEU:HB2	1:D:259:LEU:HD13	1.66	0.77
1:F:150:ILE:CD1	1:F:493:ILE:HG23	2.15	0.77
1:F:200:LEU:HD12	1:F:275:ALA:HB3	1.66	0.77
1:J:30:THR:O	1:J:35:GLY:HA3	1.84	0.77
1:J:301:ILE:HD12	1:J:312:ALA:HB2	1.65	0.77
1:L:295:LEU:HA	1:L:342:ILE:HD11	1.66	0.77
1:N:187:LEU:HD12	1:N:378:VAL:O	1.85	0.77
1:D:150:ILE:CD1	1:D:493:ILE:HG23	2.15	0.77
1:G:200:LEU:CG	1:G:254:VAL:HG11	2.14	0.77
1:G:249:ILE:HD13	1:G:262:LEU:HD11	1.62	0.77
1:K:177:VAL:HG22	1:K:379:ILE:HB	1.67	0.77
1:N:30:THR:O	1:N:35:GLY:HA3	1.84	0.77
1:B:200:LEU:HB2	1:B:259:LEU:HD13	1.66	0.77
1:I:182:GLY:CA	1:I:383:ALA:H	1.98	0.77
1:B:150:ILE:CD1	1:B:493:ILE:HG23	2.15	0.76
1:E:192:GLY:HA2	1:E:332:ILE:O	1.85	0.76
1:G:150:ILE:HD13	1:G:493:ILE:HG23	1.67	0.76
1:H:519:CYS:O	1:N:38:VAL:HA	1.85	0.76
1:I:38:VAL:HA	1:J:519:CYS:O	1.85	0.76
1:B:356:ALA:HB1	1:B:361:ASP:HB2	1.68	0.76
1:F:23:LEU:CG	1:F:60:ILE:HD12	2.11	0.76
1:H:30:THR:O	1:H:35:GLY:HA3	1.84	0.76
1:I:295:LEU:HA	1:I:342:ILE:HD11	1.66	0.76
1:J:38:VAL:HA	1:K:519:CYS:O	1.84	0.76
1:E:150:ILE:HD13	1:E:493:ILE:HG23	1.67	0.76
1:B:200:LEU:HD12	1:B:275:ALA:HB3	1.66	0.76
1:C:356:ALA:HB1	1:C:361:ASP:HB2	1.68	0.76
1:D:192:GLY:HA2	1:D:332:ILE:O	1.85	0.76
1:K:38:VAL:HA	1:L:519:CYS:O	1.85	0.76
1:A:192:GLY:HA2	1:A:332:ILE:O	1.85	0.76
1:D:200:LEU:HD12	1:D:275:ALA:CB	2.16	0.76
1:L:249:ILE:HB	1:L:275:ALA:HB2	1.68	0.76
1:C:200:LEU:HB2	1:C:259:LEU:HD13	1.66	0.76
1:E:193:MET:HE3	1:E:332:ILE:CD1	2.12	0.76
1:G:192:GLY:HA2	1:G:332:ILE:O	1.85	0.76
1:G:193:MET:SD	1:G:292:ILE:HA	2.26	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:249:ILE:HB	1:H:275:ALA:HB2	1.68	0.76
1:A:240:VAL:HG11	1:A:247:LEU:HB2	1.68	0.76
1:C:200:LEU:HD12	1:C:275:ALA:CB	2.16	0.76
1:F:150:ILE:HD13	1:F:493:ILE:HG23	1.68	0.76
1:F:200:LEU:HD12	1:F:275:ALA:CB	2.16	0.76
1:G:199:TYR:HB3	1:G:325:ILE:CD1	2.12	0.76
1:M:249:ILE:HB	1:M:275:ALA:HB2	1.68	0.76
1:N:206:ASN:OD1	1:N:213:VAL:HG23	1.84	0.76
1:D:150:ILE:HD13	1:D:493:ILE:HG23	1.68	0.76
1:E:200:LEU:HD12	1:E:275:ALA:CB	2.16	0.76
1:H:37:ASN:N	1:I:518:GLU:CA	2.36	0.76
1:J:182:GLY:CA	1:J:383:ALA:H	1.98	0.76
1:L:38:VAL:HA	1:M:519:CYS:O	1.85	0.76
1:L:279:PRO:O	1:L:285:ARG:HA	1.85	0.76
1:M:169:VAL:CG1	1:M:377:ALA:HB3	2.16	0.76
1:N:249:ILE:HB	1:N:275:ALA:HB2	1.68	0.76
1:A:200:LEU:HD12	1:A:275:ALA:CB	2.16	0.76
1:A:356:ALA:HB1	1:A:361:ASP:HB2	1.68	0.76
1:B:192:GLY:HA2	1:B:332:ILE:O	1.85	0.76
1:E:200:LEU:HD12	1:E:275:ALA:HB3	1.66	0.76
1:K:137:PRO:HA	1:K:410:GLY:HA3	1.66	0.76
1:K:249:ILE:HB	1:K:275:ALA:HB2	1.68	0.76
1:K:279:PRO:O	1:K:285:ARG:HA	1.85	0.76
1:L:137:PRO:HA	1:L:410:GLY:HA3	1.66	0.76
1:L:182:GLY:CA	1:L:383:ALA:H	1.98	0.76
1:M:38:VAL:HA	1:N:519:CYS:O	1.85	0.76
1:M:137:PRO:HA	1:M:410:GLY:HA3	1.66	0.76
1:M:279:PRO:O	1:M:285:ARG:HA	1.85	0.76
1:B:200:LEU:HD12	1:B:275:ALA:CB	2.16	0.76
1:B:240:VAL:HG11	1:B:247:LEU:HB2	1.68	0.76
1:D:249:ILE:HD13	1:D:262:LEU:HD11	1.62	0.76
1:H:137:PRO:HA	1:H:410:GLY:HA3	1.66	0.76
1:I:137:PRO:HA	1:I:410:GLY:HA3	1.66	0.76
1:I:279:PRO:O	1:I:285:ARG:HA	1.86	0.76
1:J:137:PRO:HA	1:J:410:GLY:HA3	1.66	0.76
1:K:295:LEU:HA	1:K:342:ILE:HD11	1.66	0.76
1:M:38:VAL:CA	1:N:519:CYS:H	1.94	0.76
1:N:137:PRO:HA	1:N:410:GLY:HA3	1.66	0.76
1:C:23:LEU:CG	1:C:60:ILE:HD12	2.11	0.75
1:J:279:PRO:O	1:J:285:ARG:HA	1.86	0.75
1:J:295:LEU:HA	1:J:342:ILE:HD11	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:182:GLY:CA	1:M:383:ALA:H	1.98	0.75
1:B:193:MET:HE3	1:B:332:ILE:CD1	2.13	0.75
1:G:240:VAL:HG11	1:G:247:LEU:HB2	1.68	0.75
1:N:182:GLY:CA	1:N:383:ALA:H	1.98	0.75
1:D:356:ALA:HB1	1:D:361:ASP:HB2	1.68	0.75
1:J:169:VAL:CG1	1:J:377:ALA:HB3	2.16	0.75
1:H:182:GLY:CA	1:H:383:ALA:H	1.98	0.75
1:H:279:PRO:O	1:H:285:ARG:HA	1.85	0.75
1:I:169:VAL:CG1	1:I:377:ALA:HB3	2.16	0.75
1:K:169:VAL:CG1	1:K:377:ALA:HB3	2.16	0.75
1:C:207:LYS:HB2	1:C:208:PRO:HD3	1.68	0.75
1:L:169:VAL:CG1	1:L:377:ALA:HB3	2.16	0.75
1:H:169:VAL:CG1	1:H:377:ALA:HB3	2.16	0.75
1:D:240:VAL:HG11	1:D:247:LEU:HB2	1.68	0.75
1:G:356:ALA:HB1	1:G:361:ASP:HB2	1.68	0.75
1:I:249:ILE:HB	1:I:275:ALA:HB2	1.68	0.75
1:M:301:ILE:HD12	1:M:312:ALA:HB2	1.65	0.75
1:N:169:VAL:CG1	1:N:377:ALA:HB3	2.16	0.75
1:B:150:ILE:HD13	1:B:493:ILE:HG23	1.68	0.74
1:H:138:CYS:H	1:H:410:GLY:HA2	1.52	0.74
1:J:249:ILE:HB	1:J:275:ALA:HB2	1.68	0.74
1:N:138:CYS:H	1:N:410:GLY:HA2	1.52	0.74
1:F:240:VAL:HG11	1:F:247:LEU:HB2	1.68	0.74
1:A:150:ILE:HD13	1:A:493:ILE:HG23	1.67	0.74
1:D:150:ILE:HD11	1:D:493:ILE:HA	1.68	0.74
1:E:240:VAL:HG11	1:E:247:LEU:HB2	1.68	0.74
1:E:356:ALA:HB1	1:E:361:ASP:HB2	1.68	0.74
1:M:138:CYS:H	1:M:410:GLY:HA2	1.52	0.74
1:N:204:PHE:HA	1:N:207:LYS:HZ1	1.49	0.74
1:C:240:VAL:HG11	1:C:247:LEU:HB2	1.68	0.74
1:E:381:VAL:HG21	1:E:393:LYS:N	2.03	0.74
1:F:356:ALA:HB1	1:F:361:ASP:HB2	1.68	0.74
1:E:23:LEU:CG	1:E:60:ILE:HD12	2.11	0.74
1:N:279:PRO:O	1:N:285:ARG:HA	1.85	0.74
1:D:381:VAL:HG21	1:D:393:LYS:N	2.03	0.74
1:A:38:VAL:HG21	1:A:56:VAL:CG2	2.18	0.74
1:B:38:VAL:HG21	1:B:56:VAL:CG2	2.18	0.74
1:C:38:VAL:HG21	1:C:56:VAL:CG2	2.18	0.74
1:D:38:VAL:HG21	1:D:56:VAL:CG2	2.18	0.74
1:G:38:VAL:HG21	1:G:56:VAL:CG2	2.18	0.74
1:N:301:ILE:HD12	1:N:312:ALA:HB2	1.65	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:HD11	1:A:493:ILE:HA	1.69	0.73
1:B:222:LEU:HD21	1:B:292:ILE:HG22	1.70	0.73
1:E:38:VAL:HG21	1:E:56:VAL:CG2	2.18	0.73
1:F:222:LEU:HD21	1:F:292:ILE:HG22	1.70	0.73
1:G:150:ILE:HD11	1:G:493:ILE:HA	1.69	0.73
1:B:23:LEU:CG	1:B:60:ILE:HD12	2.11	0.73
1:B:150:ILE:HD11	1:B:493:ILE:HA	1.68	0.73
1:C:381:VAL:HG21	1:C:393:LYS:N	2.03	0.73
1:F:38:VAL:HG21	1:F:56:VAL:CG2	2.18	0.73
1:I:301:ILE:CD1	1:I:312:ALA:HB1	2.18	0.73
1:C:222:LEU:HD21	1:C:292:ILE:HG22	1.70	0.73
1:G:222:LEU:HD21	1:G:292:ILE:HG22	1.70	0.73
1:K:301:ILE:CD1	1:K:312:ALA:HB1	2.18	0.73
1:L:301:ILE:CD1	1:L:312:ALA:HB1	2.18	0.73
1:A:222:LEU:HD21	1:A:292:ILE:HG22	1.70	0.73
1:C:262:LEU:HD22	1:C:273:VAL:HG11	1.71	0.73
1:E:222:LEU:HD21	1:E:292:ILE:HG22	1.70	0.73
1:F:381:VAL:HG21	1:F:393:LYS:N	2.03	0.73
1:H:301:ILE:CD1	1:H:312:ALA:HB1	2.18	0.73
1:A:313:THR:H	1:A:316:ASP:HB3	1.54	0.73
1:B:313:THR:H	1:B:316:ASP:HB3	1.54	0.73
1:G:313:THR:H	1:G:316:ASP:HB3	1.54	0.73
1:I:138:CYS:H	1:I:410:GLY:HA2	1.52	0.73
1:F:150:ILE:HD11	1:F:493:ILE:HA	1.68	0.73
1:A:262:LEU:HD22	1:A:273:VAL:HG11	1.71	0.73
1:A:381:VAL:HG21	1:A:393:LYS:N	2.03	0.73
1:B:381:VAL:HG21	1:B:393:LYS:N	2.03	0.73
1:D:222:LEU:HD21	1:D:292:ILE:HG22	1.71	0.73
1:I:37:ASN:N	1:J:518:GLU:CA	2.36	0.73
1:G:262:LEU:HD22	1:G:273:VAL:HG11	1.71	0.73
1:L:138:CYS:H	1:L:410:GLY:HA2	1.52	0.73
1:C:313:THR:H	1:C:316:ASP:HB3	1.54	0.72
1:G:381:VAL:HG21	1:G:393:LYS:N	2.03	0.72
1:F:313:THR:H	1:F:316:ASP:HB3	1.54	0.72
1:E:313:THR:H	1:E:316:ASP:HB3	1.54	0.72
1:N:301:ILE:CD1	1:N:312:ALA:HB1	2.18	0.72
1:G:150:ILE:CD1	1:G:493:ILE:HG23	2.20	0.72
1:K:207:LYS:HA	1:K:207:LYS:HE3	1.70	0.72
1:C:150:ILE:CD1	1:C:493:ILE:HG23	2.20	0.72
1:D:262:LEU:HD22	1:D:273:VAL:HG11	1.71	0.72
1:D:313:THR:H	1:D:316:ASP:HB3	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:ILE:CD1	1:E:493:ILE:HG23	2.20	0.72
1:G:193:MET:HE1	1:G:295:LEU:HB3	1.72	0.72
1:G:193:MET:HG2	1:G:295:LEU:HG	1.71	0.72
1:M:301:ILE:CD1	1:M:312:ALA:HB1	2.18	0.72
1:N:205:ILE:O	1:N:207:LYS:HG2	1.89	0.72
1:A:162:ILE:HD13	1:A:400:LEU:CA	2.20	0.72
1:J:223:ALA:HB1	1:J:225:LYS:HD2	1.72	0.72
1:G:200:LEU:CD1	1:G:254:VAL:CG1	2.68	0.72
1:B:206:ASN:HB3	1:B:208:PRO:HD2	1.70	0.71
1:B:262:LEU:HD22	1:B:273:VAL:HG11	1.71	0.71
1:A:23:LEU:CG	1:A:60:ILE:HD12	2.11	0.71
1:K:243:ALA:HB2	1:L:256:GLY:O	1.90	0.71
1:A:150:ILE:CD1	1:A:493:ILE:HG23	2.20	0.71
1:H:243:ALA:HB2	1:I:256:GLY:O	1.90	0.71
1:J:138:CYS:H	1:J:410:GLY:HA2	1.52	0.71
1:L:243:ALA:HB2	1:M:256:GLY:O	1.90	0.71
1:M:243:ALA:HB2	1:N:256:GLY:O	1.90	0.71
1:C:162:ILE:HD13	1:C:400:LEU:CA	2.20	0.71
1:E:162:ILE:HD13	1:E:400:LEU:CA	2.20	0.71
1:H:256:GLY:O	1:N:243:ALA:HB2	1.90	0.71
1:F:162:ILE:HD13	1:F:400:LEU:CA	2.20	0.71
1:F:262:LEU:HD22	1:F:273:VAL:HG11	1.71	0.71
1:I:223:ALA:HB1	1:I:225:LYS:HD2	1.72	0.71
1:N:23:LEU:HD13	1:N:60:ILE:HD12	1.70	0.71
1:E:150:ILE:HD11	1:E:493:ILE:HA	1.70	0.71
1:F:249:ILE:CD1	1:F:262:LEU:CG	2.67	0.71
1:H:199:TYR:HB3	1:H:325:ILE:HD11	1.72	0.71
1:D:162:ILE:HD13	1:D:400:LEU:CA	2.20	0.70
1:E:262:LEU:HD22	1:E:273:VAL:HG11	1.71	0.70
1:J:301:ILE:CD1	1:J:312:ALA:HB1	2.18	0.70
1:C:150:ILE:HD11	1:C:493:ILE:HA	1.70	0.70
1:H:217:SER:HA	1:H:320:ALA:O	1.91	0.70
1:K:223:ALA:HB1	1:K:225:LYS:HD2	1.73	0.70
1:J:243:ALA:HB2	1:K:256:GLY:O	1.90	0.70
1:H:301:ILE:HD12	1:H:312:ALA:HB2	1.65	0.70
1:J:23:LEU:HD13	1:J:60:ILE:HD12	1.70	0.70
1:B:162:ILE:HD13	1:B:400:LEU:CA	2.20	0.70
1:B:195:PHE:CE1	1:B:330:THR:HB	2.26	0.70
2:C:1525:PO4:P	4:C:1527:ATP:O1G	2.50	0.70
1:K:138:CYS:H	1:K:410:GLY:HA2	1.52	0.70
1:B:200:LEU:CB	1:B:259:LEU:HD13	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1525:PO4:P	4:D:1527:ATP:O1G	2.49	0.70
1:C:200:LEU:CB	1:C:259:LEU:HD13	2.22	0.70
1:F:207:LYS:H	1:F:207:LYS:HE2	1.55	0.70
1:H:223:ALA:HB1	1:H:225:LYS:HD2	1.73	0.70
1:K:153:ASN:N	1:K:154:SER:HA	2.06	0.70
1:N:223:ALA:O	1:N:251:ALA:HA	1.92	0.70
1:A:200:LEU:CB	1:A:259:LEU:HD13	2.22	0.70
1:A:220:ILE:HD12	1:A:296:THR:HG21	1.74	0.70
2:F:1525:PO4:P	4:F:1527:ATP:O1G	2.49	0.70
1:H:153:ASN:N	1:H:154:SER:HA	2.06	0.70
1:D:199:TYR:HB3	1:D:325:ILE:CD1	2.16	0.70
1:F:200:LEU:CB	1:F:259:LEU:HD13	2.22	0.70
1:I:223:ALA:O	1:I:251:ALA:HA	1.92	0.70
1:G:162:ILE:HD13	1:G:400:LEU:CA	2.20	0.70
1:N:153:ASN:N	1:N:154:SER:HA	2.06	0.70
1:N:217:SER:HA	1:N:320:ALA:O	1.91	0.70
2:A:1525:PO4:P	4:A:1527:ATP:O1G	2.50	0.69
1:G:309:LEU:HD22	1:G:312:ALA:HB3	1.74	0.69
1:K:52:ASP:OD1	2:K:1525:PO4:P	2.50	0.69
1:K:192:GLY:O	1:K:375:GLY:HA2	1.92	0.69
1:L:223:ALA:O	1:L:251:ALA:HA	1.92	0.69
1:A:309:LEU:HD22	1:A:312:ALA:HB3	1.74	0.69
1:C:192:GLY:HA3	1:C:376:VAL:HG23	1.73	0.69
1:G:220:ILE:HD12	1:G:296:THR:HG21	1.74	0.69
1:I:243:ALA:HB2	1:J:256:GLY:O	1.90	0.69
1:K:223:ALA:O	1:K:251:ALA:HA	1.92	0.69
1:L:242:LYS:HB2	1:M:257:GLU:O	1.92	0.69
1:N:52:ASP:OD1	2:N:1525:PO4:P	2.50	0.69
1:B:220:ILE:HD12	1:B:296:THR:HG21	1.74	0.69
1:C:309:LEU:HD22	1:C:312:ALA:HB3	1.74	0.69
2:E:1525:PO4:P	4:E:1527:ATP:O1G	2.50	0.69
1:L:52:ASP:OD1	2:L:1525:PO4:P	2.50	0.69
1:M:153:ASN:N	1:M:154:SER:HA	2.06	0.69
1:D:200:LEU:CB	1:D:259:LEU:HD13	2.22	0.69
1:E:200:LEU:CB	1:E:259:LEU:HD13	2.22	0.69
1:I:217:SER:HA	1:I:320:ALA:O	1.91	0.69
1:J:217:SER:HA	1:J:320:ALA:O	1.91	0.69
2:B:1525:PO4:P	4:B:1527:ATP:O1G	2.50	0.69
1:D:309:LEU:HD22	1:D:312:ALA:HB3	1.74	0.69
1:E:202:PRO:O	1:E:205:ILE:HG13	1.92	0.69
1:F:309:LEU:HD22	1:F:312:ALA:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:ILE:CD1	1:G:262:LEU:CG	2.67	0.69
1:I:52:ASP:OD1	2:I:1525:PO4:P	2.50	0.69
1:M:52:ASP:OD1	2:M:1525:PO4:P	2.50	0.69
1:B:309:LEU:HD22	1:B:312:ALA:HB3	1.75	0.69
1:D:249:ILE:CD1	1:D:262:LEU:CG	2.67	0.69
1:L:223:ALA:HB2	1:L:309:LEU:CD2	2.20	0.69
2:G:1525:PO4:P	4:G:1527:ATP:O1G	2.50	0.69
1:H:23:LEU:HD13	1:H:60:ILE:HD12	1.71	0.69
1:L:153:ASN:N	1:L:154:SER:HA	2.06	0.69
1:M:217:SER:HA	1:M:320:ALA:O	1.91	0.69
1:E:309:LEU:HD22	1:E:312:ALA:HB3	1.74	0.69
1:H:223:ALA:O	1:H:251:ALA:HA	1.92	0.69
1:H:257:GLU:O	1:N:242:LYS:HB2	1.93	0.69
1:J:153:ASN:N	1:J:154:SER:HA	2.06	0.69
1:J:223:ALA:O	1:J:251:ALA:HA	1.92	0.69
1:L:137:PRO:HA	1:L:410:GLY:CA	2.23	0.69
1:M:223:ALA:O	1:M:251:ALA:HA	1.92	0.69
1:J:242:LYS:HB2	1:K:257:GLU:O	1.93	0.69
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.75	0.69
1:C:220:ILE:HD12	1:C:296:THR:HG21	1.74	0.69
1:H:52:ASP:OD1	2:H:1525:PO4:P	2.50	0.69
1:K:217:SER:HA	1:K:320:ALA:O	1.91	0.69
1:L:217:SER:HA	1:L:320:ALA:O	1.91	0.69
1:M:36:ARG:C	1:N:518:GLU:CA	2.62	0.69
1:M:223:ALA:HB2	1:M:309:LEU:CD2	2.20	0.69
1:I:36:ARG:C	1:J:518:GLU:CA	2.62	0.68
1:K:177:VAL:HG22	1:K:379:ILE:CG2	2.23	0.68
1:L:37:ASN:N	1:M:518:GLU:CA	2.36	0.68
1:B:270:ILE:HG22	1:B:271:VAL:HG23	1.76	0.68
1:K:36:ARG:C	1:L:518:GLU:CA	2.62	0.68
1:N:223:ALA:HB2	1:N:309:LEU:CD2	2.20	0.68
1:E:249:ILE:CD1	1:E:262:LEU:CG	2.67	0.68
1:G:193:MET:CG	1:G:295:LEU:HG	2.22	0.68
1:H:518:GLU:CA	1:N:36:ARG:C	2.62	0.68
1:I:153:ASN:N	1:I:154:SER:HA	2.06	0.68
1:K:137:PRO:HA	1:K:410:GLY:CA	2.23	0.68
1:L:23:LEU:HD13	1:L:60:ILE:HD12	1.71	0.68
1:C:270:ILE:HG22	1:C:271:VAL:HG23	1.75	0.68
1:F:220:ILE:HD12	1:F:296:THR:HG21	1.74	0.68
1:G:183:LEU:HA	1:G:383:ALA:H	1.59	0.68
1:G:270:ILE:HG22	1:G:271:VAL:HG23	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:52:ASP:OD1	2:J:1525:PO4:P	2.50	0.68
1:K:223:ALA:HB2	1:K:309:LEU:CD2	2.21	0.68
1:D:220:ILE:HD12	1:D:296:THR:HG21	1.74	0.68
1:E:220:ILE:HD12	1:E:296:THR:HG21	1.74	0.68
1:H:169:VAL:HG23	1:H:170:GLY:O	1.93	0.68
1:A:183:LEU:HA	1:A:383:ALA:H	1.59	0.68
1:F:183:LEU:HA	1:F:383:ALA:H	1.59	0.68
1:H:137:PRO:HA	1:H:410:GLY:CA	2.23	0.68
1:I:242:LYS:HB2	1:J:257:GLU:O	1.93	0.68
1:M:178:GLU:O	1:M:380:LYS:HA	1.94	0.68
1:N:137:PRO:HA	1:N:410:GLY:CA	2.23	0.68
1:G:193:MET:CE	1:G:296:THR:HG23	2.24	0.68
1:I:178:GLU:O	1:I:380:LYS:HA	1.94	0.68
1:K:178:GLU:O	1:K:380:LYS:HA	1.94	0.68
1:L:178:GLU:O	1:L:380:LYS:HA	1.94	0.68
1:M:223:ALA:HB1	1:M:225:LYS:HD2	1.76	0.68
1:N:223:ALA:HB1	1:N:225:LYS:HD2	1.76	0.68
1:E:183:LEU:HA	1:E:383:ALA:H	1.59	0.68
1:I:137:PRO:HA	1:I:410:GLY:CA	2.23	0.68
1:J:168:LYS:CG	1:J:187:LEU:HD21	2.24	0.68
1:H:203:TYR:CD1	1:H:267:MET:SD	2.88	0.67
1:I:169:VAL:HG23	1:I:170:GLY:O	1.93	0.67
1:J:137:PRO:HA	1:J:410:GLY:CA	2.23	0.67
1:J:169:VAL:HG23	1:J:170:GLY:O	1.93	0.67
1:I:203:TYR:CD1	1:I:267:MET:SD	2.87	0.67
1:L:223:ALA:HB1	1:L:225:LYS:HD2	1.76	0.67
1:B:183:LEU:HA	1:B:383:ALA:H	1.59	0.67
1:D:183:LEU:HA	1:D:383:ALA:H	1.59	0.67
1:F:270:ILE:HG22	1:F:271:VAL:HG23	1.75	0.67
1:G:312:ALA:HB1	1:G:316:ASP:CG	2.15	0.67
1:J:223:ALA:HB2	1:J:309:LEU:CD2	2.22	0.67
1:K:169:VAL:HG23	1:K:170:GLY:O	1.93	0.67
1:M:137:PRO:HA	1:M:410:GLY:CA	2.23	0.67
1:N:203:TYR:CD1	1:N:267:MET:SD	2.87	0.67
1:D:270:ILE:HG22	1:D:271:VAL:HG23	1.75	0.67
1:H:36:ARG:C	1:I:518:GLU:CA	2.62	0.67
1:L:169:VAL:HG23	1:L:170:GLY:O	1.93	0.67
1:G:227:ILE:HB	1:G:258:ALA:HB2	1.77	0.67
1:K:203:TYR:CD1	1:K:267:MET:SD	2.87	0.67
1:K:243:ALA:HA	1:L:260:ALA:HB2	1.77	0.67
1:M:169:VAL:HG23	1:M:170:GLY:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:HD13	1:A:400:LEU:HA	1.77	0.67
1:A:249:ILE:CD1	1:A:262:LEU:CG	2.67	0.67
1:C:183:LEU:HA	1:C:383:ALA:H	1.59	0.67
1:G:162:ILE:HD13	1:G:400:LEU:HA	1.77	0.67
1:A:227:ILE:HB	1:A:258:ALA:HB2	1.77	0.67
1:B:227:ILE:HB	1:B:258:ALA:HB2	1.77	0.67
1:E:162:ILE:HD13	1:E:400:LEU:HA	1.77	0.67
1:H:178:GLU:O	1:H:380:LYS:HA	1.94	0.67
1:H:243:ALA:HA	1:I:260:ALA:HB2	1.77	0.67
1:N:178:GLU:O	1:N:380:LYS:HA	1.94	0.67
1:E:270:ILE:HG22	1:E:271:VAL:HG23	1.75	0.67
1:H:223:ALA:HB2	1:H:309:LEU:CD2	2.21	0.67
1:B:312:ALA:HB1	1:B:316:ASP:CG	2.15	0.67
1:C:227:ILE:HB	1:C:258:ALA:HB2	1.77	0.67
1:F:312:ALA:HB1	1:F:316:ASP:CG	2.15	0.67
1:L:243:ALA:CA	1:M:256:GLY:O	2.43	0.67
1:B:193:MET:CE	1:B:332:ILE:HD12	2.18	0.67
1:B:194:GLN:CG	1:B:329:THR:HG21	2.25	0.67
1:C:249:ILE:CD1	1:C:262:LEU:CG	2.67	0.67
1:C:312:ALA:HB1	1:C:316:ASP:CG	2.15	0.67
1:D:213:VAL:HG13	1:D:325:ILE:HG12	1.76	0.67
1:E:312:ALA:HB1	1:E:316:ASP:CG	2.15	0.67
1:L:203:TYR:CD1	1:L:267:MET:SD	2.87	0.67
1:M:203:TYR:CD1	1:M:267:MET:SD	2.87	0.67
1:J:36:ARG:C	1:K:518:GLU:CA	2.62	0.66
1:F:162:ILE:HD13	1:F:400:LEU:HA	1.77	0.66
1:F:213:VAL:HG13	1:F:325:ILE:HG12	1.77	0.66
1:F:227:ILE:HB	1:F:258:ALA:HB2	1.77	0.66
1:H:256:GLY:O	1:N:243:ALA:CA	2.43	0.66
1:H:295:LEU:HD23	1:H:342:ILE:HD13	1.78	0.66
1:N:295:LEU:HD23	1:N:342:ILE:HD13	1.77	0.66
1:B:162:ILE:HD13	1:B:400:LEU:HA	1.77	0.66
1:B:271:VAL:HG12	1:B:273:VAL:CG2	2.26	0.66
1:D:162:ILE:HD13	1:D:400:LEU:HA	1.77	0.66
1:E:279:PRO:O	1:E:285:ARG:HA	1.95	0.66
1:F:279:PRO:O	1:F:285:ARG:HA	1.95	0.66
1:I:223:ALA:HB2	1:I:309:LEU:CD2	2.22	0.66
1:J:203:TYR:CD1	1:J:267:MET:SD	2.87	0.66
1:K:243:ALA:CA	1:L:256:GLY:O	2.43	0.66
1:L:36:ARG:C	1:M:518:GLU:CA	2.62	0.66
1:A:271:VAL:HG12	1:A:273:VAL:CG2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ALA:HB1	1:A:316:ASP:CG	2.15	0.66
1:D:227:ILE:HB	1:D:258:ALA:HB2	1.77	0.66
1:M:243:ALA:CA	1:N:256:GLY:O	2.43	0.66
1:C:271:VAL:HG12	1:C:273:VAL:CG2	2.26	0.66
1:C:279:PRO:O	1:C:285:ARG:HA	1.95	0.66
1:D:271:VAL:HG12	1:D:273:VAL:CG2	2.26	0.66
1:D:312:ALA:HB1	1:D:316:ASP:CG	2.15	0.66
1:E:271:VAL:HG12	1:E:273:VAL:CG2	2.26	0.66
1:G:213:VAL:HG13	1:G:325:ILE:HG12	1.76	0.66
1:H:243:ALA:CA	1:I:256:GLY:O	2.43	0.66
1:N:206:ASN:CA	1:N:207:LYS:HG2	2.24	0.66
1:A:200:LEU:HB2	1:A:259:LEU:CD1	2.25	0.66
1:E:227:ILE:HB	1:E:258:ALA:HB2	1.77	0.66
1:F:271:VAL:HG12	1:F:273:VAL:CG2	2.26	0.66
1:G:271:VAL:HG12	1:G:273:VAL:CG2	2.26	0.66
1:H:199:TYR:CE1	1:H:202:PRO:HA	2.31	0.66
1:K:223:ALA:CB	1:K:309:LEU:HD21	2.25	0.66
1:D:200:LEU:HB2	1:D:259:LEU:CD1	2.25	0.66
1:B:249:ILE:CD1	1:B:262:LEU:CG	2.67	0.66
1:E:200:LEU:HB2	1:E:259:LEU:CD1	2.25	0.66
1:B:213:VAL:HG13	1:B:325:ILE:HG12	1.76	0.66
1:C:162:ILE:HD13	1:C:400:LEU:HA	1.77	0.66
1:I:295:LEU:HD23	1:I:342:ILE:HD13	1.78	0.66
1:B:200:LEU:HB2	1:B:259:LEU:CD1	2.26	0.65
1:B:279:PRO:O	1:B:285:ARG:HA	1.95	0.65
1:D:279:PRO:O	1:D:285:ARG:HA	1.95	0.65
1:E:195:PHE:CE2	1:E:292:ILE:HD13	2.31	0.65
1:G:279:PRO:O	1:G:285:ARG:HA	1.95	0.65
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.78	0.65
1:I:243:ALA:CA	1:J:256:GLY:O	2.43	0.65
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.78	0.65
1:E:213:VAL:HG13	1:E:325:ILE:HG12	1.76	0.65
1:H:149:THR:O	1:H:154:SER:HA	1.97	0.65
1:I:249:ILE:O	1:I:275:ALA:HA	1.97	0.65
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.78	0.65
1:J:243:ALA:CA	1:K:256:GLY:O	2.43	0.65
1:L:149:THR:O	1:L:154:SER:HA	1.97	0.65
1:M:249:ILE:O	1:M:275:ALA:HA	1.97	0.65
1:A:162:ILE:HD13	1:A:400:LEU:N	2.12	0.65
1:B:162:ILE:HD13	1:B:400:LEU:N	2.12	0.65
1:G:193:MET:SD	1:G:295:LEU:HG	2.36	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:149:THR:O	1:K:154:SER:HA	1.97	0.65
1:H:249:ILE:O	1:H:275:ALA:HA	1.97	0.65
1:J:249:ILE:O	1:J:275:ALA:HA	1.97	0.65
1:C:200:LEU:HB2	1:C:259:LEU:CD1	2.26	0.65
1:F:200:LEU:HB2	1:F:259:LEU:CD1	2.25	0.65
1:J:149:THR:O	1:J:154:SER:HA	1.97	0.65
1:K:249:ILE:O	1:K:275:ALA:HA	1.97	0.65
1:M:295:LEU:HD23	1:M:342:ILE:HD13	1.78	0.65
1:A:279:PRO:O	1:A:285:ARG:HA	1.95	0.65
1:J:295:LEU:HD23	1:J:342:ILE:HD13	1.78	0.65
1:M:223:ALA:CB	1:M:309:LEU:HD21	2.23	0.65
1:C:195:PHE:CE2	1:C:292:ILE:HD13	2.31	0.65
1:M:149:THR:O	1:M:154:SER:HA	1.97	0.65
1:A:195:PHE:CE2	1:A:292:ILE:HD13	2.31	0.65
1:D:195:PHE:CE2	1:D:292:ILE:HD13	2.31	0.65
1:G:161:LEU:HD11	1:G:185:ASP:HB3	1.79	0.65
1:G:195:PHE:CE2	1:G:292:ILE:HD13	2.31	0.65
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.78	0.65
1:D:223:ALA:HA	1:D:309:LEU:HD23	1.79	0.64
1:I:23:LEU:HD13	1:I:60:ILE:HD12	1.70	0.64
1:J:168:LYS:HG3	1:J:187:LEU:HD21	1.78	0.64
1:C:162:ILE:HD13	1:C:400:LEU:N	2.12	0.64
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.78	0.64
1:N:149:THR:O	1:N:154:SER:HA	1.97	0.64
1:C:223:ALA:HA	1:C:309:LEU:HD23	1.79	0.64
1:K:223:ALA:HB3	1:K:251:ALA:CB	2.25	0.64
1:E:162:ILE:HD13	1:E:400:LEU:N	2.12	0.64
1:L:249:ILE:O	1:L:275:ALA:HA	1.97	0.64
1:M:223:ALA:HB3	1:M:251:ALA:CB	2.26	0.64
1:N:223:ALA:CB	1:N:309:LEU:HD21	2.23	0.64
1:B:197:ARG:HG3	1:B:198:GLY:O	1.97	0.64
1:E:223:ALA:HA	1:E:309:LEU:HD23	1.79	0.64
1:L:223:ALA:CB	1:L:309:LEU:HD21	2.23	0.64
1:G:162:ILE:HD13	1:G:400:LEU:N	2.12	0.64
1:M:301:ILE:HD11	1:M:316:ASP:OD2	1.98	0.64
1:N:202:PRO:O	1:N:205:ILE:HG13	1.98	0.64
1:C:213:VAL:HG13	1:C:325:ILE:HG12	1.76	0.64
1:J:202:PRO:O	1:J:205:ILE:HG13	1.98	0.64
1:L:202:PRO:O	1:L:205:ILE:HG13	1.98	0.64
1:L:223:ALA:HB3	1:L:251:ALA:CB	2.26	0.64
1:L:295:LEU:HD23	1:L:342:ILE:HD13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:301:ILE:HD11	1:L:316:ASP:OD2	1.97	0.64
1:A:223:ALA:HA	1:A:309:LEU:HD23	1.79	0.64
1:D:162:ILE:HD13	1:D:400:LEU:N	2.12	0.64
1:G:202:PRO:O	1:G:205:ILE:HG13	1.98	0.64
1:J:223:ALA:CB	1:J:309:LEU:HD21	2.26	0.64
1:K:295:LEU:HD23	1:K:342:ILE:HD13	1.77	0.64
1:G:223:ALA:HA	1:G:309:LEU:HD23	1.79	0.64
1:J:223:ALA:HB3	1:J:251:ALA:CB	2.25	0.64
1:K:295:LEU:HA	1:K:342:ILE:CD1	2.27	0.64
1:K:301:ILE:HD11	1:K:316:ASP:OD2	1.98	0.64
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.78	0.64
1:N:249:ILE:O	1:N:275:ALA:HA	1.97	0.64
1:C:221:LEU:HD11	1:C:309:LEU:HD21	1.80	0.64
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.78	0.64
2:H:1525:PO4:P	4:H:1527:ATP:O3G	2.56	0.64
1:A:227:ILE:HD12	1:A:258:ALA:CB	2.29	0.63
1:B:223:ALA:HA	1:B:309:LEU:HD23	1.79	0.63
1:C:202:PRO:O	1:C:205:ILE:HG13	1.98	0.63
1:D:221:LEU:HD11	1:D:309:LEU:HD21	1.80	0.63
1:F:162:ILE:HD13	1:F:400:LEU:N	2.12	0.63
1:I:149:THR:O	1:I:154:SER:HA	1.97	0.63
1:I:202:PRO:O	1:I:205:ILE:HG13	1.98	0.63
1:K:23:LEU:HD13	1:K:60:ILE:HD12	1.71	0.63
1:N:223:ALA:HB3	1:N:251:ALA:CB	2.26	0.63
1:N:295:LEU:HA	1:N:342:ILE:CD1	2.27	0.63
1:G:200:LEU:HD13	1:G:254:VAL:HG11	1.79	0.63
1:H:295:LEU:HA	1:H:342:ILE:CD1	2.27	0.63
1:J:295:LEU:HA	1:J:342:ILE:CD1	2.27	0.63
2:L:1525:PO4:P	4:L:1527:ATP:O3G	2.56	0.63
1:M:295:LEU:HA	1:M:342:ILE:CD1	2.27	0.63
2:M:1525:PO4:P	4:M:1527:ATP:O3G	2.56	0.63
2:N:1525:PO4:P	4:N:1527:ATP:O3G	2.56	0.63
1:B:202:PRO:O	1:B:205:ILE:HG13	1.98	0.63
1:G:221:LEU:HD11	1:G:309:LEU:HD21	1.80	0.63
1:H:301:ILE:HD11	1:H:316:ASP:OD2	1.99	0.63
2:K:1525:PO4:P	4:K:1527:ATP:O3G	2.56	0.63
1:L:221:LEU:HA	1:L:317:LEU:HG	1.80	0.63
1:A:199:TYR:CB	1:A:325:ILE:HD11	2.21	0.63
1:F:221:LEU:HD11	1:F:309:LEU:HD21	1.80	0.63
1:M:202:PRO:O	1:M:205:ILE:HG13	1.98	0.63
1:M:242:LYS:CB	1:N:257:GLU:HA	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:HD11	1:B:309:LEU:HD21	1.80	0.63
1:F:223:ALA:HA	1:F:309:LEU:HD23	1.79	0.63
1:F:227:ILE:HD12	1:F:258:ALA:CB	2.29	0.63
1:N:196:ASP:OD1	1:N:329:THR:HG22	1.99	0.63
1:N:221:LEU:HA	1:N:317:LEU:HG	1.79	0.63
1:D:227:ILE:HD12	1:D:258:ALA:CB	2.29	0.63
1:H:202:PRO:O	1:H:205:ILE:HG13	1.98	0.63
1:I:223:ALA:HB3	1:I:251:ALA:CB	2.25	0.63
2:J:1525:PO4:P	4:J:1527:ATP:O3G	2.56	0.63
1:L:295:LEU:HA	1:L:342:ILE:CD1	2.27	0.63
1:M:221:LEU:HA	1:M:317:LEU:HG	1.80	0.63
1:N:301:ILE:HD11	1:N:316:ASP:OD2	1.98	0.63
1:E:227:ILE:HD12	1:E:258:ALA:CB	2.29	0.63
1:F:224:ASP:O	1:F:303:GLU:HB2	1.99	0.63
1:G:227:ILE:HD12	1:G:258:ALA:CB	2.29	0.63
1:C:145:ALA:HA	1:C:159:GLY:O	1.99	0.63
1:D:197:ARG:HG3	1:D:198:GLY:O	1.99	0.63
1:E:224:ASP:O	1:E:303:GLU:HB2	1.99	0.63
1:D:145:ALA:HA	1:D:159:GLY:O	1.99	0.63
1:D:224:ASP:O	1:D:303:GLU:HB2	1.99	0.63
1:G:224:ASP:O	1:G:303:GLU:HB2	1.99	0.63
1:H:223:ALA:HB3	1:H:251:ALA:CB	2.25	0.63
1:I:295:LEU:HA	1:I:342:ILE:CD1	2.27	0.63
1:I:301:ILE:HD11	1:I:316:ASP:OD2	1.98	0.63
1:J:301:ILE:HD11	1:J:316:ASP:OD2	1.99	0.63
1:K:202:PRO:O	1:K:205:ILE:HG13	1.98	0.63
1:C:224:ASP:O	1:C:303:GLU:HB2	1.99	0.62
1:E:145:ALA:HA	1:E:159:GLY:O	1.99	0.62
1:I:149:THR:HA	1:I:155:ASP:O	1.99	0.62
1:A:511:ALA:O	1:A:515:ILE:HG13	2.00	0.62
1:B:227:ILE:HD12	1:B:258:ALA:CB	2.29	0.62
1:D:202:PRO:O	1:D:205:ILE:HG13	1.98	0.62
1:E:221:LEU:HD11	1:E:309:LEU:HD21	1.80	0.62
1:K:203:TYR:CD1	1:K:267:MET:HE1	2.34	0.62
1:N:149:THR:HA	1:N:155:ASP:O	2.00	0.62
1:B:224:ASP:O	1:B:303:GLU:HB2	1.99	0.62
1:C:227:ILE:HD12	1:C:258:ALA:CB	2.29	0.62
1:E:511:ALA:O	1:E:515:ILE:HG13	2.00	0.62
1:F:511:ALA:O	1:F:515:ILE:HG13	2.00	0.62
1:G:511:ALA:O	1:G:515:ILE:HG13	2.00	0.62
1:K:221:LEU:HA	1:K:317:LEU:HG	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD11	1:A:309:LEU:HD21	1.80	0.62
1:B:145:ALA:HA	1:B:159:GLY:O	1.99	0.62
1:I:223:ALA:CB	1:I:309:LEU:HD21	2.26	0.62
1:J:192:GLY:O	1:J:375:GLY:HA2	1.99	0.62
1:A:145:ALA:HA	1:A:159:GLY:O	1.99	0.62
1:H:149:THR:HA	1:H:155:ASP:O	2.00	0.62
1:N:240:VAL:CG2	1:N:317:LEU:HD22	2.30	0.62
1:F:145:ALA:HA	1:F:159:GLY:O	1.99	0.62
1:F:207:LYS:H	1:F:207:LYS:CE	2.12	0.62
2:I:1525:PO4:P	4:I:1527:ATP:O3G	2.56	0.62
1:J:149:THR:HA	1:J:155:ASP:O	2.00	0.62
1:J:151:SER:CB	1:J:399:ALA:HA	2.30	0.62
1:M:149:THR:HA	1:M:155:ASP:O	2.00	0.62
1:A:224:ASP:O	1:A:303:GLU:HB2	1.99	0.62
1:B:511:ALA:O	1:B:515:ILE:HG13	2.00	0.62
1:N:204:PHE:C	1:N:207:LYS:HE2	2.20	0.62
1:C:511:ALA:O	1:C:515:ILE:HG13	2.00	0.62
1:D:240:VAL:CG1	1:D:271:VAL:HG13	2.30	0.62
1:G:145:ALA:HA	1:G:159:GLY:O	1.99	0.62
1:G:240:VAL:CG1	1:G:271:VAL:HG13	2.30	0.62
1:J:240:VAL:CG2	1:J:317:LEU:HD22	2.30	0.62
1:K:72:GLN:HA	1:K:75:LYS:HD2	1.82	0.62
1:L:192:GLY:O	1:L:375:GLY:HA2	1.99	0.62
1:D:511:ALA:O	1:D:515:ILE:HG13	2.00	0.62
1:M:240:VAL:CG2	1:M:317:LEU:HD22	2.30	0.62
1:B:204:PHE:CE1	1:B:273:VAL:O	2.53	0.61
1:E:240:VAL:CG1	1:E:271:VAL:HG13	2.30	0.61
1:F:165:ALA:HB2	1:F:187:LEU:HD11	1.82	0.61
1:F:240:VAL:CG1	1:F:271:VAL:HG13	2.30	0.61
1:I:151:SER:CB	1:I:399:ALA:HA	2.30	0.61
1:J:72:GLN:HA	1:J:75:LYS:HD2	1.82	0.61
1:L:72:GLN:HA	1:L:75:LYS:HD2	1.82	0.61
1:H:223:ALA:CB	1:H:309:LEU:HD21	2.25	0.61
1:I:72:GLN:HA	1:I:75:LYS:HD2	1.82	0.61
1:K:151:SER:CB	1:K:399:ALA:HA	2.30	0.61
1:M:151:SER:CB	1:M:399:ALA:HA	2.30	0.61
1:N:151:SER:CB	1:N:399:ALA:HA	2.30	0.61
1:N:192:GLY:O	1:N:375:GLY:HA2	1.99	0.61
1:C:204:PHE:CE1	1:C:273:VAL:O	2.53	0.61
1:F:204:PHE:CE1	1:F:273:VAL:O	2.53	0.61
1:H:192:GLY:O	1:H:375:GLY:HA2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:151:SER:CB	1:L:399:ALA:HA	2.30	0.61
1:H:151:SER:CB	1:H:399:ALA:HA	2.30	0.61
1:B:240:VAL:CG1	1:B:271:VAL:HG13	2.30	0.61
1:H:72:GLN:HA	1:H:75:LYS:HD2	1.82	0.61
1:H:221:LEU:HA	1:H:317:LEU:HG	1.81	0.61
1:K:177:VAL:HG22	1:K:379:ILE:CB	2.30	0.61
1:K:240:VAL:CG2	1:K:317:LEU:HD22	2.30	0.61
1:L:149:THR:HA	1:L:155:ASP:O	1.99	0.61
1:L:189:VAL:HA	1:L:377:ALA:HA	1.83	0.61
1:L:240:VAL:CG2	1:L:317:LEU:HD22	2.30	0.61
1:D:169:VAL:HB	1:D:173:GLY:HA3	1.82	0.61
1:I:192:GLY:O	1:I:375:GLY:HA2	1.99	0.61
1:A:204:PHE:CE1	1:A:273:VAL:O	2.53	0.61
1:H:189:VAL:HA	1:H:377:ALA:HA	1.83	0.61
1:M:23:LEU:HD13	1:M:60:ILE:HD12	1.70	0.61
1:E:169:VAL:HB	1:E:173:GLY:HA3	1.82	0.61
1:G:204:PHE:CE1	1:G:273:VAL:O	2.53	0.61
1:N:189:VAL:HA	1:N:377:ALA:HA	1.83	0.61
1:C:169:VAL:HB	1:C:173:GLY:HA3	1.83	0.61
1:D:204:PHE:CE1	1:D:273:VAL:O	2.53	0.61
1:H:203:TYR:CD1	1:H:267:MET:HE1	2.36	0.61
1:I:221:LEU:HA	1:I:317:LEU:HG	1.81	0.61
1:J:221:LEU:HA	1:J:317:LEU:HG	1.80	0.61
1:M:203:TYR:CD1	1:M:267:MET:HE1	2.36	0.61
1:B:200:LEU:CD1	1:B:259:LEU:HD13	2.31	0.61
1:E:220:ILE:HD13	1:E:332:ILE:CD1	2.27	0.61
1:F:220:ILE:HD13	1:F:332:ILE:CD1	2.27	0.61
1:K:189:VAL:HA	1:K:377:ALA:HA	1.83	0.61
1:K:480:ALA:O	1:K:483:GLU:HG2	2.01	0.61
1:M:192:GLY:O	1:M:375:GLY:HA2	1.99	0.61
1:N:72:GLN:HA	1:N:75:LYS:HD2	1.82	0.61
1:B:169:VAL:HB	1:B:173:GLY:HA3	1.82	0.60
1:I:240:VAL:CG2	1:I:317:LEU:HD22	2.30	0.60
1:K:149:THR:HA	1:K:155:ASP:O	2.00	0.60
1:A:169:VAL:HB	1:A:173:GLY:HA3	1.82	0.60
1:D:200:LEU:CD1	1:D:259:LEU:HD13	2.31	0.60
1:H:240:VAL:HG22	1:H:317:LEU:HD22	1.84	0.60
1:J:203:TYR:CD1	1:J:267:MET:HE1	2.35	0.60
1:L:480:ALA:O	1:L:483:GLU:HG2	2.01	0.60
1:M:72:GLN:HA	1:M:75:LYS:HD2	1.82	0.60
1:N:480:ALA:O	1:N:483:GLU:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:TYR:CB	1:B:325:ILE:HD11	2.21	0.60
1:D:52:ASP:OD1	2:D:1525:PO4:P	2.60	0.60
1:F:169:VAL:HB	1:F:173:GLY:HA3	1.83	0.60
1:G:169:VAL:HB	1:G:173:GLY:HA3	1.82	0.60
1:G:217:SER:HA	1:G:320:ALA:O	2.02	0.60
1:H:240:VAL:CG2	1:H:317:LEU:HD22	2.30	0.60
1:M:480:ALA:O	1:M:483:GLU:HG2	2.01	0.60
1:I:169:VAL:HG12	1:I:377:ALA:HB3	1.83	0.60
1:I:240:VAL:HG22	1:I:317:LEU:HD22	1.84	0.60
1:J:169:VAL:HG12	1:J:377:ALA:HB3	1.83	0.60
1:J:189:VAL:HA	1:J:377:ALA:HA	1.83	0.60
1:A:217:SER:HA	1:A:320:ALA:O	2.02	0.60
1:C:200:LEU:CD1	1:C:259:LEU:HD13	2.31	0.60
1:C:240:VAL:CG1	1:C:271:VAL:HG13	2.30	0.60
1:D:199:TYR:CB	1:D:325:ILE:HD11	2.20	0.60
1:F:217:SER:HA	1:F:320:ALA:O	2.02	0.60
1:L:203:TYR:CD1	1:L:267:MET:HE1	2.37	0.60
1:A:240:VAL:CG1	1:A:271:VAL:HG13	2.30	0.60
1:D:220:ILE:HD13	1:D:332:ILE:CD1	2.27	0.60
1:E:200:LEU:CD1	1:E:259:LEU:HD13	2.31	0.60
1:F:52:ASP:OD1	2:F:1525:PO4:P	2.60	0.60
1:G:220:ILE:HD13	1:G:332:ILE:CD1	2.27	0.60
1:K:192:GLY:HA3	1:K:332:ILE:O	2.02	0.60
1:A:200:LEU:CD1	1:A:259:LEU:HD13	2.31	0.60
1:H:480:ALA:O	1:H:483:GLU:HG2	2.01	0.60
1:I:480:ALA:O	1:I:483:GLU:HG2	2.01	0.60
1:B:52:ASP:OD1	2:B:1525:PO4:P	2.60	0.60
1:F:200:LEU:CD1	1:F:259:LEU:HD13	2.31	0.60
1:K:127:ALA:HB2	1:K:426:LEU:HD11	1.84	0.60
1:A:200:LEU:HB3	1:A:259:LEU:HD22	1.84	0.60
1:F:199:TYR:CB	1:F:325:ILE:HD11	2.21	0.60
1:J:240:VAL:HG22	1:J:317:LEU:HD22	1.84	0.60
1:M:193:MET:SD	1:M:292:ILE:HA	2.42	0.60
1:N:240:VAL:HG22	1:N:317:LEU:HD22	1.83	0.60
1:A:220:ILE:HD13	1:A:332:ILE:CD1	2.27	0.59
1:B:217:SER:HA	1:B:320:ALA:O	2.02	0.59
1:B:220:ILE:HD13	1:B:332:ILE:CD1	2.27	0.59
1:J:193:MET:SD	1:J:292:ILE:HA	2.42	0.59
1:M:127:ALA:HB2	1:M:426:LEU:HD11	1.84	0.59
1:N:127:ALA:HB2	1:N:426:LEU:HD11	1.84	0.59
1:C:220:ILE:HD13	1:C:332:ILE:CD1	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:127:ALA:HB2	1:J:426:LEU:HD11	1.84	0.59
1:K:204:PHE:CD1	1:K:273:VAL:O	2.55	0.59
1:L:127:ALA:HB2	1:L:426:LEU:HD11	1.84	0.59
1:M:242:LYS:HB3	1:N:257:GLU:HA	1.83	0.59
1:N:204:PHE:CD1	1:N:273:VAL:O	2.55	0.59
1:D:200:LEU:HB3	1:D:259:LEU:HD22	1.84	0.59
1:G:193:MET:HE1	1:G:296:THR:HG23	1.84	0.59
1:J:204:PHE:CD1	1:J:273:VAL:O	2.55	0.59
1:L:193:MET:SD	1:L:292:ILE:HA	2.42	0.59
1:C:200:LEU:HB3	1:C:259:LEU:HD22	1.84	0.59
1:E:217:SER:HA	1:E:320:ALA:O	2.02	0.59
1:I:193:MET:SD	1:I:292:ILE:HA	2.42	0.59
1:I:204:PHE:CD1	1:I:273:VAL:O	2.55	0.59
1:L:174:VAL:HG12	1:L:376:VAL:HG13	1.83	0.59
1:H:193:MET:SD	1:H:292:ILE:HA	2.42	0.59
1:H:301:ILE:HD11	1:H:312:ALA:CB	2.32	0.59
1:I:127:ALA:HB2	1:I:426:LEU:HD11	1.84	0.59
1:J:192:GLY:HA3	1:J:332:ILE:O	2.03	0.59
1:K:169:VAL:HG12	1:K:377:ALA:HB3	1.83	0.59
1:K:240:VAL:HG22	1:K:317:LEU:HD22	1.83	0.59
1:N:193:MET:SD	1:N:292:ILE:HA	2.42	0.59
1:G:52:ASP:OD1	2:G:1525:PO4:P	2.61	0.59
1:I:203:TYR:CD1	1:I:267:MET:HE1	2.37	0.59
1:J:480:ALA:O	1:J:483:GLU:HG2	2.01	0.59
1:L:204:PHE:CD1	1:L:273:VAL:O	2.55	0.59
1:M:23:LEU:HD23	1:M:74:VAL:HG13	1.85	0.59
1:M:204:PHE:CD1	1:M:273:VAL:O	2.55	0.59
1:A:52:ASP:OD1	2:A:1525:PO4:P	2.61	0.59
1:H:127:ALA:HB2	1:H:426:LEU:HD11	1.84	0.59
1:H:169:VAL:HG12	1:H:377:ALA:HB3	1.83	0.59
1:N:23:LEU:HD23	1:N:74:VAL:HG13	1.84	0.59
1:H:23:LEU:HD23	1:H:74:VAL:HG13	1.84	0.59
1:K:242:LYS:HG3	1:L:257:GLU:O	2.03	0.59
1:L:192:GLY:HA3	1:L:332:ILE:O	2.03	0.59
1:H:165:ALA:O	1:H:169:VAL:HG22	2.03	0.59
1:H:204:PHE:CD1	1:H:273:VAL:O	2.55	0.59
2:J:1525:PO4:P	4:J:1527:ATP:O1A	2.61	0.59
1:M:165:ALA:O	1:M:169:VAL:HG22	2.03	0.59
1:M:240:VAL:HG22	1:M:317:LEU:HD22	1.83	0.59
1:M:243:ALA:CB	1:N:256:GLY:O	2.51	0.59
2:N:1525:PO4:P	4:N:1527:ATP:O1A	2.61	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:TYR:CB	1:G:325:ILE:HD11	2.21	0.59
1:L:165:ALA:O	1:L:169:VAL:HG22	2.03	0.59
1:M:169:VAL:HG12	1:M:377:ALA:HB3	1.83	0.59
1:M:420:ILE:HD12	1:M:451:LEU:HD13	1.85	0.59
2:M:1525:PO4:P	4:M:1527:ATP:O1A	2.61	0.59
1:N:165:ALA:O	1:N:169:VAL:HG22	2.03	0.59
1:E:52:ASP:OD1	2:E:1525:PO4:P	2.61	0.58
1:H:256:GLY:O	1:N:243:ALA:CB	2.51	0.58
1:H:298:GLY:HA3	1:H:318:GLY:HA3	1.86	0.58
1:I:243:ALA:CB	1:J:256:GLY:O	2.51	0.58
1:J:243:ALA:CB	1:K:256:GLY:O	2.51	0.58
1:J:298:GLY:HA3	1:J:318:GLY:HA3	1.85	0.58
1:K:165:ALA:O	1:K:169:VAL:HG22	2.03	0.58
1:L:175:ILE:HG22	1:L:176:THR:N	2.17	0.58
1:M:242:LYS:HB3	1:N:257:GLU:CA	2.31	0.58
1:N:169:VAL:HG12	1:N:377:ALA:HB3	1.83	0.58
1:B:195:PHE:CZ	1:B:330:THR:HB	2.38	0.58
1:H:243:ALA:CB	1:I:256:GLY:O	2.51	0.58
2:I:1525:PO4:P	4:I:1527:ATP:O1A	2.61	0.58
1:K:301:ILE:HD12	1:K:312:ALA:HB2	1.65	0.58
2:K:1525:PO4:P	4:K:1527:ATP:O1A	2.61	0.58
1:L:23:LEU:HD23	1:L:74:VAL:HG13	1.85	0.58
1:L:240:VAL:HG22	1:L:317:LEU:HD22	1.84	0.58
2:L:1525:PO4:P	4:L:1527:ATP:O1A	2.61	0.58
1:N:192:GLY:HA3	1:N:332:ILE:O	2.03	0.58
1:I:169:VAL:HB	1:I:173:GLY:HA3	1.85	0.58
1:N:420:ILE:HD12	1:N:451:LEU:HD13	1.86	0.58
1:C:52:ASP:OD1	2:C:1525:PO4:P	2.61	0.58
1:G:221:LEU:HD13	1:G:236:VAL:HG21	1.86	0.58
1:H:169:VAL:HB	1:H:173:GLY:HA3	1.85	0.58
2:H:1525:PO4:P	4:H:1527:ATP:O1A	2.61	0.58
1:I:298:GLY:HA3	1:I:318:GLY:HA3	1.85	0.58
1:J:169:VAL:HB	1:J:173:GLY:HA3	1.85	0.58
1:N:203:TYR:CD1	1:N:267:MET:HE1	2.39	0.58
1:A:221:LEU:HD13	1:A:236:VAL:HG21	1.86	0.58
1:D:217:SER:HA	1:D:320:ALA:O	2.02	0.58
1:E:199:TYR:CB	1:E:325:ILE:HD11	2.21	0.58
1:G:200:LEU:CD1	1:G:200:LEU:N	2.64	0.58
1:I:165:ALA:O	1:I:169:VAL:HG22	2.03	0.58
1:K:298:GLY:HA3	1:K:318:GLY:HA3	1.86	0.58
1:B:200:LEU:HB3	1:B:259:LEU:HD22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:TYR:CB	1:C:325:ILE:HD11	2.21	0.58
1:E:200:LEU:HB3	1:E:259:LEU:HD22	1.84	0.58
1:F:200:LEU:HB3	1:F:259:LEU:HD22	1.84	0.58
1:F:221:LEU:HD13	1:F:236:VAL:HG21	1.86	0.58
1:H:192:GLY:HA3	1:H:332:ILE:O	2.03	0.58
1:L:152:ALA:HB3	1:L:155:ASP:H	1.69	0.58
1:L:169:VAL:HG12	1:L:377:ALA:HB3	1.83	0.58
1:L:243:ALA:CB	1:M:256:GLY:O	2.51	0.58
1:L:420:ILE:HD12	1:L:451:LEU:HD13	1.86	0.58
1:N:199:TYR:CB	1:N:325:ILE:HD11	2.34	0.58
1:N:298:GLY:HA3	1:N:318:GLY:HA3	1.85	0.58
1:E:193:MET:CE	1:E:332:ILE:HD12	2.19	0.58
1:I:192:GLY:HA3	1:I:332:ILE:O	2.02	0.58
1:J:162:ILE:HD13	1:J:400:LEU:CA	2.34	0.58
1:C:217:SER:HA	1:C:320:ALA:O	2.02	0.58
1:H:519:CYS:O	1:N:39:VAL:N	2.37	0.58
1:I:301:ILE:HD11	1:I:312:ALA:CB	2.32	0.58
1:K:169:VAL:HB	1:K:173:GLY:HA3	1.85	0.58
1:G:200:LEU:HD11	1:G:254:VAL:CG1	2.33	0.58
1:H:38:VAL:CA	1:I:519:CYS:O	2.52	0.58
1:I:152:ALA:HB3	1:I:155:ASP:H	1.69	0.58
1:J:23:LEU:HD23	1:J:74:VAL:HG13	1.84	0.58
1:J:152:ALA:HB3	1:J:155:ASP:H	1.69	0.58
1:J:165:ALA:O	1:J:169:VAL:HG22	2.03	0.58
1:K:162:ILE:HD13	1:K:400:LEU:CA	2.34	0.58
1:N:169:VAL:HB	1:N:173:GLY:HA3	1.85	0.58
1:B:293:ALA:HB1	1:B:299:THR:HA	1.85	0.58
1:F:293:ALA:HB1	1:F:299:THR:HA	1.86	0.58
1:G:293:ALA:HB1	1:G:299:THR:HA	1.85	0.58
1:H:420:ILE:HD12	1:H:451:LEU:HD13	1.85	0.58
1:I:23:LEU:HD23	1:I:74:VAL:HG13	1.84	0.58
1:K:23:LEU:HD23	1:K:74:VAL:HG13	1.84	0.58
1:K:39:VAL:N	1:L:519:CYS:O	2.37	0.58
1:K:242:LYS:CB	1:L:257:GLU:HA	2.34	0.58
1:K:420:ILE:HD12	1:K:451:LEU:HD13	1.85	0.58
1:M:192:GLY:HA3	1:M:332:ILE:O	2.03	0.58
1:C:293:ALA:HB1	1:C:299:THR:HA	1.85	0.57
1:H:39:VAL:N	1:I:519:CYS:O	2.37	0.57
1:I:38:VAL:CA	1:J:519:CYS:O	2.52	0.57
1:K:152:ALA:HB3	1:K:155:ASP:H	1.69	0.57
1:L:298:GLY:HA3	1:L:318:GLY:HA3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:199:TYR:CB	1:M:325:ILE:HD11	2.34	0.57
1:I:162:ILE:HD13	1:I:400:LEU:CA	2.34	0.57
1:M:298:GLY:HA3	1:M:318:GLY:HA3	1.85	0.57
1:B:221:LEU:HD13	1:B:236:VAL:HG21	1.86	0.57
1:C:224:ASP:HA	1:C:289:LEU:HD13	1.86	0.57
1:F:381:VAL:HG22	1:F:382:GLY:N	2.20	0.57
1:G:300:VAL:CG2	1:G:312:ALA:HB2	2.33	0.57
1:H:353:ILE:HD11	1:H:369:VAL:CG2	2.35	0.57
1:I:353:ILE:HD11	1:I:369:VAL:CG2	2.35	0.57
1:I:420:ILE:HD12	1:I:451:LEU:HD13	1.85	0.57
1:J:39:VAL:N	1:K:519:CYS:O	2.37	0.57
1:D:224:ASP:HA	1:D:289:LEU:HD13	1.86	0.57
1:F:193:MET:CE	1:F:332:ILE:HD12	2.19	0.57
1:G:381:VAL:HG22	1:G:382:GLY:N	2.20	0.57
1:I:301:ILE:HD11	1:I:312:ALA:HB1	1.85	0.57
1:I:524:LEU:HG	1:I:525:PRO:N	2.20	0.57
1:K:243:ALA:CB	1:L:256:GLY:O	2.51	0.57
1:N:152:ALA:HB3	1:N:155:ASP:H	1.69	0.57
1:E:221:LEU:HD13	1:E:236:VAL:HG21	1.86	0.57
1:E:300:VAL:CG2	1:E:312:ALA:HB2	2.33	0.57
1:F:300:VAL:CG2	1:F:312:ALA:HB2	2.33	0.57
1:G:200:LEU:CD1	1:G:254:VAL:HG21	2.22	0.57
1:I:39:VAL:N	1:J:519:CYS:O	2.37	0.57
1:J:207:LYS:HE2	1:J:207:LYS:CA	2.34	0.57
1:L:301:ILE:HD12	1:L:312:ALA:HB2	1.65	0.57
1:M:39:VAL:N	1:N:519:CYS:O	2.37	0.57
1:M:353:ILE:HD11	1:M:369:VAL:CG2	2.35	0.57
1:E:381:VAL:HG22	1:E:382:GLY:N	2.20	0.57
1:J:301:ILE:HD11	1:J:312:ALA:HB1	1.85	0.57
1:J:420:ILE:HD12	1:J:451:LEU:HD13	1.86	0.57
1:K:353:ILE:HD11	1:K:369:VAL:CG2	2.35	0.57
1:L:36:ARG:O	1:M:518:GLU:HB2	2.05	0.57
1:L:384:ALA:HA	1:L:385:THR:C	2.25	0.57
1:A:300:VAL:CG2	1:A:312:ALA:HB2	2.33	0.57
1:E:200:LEU:HB3	1:E:259:LEU:CD2	2.35	0.57
1:E:293:ALA:HB1	1:E:299:THR:HA	1.86	0.57
1:F:23:LEU:HA	1:F:60:ILE:CD1	2.32	0.57
1:H:301:ILE:HD11	1:H:312:ALA:HB1	1.85	0.57
1:I:240:VAL:HG11	1:I:247:LEU:HA	1.87	0.57
1:J:36:ARG:O	1:K:518:GLU:HB2	2.05	0.57
1:J:240:VAL:HG11	1:J:247:LEU:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:524:LEU:HG	1:J:525:PRO:N	2.20	0.57
1:K:301:ILE:HD11	1:K:312:ALA:CB	2.32	0.57
1:K:524:LEU:HG	1:K:525:PRO:N	2.20	0.57
1:L:199:TYR:CB	1:L:325:ILE:HD11	2.34	0.57
1:M:524:LEU:HG	1:M:525:PRO:N	2.20	0.57
1:N:240:VAL:HG11	1:N:247:LEU:HA	1.87	0.57
1:N:353:ILE:HD11	1:N:369:VAL:CG2	2.35	0.57
1:C:221:LEU:HD13	1:C:236:VAL:HG21	1.86	0.57
1:D:293:ALA:HB1	1:D:299:THR:HA	1.86	0.57
1:E:240:VAL:HG21	1:E:247:LEU:HB2	1.87	0.57
1:F:192:GLY:HA3	1:F:376:VAL:HG23	1.86	0.57
1:F:240:VAL:HG21	1:F:247:LEU:HB2	1.87	0.57
1:G:224:ASP:HA	1:G:289:LEU:HD13	1.86	0.57
1:G:240:VAL:HG21	1:G:247:LEU:HB2	1.87	0.57
1:H:518:GLU:HB2	1:N:36:ARG:O	2.05	0.57
1:L:524:LEU:HG	1:L:525:PRO:N	2.20	0.57
1:A:240:VAL:HG21	1:A:247:LEU:HB2	1.87	0.57
1:D:221:LEU:HD13	1:D:236:VAL:HG21	1.86	0.57
1:D:240:VAL:HG21	1:D:247:LEU:HB2	1.87	0.57
1:E:192:GLY:HA3	1:E:376:VAL:HG23	1.86	0.57
1:H:240:VAL:HG11	1:H:247:LEU:HA	1.87	0.57
1:H:524:LEU:HG	1:H:525:PRO:N	2.20	0.57
1:A:293:ALA:HB1	1:A:299:THR:HA	1.86	0.57
1:D:381:VAL:HG22	1:D:382:GLY:N	2.20	0.57
1:E:38:VAL:HG21	1:E:56:VAL:HG22	1.87	0.57
1:G:192:GLY:HA3	1:G:376:VAL:HG23	1.86	0.57
1:H:519:CYS:O	1:N:38:VAL:CA	2.52	0.57
1:I:384:ALA:HA	1:I:385:THR:C	2.25	0.57
1:I:518:GLU:HB3	1:I:519:CYS:N	2.19	0.57
1:J:353:ILE:HD11	1:J:369:VAL:CG2	2.35	0.57
1:J:518:GLU:HB3	1:J:519:CYS:N	2.19	0.57
1:L:39:VAL:N	1:M:519:CYS:O	2.37	0.57
1:L:162:ILE:HD13	1:L:400:LEU:CA	2.34	0.57
1:L:206:ASN:OD1	1:L:207:LYS:HD2	2.05	0.57
1:B:300:VAL:CG2	1:B:312:ALA:HB2	2.33	0.56
1:D:300:VAL:CG2	1:D:312:ALA:HB2	2.33	0.56
1:F:224:ASP:HA	1:F:289:LEU:HD13	1.86	0.56
1:H:36:ARG:O	1:I:518:GLU:HB2	2.05	0.56
1:I:36:ARG:O	1:J:518:GLU:HB2	2.05	0.56
1:N:524:LEU:HG	1:N:525:LEU:N	2.20	0.56
1:B:192:GLY:HA3	1:B:376:VAL:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ASP:HA	1:B:289:LEU:HD13	1.86	0.56
1:C:200:LEU:HB3	1:C:259:LEU:CD2	2.35	0.56
1:H:152:ALA:HB3	1:H:155:ASP:H	1.69	0.56
1:N:518:GLU:HB3	1:N:519:CYS:N	2.19	0.56
1:A:224:ASP:HA	1:A:289:LEU:HD13	1.86	0.56
1:B:38:VAL:HG21	1:B:56:VAL:HG22	1.87	0.56
1:B:200:LEU:HB3	1:B:259:LEU:CD2	2.35	0.56
1:C:38:VAL:HG21	1:C:56:VAL:HG22	1.86	0.56
1:D:200:LEU:HB3	1:D:259:LEU:CD2	2.35	0.56
1:F:38:VAL:HG21	1:F:56:VAL:HG22	1.87	0.56
1:J:384:ALA:HA	1:J:385:THR:C	2.25	0.56
1:K:384:ALA:HA	1:K:385:THR:C	2.25	0.56
1:K:518:GLU:HB3	1:K:519:CYS:N	2.19	0.56
1:L:38:VAL:CA	1:M:519:CYS:O	2.52	0.56
1:M:240:VAL:HG11	1:M:247:LEU:HA	1.87	0.56
1:M:384:ALA:HA	1:M:385:THR:C	2.25	0.56
1:A:207:LYS:HB2	1:A:208:PRO:HD3	1.87	0.56
1:A:381:VAL:HG22	1:A:382:GLY:N	2.20	0.56
1:B:240:VAL:HG21	1:B:247:LEU:HB2	1.87	0.56
1:C:23:LEU:HA	1:C:60:ILE:CD1	2.32	0.56
1:E:200:LEU:HD12	1:E:259:LEU:HD13	1.88	0.56
1:E:224:ASP:HA	1:E:289:LEU:HD13	1.86	0.56
1:F:200:LEU:HD12	1:F:259:LEU:HD13	1.88	0.56
1:K:36:ARG:O	1:L:518:GLU:HB2	2.05	0.56
1:K:38:VAL:CA	1:L:519:CYS:O	2.52	0.56
1:K:240:VAL:HG11	1:K:247:LEU:HA	1.87	0.56
1:L:169:VAL:HB	1:L:173:GLY:HA3	1.85	0.56
1:M:152:ALA:HB3	1:M:155:ASP:H	1.69	0.56
1:A:38:VAL:HG21	1:A:56:VAL:HG22	1.87	0.56
1:C:300:VAL:CG2	1:C:312:ALA:HB2	2.33	0.56
1:H:518:GLU:HB3	1:H:519:CYS:N	2.19	0.56
1:J:100:ILE:HD13	1:J:514:MET:SD	2.46	0.56
1:L:100:ILE:HD13	1:L:514:MET:SD	2.46	0.56
1:D:150:ILE:HD11	1:D:493:ILE:HG23	1.88	0.56
1:D:192:GLY:HA3	1:D:376:VAL:HG23	1.86	0.56
1:D:193:MET:CE	1:D:332:ILE:HD12	2.19	0.56
1:H:240:VAL:HG21	1:H:247:LEU:HD13	1.88	0.56
1:K:301:ILE:HD11	1:K:312:ALA:HB1	1.85	0.56
1:M:36:ARG:O	1:N:518:GLU:HB2	2.05	0.56
1:A:192:GLY:HA3	1:A:376:VAL:HG23	1.86	0.56
1:D:38:VAL:HG21	1:D:56:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:521:VAL:CG1	1:E:59:GLU:HB3	2.36	0.56
1:E:521:VAL:CG1	1:F:59:GLU:HB3	2.36	0.56
1:F:187:LEU:CD1	1:F:379:ILE:HG12	2.35	0.56
1:F:200:LEU:HB3	1:F:259:LEU:CD2	2.35	0.56
1:H:100:ILE:HD13	1:H:514:MET:SD	2.46	0.56
1:L:240:VAL:HG11	1:L:247:LEU:HA	1.87	0.56
1:N:301:ILE:HD11	1:N:312:ALA:HB1	1.86	0.56
1:B:31:LEU:HB2	1:B:90:THR:HG21	1.88	0.56
1:C:240:VAL:HG21	1:C:247:LEU:HB2	1.87	0.56
1:C:312:ALA:HB1	1:C:316:ASP:OD2	2.06	0.56
1:D:200:LEU:HD12	1:D:259:LEU:HD13	1.88	0.56
1:F:521:VAL:CG1	1:G:59:GLU:HB3	2.36	0.56
1:H:384:ALA:HA	1:H:385:THR:C	2.25	0.56
1:J:243:ALA:HA	1:K:260:ALA:HB2	1.88	0.56
1:L:301:ILE:HD11	1:L:312:ALA:HB1	1.86	0.56
1:M:518:GLU:HB3	1:M:519:CYS:N	2.19	0.56
1:A:200:LEU:HB3	1:A:259:LEU:CD2	2.35	0.56
1:B:312:ALA:HB1	1:B:316:ASP:OD2	2.06	0.56
1:H:302:SER:HB2	1:H:305:ILE:H	1.71	0.56
1:I:240:VAL:HG21	1:I:247:LEU:HD13	1.88	0.56
1:K:206:ASN:HB2	1:K:213:VAL:HG23	1.88	0.56
1:L:353:ILE:HD11	1:L:369:VAL:CG2	2.35	0.56
1:B:381:VAL:HG22	1:B:382:GLY:N	2.19	0.56
1:F:150:ILE:HD11	1:F:493:ILE:HG23	1.87	0.56
1:F:312:ALA:HB1	1:F:316:ASP:OD2	2.06	0.56
1:H:239:ALA:HB1	1:H:314:LEU:HB3	1.88	0.56
1:M:38:VAL:CA	1:N:519:CYS:O	2.52	0.56
1:M:100:ILE:HD13	1:M:514:MET:SD	2.46	0.56
1:M:301:ILE:HD11	1:M:312:ALA:HB1	1.86	0.56
1:N:240:VAL:HG21	1:N:247:LEU:HD13	1.87	0.56
1:C:200:LEU:HD12	1:C:259:LEU:HD13	1.88	0.55
1:C:521:VAL:CG1	1:D:59:GLU:HB3	2.36	0.55
1:I:239:ALA:HB1	1:I:314:LEU:HB3	1.88	0.55
1:J:240:VAL:HG21	1:J:247:LEU:HD13	1.88	0.55
1:A:59:GLU:HB3	1:G:521:VAL:CG1	2.36	0.55
1:A:200:LEU:HD21	1:A:254:VAL:HG21	1.04	0.55
1:D:191:GLU:HG3	1:D:342:ILE:CD1	2.37	0.55
1:F:202:PRO:O	1:F:205:ILE:HG13	2.05	0.55
1:G:38:VAL:HG21	1:G:56:VAL:HG22	1.87	0.55
1:G:312:ALA:HB1	1:G:316:ASP:OD2	2.06	0.55
1:K:193:MET:HE1	1:K:295:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:183:LEU:HG	1:L:183:LEU:O	2.06	0.55
1:N:239:ALA:HB1	1:N:314:LEU:HB3	1.88	0.55
1:D:312:ALA:HB1	1:D:316:ASP:OD2	2.06	0.55
1:J:290:GLN:HA	1:J:300:VAL:CG2	2.37	0.55
1:K:100:ILE:HD13	1:K:514:MET:SD	2.46	0.55
1:K:302:SER:HB2	1:K:305:ILE:H	1.71	0.55
1:M:162:ILE:HD13	1:M:400:LEU:CA	2.34	0.55
1:B:150:ILE:HD11	1:B:493:ILE:HG23	1.88	0.55
1:I:100:ILE:HD13	1:I:514:MET:SD	2.46	0.55
1:N:384:ALA:HA	1:N:385:THR:C	2.25	0.55
1:C:381:VAL:HG22	1:C:382:GLY:N	2.20	0.55
1:K:240:VAL:HG11	1:K:247:LEU:CB	2.37	0.55
1:K:240:VAL:HG21	1:K:247:LEU:HD13	1.88	0.55
1:L:518:GLU:HB3	1:L:519:CYS:N	2.19	0.55
1:N:100:ILE:HD13	1:N:514:MET:SD	2.46	0.55
1:N:221:LEU:HD13	1:N:317:LEU:HD11	1.89	0.55
1:B:200:LEU:HD12	1:B:259:LEU:HD13	1.88	0.55
1:I:243:ALA:HA	1:J:260:ALA:HB2	1.88	0.55
1:J:38:VAL:CA	1:K:519:CYS:O	2.52	0.55
1:J:240:VAL:HG11	1:J:247:LEU:CB	2.37	0.55
1:K:193:MET:CE	1:K:295:LEU:HD12	2.36	0.55
1:A:521:VAL:CG1	1:B:59:GLU:HB3	2.36	0.55
1:B:521:VAL:CG1	1:C:59:GLU:HB3	2.36	0.55
1:D:23:LEU:HA	1:D:60:ILE:CD1	2.32	0.55
1:D:190:VAL:HB	1:D:334:ASP:HB2	1.89	0.55
1:D:406:ALA:HB1	1:D:411:VAL:HG13	1.89	0.55
1:M:240:VAL:HG11	1:M:247:LEU:CB	2.37	0.55
1:E:312:ALA:HB1	1:E:316:ASP:OD2	2.06	0.55
1:F:31:LEU:HB2	1:F:90:THR:HG21	1.89	0.55
1:N:240:VAL:HG11	1:N:247:LEU:CB	2.35	0.55
1:A:200:LEU:HD12	1:A:259:LEU:HD13	1.88	0.55
1:A:312:ALA:HB1	1:A:316:ASP:OD2	2.06	0.55
1:D:31:LEU:HB2	1:D:90:THR:HG21	1.89	0.55
1:F:207:LYS:HE2	1:F:207:LYS:N	2.21	0.55
1:G:193:MET:CE	1:G:295:LEU:HB3	2.37	0.55
1:H:240:VAL:HG11	1:H:247:LEU:CB	2.37	0.55
1:H:243:ALA:CA	1:I:260:ALA:HB2	2.37	0.55
1:J:199:TYR:CB	1:J:325:ILE:HD11	2.34	0.55
1:A:197:ARG:HG3	1:A:198:GLY:O	2.07	0.54
1:I:181:THR:O	1:I:383:ALA:HB3	2.08	0.54
1:I:240:VAL:HG11	1:I:247:LEU:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:239:ALA:HB1	1:J:314:LEU:HB3	1.88	0.54
1:L:240:VAL:HG21	1:L:247:LEU:HD13	1.87	0.54
1:A:213:VAL:HG13	1:A:325:ILE:HG12	1.89	0.54
1:E:406:ALA:HB1	1:E:411:VAL:HG13	1.89	0.54
1:F:150:ILE:CD1	1:F:493:ILE:CA	2.74	0.54
1:F:150:ILE:HD13	1:F:493:ILE:CG2	2.36	0.54
1:L:301:ILE:HD11	1:L:312:ALA:CB	2.32	0.54
1:M:239:ALA:HB1	1:M:314:LEU:HB3	1.88	0.54
1:H:207:LYS:HE2	1:H:207:LYS:CA	2.38	0.54
1:I:221:LEU:HD13	1:I:317:LEU:HD11	1.89	0.54
1:M:240:VAL:HG21	1:M:247:LEU:HD13	1.87	0.54
1:M:290:GLN:HA	1:M:300:VAL:CG2	2.38	0.54
1:K:221:LEU:HD13	1:K:317:LEU:HD11	1.90	0.54
1:N:221:LEU:HD21	1:N:309:LEU:HD22	1.88	0.54
1:B:137:PRO:HA	1:B:410:GLY:HA3	1.90	0.54
1:C:406:ALA:HB1	1:C:411:VAL:HG13	1.89	0.54
1:F:206:ASN:HB3	1:F:208:PRO:HD2	1.90	0.54
1:G:241:ALA:HA	1:G:271:VAL:HG22	1.90	0.54
1:L:240:VAL:HG11	1:L:247:LEU:CB	2.37	0.54
1:I:290:GLN:HA	1:I:300:VAL:CG2	2.37	0.54
1:J:302:SER:HB2	1:J:305:ILE:H	1.72	0.54
1:K:137:PRO:CA	1:K:410:GLY:HA3	2.36	0.54
1:A:241:ALA:HA	1:A:271:VAL:HG22	1.90	0.54
1:B:150:ILE:HD13	1:B:493:ILE:CG2	2.37	0.54
1:E:200:LEU:CB	1:E:259:LEU:CD1	2.86	0.54
1:H:260:ALA:HB2	1:N:243:ALA:CA	2.38	0.54
1:H:260:ALA:HB2	1:N:243:ALA:HA	1.88	0.54
1:J:221:LEU:HD13	1:J:317:LEU:HD11	1.90	0.54
1:N:221:LEU:HD22	1:N:236:VAL:HG11	1.90	0.54
1:C:464:VAL:HG22	1:J:464:VAL:HG22	1.90	0.54
1:D:150:ILE:CD1	1:D:493:ILE:CA	2.74	0.54
1:I:189:VAL:HA	1:I:377:ALA:HA	1.89	0.54
1:L:239:ALA:HB1	1:L:314:LEU:HB3	1.88	0.54
1:M:60:ILE:HA	1:N:6:VAL:HG21	1.90	0.54
1:A:150:ILE:HD13	1:A:493:ILE:CG2	2.37	0.54
1:C:31:LEU:HB2	1:C:90:THR:HG21	1.90	0.54
1:C:144:ILE:HG23	1:C:403:THR:CG2	2.38	0.54
1:D:464:VAL:HG22	1:K:464:VAL:HG22	1.90	0.54
1:E:23:LEU:HA	1:E:60:ILE:CD1	2.32	0.54
1:H:6:VAL:HG21	1:N:60:ILE:HA	1.90	0.54
1:H:242:LYS:HG3	1:I:257:GLU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:221:LEU:HD13	1:L:317:LEU:HD11	1.90	0.54
1:A:31:LEU:HB2	1:A:90:THR:HG21	1.90	0.54
1:E:31:LEU:HB2	1:E:90:THR:HG21	1.90	0.54
1:E:213:VAL:HG11	1:E:325:ILE:HG12	1.87	0.54
1:F:193:MET:SD	1:F:292:ILE:HG23	2.48	0.54
1:H:221:LEU:HD13	1:H:317:LEU:HD11	1.90	0.54
1:I:243:ALA:CA	1:J:260:ALA:HB2	2.38	0.54
1:J:243:ALA:CA	1:K:260:ALA:HB2	2.38	0.54
1:D:137:PRO:HA	1:D:410:GLY:HA3	1.90	0.53
1:F:406:ALA:HB1	1:F:411:VAL:HG13	1.88	0.53
1:G:31:LEU:HB2	1:G:90:THR:HG21	1.90	0.53
1:G:193:MET:SD	1:G:295:LEU:HB3	2.48	0.53
1:I:23:LEU:HA	1:I:60:ILE:HD13	1.90	0.53
1:K:150:ILE:CD1	1:K:494:LEU:H	2.22	0.53
1:N:290:GLN:HA	1:N:300:VAL:CG2	2.38	0.53
1:A:23:LEU:HA	1:A:60:ILE:CD1	2.32	0.53
1:B:144:ILE:HG23	1:B:403:THR:CG2	2.39	0.53
1:B:464:VAL:HG22	1:I:464:VAL:HG22	1.90	0.53
1:D:144:ILE:HG23	1:D:403:THR:CG2	2.39	0.53
1:F:241:ALA:HA	1:F:271:VAL:HG22	1.90	0.53
1:I:199:TYR:CB	1:I:325:ILE:HD11	2.34	0.53
1:I:206:ASN:CG	1:I:207:LYS:H	2.12	0.53
1:J:23:LEU:HA	1:J:60:ILE:HD13	1.90	0.53
1:J:221:LEU:HD21	1:J:309:LEU:HD22	1.90	0.53
1:K:243:ALA:CA	1:L:260:ALA:HB2	2.37	0.53
1:K:290:GLN:HA	1:K:300:VAL:CG2	2.38	0.53
1:N:162:ILE:HD13	1:N:400:LEU:CA	2.34	0.53
1:A:144:ILE:HG23	1:A:403:THR:CG2	2.38	0.53
1:D:193:MET:SD	1:D:292:ILE:HG23	2.48	0.53
1:E:144:ILE:HG23	1:E:403:THR:CG2	2.38	0.53
1:E:193:MET:SD	1:E:292:ILE:HA	2.49	0.53
1:G:150:ILE:HD13	1:G:493:ILE:CG2	2.37	0.53
1:H:290:GLN:HA	1:H:300:VAL:CG2	2.38	0.53
1:L:221:LEU:HD22	1:L:236:VAL:HG11	1.90	0.53
1:L:290:GLN:HA	1:L:300:VAL:CG2	2.38	0.53
1:M:221:LEU:HD13	1:M:317:LEU:HD11	1.90	0.53
1:A:200:LEU:HD11	1:A:254:VAL:CA	2.12	0.53
1:A:406:ALA:HB1	1:A:411:VAL:HG13	1.89	0.53
1:B:193:MET:SD	1:B:292:ILE:HG23	2.48	0.53
1:C:38:VAL:HG11	1:C:56:VAL:HG22	1.91	0.53
1:F:137:PRO:HA	1:F:410:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:LEU:CB	1:F:259:LEU:CD1	2.86	0.53
1:H:137:PRO:CA	1:H:410:GLY:HA3	2.36	0.53
1:H:221:LEU:HD21	1:H:309:LEU:HD22	1.90	0.53
1:I:221:LEU:HD21	1:I:309:LEU:HD22	1.90	0.53
1:K:221:LEU:HD21	1:K:309:LEU:HD22	1.89	0.53
1:L:150:ILE:CD1	1:L:494:LEU:H	2.22	0.53
1:L:243:ALA:CA	1:M:260:ALA:HB2	2.39	0.53
1:A:193:MET:SD	1:A:292:ILE:HG23	2.48	0.53
1:B:406:ALA:HB1	1:B:411:VAL:HG13	1.88	0.53
1:H:60:ILE:HA	1:I:6:VAL:HG21	1.90	0.53
1:L:60:ILE:HA	1:M:6:VAL:HG21	1.90	0.53
1:M:229:ASN:HD22	1:M:230:ILE:H	1.56	0.53
1:M:518:GLU:CB	1:M:518:GLU:O	2.54	0.53
1:N:137:PRO:CA	1:N:410:GLY:HA3	2.36	0.53
1:D:200:LEU:CB	1:D:259:LEU:CD1	2.86	0.53
1:D:213:VAL:HG11	1:D:325:ILE:HG12	1.88	0.53
1:D:241:ALA:HA	1:D:271:VAL:HG22	1.90	0.53
1:H:31:LEU:CB	1:H:90:THR:HG21	2.39	0.53
1:H:242:LYS:CB	1:I:257:GLU:HA	2.38	0.53
1:J:221:LEU:CG	1:J:309:LEU:HD22	2.39	0.53
1:K:221:LEU:HD22	1:K:236:VAL:HG11	1.91	0.53
1:K:239:ALA:HB1	1:K:314:LEU:HB3	1.89	0.53
1:L:221:LEU:HD21	1:L:309:LEU:HD22	1.89	0.53
1:M:221:LEU:HD21	1:M:309:LEU:HD22	1.89	0.53
1:B:193:MET:SD	1:B:292:ILE:HA	2.49	0.53
1:G:406:ALA:HB1	1:G:411:VAL:HG13	1.89	0.53
1:I:31:LEU:CB	1:I:90:THR:HG21	2.39	0.53
1:I:302:SER:HB2	1:I:305:ILE:H	1.72	0.53
1:A:137:PRO:HA	1:A:410:GLY:HA3	1.90	0.53
1:C:241:ALA:HA	1:C:271:VAL:HG22	1.90	0.53
1:E:241:ALA:HA	1:E:271:VAL:HG22	1.90	0.53
1:E:464:VAL:HG22	1:L:464:VAL:HG22	1.91	0.53
1:F:193:MET:SD	1:F:292:ILE:HA	2.49	0.53
1:K:31:LEU:CB	1:K:90:THR:HG21	2.39	0.53
1:M:150:ILE:CD1	1:M:494:LEU:H	2.22	0.53
1:M:221:LEU:HD22	1:M:236:VAL:HG11	1.91	0.53
1:M:243:ALA:CA	1:N:260:ALA:HB2	2.39	0.53
1:N:31:LEU:CB	1:N:90:THR:HG21	2.39	0.53
1:N:518:GLU:CB	1:N:518:GLU:O	2.54	0.53
1:A:193:MET:SD	1:A:292:ILE:HA	2.49	0.53
1:B:200:LEU:CB	1:B:259:LEU:CD1	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ALA:HA	1:B:271:VAL:HG22	1.90	0.53
1:D:38:VAL:HG11	1:D:56:VAL:HG22	1.91	0.53
1:D:196:ASP:OD1	1:D:329:THR:HG22	2.08	0.53
1:E:193:MET:SD	1:E:292:ILE:HG23	2.48	0.53
1:F:144:ILE:HG23	1:F:403:THR:CG2	2.39	0.53
1:G:144:ILE:HG23	1:G:403:THR:CG2	2.38	0.53
1:I:60:ILE:HA	1:J:6:VAL:HG21	1.90	0.53
1:J:60:ILE:HA	1:K:6:VAL:HG21	1.90	0.53
1:M:302:SER:HB2	1:M:305:ILE:H	1.74	0.53
1:G:199:TYR:C	1:G:200:LEU:HD12	2.29	0.53
1:G:240:VAL:HG12	1:G:271:VAL:HG13	1.91	0.53
1:L:23:LEU:HA	1:L:60:ILE:HD13	1.90	0.53
1:M:23:LEU:HA	1:M:60:ILE:HD13	1.90	0.53
1:A:174:VAL:H	1:A:376:VAL:HG22	1.74	0.52
1:A:464:VAL:HG22	1:H:464:VAL:HG22	1.91	0.52
1:E:240:VAL:HG12	1:E:271:VAL:HG13	1.91	0.52
1:H:23:LEU:HA	1:H:60:ILE:HD13	1.90	0.52
1:H:162:ILE:HD13	1:H:400:LEU:CA	2.34	0.52
1:J:31:LEU:CB	1:J:90:THR:HG21	2.39	0.52
1:J:150:ILE:CD1	1:J:494:LEU:H	2.22	0.52
1:D:193:MET:SD	1:D:292:ILE:HA	2.49	0.52
1:F:174:VAL:H	1:F:376:VAL:HG22	1.74	0.52
1:I:221:LEU:CG	1:I:309:LEU:HD22	2.39	0.52
1:N:150:ILE:CD1	1:N:494:LEU:H	2.22	0.52
1:D:150:ILE:HD13	1:D:493:ILE:CG2	2.37	0.52
1:I:137:PRO:CA	1:I:410:GLY:HA3	2.36	0.52
1:K:60:ILE:HA	1:L:6:VAL:HG21	1.90	0.52
1:L:31:LEU:CB	1:L:90:THR:HG21	2.39	0.52
1:L:243:ALA:HA	1:M:260:ALA:HB2	1.90	0.52
1:E:220:ILE:CD1	1:E:332:ILE:HD13	2.33	0.52
1:F:213:VAL:HG11	1:F:325:ILE:HG12	1.88	0.52
1:G:197:ARG:HG3	1:G:198:GLY:O	2.10	0.52
1:H:150:ILE:CD1	1:H:494:LEU:H	2.22	0.52
1:K:23:LEU:HA	1:K:60:ILE:HD13	1.90	0.52
1:M:31:LEU:CB	1:M:90:THR:HG21	2.39	0.52
1:N:221:LEU:HB2	1:N:317:LEU:HD21	1.91	0.52
1:A:328:ASP:O	1:A:329:THR:HG23	2.10	0.52
1:B:328:ASP:O	1:B:329:THR:HG23	2.10	0.52
1:B:381:VAL:HB	1:B:393:LYS:HA	1.92	0.52
1:C:381:VAL:HB	1:C:393:LYS:HA	1.92	0.52
1:E:150:ILE:HD13	1:E:493:ILE:CG2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:LEU:HA	1:F:383:ALA:N	2.25	0.52
1:H:220:ILE:HD12	1:H:296:THR:CG2	2.40	0.52
1:B:38:VAL:HG11	1:B:56:VAL:HG22	1.91	0.52
1:D:521:VAL:O	1:E:41:ASP:CB	2.58	0.52
1:E:174:VAL:H	1:E:376:VAL:HG22	1.74	0.52
1:F:464:VAL:HG22	1:M:464:VAL:HG22	1.91	0.52
1:J:221:LEU:HD22	1:J:236:VAL:HG11	1.92	0.52
1:L:191:GLU:CG	1:L:192:GLY:H	2.21	0.52
1:L:220:ILE:HD12	1:L:296:THR:CG2	2.40	0.52
1:M:137:PRO:CA	1:M:410:GLY:HA3	2.36	0.52
1:N:23:LEU:HA	1:N:60:ILE:HD13	1.89	0.52
1:N:221:LEU:CG	1:N:309:LEU:HD22	2.40	0.52
1:A:521:VAL:O	1:B:41:ASP:CB	2.58	0.52
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.92	0.52
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.92	0.52
1:G:183:LEU:HA	1:G:383:ALA:N	2.25	0.52
1:I:247:LEU:O	1:I:273:VAL:HA	2.10	0.52
1:E:38:VAL:HG11	1:E:56:VAL:HG22	1.91	0.52
1:G:328:ASP:O	1:G:329:THR:HG23	2.10	0.52
1:J:194:GLN:OE1	1:J:329:THR:HG21	2.09	0.52
1:K:207:LYS:HA	1:K:207:LYS:CE	2.35	0.52
1:K:221:LEU:HB2	1:K:317:LEU:HD21	1.92	0.52
1:K:247:LEU:O	1:K:273:VAL:HA	2.10	0.52
1:L:233:MET:HE2	1:L:249:ILE:HD11	1.90	0.52
1:L:247:LEU:O	1:L:273:VAL:HA	2.10	0.52
1:M:247:LEU:O	1:M:273:VAL:HA	2.10	0.52
1:A:200:LEU:CB	1:A:259:LEU:CD1	2.86	0.52
1:B:37:ASN:ND2	1:B:49:ILE:HG23	2.25	0.52
1:B:521:VAL:O	1:C:41:ASP:CB	2.58	0.52
1:C:328:ASP:O	1:C:329:THR:HG23	2.10	0.52
1:E:183:LEU:HA	1:E:383:ALA:N	2.25	0.52
1:F:521:VAL:O	1:G:41:ASP:CB	2.58	0.52
1:G:464:VAL:HG22	1:N:464:VAL:HG22	1.91	0.52
1:H:221:LEU:CG	1:H:309:LEU:HD22	2.39	0.52
1:K:221:LEU:CG	1:K:309:LEU:HD22	2.39	0.52
1:L:221:LEU:HB2	1:L:317:LEU:HD21	1.92	0.52
1:N:302:SER:HB2	1:N:305:ILE:H	1.74	0.52
1:A:37:ASN:ND2	1:A:49:ILE:HG23	2.25	0.52
1:A:41:ASP:CB	1:G:521:VAL:O	2.58	0.52
1:C:37:ASN:ND2	1:C:49:ILE:HG23	2.25	0.52
1:K:220:ILE:HD12	1:K:296:THR:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:518:GLU:CB	1:L:518:GLU:O	2.54	0.52
1:M:221:LEU:CG	1:M:309:LEU:HD22	2.40	0.52
1:C:521:VAL:O	1:D:41:ASP:CB	2.58	0.51
1:D:381:VAL:HB	1:D:393:LYS:HA	1.92	0.51
1:J:221:LEU:HB2	1:J:317:LEU:HD21	1.92	0.51
1:A:193:MET:CE	1:A:332:ILE:HD12	2.18	0.51
1:B:158:VAL:HG22	1:B:396:VAL:HG22	1.92	0.51
1:D:37:ASN:ND2	1:D:49:ILE:HG23	2.25	0.51
1:D:521:VAL:HG11	1:E:59:GLU:HB3	1.93	0.51
1:E:150:ILE:CD1	1:E:493:ILE:CA	2.74	0.51
1:E:521:VAL:HG11	1:F:59:GLU:HB3	1.92	0.51
1:E:521:VAL:O	1:F:41:ASP:CB	2.58	0.51
1:N:204:PHE:HA	1:N:207:LYS:CE	2.40	0.51
1:A:34:LYS:HB2	1:A:458:CYS:HA	1.92	0.51
1:A:521:VAL:HG11	1:B:59:GLU:HB3	1.93	0.51
1:C:174:VAL:H	1:C:376:VAL:HG22	1.74	0.51
1:C:521:VAL:HG11	1:D:59:GLU:HB3	1.93	0.51
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.92	0.51
1:D:174:VAL:H	1:D:376:VAL:HG22	1.74	0.51
1:G:174:VAL:H	1:G:376:VAL:HG22	1.74	0.51
1:H:247:LEU:O	1:H:273:VAL:HA	2.10	0.51
1:I:221:LEU:HD22	1:I:236:VAL:HG11	1.91	0.51
1:J:511:ALA:O	1:J:515:ILE:HG13	2.11	0.51
1:B:207:LYS:HB2	1:B:208:PRO:HD3	1.92	0.51
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.93	0.51
1:C:150:ILE:HD13	1:C:493:ILE:CG2	2.37	0.51
1:C:207:LYS:CB	1:C:208:PRO:HD3	2.40	0.51
1:G:34:LYS:HB2	1:G:458:CYS:HA	1.92	0.51
1:H:221:LEU:HD22	1:H:236:VAL:HG11	1.91	0.51
1:I:221:LEU:HB2	1:I:317:LEU:HD21	1.92	0.51
1:N:247:LEU:O	1:N:273:VAL:HA	2.10	0.51
1:B:174:VAL:H	1:B:376:VAL:HG22	1.74	0.51
1:B:195:PHE:CZ	1:B:330:THR:CB	2.94	0.51
1:B:521:VAL:HG11	1:C:59:GLU:HB3	1.93	0.51
1:E:37:ASN:ND2	1:E:49:ILE:HG23	2.25	0.51
1:E:475:ASN:ND2	1:E:489:ILE:HD11	2.26	0.51
1:F:161:LEU:HD11	1:F:185:ASP:HB3	1.93	0.51
1:G:23:LEU:HA	1:G:60:ILE:CD1	2.32	0.51
1:G:38:VAL:HG11	1:G:56:VAL:HG22	1.91	0.51
1:G:52:ASP:CB	1:G:55:SER:H	2.24	0.51
1:H:221:LEU:HB2	1:H:317:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:511:ALA:O	1:H:515:ILE:HG13	2.11	0.51
1:J:220:ILE:HD12	1:J:296:THR:CG2	2.40	0.51
2:K:1525:PO4:P	4:K:1527:ATP:PG	3.09	0.51
1:L:137:PRO:CA	1:L:410:GLY:HA3	2.36	0.51
1:M:220:ILE:HD12	1:M:296:THR:CG2	2.40	0.51
1:M:221:LEU:HB2	1:M:317:LEU:HD21	1.92	0.51
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.93	0.51
1:A:59:GLU:HB3	1:G:521:VAL:HG11	1.93	0.51
1:A:183:LEU:HA	1:A:383:ALA:N	2.25	0.51
1:B:240:VAL:HG12	1:B:271:VAL:HG13	1.91	0.51
1:C:141:SER:O	1:C:163:ALA:HB1	2.11	0.51
1:C:158:VAL:HG22	1:C:396:VAL:HG22	1.93	0.51
1:C:213:VAL:HG11	1:C:325:ILE:HG12	1.87	0.51
1:D:34:LYS:HB2	1:D:458:CYS:HA	1.92	0.51
1:D:158:VAL:HG22	1:D:396:VAL:HG22	1.93	0.51
1:D:183:LEU:HA	1:D:383:ALA:N	2.25	0.51
1:F:52:ASP:HB3	1:F:55:SER:H	1.75	0.51
1:F:328:ASP:O	1:F:329:THR:HG23	2.10	0.51
1:F:521:VAL:HG11	1:G:59:GLU:HB3	1.92	0.51
1:G:37:ASN:ND2	1:G:49:ILE:HG23	2.25	0.51
2:I:1525:PO4:P	4:I:1527:ATP:PG	3.09	0.51
2:J:1525:PO4:P	4:J:1527:ATP:PG	3.09	0.51
1:K:183:LEU:H	1:K:183:LEU:HD23	1.76	0.51
1:A:158:VAL:HG22	1:A:396:VAL:HG22	1.93	0.51
1:A:475:ASN:ND2	1:A:489:ILE:HD11	2.26	0.51
1:C:34:LYS:HB2	1:C:458:CYS:HA	1.92	0.51
1:D:225:LYS:CB	1:D:308:GLU:HA	2.41	0.51
1:D:328:ASP:O	1:D:329:THR:HG23	2.10	0.51
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.93	0.51
1:H:77:VAL:HG22	1:H:510:VAL:HB	1.92	0.51
1:I:150:ILE:CD1	1:I:494:LEU:H	2.22	0.51
1:J:137:PRO:CA	1:J:410:GLY:HA3	2.37	0.51
1:K:511:ALA:O	1:K:515:ILE:HG13	2.11	0.51
2:L:1525:PO4:P	4:L:1527:ATP:PG	3.09	0.51
1:M:189:VAL:HA	1:M:377:ALA:HA	1.93	0.51
1:N:77:VAL:HG22	1:N:510:VAL:HB	1.92	0.51
1:N:169:VAL:HG23	1:N:170:GLY:O	2.10	0.51
1:N:240:VAL:HG11	1:N:247:LEU:CA	2.40	0.51
1:A:141:SER:O	1:A:163:ALA:HB1	2.11	0.51
1:C:183:LEU:HA	1:C:383:ALA:N	2.25	0.51
1:C:225:LYS:CB	1:C:308:GLU:HA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:ASN:ND2	1:C:489:ILE:HD11	2.26	0.51
1:D:52:ASP:HB3	1:D:55:SER:H	1.75	0.51
1:E:52:ASP:CB	1:E:55:SER:H	2.24	0.51
1:E:141:SER:O	1:E:163:ALA:HB1	2.11	0.51
1:E:328:ASP:O	1:E:329:THR:HG23	2.10	0.51
1:F:34:LYS:HB2	1:F:458:CYS:HA	1.92	0.51
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.93	0.51
2:H:1525:PO4:P	4:H:1527:ATP:PG	3.09	0.51
1:I:220:ILE:HD12	1:I:296:THR:CG2	2.40	0.51
1:L:240:VAL:HG11	1:L:247:LEU:CA	2.41	0.51
1:N:240:VAL:HG11	1:N:247:LEU:HB2	1.93	0.51
1:B:141:SER:O	1:B:163:ALA:HB1	2.11	0.51
1:B:225:LYS:CB	1:B:308:GLU:HA	2.41	0.51
1:C:240:VAL:HG12	1:C:271:VAL:HG13	1.91	0.51
1:E:225:LYS:CB	1:E:308:GLU:HA	2.41	0.51
1:F:37:ASN:ND2	1:F:49:ILE:HG23	2.25	0.51
1:F:240:VAL:HG12	1:F:271:VAL:HG13	1.91	0.51
1:G:475:ASN:ND2	1:G:489:ILE:HD11	2.26	0.51
1:H:207:LYS:HE2	1:H:207:LYS:N	2.24	0.51
1:H:518:GLU:CB	1:H:518:GLU:O	2.54	0.51
1:J:183:LEU:HD23	1:J:183:LEU:H	1.76	0.51
1:L:302:SER:HB2	1:L:305:ILE:H	1.74	0.51
1:M:77:VAL:HG22	1:M:510:VAL:HB	1.92	0.51
1:N:511:ALA:O	1:N:515:ILE:HG13	2.11	0.51
1:A:381:VAL:HB	1:A:393:LYS:HA	1.92	0.51
1:B:52:ASP:CB	1:B:55:SER:H	2.24	0.51
1:C:52:ASP:CB	1:C:55:SER:H	2.24	0.51
1:C:194:GLN:CG	1:C:329:THR:HG21	2.41	0.51
1:C:200:LEU:CB	1:C:259:LEU:CD1	2.86	0.51
1:F:381:VAL:HB	1:F:393:LYS:HA	1.92	0.51
1:G:141:SER:O	1:G:163:ALA:HB1	2.11	0.51
1:L:221:LEU:CG	1:L:309:LEU:HD22	2.40	0.51
1:N:220:ILE:HD12	1:N:296:THR:CG2	2.40	0.51
1:N:221:LEU:CD2	1:N:309:LEU:HD22	2.41	0.51
1:A:38:VAL:HG11	1:A:56:VAL:HG22	1.91	0.50
1:D:475:ASN:ND2	1:D:489:ILE:HD11	2.26	0.50
1:E:161:LEU:HD11	1:E:185:ASP:HB3	1.93	0.50
1:F:38:VAL:HG11	1:F:56:VAL:HG22	1.91	0.50
1:F:141:SER:O	1:F:163:ALA:HB1	2.11	0.50
1:H:240:VAL:HG11	1:H:247:LEU:CA	2.42	0.50
1:J:247:LEU:O	1:J:273:VAL:HA	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:249:ILE:HB	1:M:275:ALA:CB	2.40	0.50
1:A:161:LEU:HD11	1:A:185:ASP:HB3	1.93	0.50
1:B:34:LYS:HB2	1:B:458:CYS:HA	1.92	0.50
1:B:100:ILE:HD13	1:B:514:MET:SD	2.52	0.50
1:D:194:GLN:CG	1:D:329:THR:HG21	2.41	0.50
1:G:100:ILE:HD13	1:G:514:MET:SD	2.52	0.50
1:I:206:ASN:HB3	1:I:208:PRO:HD2	1.93	0.50
1:J:206:ASN:CG	1:J:207:LYS:H	2.15	0.50
1:J:240:VAL:HG11	1:J:247:LEU:CA	2.41	0.50
1:K:177:VAL:HG12	1:K:393:LYS:HE2	1.93	0.50
1:M:183:LEU:HD23	1:M:183:LEU:H	1.76	0.50
1:M:240:VAL:HG11	1:M:247:LEU:CA	2.41	0.50
1:A:100:ILE:HD13	1:A:514:MET:SD	2.52	0.50
1:G:158:VAL:HG22	1:G:396:VAL:HG22	1.93	0.50
1:L:77:VAL:HG22	1:L:510:VAL:HB	1.92	0.50
1:L:511:ALA:O	1:L:515:ILE:HG13	2.11	0.50
1:A:240:VAL:HG12	1:A:271:VAL:HG13	1.91	0.50
1:C:100:ILE:HD13	1:C:514:MET:SD	2.52	0.50
1:C:137:PRO:HA	1:C:410:GLY:HA3	1.90	0.50
1:D:166:MET:O	1:D:170:GLY:HA2	2.12	0.50
1:F:158:VAL:HG22	1:F:396:VAL:HG22	1.93	0.50
1:G:166:MET:O	1:G:170:GLY:HA2	2.12	0.50
1:G:213:VAL:HG11	1:G:325:ILE:HG12	1.88	0.50
2:M:1525:PO4:P	4:M:1527:ATP:PG	3.09	0.50
2:N:1525:PO4:P	4:N:1527:ATP:PG	3.09	0.50
1:A:166:MET:O	1:A:170:GLY:HA2	2.12	0.50
1:A:200:LEU:HD11	1:A:254:VAL:HA	1.94	0.50
1:B:183:LEU:HA	1:B:383:ALA:N	2.25	0.50
1:B:194:GLN:O	1:B:371:LYS:HB3	2.12	0.50
1:D:161:LEU:HD11	1:D:185:ASP:HB3	1.93	0.50
1:D:240:VAL:HG12	1:D:271:VAL:HG13	1.91	0.50
1:E:158:VAL:HG22	1:E:396:VAL:HG22	1.93	0.50
1:F:100:ILE:HD13	1:F:514:MET:SD	2.52	0.50
1:F:475:ASN:ND2	1:F:489:ILE:HD11	2.26	0.50
1:G:194:GLN:CG	1:G:329:THR:HG21	2.41	0.50
1:G:381:VAL:HB	1:G:393:LYS:HA	1.92	0.50
1:K:190:VAL:HG21	1:K:333:ILE:HD13	1.94	0.50
1:B:52:ASP:HB3	1:B:55:SER:H	1.76	0.50
1:G:225:LYS:CB	1:G:308:GLU:HA	2.41	0.50
1:G:255:GLU:HB2	1:G:259:LEU:H	1.77	0.50
1:I:77:VAL:HG22	1:I:510:VAL:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:77:VAL:HG22	1:J:510:VAL:HB	1.92	0.50
1:K:221:LEU:CD2	1:K:309:LEU:HD22	2.42	0.50
1:L:191:GLU:HG2	1:L:192:GLY:H	1.75	0.50
1:L:221:LEU:CD2	1:L:309:LEU:HD22	2.42	0.50
1:N:204:PHE:HD1	1:N:207:LYS:NZ	2.06	0.50
1:N:249:ILE:HB	1:N:275:ALA:CB	2.40	0.50
1:A:194:GLN:CG	1:A:329:THR:HG21	2.41	0.50
1:B:255:GLU:HB2	1:B:259:LEU:H	1.77	0.50
1:C:166:MET:O	1:C:170:GLY:HA2	2.12	0.50
1:E:34:LYS:HB2	1:E:458:CYS:HA	1.92	0.50
1:E:194:GLN:CG	1:E:329:THR:HG21	2.41	0.50
1:E:381:VAL:HB	1:E:393:LYS:HA	1.92	0.50
1:F:200:LEU:HD12	1:F:275:ALA:HB1	1.93	0.50
1:G:150:ILE:CD1	1:G:493:ILE:CA	2.74	0.50
1:G:406:ALA:HB1	1:G:411:VAL:CG1	2.42	0.50
1:J:168:LYS:HG2	1:J:187:LEU:HD21	1.93	0.50
1:M:511:ALA:O	1:M:515:ILE:HG13	2.11	0.50
1:N:183:LEU:HD23	1:N:183:LEU:H	1.76	0.50
1:C:224:ASP:HA	1:C:289:LEU:CD1	2.42	0.50
1:C:249:ILE:HD11	1:C:262:LEU:HD22	1.87	0.50
1:D:255:GLU:HB2	1:D:259:LEU:H	1.77	0.50
1:E:147:VAL:HG22	1:E:494:LEU:HB2	1.94	0.50
1:E:166:MET:O	1:E:170:GLY:HA2	2.12	0.50
1:F:147:VAL:HG22	1:F:494:LEU:HB2	1.94	0.50
1:G:382:GLY:O	1:G:389:MET:HA	2.12	0.50
1:I:511:ALA:O	1:I:515:ILE:HG13	2.11	0.50
1:J:190:VAL:HG21	1:J:333:ILE:HD13	1.94	0.50
1:J:242:LYS:CB	1:K:257:GLU:HA	2.41	0.50
1:K:182:GLY:HA3	1:K:383:ALA:N	2.09	0.50
1:A:52:ASP:CB	1:A:55:SER:H	2.24	0.50
1:A:224:ASP:HA	1:A:289:LEU:CD1	2.42	0.50
1:A:225:LYS:CB	1:A:308:GLU:HA	2.41	0.50
1:B:147:VAL:HG22	1:B:494:LEU:HB2	1.94	0.50
1:B:213:VAL:HG11	1:B:325:ILE:HG12	1.88	0.50
1:B:406:ALA:HB1	1:B:411:VAL:CG1	2.42	0.50
1:C:382:GLY:O	1:C:389:MET:HA	2.12	0.50
1:D:141:SER:O	1:D:163:ALA:HB1	2.11	0.50
1:E:240:VAL:HG21	1:E:247:LEU:HD13	1.94	0.50
1:E:382:GLY:O	1:E:389:MET:HA	2.12	0.50
1:F:224:ASP:HA	1:F:289:LEU:CD1	2.42	0.50
1:K:240:VAL:HG11	1:K:247:LEU:CA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:221:LEU:CD2	1:M:309:LEU:HD22	2.42	0.50
1:A:225:LYS:HB2	1:A:308:GLU:HA	1.94	0.49
1:B:475:ASN:ND2	1:B:489:ILE:HD11	2.26	0.49
1:C:224:ASP:CG	1:C:302:SER:HA	2.33	0.49
1:D:100:ILE:HD13	1:D:514:MET:SD	2.52	0.49
1:D:191:GLU:HG3	1:D:342:ILE:HD12	1.93	0.49
1:G:200:LEU:CD2	1:G:254:VAL:CG1	2.86	0.49
1:I:190:VAL:HG21	1:I:333:ILE:HD13	1.94	0.49
1:I:221:LEU:HG	1:I:309:LEU:HD22	1.94	0.49
1:K:152:ALA:HB3	1:K:155:ASP:N	2.27	0.49
1:M:152:ALA:HB3	1:M:155:ASP:N	2.27	0.49
1:M:190:VAL:HG21	1:M:333:ILE:HD13	1.94	0.49
1:M:301:ILE:HD11	1:M:312:ALA:CB	2.32	0.49
1:A:147:VAL:HG22	1:A:494:LEU:HB2	1.94	0.49
1:A:224:ASP:CG	1:A:302:SER:HA	2.33	0.49
1:B:161:LEU:HD11	1:B:185:ASP:HB3	1.93	0.49
1:B:224:ASP:HA	1:B:289:LEU:CD1	2.42	0.49
1:B:225:LYS:HB2	1:B:308:GLU:HA	1.94	0.49
1:C:25:ASP:CG	1:C:28:LYS:HZ3	2.16	0.49
1:C:161:LEU:HD11	1:C:185:ASP:HB3	1.93	0.49
1:C:192:GLY:HA3	1:C:376:VAL:CG2	2.40	0.49
1:D:220:ILE:CD1	1:D:332:ILE:HD13	2.33	0.49
1:F:225:LYS:CB	1:F:308:GLU:HA	2.41	0.49
1:F:240:VAL:HG21	1:F:247:LEU:HD13	1.94	0.49
1:G:225:LYS:HB2	1:G:308:GLU:HA	1.94	0.49
1:J:224:ASP:HB2	1:J:303:GLU:H	1.77	0.49
1:K:240:VAL:HG11	1:K:247:LEU:HB2	1.94	0.49
1:L:31:LEU:HB2	1:L:90:THR:HG21	1.95	0.49
1:L:249:ILE:HB	1:L:275:ALA:CB	2.40	0.49
1:M:243:ALA:HA	1:N:260:ALA:HB2	1.93	0.49
1:N:182:GLY:HA3	1:N:383:ALA:N	2.09	0.49
1:B:166:MET:O	1:B:170:GLY:HA2	2.12	0.49
1:B:240:VAL:HG21	1:B:247:LEU:HD13	1.94	0.49
1:C:147:VAL:HG22	1:C:494:LEU:HB2	1.94	0.49
1:D:190:VAL:HG23	1:D:333:ILE:CG2	2.42	0.49
1:D:224:ASP:HA	1:D:289:LEU:CD1	2.42	0.49
1:D:240:VAL:HG21	1:D:247:LEU:HD13	1.94	0.49
1:D:382:GLY:O	1:D:389:MET:HA	2.12	0.49
1:E:25:ASP:CG	1:E:28:LYS:HZ3	2.15	0.49
1:F:225:LYS:HB2	1:F:308:GLU:HA	1.94	0.49
1:H:152:ALA:HB3	1:H:155:ASP:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:257:GLU:HA	1:N:242:LYS:CB	2.41	0.49
1:J:178:GLU:O	1:J:380:LYS:HA	2.12	0.49
1:K:77:VAL:HG22	1:K:510:VAL:HB	1.92	0.49
1:K:518:GLU:CB	1:K:518:GLU:O	2.54	0.49
1:C:240:VAL:HG21	1:C:247:LEU:HD13	1.94	0.49
1:D:52:ASP:CB	1:D:55:SER:H	2.25	0.49
1:E:221:LEU:HD21	1:E:309:LEU:HD11	1.95	0.49
1:F:166:MET:O	1:F:170:GLY:HA2	2.12	0.49
1:F:255:GLU:HB2	1:F:259:LEU:H	1.77	0.49
1:F:406:ALA:HB1	1:F:411:VAL:CG1	2.42	0.49
1:H:236:VAL:O	1:H:240:VAL:HG23	2.13	0.49
1:I:31:LEU:HB2	1:I:90:THR:HG21	1.95	0.49
1:I:243:ALA:N	1:J:256:GLY:C	2.66	0.49
1:K:31:LEU:HB2	1:K:90:THR:HG21	1.95	0.49
1:K:249:ILE:HB	1:K:275:ALA:CB	2.40	0.49
1:N:224:ASP:HB2	1:N:303:GLU:H	1.78	0.49
1:A:240:VAL:HG21	1:A:247:LEU:HD13	1.94	0.49
1:A:382:GLY:O	1:A:389:MET:HA	2.12	0.49
1:A:406:ALA:HB1	1:A:411:VAL:CG1	2.42	0.49
1:B:200:LEU:HD11	1:B:254:VAL:HA	1.94	0.49
1:C:193:MET:CE	1:C:332:ILE:HD12	2.36	0.49
1:C:221:LEU:HD21	1:C:309:LEU:HD11	1.95	0.49
1:D:147:VAL:HG22	1:D:494:LEU:HB2	1.94	0.49
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.95	0.49
1:G:25:ASP:CG	1:G:28:LYS:HZ3	2.15	0.49
1:G:224:ASP:CG	1:G:302:SER:HA	2.33	0.49
1:I:183:LEU:HD23	1:I:183:LEU:H	1.76	0.49
1:J:227:ILE:CD1	1:J:233:MET:SD	2.92	0.49
1:J:240:VAL:HG11	1:J:247:LEU:HB2	1.94	0.49
1:J:242:LYS:HG3	1:K:257:GLU:HB2	1.94	0.49
1:K:406:ALA:HB1	1:K:411:VAL:CG1	2.43	0.49
1:L:406:ALA:HB1	1:L:411:VAL:CG1	2.43	0.49
1:B:224:ASP:CG	1:B:302:SER:HA	2.33	0.49
1:C:200:LEU:HD12	1:C:275:ALA:HB1	1.93	0.49
1:C:406:ALA:HB1	1:C:411:VAL:CG1	2.42	0.49
1:D:521:VAL:HG21	1:E:59:GLU:CB	2.43	0.49
1:E:100:ILE:HD13	1:E:514:MET:SD	2.52	0.49
1:E:137:PRO:HA	1:E:410:GLY:HA3	1.90	0.49
1:F:194:GLN:CG	1:F:329:THR:HG21	2.41	0.49
1:H:221:LEU:HG	1:H:309:LEU:HD22	1.95	0.49
1:H:406:ALA:HB1	1:H:411:VAL:CG1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:240:VAL:HG11	1:I:247:LEU:CA	2.41	0.49
1:I:242:LYS:CB	1:J:257:GLU:HA	2.41	0.49
1:I:242:LYS:HG3	1:J:257:GLU:HB2	1.93	0.49
1:J:31:LEU:HB2	1:J:90:THR:HG21	1.95	0.49
1:J:221:LEU:HG	1:J:309:LEU:HD22	1.95	0.49
1:A:255:GLU:HB2	1:A:259:LEU:H	1.77	0.49
1:D:383:ALA:HA	1:D:389:MET:HB2	1.95	0.49
1:E:224:ASP:CG	1:E:302:SER:HA	2.33	0.49
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.95	0.49
1:F:383:ALA:HA	1:F:389:MET:HB2	1.95	0.49
1:G:240:VAL:HG21	1:G:247:LEU:HD13	1.94	0.49
1:H:190:VAL:HG21	1:H:333:ILE:HD13	1.94	0.49
1:H:249:ILE:HB	1:H:275:ALA:CB	2.40	0.49
1:H:256:GLY:C	1:N:243:ALA:N	2.66	0.49
1:J:290:GLN:HA	1:J:300:VAL:HG21	1.95	0.49
1:K:242:LYS:C	1:L:257:GLU:CA	2.78	0.49
1:L:182:GLY:HA3	1:L:383:ALA:N	2.09	0.49
1:L:224:ASP:HB2	1:L:303:GLU:H	1.78	0.49
1:B:200:LEU:HD12	1:B:275:ALA:HB1	1.93	0.49
1:B:382:GLY:O	1:B:389:MET:HA	2.12	0.49
1:C:225:LYS:HB2	1:C:308:GLU:HA	1.94	0.49
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.95	0.49
1:D:224:ASP:CG	1:D:302:SER:HA	2.33	0.49
1:E:383:ALA:HA	1:E:389:MET:HB2	1.95	0.49
1:F:52:ASP:CB	1:F:55:SER:H	2.25	0.49
1:F:227:ILE:HG12	1:F:309:LEU:HG	1.95	0.49
1:I:236:VAL:O	1:I:240:VAL:HG23	2.13	0.49
1:J:243:ALA:N	1:K:256:GLY:C	2.66	0.49
1:J:406:ALA:HB1	1:J:411:VAL:CG1	2.43	0.49
1:M:31:LEU:HB2	1:M:90:THR:HG21	1.95	0.49
1:N:206:ASN:HB2	1:N:213:VAL:HA	1.94	0.49
1:A:220:ILE:CD1	1:A:332:ILE:HD13	2.33	0.49
1:B:221:LEU:HD21	1:B:309:LEU:HD11	1.95	0.49
1:C:255:GLU:HB2	1:C:259:LEU:H	1.77	0.49
1:D:406:ALA:HB1	1:D:411:VAL:CG1	2.42	0.49
1:E:225:LYS:HB2	1:E:308:GLU:HA	1.94	0.49
1:E:249:ILE:HD11	1:E:262:LEU:HD22	1.87	0.49
1:E:521:VAL:HG21	1:F:59:GLU:CB	2.43	0.49
1:G:137:PRO:HA	1:G:410:GLY:HA3	1.90	0.49
1:H:31:LEU:HB2	1:H:90:THR:HG21	1.95	0.49
1:H:136:VAL:O	1:H:410:GLY:HA3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:221:LEU:HD13	1:I:317:LEU:CD1	2.43	0.49
1:I:290:GLN:HA	1:I:300:VAL:HG21	1.95	0.49
1:J:242:LYS:C	1:K:257:GLU:CA	2.78	0.49
1:K:243:ALA:N	1:L:256:GLY:C	2.66	0.49
1:M:182:GLY:HA3	1:M:383:ALA:N	2.09	0.49
1:A:383:ALA:HA	1:A:389:MET:HB2	1.95	0.49
1:B:383:ALA:HA	1:B:389:MET:HB2	1.95	0.49
1:C:383:ALA:HA	1:C:389:MET:HB2	1.95	0.49
1:D:221:LEU:HD21	1:D:309:LEU:HD11	1.95	0.49
1:E:240:VAL:CG1	1:E:247:LEU:HB2	2.42	0.49
1:G:227:ILE:HG12	1:G:309:LEU:HG	1.94	0.49
1:H:221:LEU:CD2	1:H:309:LEU:HD22	2.42	0.49
1:H:257:GLU:HB2	1:N:242:LYS:HG3	1.94	0.49
1:H:427:ALA:HA	1:H:444:LEU:HD11	1.95	0.49
1:L:240:VAL:HG11	1:L:247:LEU:HB2	1.94	0.49
1:M:136:VAL:O	1:M:410:GLY:HA3	2.13	0.49
1:M:243:ALA:N	1:N:256:GLY:C	2.66	0.49
1:N:206:ASN:C	1:N:208:PRO:N	2.66	0.49
1:C:247:LEU:HB3	1:C:273:VAL:HG22	1.96	0.48
1:E:227:ILE:HG12	1:E:309:LEU:HG	1.94	0.48
1:G:383:ALA:HA	1:G:389:MET:HB2	1.95	0.48
1:I:224:ASP:HB2	1:I:303:GLU:H	1.78	0.48
1:K:221:LEU:HG	1:K:309:LEU:HD22	1.95	0.48
1:L:243:ALA:N	1:M:256:GLY:C	2.66	0.48
1:L:255:GLU:CD	1:L:256:GLY:H	2.16	0.48
1:L:290:GLN:HA	1:L:300:VAL:HG21	1.95	0.48
1:M:240:VAL:HG11	1:M:247:LEU:HB2	1.94	0.48
1:M:290:GLN:HA	1:M:300:VAL:HG21	1.95	0.48
1:M:406:ALA:HB1	1:M:411:VAL:CG1	2.43	0.48
1:N:31:LEU:HB2	1:N:90:THR:HG21	1.95	0.48
1:N:152:ALA:HB3	1:N:155:ASP:N	2.27	0.48
1:N:190:VAL:HG21	1:N:333:ILE:HD13	1.94	0.48
1:A:59:GLU:CB	1:G:521:VAL:HG21	2.43	0.48
1:D:225:LYS:HB2	1:D:308:GLU:HA	1.94	0.48
1:E:200:LEU:HD12	1:E:275:ALA:HB1	1.93	0.48
1:E:224:ASP:HA	1:E:289:LEU:CD1	2.42	0.48
1:G:206:ASN:HB3	1:G:208:PRO:HD2	1.94	0.48
1:H:243:ALA:N	1:I:256:GLY:C	2.66	0.48
1:I:152:ALA:HB3	1:I:155:ASP:N	2.27	0.48
1:I:427:ALA:HA	1:I:444:LEU:HD11	1.95	0.48
1:J:221:LEU:HD13	1:J:317:LEU:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:350:ARG:HD2	1:N:353:ILE:HD12	1.96	0.48
1:N:427:ALA:HA	1:N:444:LEU:HD11	1.95	0.48
1:B:247:LEU:HB3	1:B:273:VAL:HG22	1.96	0.48
1:E:255:GLU:HB2	1:E:259:LEU:H	1.77	0.48
1:F:382:GLY:O	1:F:389:MET:HA	2.12	0.48
1:G:220:ILE:CD1	1:G:332:ILE:HD13	2.33	0.48
1:H:350:ARG:HD2	1:H:353:ILE:HD12	1.95	0.48
1:I:221:LEU:CD2	1:I:309:LEU:HD22	2.42	0.48
1:I:518:GLU:CB	1:I:518:GLU:O	2.54	0.48
1:J:152:ALA:HB3	1:J:155:ASP:N	2.27	0.48
1:N:290:GLN:HA	1:N:300:VAL:HG21	1.95	0.48
1:B:521:VAL:HG21	1:C:59:GLU:CB	2.43	0.48
1:E:200:LEU:HD11	1:E:254:VAL:CA	2.12	0.48
1:E:406:ALA:HB1	1:E:411:VAL:CG1	2.42	0.48
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.95	0.48
1:I:240:VAL:HG11	1:I:247:LEU:HB2	1.94	0.48
1:K:221:LEU:HD13	1:K:317:LEU:CD1	2.44	0.48
1:L:152:ALA:HB3	1:L:155:ASP:N	2.27	0.48
1:M:350:ARG:HD2	1:M:353:ILE:HD12	1.96	0.48
1:A:247:LEU:HB3	1:A:273:VAL:HG22	1.96	0.48
1:D:190:VAL:HG23	1:D:333:ILE:HG23	1.96	0.48
1:G:147:VAL:HG22	1:G:494:LEU:HB2	1.94	0.48
1:K:290:GLN:HA	1:K:300:VAL:HG21	1.95	0.48
1:A:227:ILE:HG12	1:A:309:LEU:HG	1.95	0.48
1:A:311:LYS:HD3	1:A:311:LYS:HA	1.93	0.48
1:B:23:LEU:HA	1:B:60:ILE:CD1	2.32	0.48
1:B:150:ILE:CD1	1:B:493:ILE:CA	2.74	0.48
1:D:200:LEU:HD11	1:D:254:VAL:CA	2.12	0.48
1:D:240:VAL:CG1	1:D:247:LEU:HB2	2.42	0.48
1:F:224:ASP:CG	1:F:302:SER:HA	2.33	0.48
1:F:247:LEU:HB3	1:F:273:VAL:HG22	1.95	0.48
1:F:521:VAL:HG21	1:G:59:GLU:CB	2.43	0.48
1:G:162:ILE:CD1	1:G:400:LEU:N	2.77	0.48
1:G:224:ASP:HA	1:G:289:LEU:CD1	2.42	0.48
1:H:221:LEU:HD13	1:H:317:LEU:CD1	2.44	0.48
1:H:240:VAL:HG11	1:H:247:LEU:HB2	1.95	0.48
1:H:290:GLN:HA	1:H:300:VAL:HG21	1.95	0.48
1:J:221:LEU:CD2	1:J:309:LEU:HD22	2.42	0.48
1:J:249:ILE:HB	1:J:275:ALA:CB	2.40	0.48
1:J:427:ALA:HA	1:J:444:LEU:HD11	1.95	0.48
1:K:274:ALA:HB1	1:K:325:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:224:ASP:HB2	1:M:303:GLU:H	1.78	0.48
1:A:227:ILE:HD12	1:A:258:ALA:HB1	1.96	0.48
1:B:222:LEU:CD2	1:B:292:ILE:HG22	2.42	0.48
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.95	0.48
1:C:162:ILE:CD1	1:C:400:LEU:N	2.77	0.48
1:D:25:ASP:CG	1:D:28:LYS:HZ3	2.17	0.48
1:D:309:LEU:O	1:D:312:ALA:HB3	2.14	0.48
1:E:158:VAL:HG13	1:E:396:VAL:HA	1.96	0.48
1:F:309:LEU:O	1:F:312:ALA:HB3	2.14	0.48
1:G:241:ALA:CA	1:G:271:VAL:HG22	2.44	0.48
1:G:247:LEU:HB3	1:G:273:VAL:HG22	1.96	0.48
1:I:136:VAL:O	1:I:410:GLY:HA3	2.13	0.48
1:I:182:GLY:HA3	1:I:383:ALA:N	2.09	0.48
1:L:236:VAL:O	1:L:240:VAL:HG23	2.13	0.48
1:M:236:VAL:O	1:M:240:VAL:HG23	2.13	0.48
1:A:200:LEU:HD12	1:A:275:ALA:HB1	1.93	0.48
1:D:158:VAL:HG13	1:D:396:VAL:HA	1.96	0.48
1:D:190:VAL:CG2	1:D:333:ILE:HG22	2.43	0.48
1:D:247:LEU:HB3	1:D:273:VAL:HG22	1.96	0.48
1:F:158:VAL:HG13	1:F:396:VAL:HA	1.96	0.48
1:G:184:GLN:HG2	1:G:185:ASP:O	2.14	0.48
1:H:203:TYR:CD1	1:H:267:MET:CE	2.97	0.48
1:L:136:VAL:O	1:L:410:GLY:HA3	2.13	0.48
1:L:196:ASP:OD1	1:L:329:THR:HG22	2.14	0.48
1:A:222:LEU:CD2	1:A:292:ILE:HG22	2.42	0.48
1:D:162:ILE:CD1	1:D:400:LEU:N	2.77	0.48
1:E:222:LEU:CD2	1:E:292:ILE:HG22	2.42	0.48
1:E:247:LEU:HB3	1:E:273:VAL:HG22	1.96	0.48
1:J:207:LYS:HE2	1:J:207:LYS:N	2.28	0.48
1:J:518:GLU:CB	1:J:518:GLU:O	2.54	0.48
1:L:298:GLY:HA3	1:L:318:GLY:CA	2.44	0.48
1:M:183:LEU:HA	1:M:382:GLY:CA	2.44	0.48
1:N:236:VAL:O	1:N:240:VAL:HG23	2.14	0.48
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.95	0.48
1:A:99:ILE:CG2	1:A:120:ILE:HD13	2.44	0.48
1:A:249:ILE:HD11	1:A:262:LEU:HD22	1.87	0.48
1:A:309:LEU:O	1:A:312:ALA:HB3	2.14	0.48
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.95	0.48
1:C:213:VAL:CG2	1:C:214:GLU:N	2.77	0.48
1:E:309:LEU:O	1:E:312:ALA:HB3	2.14	0.48
1:F:221:LEU:HD21	1:F:309:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:LYS:HE2	1:G:207:LYS:HB2	1.49	0.48
1:G:311:LYS:HD3	1:G:311:LYS:HA	1.93	0.48
1:I:350:ARG:HD2	1:I:353:ILE:HD12	1.95	0.48
1:K:236:VAL:O	1:K:240:VAL:HG23	2.13	0.48
1:L:183:LEU:HD23	1:L:183:LEU:N	2.22	0.48
1:L:350:ARG:HD2	1:L:353:ILE:HD12	1.96	0.48
1:B:99:ILE:CG2	1:B:120:ILE:HD13	2.44	0.47
1:B:220:ILE:CD1	1:B:332:ILE:HD13	2.33	0.47
1:C:200:LEU:HD11	1:C:254:VAL:HA	1.94	0.47
1:C:521:VAL:HG21	1:D:59:GLU:CB	2.43	0.47
1:D:190:VAL:HB	1:D:334:ASP:CB	2.44	0.47
1:D:241:ALA:CA	1:D:271:VAL:HG22	2.44	0.47
1:E:180:GLY:HA2	1:E:380:LYS:HB3	1.96	0.47
1:E:240:VAL:HG11	1:E:247:LEU:CB	2.43	0.47
1:F:25:ASP:CG	1:F:28:LYS:HZ3	2.18	0.47
1:G:200:LEU:HD22	1:G:259:LEU:CD2	2.30	0.47
1:J:183:LEU:HA	1:J:382:GLY:CA	2.44	0.47
1:K:427:ALA:HA	1:K:444:LEU:HD11	1.95	0.47
1:L:427:ALA:HA	1:L:444:LEU:HD11	1.95	0.47
1:N:221:LEU:HD13	1:N:317:LEU:CD1	2.44	0.47
1:A:162:ILE:CD1	1:A:400:LEU:N	2.77	0.47
1:A:384:ALA:HA	1:A:385:THR:HA	1.68	0.47
1:B:25:ASP:CG	1:B:28:LYS:HZ3	2.16	0.47
1:B:162:ILE:CD1	1:B:400:LEU:N	2.77	0.47
1:B:180:GLY:HA2	1:B:380:LYS:HB3	1.96	0.47
1:B:203:TYR:N	1:B:203:TYR:HD1	2.12	0.47
1:B:227:ILE:HD12	1:B:258:ALA:HB1	1.96	0.47
1:C:220:ILE:CD1	1:C:332:ILE:HD13	2.33	0.47
1:D:200:LEU:HD12	1:D:275:ALA:HB1	1.93	0.47
1:D:222:LEU:CD2	1:D:292:ILE:HG22	2.42	0.47
1:E:99:ILE:CG2	1:E:120:ILE:HD13	2.44	0.47
1:F:311:LYS:HD3	1:F:311:LYS:HA	1.93	0.47
1:J:301:ILE:HD11	1:J:312:ALA:CB	2.32	0.47
1:B:309:LEU:O	1:B:312:ALA:HB3	2.14	0.47
1:D:99:ILE:CG2	1:D:120:ILE:HD13	2.44	0.47
1:D:213:VAL:O	1:D:324:VAL:HA	2.15	0.47
1:D:240:VAL:HG11	1:D:247:LEU:CB	2.43	0.47
1:D:278:ALA:HB2	1:D:289:LEU:CD1	2.45	0.47
1:E:213:VAL:CG2	1:E:214:GLU:N	2.77	0.47
1:E:278:ALA:HB2	1:E:289:LEU:CD1	2.45	0.47
1:F:180:GLY:HA2	1:F:380:LYS:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:ALA:CA	1:F:271:VAL:HG22	2.44	0.47
1:G:158:VAL:HG13	1:G:396:VAL:HA	1.96	0.47
1:G:222:LEU:CD2	1:G:292:ILE:HG22	2.42	0.47
1:I:189:VAL:HG22	1:I:377:ALA:HB2	1.95	0.47
1:K:136:VAL:O	1:K:410:GLY:HA3	2.13	0.47
1:K:183:LEU:HA	1:K:382:GLY:CA	2.44	0.47
1:K:350:ARG:HD2	1:K:353:ILE:HD12	1.96	0.47
1:M:298:GLY:HA3	1:M:318:GLY:CA	2.44	0.47
1:N:136:VAL:O	1:N:410:GLY:HA3	2.13	0.47
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.96	0.47
1:A:221:LEU:HD21	1:A:309:LEU:HD11	1.95	0.47
1:A:241:ALA:CA	1:A:271:VAL:HG22	2.44	0.47
1:A:278:ALA:HB2	1:A:289:LEU:CD1	2.45	0.47
1:A:521:VAL:HG21	1:B:59:GLU:CB	2.43	0.47
1:B:227:ILE:HG12	1:B:309:LEU:HG	1.95	0.47
1:B:353:ILE:HD13	1:B:366:GLN:HG2	1.97	0.47
1:C:99:ILE:CG2	1:C:120:ILE:HD13	2.44	0.47
1:C:158:VAL:HG13	1:C:396:VAL:HA	1.96	0.47
1:C:227:ILE:HG12	1:C:309:LEU:HG	1.95	0.47
1:C:353:ILE:HD13	1:C:366:GLN:HG2	1.97	0.47
1:D:150:ILE:CD1	1:D:493:ILE:CG2	2.91	0.47
1:D:180:GLY:HA2	1:D:380:LYS:HB3	1.97	0.47
1:E:241:ALA:CA	1:E:271:VAL:HG22	2.44	0.47
1:E:311:LYS:HD3	1:E:311:LYS:HA	1.93	0.47
1:F:222:LEU:CD2	1:F:292:ILE:HG22	2.42	0.47
1:H:298:GLY:HA3	1:H:318:GLY:CA	2.44	0.47
1:J:136:VAL:O	1:J:410:GLY:HA3	2.13	0.47
1:L:207:LYS:HA	1:L:207:LYS:CE	2.36	0.47
1:L:221:LEU:HG	1:L:309:LEU:HD22	1.96	0.47
1:M:196:ASP:OD2	1:M:329:THR:HG22	2.14	0.47
1:M:237:LEU:CD2	1:M:247:LEU:HD23	2.44	0.47
1:M:314:LEU:O	1:M:317:LEU:HB2	2.14	0.47
1:M:427:ALA:HA	1:M:444:LEU:HD11	1.95	0.47
1:N:183:LEU:HA	1:N:382:GLY:CA	2.44	0.47
1:N:237:LEU:CD2	1:N:247:LEU:HD23	2.44	0.47
1:B:384:ALA:HA	1:B:385:THR:HA	1.68	0.47
1:C:150:ILE:CD1	1:C:493:ILE:CA	2.74	0.47
1:C:180:GLY:HA2	1:C:380:LYS:HB3	1.96	0.47
1:C:240:VAL:CG1	1:C:247:LEU:HB2	2.42	0.47
1:C:241:ALA:CA	1:C:271:VAL:HG22	2.44	0.47
1:D:353:ILE:HD13	1:D:366:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:VAL:O	1:E:324:VAL:HA	2.14	0.47
1:E:381:VAL:CG2	1:E:393:LYS:N	2.77	0.47
1:F:223:ALA:CA	1:F:309:LEU:HD23	2.45	0.47
1:G:99:ILE:CG2	1:G:120:ILE:HD13	2.44	0.47
1:H:237:LEU:CD2	1:H:247:LEU:HD23	2.45	0.47
2:H:1525:PO4:P	4:H:1527:ATP:O1G	2.73	0.47
1:J:237:LEU:CD2	1:J:247:LEU:HD23	2.45	0.47
1:K:298:GLY:HA3	1:K:318:GLY:CA	2.44	0.47
1:A:223:ALA:CA	1:A:309:LEU:HD23	2.45	0.47
1:A:353:ILE:HD13	1:A:366:GLN:HG2	1.97	0.47
1:C:213:VAL:O	1:C:324:VAL:HA	2.15	0.47
1:C:222:LEU:CD2	1:C:292:ILE:HG22	2.42	0.47
1:D:213:VAL:CG2	1:D:214:GLU:N	2.77	0.47
1:D:221:LEU:CD1	1:D:309:LEU:HD21	2.45	0.47
1:F:99:ILE:CG2	1:F:120:ILE:HD13	2.44	0.47
1:G:180:GLY:HA2	1:G:380:LYS:HB3	1.96	0.47
1:G:221:LEU:HD21	1:G:309:LEU:HD11	1.95	0.47
1:G:278:ALA:HB2	1:G:289:LEU:CD1	2.45	0.47
1:H:220:ILE:HD12	1:H:296:THR:HG21	1.96	0.47
1:I:237:LEU:CD2	1:I:247:LEU:HD23	2.44	0.47
1:J:350:ARG:HD2	1:J:353:ILE:HD12	1.96	0.47
1:L:221:LEU:HD13	1:L:317:LEU:CD1	2.45	0.47
2:L:1525:PO4:P	4:L:1527:ATP:O1G	2.73	0.47
1:N:221:LEU:HG	1:N:309:LEU:HD22	1.96	0.47
1:B:203:TYR:N	1:B:203:TYR:CD1	2.83	0.47
1:B:221:LEU:CD1	1:B:309:LEU:HD21	2.45	0.47
1:B:278:ALA:HB2	1:B:289:LEU:CD1	2.45	0.47
1:C:309:LEU:O	1:C:312:ALA:HB3	2.14	0.47
1:D:227:ILE:HG12	1:D:309:LEU:HG	1.95	0.47
1:F:213:VAL:CG2	1:F:214:GLU:N	2.77	0.47
1:F:262:LEU:O	1:F:266:THR:HG23	2.15	0.47
1:G:213:VAL:O	1:G:324:VAL:HA	2.14	0.47
1:G:309:LEU:O	1:G:312:ALA:HB3	2.14	0.47
1:H:237:LEU:HA	1:H:247:LEU:HD22	1.97	0.47
1:I:183:LEU:HA	1:I:382:GLY:CA	2.44	0.47
1:I:220:ILE:HD12	1:I:296:THR:HG21	1.96	0.47
2:I:1525:PO4:P	4:I:1527:ATP:O1G	2.73	0.47
1:K:227:ILE:CD1	1:K:233:MET:SD	2.92	0.47
2:K:1525:PO4:P	4:K:1527:ATP:O1G	2.73	0.47
1:L:237:LEU:CD2	1:L:247:LEU:HD23	2.45	0.47
1:M:203:TYR:CD1	1:M:267:MET:CE	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:221:LEU:HD13	1:M:317:LEU:CD1	2.45	0.47
1:N:34:LYS:HB2	1:N:457:ASN:HB3	1.97	0.47
1:N:205:ILE:O	1:N:207:LYS:CG	2.62	0.47
2:N:1525:PO4:P	4:N:1527:ATP:O1G	2.73	0.47
1:A:158:VAL:HG13	1:A:396:VAL:HA	1.96	0.47
1:C:192:GLY:H	1:C:375:GLY:HA2	1.80	0.47
1:C:221:LEU:CD1	1:C:309:LEU:HD21	2.45	0.47
1:D:223:ALA:CA	1:D:309:LEU:HD23	2.45	0.47
1:E:353:ILE:HD13	1:E:366:GLN:HG2	1.97	0.47
1:F:240:VAL:HG11	1:F:247:LEU:CB	2.43	0.47
1:G:227:ILE:HD12	1:G:258:ALA:HB1	1.96	0.47
1:H:314:LEU:O	1:H:317:LEU:HB2	2.14	0.47
1:J:194:GLN:HG3	1:J:329:THR:HB	1.97	0.47
1:J:203:TYR:CD1	1:J:267:MET:CE	2.97	0.47
1:L:206:ASN:HB2	1:L:213:VAL:HG23	1.96	0.47
1:L:242:LYS:CB	1:M:257:GLU:HA	2.43	0.47
1:N:50:THR:HB	1:N:51:LYS:HA	1.97	0.47
1:N:237:LEU:HA	1:N:247:LEU:HD22	1.97	0.47
1:B:213:VAL:CG2	1:B:214:GLU:N	2.77	0.47
1:B:262:LEU:O	1:B:266:THR:HG23	2.15	0.47
1:C:227:ILE:HD12	1:C:258:ALA:HB1	1.96	0.47
1:C:278:ALA:HB2	1:C:289:LEU:CD1	2.45	0.47
1:F:226:LYS:HB2	1:F:252:GLU:HG3	1.96	0.47
1:G:200:LEU:HD22	1:G:254:VAL:HG11	1.96	0.47
1:G:262:LEU:O	1:G:266:THR:HG23	2.15	0.47
1:H:203:TYR:CE2	1:H:267:MET:SD	3.08	0.47
1:I:237:LEU:HA	1:I:247:LEU:HD22	1.97	0.47
1:J:236:VAL:O	1:J:240:VAL:HG23	2.13	0.47
1:K:144:ILE:HG23	1:K:403:THR:HG21	1.97	0.47
1:K:314:LEU:O	1:K:317:LEU:HB2	2.14	0.47
1:L:144:ILE:HG23	1:L:403:THR:HG21	1.97	0.47
1:A:204:PHE:CD1	1:A:273:VAL:O	2.68	0.47
1:B:213:VAL:O	1:B:324:VAL:HA	2.15	0.47
1:C:150:ILE:HD11	1:C:493:ILE:HG23	1.97	0.47
1:D:262:LEU:O	1:D:266:THR:HG23	2.15	0.47
1:F:162:ILE:CD1	1:F:400:LEU:N	2.77	0.47
1:F:213:VAL:O	1:F:324:VAL:HA	2.14	0.47
1:G:353:ILE:HD13	1:G:366:GLN:HG2	1.97	0.47
1:I:298:GLY:HA3	1:I:318:GLY:CA	2.44	0.47
1:J:203:TYR:CE2	1:J:267:MET:SD	3.08	0.47
1:J:220:ILE:HD12	1:J:296:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:34:LYS:HB2	1:K:457:ASN:HB3	1.97	0.47
1:K:237:LEU:HD13	1:K:271:VAL:HG21	1.97	0.47
1:M:237:LEU:HA	1:M:247:LEU:HD22	1.97	0.47
1:B:241:ALA:CA	1:B:271:VAL:HG22	2.44	0.46
1:E:226:LYS:HB2	1:E:252:GLU:HG3	1.96	0.46
1:G:213:VAL:CG2	1:G:214:GLU:N	2.77	0.46
1:H:34:LYS:HB2	1:H:457:ASN:HB3	1.97	0.46
1:H:182:GLY:HA3	1:H:383:ALA:N	2.11	0.46
1:J:144:ILE:HG23	1:J:403:THR:HG21	1.97	0.46
1:K:237:LEU:CD2	1:K:247:LEU:HD23	2.44	0.46
1:L:237:LEU:HD13	1:L:271:VAL:HG21	1.97	0.46
1:M:34:LYS:HB2	1:M:457:ASN:HB3	1.97	0.46
1:M:50:THR:HB	1:M:51:LYS:HA	1.97	0.46
1:M:411:VAL:HG21	1:M:494:LEU:HD13	1.97	0.46
1:A:25:ASP:CG	1:A:28:LYS:HZ3	2.19	0.46
1:B:158:VAL:HG13	1:B:396:VAL:HA	1.96	0.46
1:B:195:PHE:N	1:B:195:PHE:CD1	2.82	0.46
1:C:226:LYS:HB2	1:C:252:GLU:HG3	1.96	0.46
1:E:162:ILE:CD1	1:E:400:LEU:N	2.77	0.46
1:E:206:ASN:HB3	1:E:208:PRO:HD2	1.96	0.46
1:E:262:LEU:O	1:E:266:THR:HG23	2.15	0.46
1:F:204:PHE:CD1	1:F:273:VAL:O	2.68	0.46
1:F:227:ILE:HD12	1:F:258:ALA:HB1	1.96	0.46
1:F:278:ALA:HB2	1:F:289:LEU:CD1	2.45	0.46
1:I:314:LEU:O	1:I:317:LEU:HB2	2.14	0.46
1:J:30:THR:C	1:J:35:GLY:HA3	2.36	0.46
1:K:220:ILE:HD12	1:K:296:THR:HG21	1.96	0.46
1:L:203:TYR:CD1	1:L:267:MET:CE	2.99	0.46
2:M:1525:PO4:P	4:M:1527:ATP:O1G	2.73	0.46
1:N:220:ILE:HD12	1:N:296:THR:HG21	1.96	0.46
1:N:233:MET:CE	1:N:249:ILE:HD11	2.42	0.46
1:N:314:LEU:O	1:N:317:LEU:HB2	2.15	0.46
1:A:353:ILE:HD13	1:A:366:GLN:CG	2.46	0.46
1:C:262:LEU:O	1:C:266:THR:HG23	2.15	0.46
1:D:204:PHE:CD1	1:D:273:VAL:O	2.68	0.46
1:D:207:LYS:N	1:D:208:PRO:HD2	2.29	0.46
1:G:207:LYS:CB	1:G:208:PRO:HD3	2.46	0.46
1:H:50:THR:HB	1:H:51:LYS:HA	1.97	0.46
1:I:144:ILE:HG23	1:I:403:THR:HG21	1.97	0.46
1:J:34:LYS:HB2	1:J:457:ASN:HB3	1.97	0.46
1:J:77:VAL:HG22	1:J:510:VAL:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:298:GLY:HA3	1:J:318:GLY:CA	2.44	0.46
1:J:314:LEU:O	1:J:317:LEU:HB2	2.14	0.46
1:L:220:ILE:HD12	1:L:296:THR:HG21	1.96	0.46
1:M:183:LEU:HA	1:M:382:GLY:HA3	1.97	0.46
1:N:183:LEU:HA	1:N:382:GLY:HA3	1.98	0.46
1:B:226:LYS:HB2	1:B:252:GLU:HG3	1.96	0.46
1:B:250:ILE:HD11	1:B:332:ILE:HD11	1.98	0.46
1:C:240:VAL:HG11	1:C:247:LEU:CB	2.43	0.46
1:C:250:ILE:HD11	1:C:332:ILE:HD11	1.98	0.46
1:D:250:ILE:HD11	1:D:332:ILE:HD11	1.98	0.46
1:D:311:LYS:HD3	1:D:311:LYS:HA	1.93	0.46
1:E:353:ILE:HD13	1:E:366:GLN:CG	2.46	0.46
1:G:226:LYS:HB2	1:G:252:GLU:HG3	1.96	0.46
1:H:411:VAL:HG21	1:H:494:LEU:HD13	1.97	0.46
1:I:50:THR:HB	1:I:51:LYS:HA	1.97	0.46
1:I:249:ILE:HB	1:I:275:ALA:CB	2.40	0.46
1:J:237:LEU:HD13	1:J:271:VAL:HG21	1.97	0.46
2:J:1525:PO4:P	4:J:1527:ATP:O1G	2.73	0.46
1:K:203:TYR:CD1	1:K:267:MET:CE	2.97	0.46
1:M:144:ILE:HG23	1:M:403:THR:HG21	1.97	0.46
1:M:221:LEU:HG	1:M:309:LEU:HD22	1.96	0.46
1:D:200:LEU:HD11	1:D:254:VAL:HA	1.94	0.46
1:D:226:LYS:HB2	1:D:252:GLU:HG3	1.96	0.46
1:G:353:ILE:HD13	1:G:366:GLN:CG	2.46	0.46
1:H:237:LEU:HD13	1:H:271:VAL:HG21	1.97	0.46
1:L:314:LEU:O	1:L:317:LEU:HB2	2.14	0.46
1:B:111:MET:O	1:B:113:PRO:HD3	2.16	0.46
1:B:353:ILE:HD13	1:B:366:GLN:CG	2.46	0.46
1:E:111:MET:O	1:E:113:PRO:HD3	2.16	0.46
1:F:165:ALA:CA	1:F:187:LEU:HD21	2.46	0.46
1:F:353:ILE:HD13	1:F:366:GLN:HG2	1.97	0.46
1:H:144:ILE:HG23	1:H:403:THR:HG21	1.97	0.46
1:I:237:LEU:HD13	1:I:271:VAL:HG21	1.97	0.46
1:I:242:LYS:C	1:J:257:GLU:CA	2.78	0.46
1:J:237:LEU:HA	1:J:247:LEU:HD22	1.97	0.46
1:J:411:VAL:HG21	1:J:494:LEU:HD13	1.97	0.46
1:M:220:ILE:HD12	1:M:296:THR:HG21	1.96	0.46
1:N:203:TYR:CD1	1:N:267:MET:CE	2.98	0.46
1:A:262:LEU:O	1:A:266:THR:HG23	2.15	0.46
1:B:204:PHE:CD1	1:B:273:VAL:O	2.68	0.46
1:B:223:ALA:CA	1:B:309:LEU:HD23	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ASP:OD1	1:C:329:THR:HG22	2.16	0.46
1:C:204:PHE:CD1	1:C:273:VAL:O	2.69	0.46
1:H:199:TYR:CB	1:H:325:ILE:HD11	2.41	0.46
1:K:203:TYR:CE2	1:K:267:MET:SD	3.08	0.46
1:K:233:MET:HE2	1:K:249:ILE:HD11	1.93	0.46
1:L:30:THR:C	1:L:35:GLY:HA3	2.36	0.46
1:L:40:LEU:HD21	1:L:55:SER:HB3	1.98	0.46
1:M:353:ILE:HD11	1:M:369:VAL:HG21	1.98	0.46
1:N:144:ILE:HG23	1:N:403:THR:HG21	1.97	0.46
1:A:250:ILE:HD11	1:A:332:ILE:HD11	1.98	0.46
1:B:240:VAL:CG1	1:B:247:LEU:HB2	2.42	0.46
1:C:353:ILE:HD13	1:C:366:GLN:CG	2.46	0.46
1:F:381:VAL:CG2	1:F:393:LYS:N	2.77	0.46
1:G:240:VAL:HG11	1:G:247:LEU:CB	2.43	0.46
1:H:30:THR:C	1:H:35:GLY:HA3	2.36	0.46
1:K:233:MET:CE	1:K:249:ILE:HD11	2.42	0.46
1:L:50:THR:HB	1:L:51:LYS:HA	1.97	0.46
1:L:77:VAL:HG22	1:L:510:VAL:CG2	2.46	0.46
1:L:237:LEU:HA	1:L:247:LEU:HD22	1.97	0.46
1:M:40:LEU:HD21	1:M:55:SER:HB3	1.98	0.46
1:M:182:GLY:HA2	1:M:382:GLY:HA2	1.98	0.46
1:M:237:LEU:HD13	1:M:271:VAL:HG21	1.97	0.46
1:N:353:ILE:HD11	1:N:369:VAL:HG21	1.98	0.46
1:A:111:MET:O	1:A:113:PRO:HD3	2.16	0.46
1:A:226:LYS:HB2	1:A:252:GLU:HG3	1.96	0.46
1:C:278:ALA:CB	1:C:289:LEU:HD12	2.46	0.46
1:D:278:ALA:HB2	1:D:289:LEU:HD12	1.98	0.46
1:F:220:ILE:CD1	1:F:332:ILE:HD13	2.33	0.46
1:F:353:ILE:HD13	1:F:366:GLN:CG	2.46	0.46
1:K:237:LEU:HA	1:K:247:LEU:HD22	1.97	0.46
1:M:196:ASP:CG	1:M:329:THR:HG22	2.35	0.46
1:N:169:VAL:HG21	1:N:175:ILE:HG13	1.98	0.46
1:N:298:GLY:HA3	1:N:318:GLY:CA	2.44	0.46
1:C:111:MET:O	1:C:113:PRO:HD3	2.16	0.46
1:D:191:GLU:OE1	1:D:191:GLU:HA	2.16	0.46
1:H:77:VAL:HG22	1:H:510:VAL:CG2	2.46	0.46
1:H:169:VAL:HG21	1:H:175:ILE:HG13	1.98	0.46
1:J:29:VAL:O	1:J:35:GLY:HA2	2.16	0.46
1:J:50:THR:HB	1:J:51:LYS:HA	1.97	0.46
1:K:282:GLY:O	1:K:285:ARG:HB3	2.16	0.46
1:L:182:GLY:HA2	1:L:382:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:411:VAL:HG21	1:L:494:LEU:HD13	1.97	0.46
1:M:29:VAL:O	1:M:35:GLY:HA2	2.16	0.46
1:N:77:VAL:HG22	1:N:510:VAL:CG2	2.46	0.46
1:A:150:ILE:HD11	1:A:493:ILE:HG23	1.97	0.45
1:B:521:VAL:O	1:C:41:ASP:HB3	2.16	0.45
1:C:289:LEU:HD23	1:C:289:LEU:O	2.17	0.45
1:D:353:ILE:HD13	1:D:366:GLN:CG	2.46	0.45
1:E:227:ILE:HD12	1:E:258:ALA:HB1	1.96	0.45
1:G:111:MET:O	1:G:113:PRO:HD3	2.16	0.45
1:I:30:THR:C	1:I:35:GLY:HA3	2.36	0.45
1:I:169:VAL:HG21	1:I:175:ILE:HG13	1.98	0.45
1:I:203:TYR:CD1	1:I:267:MET:CE	2.98	0.45
1:I:227:ILE:CD1	1:I:233:MET:SD	2.92	0.45
1:K:40:LEU:HD21	1:K:55:SER:HB3	1.98	0.45
1:K:199:TYR:CB	1:K:325:ILE:HD11	2.39	0.45
1:L:34:LYS:HB2	1:L:457:ASN:HB3	1.97	0.45
1:L:183:LEU:HA	1:L:382:GLY:CA	2.45	0.45
1:N:205:ILE:C	1:N:207:LYS:HG2	2.36	0.45
1:B:207:LYS:HB2	1:B:207:LYS:HE2	1.62	0.45
1:C:278:ALA:HB2	1:C:289:LEU:HD12	1.98	0.45
1:D:521:VAL:O	1:E:41:ASP:HB3	2.16	0.45
1:E:250:ILE:HD11	1:E:332:ILE:HD11	1.98	0.45
1:F:278:ALA:HB2	1:F:289:LEU:HD12	1.99	0.45
1:G:223:ALA:CA	1:G:309:LEU:HD23	2.45	0.45
1:I:40:LEU:HD21	1:I:55:SER:HB3	1.98	0.45
1:I:227:ILE:HB	1:I:262:LEU:HD11	1.98	0.45
1:J:227:ILE:HB	1:J:262:LEU:HD11	1.98	0.45
1:L:227:ILE:HB	1:L:262:LEU:HD11	1.98	0.45
1:N:40:LEU:HD21	1:N:55:SER:HB3	1.97	0.45
1:B:278:ALA:CB	1:B:289:LEU:HD12	2.46	0.45
1:D:111:MET:O	1:D:113:PRO:HD3	2.16	0.45
1:D:190:VAL:HG21	1:D:333:ILE:HG22	1.99	0.45
1:D:278:ALA:CB	1:D:289:LEU:HD12	2.46	0.45
2:D:1525:PO4:P	4:D:1527:ATP:PG	3.15	0.45
1:G:204:PHE:CD1	1:G:273:VAL:O	2.69	0.45
1:G:278:ALA:HB2	1:G:289:LEU:HD12	1.98	0.45
1:G:289:LEU:O	1:G:289:LEU:HD23	2.17	0.45
1:H:406:ALA:HB1	1:H:411:VAL:HG12	1.99	0.45
1:K:29:VAL:O	1:K:35:GLY:HA2	2.16	0.45
1:K:30:THR:C	1:K:35:GLY:HA3	2.36	0.45
1:K:50:THR:HB	1:K:51:LYS:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:77:VAL:HG22	1:K:510:VAL:CG2	2.46	0.45
1:K:183:LEU:HA	1:K:382:GLY:HA3	1.97	0.45
1:L:182:GLY:HA2	1:L:183:LEU:HA	1.57	0.45
1:M:77:VAL:HG22	1:M:510:VAL:CG2	2.46	0.45
1:N:182:GLY:HA2	1:N:382:GLY:HA2	1.98	0.45
1:C:521:VAL:O	1:D:41:ASP:HB3	2.16	0.45
1:D:402:ALA:HB1	1:D:496:PRO:HG2	1.99	0.45
1:E:200:LEU:HD11	1:E:254:VAL:HA	1.94	0.45
1:E:223:ALA:CA	1:E:309:LEU:HD23	2.45	0.45
1:F:200:LEU:HD11	1:F:254:VAL:CA	2.12	0.45
1:F:200:LEU:HD11	1:F:254:VAL:HA	1.94	0.45
1:F:272:LYS:CD	1:F:272:LYS:H	2.30	0.45
1:F:384:ALA:HA	1:F:385:THR:HA	1.68	0.45
1:G:219:PHE:HB3	1:G:317:LEU:HD11	1.98	0.45
1:H:353:ILE:HD11	1:H:369:VAL:HG21	1.98	0.45
1:I:29:VAL:O	1:I:35:GLY:HA2	2.16	0.45
1:K:227:ILE:HB	1:K:262:LEU:HD11	1.98	0.45
1:K:353:ILE:HD11	1:K:369:VAL:HG21	1.98	0.45
1:L:151:SER:HB3	1:L:399:ALA:HA	1.99	0.45
1:L:190:VAL:HG21	1:L:333:ILE:HG12	1.98	0.45
1:M:169:VAL:HG21	1:M:175:ILE:HG13	1.98	0.45
1:N:29:VAL:O	1:N:35:GLY:HA2	2.16	0.45
1:N:184:GLN:HG2	1:N:186:GLU:HG2	1.97	0.45
1:N:227:ILE:HB	1:N:262:LEU:HD11	1.97	0.45
1:N:237:LEU:HD13	1:N:271:VAL:HG21	1.97	0.45
1:A:289:LEU:HD23	1:A:289:LEU:O	2.17	0.45
1:A:521:VAL:O	1:B:41:ASP:HB3	2.16	0.45
1:B:249:ILE:HD11	1:B:262:LEU:HD22	1.87	0.45
1:E:272:LYS:H	1:E:272:LYS:CD	2.30	0.45
1:F:195:PHE:CD1	1:F:195:PHE:N	2.82	0.45
1:F:207:LYS:HB2	1:F:207:LYS:HE3	1.73	0.45
1:F:219:PHE:HB3	1:F:317:LEU:HD11	1.98	0.45
1:H:215:LEU:HB2	1:H:323:VAL:HG22	1.99	0.45
1:H:255:GLU:CD	1:H:256:GLY:H	2.20	0.45
1:I:34:LYS:HB2	1:I:457:ASN:HB3	1.97	0.45
1:I:182:GLY:HA2	1:I:382:GLY:HA2	1.98	0.45
1:J:182:GLY:HA2	1:J:382:GLY:HA2	1.98	0.45
1:J:183:LEU:HA	1:J:382:GLY:HA3	1.97	0.45
1:K:151:SER:HB3	1:K:399:ALA:HA	1.99	0.45
1:K:406:ALA:HB1	1:K:411:VAL:HG12	1.98	0.45
1:K:411:VAL:HG21	1:K:494:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:233:MET:CE	1:L:249:ILE:HD11	2.44	0.45
1:C:402:ALA:HB1	1:C:496:PRO:HG2	1.99	0.45
1:D:289:LEU:HD23	1:D:289:LEU:O	2.17	0.45
1:E:402:ALA:HB1	1:E:496:PRO:HG2	1.99	0.45
1:H:27:VAL:CG1	1:H:90:THR:HG23	2.47	0.45
1:H:207:LYS:HE2	1:H:207:LYS:HA	1.99	0.45
1:I:77:VAL:HG22	1:I:510:VAL:CG2	2.46	0.45
1:I:215:LEU:HB2	1:I:323:VAL:HG22	1.99	0.45
1:J:40:LEU:HD21	1:J:55:SER:HB3	1.98	0.45
1:K:182:GLY:HA2	1:K:183:LEU:HA	1.63	0.45
1:L:29:VAL:O	1:L:35:GLY:HA2	2.16	0.45
1:L:353:ILE:HD11	1:L:369:VAL:HG21	1.98	0.45
1:M:30:THR:C	1:M:35:GLY:HA3	2.36	0.45
1:A:240:VAL:HG11	1:A:247:LEU:CB	2.43	0.45
1:C:207:LYS:HE3	1:C:207:LYS:N	2.23	0.45
1:D:227:ILE:HD12	1:D:258:ALA:HB1	1.96	0.45
1:F:521:VAL:O	1:G:41:ASP:HB3	2.16	0.45
1:H:227:ILE:HB	1:H:262:LEU:HD11	1.98	0.45
1:J:151:SER:HB3	1:J:399:ALA:HA	1.99	0.45
1:J:169:VAL:HG21	1:J:175:ILE:HG13	1.99	0.45
1:M:151:SER:HB3	1:M:399:ALA:HA	1.99	0.45
1:M:203:TYR:CE2	1:M:267:MET:SD	3.09	0.45
1:A:278:ALA:CB	1:A:289:LEU:HD12	2.46	0.45
1:B:402:ALA:HB1	1:B:496:PRO:HG2	1.99	0.45
1:C:177:VAL:HG21	1:C:397:GLU:HG2	1.99	0.45
1:D:272:LYS:CD	1:D:272:LYS:H	2.30	0.45
1:E:278:ALA:CB	1:E:289:LEU:HD12	2.46	0.45
1:E:521:VAL:O	1:F:41:ASP:HB3	2.16	0.45
1:F:111:MET:O	1:F:113:PRO:HD3	2.16	0.45
1:G:272:LYS:H	1:G:272:LYS:CD	2.30	0.45
1:H:196:ASP:OD1	1:H:329:THR:HG22	2.17	0.45
1:J:196:ASP:HA	1:J:329:THR:HG22	1.98	0.45
1:J:215:LEU:HB2	1:J:323:VAL:HG22	1.99	0.45
1:K:255:GLU:CD	1:K:256:GLY:H	2.20	0.45
1:L:406:ALA:HB1	1:L:411:VAL:HG12	1.98	0.45
1:A:240:VAL:CG1	1:A:247:LEU:HB2	2.42	0.45
1:B:278:ALA:HB2	1:B:289:LEU:HD12	1.98	0.45
2:F:1525:PO4:P	4:F:1527:ATP:PG	3.15	0.45
1:H:242:LYS:HG3	1:I:257:GLU:C	2.38	0.45
1:H:282:GLY:O	1:H:285:ARG:HB3	2.16	0.45
1:K:19:GLY:HA2	1:K:62:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:177:VAL:CG2	1:K:379:ILE:HB	2.42	0.45
1:K:182:GLY:HA2	1:K:382:GLY:HA2	1.98	0.45
1:L:183:LEU:H	1:L:183:LEU:CD2	2.22	0.45
1:M:227:ILE:HB	1:M:262:LEU:HD11	1.98	0.45
1:F:250:ILE:HD11	1:F:332:ILE:HD11	1.98	0.45
1:G:384:ALA:HA	1:G:385:THR:HA	1.68	0.45
1:H:40:LEU:HD21	1:H:55:SER:HB3	1.98	0.45
1:H:517:THR:HG21	1:H:520:MET:HG3	1.99	0.45
1:I:183:LEU:HA	1:I:382:GLY:HA3	1.98	0.45
1:I:517:THR:HG21	1:I:520:MET:HG3	1.99	0.45
1:L:19:GLY:HA2	1:L:62:LEU:CD1	2.47	0.45
1:M:223:ALA:HB2	1:M:309:LEU:CG	2.47	0.45
1:N:215:LEU:HB2	1:N:323:VAL:HG22	1.99	0.45
1:A:41:ASP:HB3	1:G:521:VAL:O	2.16	0.44
1:A:52:ASP:HB3	1:A:55:SER:H	1.82	0.44
1:C:219:PHE:HB3	1:C:317:LEU:HD11	1.98	0.44
1:C:461:GLU:HA	1:C:462:PRO:HD3	1.87	0.44
1:E:384:ALA:HA	1:E:385:THR:HA	1.68	0.44
1:G:278:ALA:CB	1:G:289:LEU:HD12	2.46	0.44
1:I:27:VAL:CG1	1:I:90:THR:HG23	2.47	0.44
1:I:203:TYR:CE2	1:I:267:MET:SD	3.09	0.44
1:I:295:LEU:HD23	1:I:342:ILE:CD1	2.46	0.44
1:I:353:ILE:HD11	1:I:369:VAL:HG21	1.98	0.44
1:J:353:ILE:HD11	1:J:369:VAL:HG21	1.98	0.44
1:L:295:LEU:HD23	1:L:342:ILE:CD1	2.46	0.44
1:M:19:GLY:HA2	1:M:62:LEU:CD1	2.47	0.44
1:B:177:VAL:HG21	1:B:397:GLU:HG2	1.99	0.44
1:C:152:ALA:HB2	1:C:399:ALA:HB2	2.00	0.44
1:D:177:VAL:HG21	1:D:397:GLU:HG2	1.99	0.44
1:D:219:PHE:HB3	1:D:317:LEU:HD11	1.99	0.44
1:E:513:LEU:HB3	1:F:49:ILE:HD12	2.00	0.44
1:F:221:LEU:CD1	1:F:309:LEU:HD21	2.45	0.44
1:F:291:ASP:OD1	1:F:349:ILE:HD11	2.18	0.44
1:F:513:LEU:HB3	1:G:49:ILE:HD12	1.99	0.44
1:G:240:VAL:CG1	1:G:247:LEU:HB2	2.42	0.44
1:G:250:ILE:HD11	1:G:332:ILE:HD11	1.98	0.44
1:H:19:GLY:HA2	1:H:62:LEU:CD1	2.47	0.44
1:I:272:LYS:HD3	1:I:272:LYS:H	1.82	0.44
1:J:517:THR:HG21	1:J:520:MET:HG3	1.99	0.44
1:K:215:LEU:HB2	1:K:323:VAL:HG22	1.99	0.44
1:L:223:ALA:HB2	1:L:309:LEU:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ALA:HB2	1:A:289:LEU:HD12	1.98	0.44
1:A:402:ALA:HB1	1:A:496:PRO:HG2	1.99	0.44
1:B:152:ALA:HB2	1:B:399:ALA:HB2	2.00	0.44
1:B:291:ASP:OD1	1:B:349:ILE:HD11	2.18	0.44
1:B:311:LYS:HD3	1:B:311:LYS:HA	1.93	0.44
1:E:291:ASP:OD1	1:E:349:ILE:HD11	2.17	0.44
1:F:289:LEU:HD23	1:F:289:LEU:O	2.17	0.44
1:F:402:ALA:HB1	1:F:496:PRO:HG2	1.99	0.44
1:G:381:VAL:CG2	1:G:393:LYS:N	2.77	0.44
1:I:222:LEU:CD2	1:I:250:ILE:HD12	2.48	0.44
1:J:222:LEU:CD2	1:J:250:ILE:HD12	2.47	0.44
1:J:518:GLU:CB	1:J:519:CYS:N	2.74	0.44
1:K:169:VAL:HG21	1:K:175:ILE:HG13	1.98	0.44
1:L:203:TYR:CE2	1:L:267:MET:SD	3.09	0.44
1:L:272:LYS:HD3	1:L:272:LYS:H	1.82	0.44
1:M:255:GLU:CD	1:M:256:GLY:H	2.20	0.44
1:N:30:THR:C	1:N:35:GLY:HA3	2.36	0.44
1:N:203:TYR:CE2	1:N:267:MET:SD	3.09	0.44
1:A:219:PHE:HB3	1:A:317:LEU:HD11	1.98	0.44
1:B:272:LYS:H	1:B:272:LYS:CD	2.30	0.44
1:D:513:LEU:HB3	1:E:49:ILE:HD12	2.00	0.44
1:G:291:ASP:OD1	1:G:349:ILE:HD11	2.18	0.44
1:H:295:LEU:HD23	1:H:342:ILE:CD1	2.46	0.44
1:J:272:LYS:H	1:J:272:LYS:HD3	1.82	0.44
1:N:19:GLY:HA2	1:N:62:LEU:CD1	2.47	0.44
1:N:223:ALA:HB2	1:N:309:LEU:CG	2.47	0.44
1:N:255:GLU:CD	1:N:256:GLY:H	2.21	0.44
1:A:272:LYS:CD	1:A:272:LYS:H	2.30	0.44
1:B:194:GLN:HG2	1:B:329:THR:HG21	1.99	0.44
1:B:240:VAL:HG11	1:B:247:LEU:CB	2.43	0.44
1:B:289:LEU:O	1:B:289:LEU:HD23	2.17	0.44
1:E:289:LEU:O	1:E:289:LEU:HD23	2.17	0.44
1:J:206:ASN:HB3	1:J:208:PRO:HD2	1.98	0.44
1:M:27:VAL:CG1	1:M:90:THR:HG23	2.47	0.44
1:M:406:ALA:HB1	1:M:411:VAL:HG12	1.98	0.44
1:A:49:ILE:HD12	1:G:513:LEU:HB3	2.00	0.44
1:A:291:ASP:OD1	1:A:349:ILE:HD11	2.17	0.44
1:C:193:MET:SD	1:C:292:ILE:HG12	2.57	0.44
1:H:29:VAL:O	1:H:35:GLY:HA2	2.16	0.44
1:H:218:PRO:HG3	1:H:323:VAL:HG13	2.00	0.44
1:I:60:ILE:HA	1:J:6:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:255:GLU:CD	1:J:256:GLY:H	2.20	0.44
1:M:413:ALA:HB1	1:M:488:MET:HB2	2.00	0.44
1:N:215:LEU:HB3	1:N:246:PRO:HG2	2.00	0.44
1:N:517:THR:HG21	1:N:520:MET:HG3	1.99	0.44
1:C:200:LEU:HD11	1:C:254:VAL:CA	2.12	0.44
1:G:402:ALA:HB1	1:G:496:PRO:HG2	1.99	0.44
1:H:60:ILE:HA	1:I:6:VAL:CG2	2.48	0.44
1:H:215:LEU:HB3	1:H:246:PRO:HG2	2.00	0.44
1:H:224:ASP:HB2	1:H:303:GLU:H	1.82	0.44
1:J:60:ILE:HA	1:K:6:VAL:CG2	2.48	0.44
1:K:272:LYS:HD3	1:K:272:LYS:H	1.82	0.44
1:L:356:ALA:HB1	1:L:361:ASP:HB2	2.00	0.44
1:M:215:LEU:HB2	1:M:323:VAL:HG22	1.99	0.44
1:N:413:ALA:HB1	1:N:488:MET:HB2	2.00	0.44
1:A:221:LEU:CD1	1:A:309:LEU:HD21	2.45	0.44
1:C:272:LYS:CD	1:C:272:LYS:H	2.30	0.44
1:D:152:ALA:HB2	1:D:399:ALA:HB2	2.00	0.44
1:G:278:ALA:HA	1:G:279:PRO:HD3	1.72	0.44
1:I:182:GLY:HA2	1:I:183:LEU:HA	1.63	0.44
1:I:356:ALA:HB1	1:I:361:ASP:HB2	2.00	0.44
1:J:215:LEU:HB3	1:J:246:PRO:HG2	2.00	0.44
1:J:406:ALA:HB1	1:J:411:VAL:HG12	1.99	0.44
1:K:60:ILE:HA	1:L:6:VAL:CG2	2.48	0.44
1:K:215:LEU:HB3	1:K:246:PRO:HG2	2.00	0.44
1:K:356:ALA:HB1	1:K:361:ASP:HB2	2.00	0.44
1:L:215:LEU:HB3	1:L:246:PRO:HG2	2.00	0.44
1:L:240:VAL:HG21	1:L:317:LEU:HD22	2.00	0.44
1:N:272:LYS:HD3	1:N:272:LYS:H	1.82	0.44
1:A:152:ALA:HB2	1:A:399:ALA:HB2	2.00	0.44
1:A:513:LEU:HB3	1:B:49:ILE:HD12	2.00	0.44
1:B:52:ASP:HB2	1:B:55:SER:HB2	2.00	0.44
1:B:381:VAL:CG2	1:B:393:LYS:N	2.77	0.44
1:C:52:ASP:HB3	1:C:55:SER:H	1.82	0.44
1:E:219:PHE:HB3	1:E:317:LEU:HD11	1.98	0.44
1:E:278:ALA:HB2	1:E:289:LEU:HD12	1.98	0.44
1:F:52:ASP:HB2	1:F:55:SER:HB2	2.00	0.44
1:G:177:VAL:HG21	1:G:397:GLU:HG2	1.99	0.44
1:H:237:LEU:HA	1:H:247:LEU:CD2	2.48	0.44
1:I:255:GLU:CD	1:I:256:GLY:H	2.21	0.44
1:I:413:ALA:HB1	1:I:488:MET:HB2	2.00	0.44
1:J:62:LEU:HB2	1:J:68:ASN:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:215:LEU:HB2	1:L:323:VAL:HG22	1.99	0.44
1:M:215:LEU:HB3	1:M:246:PRO:HG2	2.00	0.44
1:M:227:ILE:CD1	1:M:233:MET:SD	2.93	0.44
1:B:219:PHE:HB3	1:B:317:LEU:HD11	1.98	0.43
1:C:513:LEU:HB3	1:D:49:ILE:HD12	2.00	0.43
2:C:1525:PO4:P	4:C:1527:ATP:PG	3.16	0.43
1:F:278:ALA:CB	1:F:289:LEU:HD12	2.47	0.43
1:F:524:LEU:HG	1:F:525:PRO:N	2.33	0.43
1:H:272:LYS:H	1:H:272:LYS:HD3	1.82	0.43
1:H:413:ALA:HB1	1:H:488:MET:HB2	2.00	0.43
1:J:19:GLY:HA2	1:J:62:LEU:CD1	2.47	0.43
1:J:242:LYS:HA	1:J:243:ALA:HA	1.12	0.43
1:J:356:ALA:HB1	1:J:361:ASP:HB2	2.00	0.43
1:K:218:PRO:HG3	1:K:323:VAL:HG13	1.99	0.43
1:N:218:PRO:HG3	1:N:323:VAL:HG13	2.00	0.43
1:B:513:LEU:HB3	1:C:49:ILE:HD12	2.00	0.43
1:C:291:ASP:OD1	1:C:349:ILE:HD11	2.18	0.43
1:D:52:ASP:HB2	1:D:55:SER:HB2	2.00	0.43
1:E:152:ALA:HB2	1:E:399:ALA:HB2	2.00	0.43
1:E:524:LEU:HG	1:E:525:PRO:N	2.33	0.43
1:K:240:VAL:HG21	1:K:317:LEU:HD22	2.00	0.43
1:K:517:THR:HG21	1:K:520:MET:HG3	1.99	0.43
1:L:190:VAL:HG21	1:L:333:ILE:HG23	1.98	0.43
1:M:240:VAL:HG21	1:M:317:LEU:HD22	2.00	0.43
1:D:278:ALA:HB2	1:D:289:LEU:CG	2.49	0.43
1:D:291:ASP:OD1	1:D:349:ILE:HD11	2.17	0.43
1:F:177:VAL:HG21	1:F:397:GLU:HG2	1.99	0.43
1:F:240:VAL:CG1	1:F:247:LEU:HB2	2.42	0.43
1:G:220:ILE:CD1	1:G:296:THR:HG21	2.47	0.43
1:H:62:LEU:HB2	1:H:68:ASN:HA	2.00	0.43
1:H:240:VAL:HG21	1:H:317:LEU:CD2	2.49	0.43
1:H:356:ALA:HB1	1:H:361:ASP:HB2	2.00	0.43
1:I:215:LEU:HB3	1:I:246:PRO:HG2	2.00	0.43
1:I:218:PRO:HG3	1:I:323:VAL:HG13	2.00	0.43
1:I:237:LEU:HA	1:I:247:LEU:CD2	2.49	0.43
1:L:218:PRO:HG3	1:L:323:VAL:HG13	2.00	0.43
1:L:413:ALA:HB1	1:L:488:MET:HB2	2.00	0.43
1:M:356:ALA:HB1	1:M:361:ASP:HB2	2.00	0.43
1:A:177:VAL:HA	1:A:379:ILE:O	2.19	0.43
1:A:240:VAL:HG13	1:A:245:LYS:O	2.19	0.43
1:A:278:ALA:HB2	1:A:289:LEU:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:524:LEU:HG	1:D:525:PRO:N	2.33	0.43
1:I:19:GLY:HA2	1:I:62:LEU:CD1	2.47	0.43
1:I:62:LEU:HB2	1:I:68:ASN:HA	2.00	0.43
1:J:27:VAL:CG1	1:J:90:THR:HG23	2.47	0.43
1:K:62:LEU:HB2	1:K:68:ASN:HA	2.00	0.43
1:K:77:VAL:HG22	1:K:510:VAL:CB	2.49	0.43
1:K:240:VAL:HG21	1:K:317:LEU:CD2	2.49	0.43
1:L:240:VAL:HG21	1:L:317:LEU:CD2	2.49	0.43
1:M:60:ILE:HA	1:N:6:VAL:CG2	2.48	0.43
1:M:240:VAL:HG21	1:M:317:LEU:CD2	2.49	0.43
1:N:227:ILE:CD1	1:N:233:MET:SD	2.93	0.43
1:N:301:ILE:HD11	1:N:312:ALA:CB	2.32	0.43
1:A:150:ILE:CD1	1:A:493:ILE:CA	2.74	0.43
1:C:311:LYS:HD3	1:C:311:LYS:HA	1.93	0.43
1:D:177:VAL:HA	1:D:379:ILE:O	2.18	0.43
1:E:240:VAL:HG13	1:E:245:LYS:O	2.18	0.43
1:F:150:ILE:CD1	1:F:493:ILE:CG2	2.91	0.43
1:G:152:ALA:HB2	1:G:399:ALA:HB2	2.00	0.43
1:G:177:VAL:HA	1:G:379:ILE:O	2.19	0.43
1:G:240:VAL:HG13	1:G:245:LYS:O	2.18	0.43
1:I:233:MET:CE	1:I:249:ILE:HD11	2.40	0.43
1:J:77:VAL:HG22	1:J:510:VAL:CB	2.49	0.43
1:J:240:VAL:HG21	1:J:317:LEU:CD2	2.49	0.43
1:K:169:VAL:HG21	1:K:175:ILE:CG1	2.49	0.43
1:K:223:ALA:HB2	1:K:309:LEU:CG	2.48	0.43
1:L:60:ILE:HA	1:M:6:VAL:CG2	2.48	0.43
1:N:99:ILE:CG2	1:N:120:ILE:HD13	2.49	0.43
1:N:356:ALA:HB1	1:N:361:ASP:HB2	2.00	0.43
1:B:240:VAL:HG13	1:B:245:LYS:O	2.18	0.43
1:B:381:VAL:HG11	1:B:393:LYS:HB2	2.00	0.43
1:C:197:ARG:HG3	1:C:198:GLY:O	2.18	0.43
1:C:223:ALA:CA	1:C:309:LEU:HD23	2.45	0.43
1:C:524:LEU:HG	1:C:525:PRO:N	2.33	0.43
1:F:240:VAL:HG13	1:F:245:LYS:O	2.18	0.43
1:F:381:VAL:HG11	1:F:393:LYS:HB2	2.00	0.43
1:G:221:LEU:CD1	1:G:309:LEU:HD21	2.45	0.43
2:G:1525:PO4:P	4:G:1527:ATP:PG	3.16	0.43
1:H:151:SER:HB3	1:H:399:ALA:HA	1.99	0.43
1:H:223:ALA:HB2	1:H:309:LEU:CG	2.48	0.43
1:I:181:THR:HG22	1:I:182:GLY:O	2.19	0.43
1:J:240:VAL:HG21	1:J:317:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:77:VAL:HG22	1:L:510:VAL:CB	2.49	0.43
1:M:99:ILE:CG2	1:M:120:ILE:HD13	2.49	0.43
1:M:229:ASN:HB3	1:M:231:ARG:HG3	2.01	0.43
1:M:272:LYS:H	1:M:272:LYS:HD3	1.82	0.43
1:M:517:THR:HG21	1:M:520:MET:HG3	2.00	0.43
1:N:240:VAL:HG21	1:N:317:LEU:HD22	2.00	0.43
2:A:1525:PO4:P	4:A:1527:ATP:PG	3.16	0.43
1:B:236:VAL:HG13	1:B:317:LEU:HD13	2.01	0.43
1:B:524:LEU:HG	1:B:525:PRO:N	2.33	0.43
1:E:177:VAL:HA	1:E:379:ILE:O	2.19	0.43
1:E:191:GLU:H	1:E:334:ASP:HA	1.84	0.43
1:I:169:VAL:HG21	1:I:175:ILE:CG1	2.49	0.43
1:J:218:PRO:HG3	1:J:323:VAL:HG13	2.00	0.43
1:J:413:ALA:HB1	1:J:488:MET:HB2	2.00	0.43
1:K:237:LEU:HA	1:K:247:LEU:CD2	2.48	0.43
1:K:413:ALA:HB1	1:K:488:MET:HB2	2.00	0.43
1:L:242:LYS:HG3	1:M:257:GLU:HB2	2.00	0.43
1:N:169:VAL:HG21	1:N:175:ILE:CG1	2.49	0.43
1:A:177:VAL:HG21	1:A:397:GLU:HG2	1.99	0.43
1:A:200:LEU:HD13	1:A:259:LEU:HB2	2.00	0.43
1:A:236:VAL:HG13	1:A:317:LEU:HD13	2.01	0.43
1:C:144:ILE:CG2	1:C:163:ALA:HA	2.49	0.43
1:D:240:VAL:HG13	1:D:245:LYS:O	2.18	0.43
1:H:6:VAL:CG2	1:N:60:ILE:HA	2.48	0.43
1:J:179:ASP:HB3	1:J:383:ALA:HB2	2.01	0.43
1:J:214:GLU:CD	1:J:322:ARG:HE	2.22	0.43
1:L:517:THR:HG21	1:L:520:MET:HG3	1.99	0.43
1:M:222:LEU:CD2	1:M:250:ILE:HD12	2.48	0.43
1:N:62:LEU:HB2	1:N:68:ASN:HA	2.00	0.43
1:N:295:LEU:HD23	1:N:342:ILE:CD1	2.46	0.43
1:A:381:VAL:CG2	1:A:393:LYS:N	2.77	0.43
1:A:521:VAL:HG11	1:B:59:GLU:CG	2.49	0.43
1:B:144:ILE:CG2	1:B:163:ALA:HA	2.49	0.43
1:C:236:VAL:HG13	1:C:317:LEU:HD13	2.01	0.43
1:C:240:VAL:HG13	1:C:245:LYS:O	2.18	0.43
1:C:278:ALA:HB2	1:C:289:LEU:CG	2.49	0.43
1:E:144:ILE:CG2	1:E:163:ALA:HA	2.49	0.43
1:E:513:LEU:O	1:F:49:ILE:HD13	2.19	0.43
1:F:152:ALA:HB2	1:F:399:ALA:HB2	2.00	0.43
1:G:52:ASP:HB3	1:G:55:SER:H	1.82	0.43
1:G:381:VAL:HG11	1:G:393:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:ILE:CD1	1:H:233:MET:SD	2.92	0.43
1:H:257:GLU:CA	1:N:242:LYS:C	2.78	0.43
1:I:77:VAL:HG22	1:I:510:VAL:CB	2.49	0.43
1:I:240:VAL:HG21	1:I:317:LEU:CD2	2.49	0.43
1:I:240:VAL:HG21	1:I:317:LEU:HD22	2.00	0.43
1:L:99:ILE:CG2	1:L:120:ILE:HD13	2.49	0.43
1:M:237:LEU:HA	1:M:247:LEU:CD2	2.48	0.43
1:N:282:GLY:O	1:N:285:ARG:HB3	2.19	0.43
1:A:513:LEU:O	1:B:49:ILE:HD13	2.19	0.43
1:A:524:LEU:HG	1:A:525:PRO:N	2.33	0.43
1:B:200:LEU:HD13	1:B:259:LEU:HB2	2.00	0.43
1:C:191:GLU:H	1:C:334:ASP:HA	1.84	0.43
1:C:381:VAL:HG11	1:C:393:LYS:HB2	2.00	0.43
1:D:236:VAL:HG13	1:D:317:LEU:HD13	2.01	0.43
1:E:177:VAL:HG21	1:E:397:GLU:HG2	1.99	0.43
1:F:165:ALA:HA	1:F:187:LEU:HD21	2.01	0.43
1:F:177:VAL:HA	1:F:379:ILE:O	2.19	0.43
1:F:236:VAL:HG13	1:F:317:LEU:HD13	2.01	0.43
1:F:513:LEU:O	1:G:49:ILE:HD13	2.19	0.43
1:F:521:VAL:HG11	1:G:59:GLU:CG	2.49	0.43
1:G:236:VAL:HG13	1:G:317:LEU:HD13	2.01	0.43
1:G:524:LEU:HG	1:G:525:LEU:N	2.34	0.43
1:H:518:GLU:CB	1:H:519:CYS:N	2.74	0.43
1:J:237:LEU:HA	1:J:247:LEU:CD2	2.49	0.43
1:K:224:ASP:HB2	1:K:303:GLU:H	1.82	0.43
1:K:301:ILE:HG23	1:K:307:MET:HB2	2.01	0.43
1:L:27:VAL:CG1	1:L:90:THR:HG23	2.47	0.43
1:L:237:LEU:HA	1:L:247:LEU:CD2	2.48	0.43
1:B:150:ILE:CD1	1:B:493:ILE:CG2	2.91	0.42
1:B:191:GLU:H	1:B:334:ASP:HA	1.84	0.42
1:B:206:ASN:CB	1:B:208:PRO:HD2	2.42	0.42
1:B:278:ALA:HB2	1:B:289:LEU:CG	2.49	0.42
2:B:1525:PO4:P	4:B:1527:ATP:PG	3.17	0.42
1:E:200:LEU:HD13	1:E:259:LEU:HB2	2.00	0.42
1:E:236:VAL:HG13	1:E:317:LEU:HD13	2.01	0.42
1:E:521:VAL:HG11	1:F:59:GLU:CG	2.49	0.42
2:E:1525:PO4:P	4:E:1527:ATP:PG	3.16	0.42
1:H:222:LEU:CD2	1:H:250:ILE:HD12	2.48	0.42
1:H:240:VAL:HG21	1:H:317:LEU:HD22	2.00	0.42
1:I:298:GLY:CA	1:I:318:GLY:HA3	2.49	0.42
1:J:99:ILE:CG2	1:J:120:ILE:HD13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:62:LEU:HB2	1:L:68:ASN:HA	2.00	0.42
1:M:218:PRO:HG3	1:M:323:VAL:HG13	2.00	0.42
1:M:282:GLY:O	1:M:285:ARG:HB3	2.19	0.42
1:A:220:ILE:CD1	1:A:296:THR:HG21	2.47	0.42
1:B:223:ALA:HB3	1:B:251:ALA:HA	2.02	0.42
1:C:223:ALA:HB3	1:C:251:ALA:HA	2.02	0.42
1:E:207:LYS:HB2	1:E:208:PRO:HD3	2.01	0.42
1:E:381:VAL:HG11	1:E:393:LYS:HB2	2.00	0.42
1:F:200:LEU:HD13	1:F:259:LEU:HB2	2.00	0.42
1:F:249:ILE:HD11	1:F:262:LEU:HD22	1.87	0.42
1:G:190:VAL:HB	1:G:334:ASP:HB2	2.01	0.42
1:H:182:GLY:HA2	1:H:183:LEU:HA	1.66	0.42
1:H:242:LYS:C	1:I:257:GLU:CA	2.78	0.42
1:I:214:GLU:CD	1:I:322:ARG:HE	2.22	0.42
1:I:278:ALA:HA	1:I:279:PRO:HD3	1.87	0.42
1:J:169:VAL:HG21	1:J:175:ILE:CG1	2.49	0.42
1:L:190:VAL:HG21	1:L:333:ILE:CG1	2.49	0.42
1:L:227:ILE:HG22	1:L:262:LEU:HD21	2.01	0.42
1:L:242:LYS:C	1:M:257:GLU:CA	2.78	0.42
1:M:62:LEU:HB2	1:M:68:ASN:HA	2.00	0.42
1:N:182:GLY:HA2	1:N:183:LEU:HA	1.63	0.42
1:N:240:VAL:HG21	1:N:317:LEU:CD2	2.49	0.42
1:C:278:ALA:HB2	1:C:289:LEU:HG	2.01	0.42
1:C:521:VAL:HG11	1:D:59:GLU:CG	2.49	0.42
1:D:200:LEU:HD13	1:D:259:LEU:HB2	2.00	0.42
1:E:221:LEU:CD1	1:E:309:LEU:HD21	2.45	0.42
1:F:223:ALA:HB3	1:F:251:ALA:HA	2.02	0.42
1:G:52:ASP:HB2	1:G:55:SER:HB2	2.01	0.42
1:G:278:ALA:HB2	1:G:289:LEU:CG	2.49	0.42
1:H:169:VAL:HG21	1:H:175:ILE:CG1	2.49	0.42
1:I:209:GLU:H	1:I:209:GLU:CD	2.23	0.42
1:I:223:ALA:HB2	1:I:309:LEU:CG	2.48	0.42
1:J:37:ASN:HB2	1:K:516:THR:O	2.20	0.42
1:J:223:ALA:HB2	1:J:309:LEU:CG	2.49	0.42
1:L:222:LEU:CD2	1:L:250:ILE:HD12	2.48	0.42
1:M:225:LYS:CA	1:M:303:GLU:HB2	2.50	0.42
1:A:52:ASP:HB2	1:A:55:SER:HB2	2.01	0.42
1:A:190:VAL:HB	1:A:334:ASP:HB2	2.01	0.42
1:A:381:VAL:HG11	1:A:393:LYS:HB2	2.00	0.42
1:B:521:VAL:HG11	1:C:59:GLU:CG	2.49	0.42
1:D:521:VAL:HG11	1:E:59:GLU:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:ASP:HB2	1:E:55:SER:HB2	2.01	0.42
1:E:223:ALA:HB3	1:E:251:ALA:HA	2.02	0.42
1:E:278:ALA:HB2	1:E:289:LEU:CG	2.49	0.42
1:F:190:VAL:HB	1:F:334:ASP:HB2	2.01	0.42
1:F:278:ALA:HB2	1:F:289:LEU:CG	2.49	0.42
1:G:144:ILE:CG2	1:G:163:ALA:HA	2.49	0.42
1:G:161:LEU:HD21	1:G:185:ASP:HB3	2.00	0.42
1:H:100:ILE:HD11	1:H:514:MET:HE3	2.01	0.42
1:I:99:ILE:CG2	1:I:120:ILE:HD13	2.49	0.42
1:I:301:ILE:HG23	1:I:307:MET:HB2	2.01	0.42
1:J:100:ILE:HD11	1:J:514:MET:HE3	2.02	0.42
1:K:37:ASN:HB2	1:L:516:THR:O	2.20	0.42
1:M:295:LEU:HD13	1:M:335:GLY:HA3	2.02	0.42
1:N:222:LEU:CD2	1:N:250:ILE:HD12	2.48	0.42
1:A:213:VAL:HG23	1:A:214:GLU:N	2.33	0.42
1:A:215:LEU:HB3	1:A:246:PRO:HG2	2.02	0.42
1:C:286:LYS:HD3	1:C:304:GLU:HA	2.01	0.42
1:D:278:ALA:HB2	1:D:289:LEU:HG	2.01	0.42
1:D:513:LEU:O	1:E:49:ILE:HD13	2.19	0.42
1:G:249:ILE:HD11	1:G:262:LEU:HD22	1.87	0.42
1:H:193:MET:HG2	1:H:372:LEU:HA	2.02	0.42
1:I:151:SER:HB3	1:I:399:ALA:HA	1.99	0.42
1:J:239:ALA:CB	1:J:314:LEU:HB3	2.49	0.42
1:K:99:ILE:CG2	1:K:120:ILE:HD13	2.49	0.42
1:K:214:GLU:CD	1:K:322:ARG:HE	2.22	0.42
1:L:227:ILE:CD1	1:L:233:MET:SD	2.93	0.42
1:M:169:VAL:HG21	1:M:175:ILE:CG1	2.49	0.42
1:M:298:GLY:CA	1:M:318:GLY:HA3	2.49	0.42
1:N:237:LEU:HA	1:N:247:LEU:CD2	2.49	0.42
1:N:295:LEU:HD13	1:N:335:GLY:HA3	2.02	0.42
1:A:49:ILE:HD13	1:G:513:LEU:O	2.19	0.42
1:A:59:GLU:CG	1:G:521:VAL:HG11	2.49	0.42
1:A:144:ILE:CG2	1:A:163:ALA:HA	2.49	0.42
1:A:191:GLU:H	1:A:334:ASP:HA	1.84	0.42
1:A:223:ALA:HB3	1:A:251:ALA:HA	2.02	0.42
1:B:513:LEU:O	1:C:49:ILE:HD13	2.19	0.42
1:C:52:ASP:HB2	1:C:55:SER:HB2	2.01	0.42
1:D:271:VAL:O	1:D:273:VAL:HG23	2.20	0.42
1:D:381:VAL:CG2	1:D:393:LYS:N	2.77	0.42
1:E:207:LYS:N	1:E:208:PRO:HD2	2.34	0.42
1:E:271:VAL:O	1:E:273:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:ALA:HB3	1:G:251:ALA:HA	2.02	0.42
1:H:214:GLU:CD	1:H:322:ARG:HE	2.22	0.42
1:H:295:LEU:HD13	1:H:335:GLY:HA3	2.02	0.42
1:I:37:ASN:HB2	1:J:516:THR:O	2.20	0.42
1:I:227:ILE:H	1:I:254:VAL:HG22	1.85	0.42
1:J:295:LEU:HD23	1:J:342:ILE:CD1	2.46	0.42
1:K:295:LEU:HD13	1:K:335:GLY:HA3	2.02	0.42
1:L:225:LYS:CA	1:L:303:GLU:HB2	2.50	0.42
1:L:295:LEU:HD13	1:L:335:GLY:HA3	2.02	0.42
1:M:227:ILE:HG22	1:M:262:LEU:HD21	2.01	0.42
1:M:446:ALA:O	1:M:450:PRO:HD2	2.20	0.42
1:N:193:MET:HG2	1:N:372:LEU:HA	2.02	0.42
1:B:278:ALA:HB2	1:B:289:LEU:HG	2.01	0.42
1:B:286:LYS:HD3	1:B:304:GLU:HA	2.01	0.42
1:D:144:ILE:CG2	1:D:163:ALA:HA	2.49	0.42
1:D:190:VAL:HB	1:D:334:ASP:CA	2.50	0.42
1:D:223:ALA:HB3	1:D:251:ALA:HA	2.02	0.42
1:D:270:ILE:O	1:D:271:VAL:HB	2.20	0.42
1:D:381:VAL:HG11	1:D:393:LYS:HB2	2.00	0.42
1:D:384:ALA:HA	1:D:385:THR:HA	1.68	0.42
1:E:270:ILE:O	1:E:271:VAL:HB	2.20	0.42
1:F:191:GLU:H	1:F:334:ASP:HA	1.84	0.42
1:G:150:ILE:HD11	1:G:493:ILE:HG23	1.97	0.42
1:G:191:GLU:H	1:G:334:ASP:HA	1.84	0.42
1:G:215:LEU:HB3	1:G:246:PRO:HG2	2.02	0.42
1:H:82:ASN:HA	1:H:89:THR:HG22	2.02	0.42
1:H:227:ILE:H	1:H:254:VAL:HG22	1.85	0.42
1:I:295:LEU:HD13	1:I:335:GLY:HA3	2.02	0.42
1:K:27:VAL:CG1	1:K:90:THR:HG23	2.47	0.42
1:L:82:ASN:HA	1:L:89:THR:HG22	2.02	0.42
1:L:183:LEU:HA	1:L:382:GLY:HA3	2.01	0.42
1:L:209:GLU:H	1:L:209:GLU:CD	2.23	0.42
1:M:82:ASN:HA	1:M:89:THR:HG22	2.02	0.42
1:N:239:ALA:CB	1:N:314:LEU:HB3	2.49	0.42
1:N:301:ILE:HG23	1:N:307:MET:HB2	2.01	0.42
1:N:406:ALA:HB1	1:N:411:VAL:CG1	2.49	0.42
1:N:446:ALA:O	1:N:450:PRO:HD2	2.20	0.42
1:C:177:VAL:HA	1:C:379:ILE:O	2.19	0.42
1:C:271:VAL:O	1:C:273:VAL:HG23	2.20	0.42
1:F:215:LEU:HB3	1:F:246:PRO:HG2	2.02	0.42
1:F:270:ILE:O	1:F:271:VAL:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:LYS:HD3	1:F:304:GLU:HA	2.01	0.42
1:G:165:ALA:HB2	1:G:187:LEU:HD13	2.02	0.42
1:H:225:LYS:CA	1:H:303:GLU:HB2	2.50	0.42
1:H:239:ALA:CB	1:H:314:LEU:HB3	2.49	0.42
1:H:446:ALA:O	1:H:450:PRO:HD2	2.20	0.42
1:I:82:ASN:HA	1:I:89:THR:HG22	2.02	0.42
1:I:406:ALA:HB1	1:I:411:VAL:CG1	2.50	0.42
1:I:406:ALA:HB1	1:I:411:VAL:HG12	2.02	0.42
1:J:82:ASN:HA	1:J:89:THR:HG22	2.02	0.42
1:J:295:LEU:HD13	1:J:335:GLY:HA3	2.02	0.42
1:K:222:LEU:CD2	1:K:250:ILE:HD12	2.49	0.42
1:L:100:ILE:HD11	1:L:514:MET:HE3	2.01	0.42
1:L:214:GLU:CD	1:L:322:ARG:HE	2.22	0.42
1:L:282:GLY:O	1:L:285:ARG:HB3	2.19	0.42
1:M:8:PHE:HA	1:M:9:GLY:HA3	1.82	0.42
1:M:77:VAL:HG22	1:M:510:VAL:CB	2.49	0.42
1:N:151:SER:HB3	1:N:399:ALA:HA	1.99	0.42
1:N:206:ASN:O	1:N:208:PRO:N	2.52	0.42
1:B:177:VAL:HA	1:B:379:ILE:O	2.19	0.42
1:C:270:ILE:O	1:C:271:VAL:HB	2.20	0.42
1:E:52:ASP:HB3	1:E:55:SER:H	1.83	0.42
1:F:271:VAL:O	1:F:273:VAL:HG23	2.20	0.42
1:H:227:ILE:HG22	1:H:262:LEU:HD21	2.02	0.42
1:H:298:GLY:CA	1:H:318:GLY:HA3	2.49	0.42
1:I:149:THR:HG22	1:I:154:SER:HB3	2.02	0.42
1:J:227:ILE:HG22	1:J:262:LEU:HD21	2.02	0.42
1:K:82:ASN:HA	1:K:89:THR:HG22	2.02	0.42
1:K:150:ILE:HD12	1:K:494:LEU:H	1.85	0.42
1:L:239:ALA:CB	1:L:314:LEU:HB3	2.49	0.42
1:M:240:VAL:HB	1:M:247:LEU:HD22	2.02	0.42
1:N:82:ASN:HA	1:N:89:THR:HG22	2.02	0.42
1:N:406:ALA:HB1	1:N:411:VAL:HG12	2.02	0.42
1:A:165:ALA:HB2	1:A:187:LEU:HD13	2.02	0.42
1:B:215:LEU:HB3	1:B:246:PRO:HG2	2.02	0.42
1:D:286:LYS:HD3	1:D:304:GLU:HA	2.01	0.42
1:E:190:VAL:HB	1:E:334:ASP:HB2	2.01	0.42
1:G:270:ILE:O	1:G:271:VAL:HB	2.20	0.42
1:H:77:VAL:HG22	1:H:510:VAL:CB	2.49	0.42
1:H:99:ILE:CG2	1:H:120:ILE:HD13	2.49	0.42
1:H:149:THR:HG22	1:H:154:SER:HB3	2.02	0.42
1:I:227:ILE:HG22	1:I:262:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:240:VAL:HB	1:J:247:LEU:HD22	2.02	0.42
1:K:100:ILE:HD11	1:K:514:MET:HE3	2.02	0.42
1:K:227:ILE:H	1:K:254:VAL:HG22	1.85	0.42
1:K:227:ILE:HG22	1:K:262:LEU:HD21	2.02	0.42
1:K:242:LYS:HG3	1:L:257:GLU:C	2.40	0.42
1:K:309:LEU:HD23	1:K:309:LEU:HA	1.81	0.42
1:L:37:ASN:HB2	1:M:516:THR:O	2.20	0.42
1:L:190:VAL:HG23	1:L:191:GLU:O	2.20	0.42
1:M:153:ASN:N	1:M:154:SER:CA	2.82	0.42
1:M:301:ILE:HG23	1:M:307:MET:HB2	2.01	0.42
1:M:417:VAL:HG11	1:M:477:GLY:HA3	2.02	0.42
1:N:204:PHE:CA	1:N:207:LYS:HE2	2.50	0.42
1:N:227:ILE:HG22	1:N:262:LEU:HD21	2.02	0.42
1:B:200:LEU:HD11	1:B:254:VAL:CA	2.12	0.41
1:C:513:LEU:O	1:D:49:ILE:HD13	2.19	0.41
1:E:150:ILE:HD11	1:E:493:ILE:HG23	1.97	0.41
1:E:215:LEU:HB3	1:E:246:PRO:HG2	2.02	0.41
1:F:165:ALA:HB2	1:F:187:LEU:CD1	2.50	0.41
1:F:200:LEU:HD11	1:F:254:VAL:CG2	2.20	0.41
1:H:37:ASN:HB2	1:I:516:THR:O	2.20	0.41
1:I:161:LEU:HD22	1:I:379:ILE:HG23	2.02	0.41
1:J:182:GLY:HA2	1:J:183:LEU:HA	1.63	0.41
1:K:298:GLY:CA	1:K:318:GLY:HA3	2.50	0.41
1:L:161:LEU:HD22	1:L:379:ILE:HG23	2.02	0.41
1:M:31:LEU:HB3	1:M:90:THR:HG21	2.03	0.41
1:M:214:GLU:CD	1:M:322:ARG:HE	2.22	0.41
1:N:214:GLU:CD	1:N:322:ARG:HE	2.22	0.41
1:A:193:MET:CE	1:A:292:ILE:HG23	2.51	0.41
1:C:200:LEU:HD13	1:C:259:LEU:HB2	2.00	0.41
1:F:144:ILE:CG2	1:F:163:ALA:HA	2.49	0.41
1:G:286:LYS:HD3	1:G:304:GLU:HA	2.01	0.41
1:I:240:VAL:HB	1:I:247:LEU:HD22	2.02	0.41
1:L:417:VAL:HG11	1:L:477:GLY:HA3	2.02	0.41
1:A:270:ILE:O	1:A:271:VAL:HB	2.20	0.41
1:A:278:ALA:HB2	1:A:289:LEU:HG	2.02	0.41
1:A:286:LYS:HD3	1:A:304:GLU:HA	2.01	0.41
1:B:190:VAL:HB	1:B:334:ASP:HB2	2.01	0.41
1:B:270:ILE:O	1:B:271:VAL:HB	2.20	0.41
1:C:254:VAL:HG12	1:C:259:LEU:HB2	2.03	0.41
1:C:381:VAL:CG2	1:C:393:LYS:N	2.77	0.41
1:D:193:MET:CE	1:D:292:ILE:HG23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:MET:CE	1:E:292:ILE:HG23	2.50	0.41
1:E:286:LYS:HD3	1:E:304:GLU:HA	2.01	0.41
1:F:209:GLU:H	1:F:209:GLU:CD	2.24	0.41
1:H:182:GLY:HA2	1:H:382:GLY:HA2	2.02	0.41
1:H:242:LYS:HA	1:H:243:ALA:HA	1.16	0.41
1:I:239:ALA:CB	1:I:314:LEU:HB3	2.49	0.41
1:I:417:VAL:HG11	1:I:477:GLY:HA3	2.02	0.41
1:J:233:MET:CE	1:J:249:ILE:HD11	2.40	0.41
1:J:301:ILE:HG23	1:J:307:MET:HB2	2.01	0.41
1:K:161:LEU:HD22	1:K:379:ILE:HG23	2.02	0.41
1:K:225:LYS:CA	1:K:303:GLU:HB2	2.50	0.41
1:L:31:LEU:HB3	1:L:90:THR:HG21	2.03	0.41
1:L:227:ILE:H	1:L:254:VAL:HG22	1.85	0.41
1:M:150:ILE:HD12	1:M:494:LEU:H	1.85	0.41
1:M:295:LEU:HD23	1:M:342:ILE:CD1	2.46	0.41
1:N:417:VAL:HG11	1:N:477:GLY:HA3	2.02	0.41
1:B:193:MET:CE	1:B:292:ILE:HG23	2.51	0.41
1:B:220:ILE:CD1	1:B:296:THR:HG21	2.47	0.41
1:E:165:ALA:HB2	1:E:187:LEU:HD13	2.02	0.41
1:E:278:ALA:HB2	1:E:289:LEU:HG	2.01	0.41
1:F:254:VAL:HG12	1:F:259:LEU:HB2	2.03	0.41
1:G:278:ALA:HB2	1:G:289:LEU:HG	2.01	0.41
1:H:161:LEU:HD22	1:H:379:ILE:HG23	2.02	0.41
1:H:417:VAL:HG11	1:H:477:GLY:HA3	2.03	0.41
1:J:161:LEU:HD22	1:J:379:ILE:HG23	2.02	0.41
1:J:225:LYS:CA	1:J:303:GLU:HB2	2.50	0.41
1:L:446:ALA:O	1:L:450:PRO:HD2	2.20	0.41
1:M:100:ILE:HD11	1:M:514:MET:HE3	2.02	0.41
1:M:161:LEU:HD22	1:M:379:ILE:HG23	2.03	0.41
1:M:278:ALA:HA	1:M:279:PRO:HD3	1.87	0.41
1:N:150:ILE:HD12	1:N:494:LEU:H	1.85	0.41
1:C:250:ILE:HD13	1:C:292:ILE:HG21	2.02	0.41
1:D:215:LEU:HB3	1:D:246:PRO:HG2	2.02	0.41
1:D:254:VAL:HG12	1:D:259:LEU:HB2	2.03	0.41
1:E:197:ARG:HG3	1:E:198:GLY:O	2.20	0.41
1:E:254:VAL:HG12	1:E:259:LEU:HB2	2.03	0.41
1:F:278:ALA:HA	1:F:279:PRO:HD3	1.72	0.41
1:I:31:LEU:HB3	1:I:90:THR:HG21	2.02	0.41
1:I:193:MET:HG2	1:I:372:LEU:HA	2.02	0.41
1:K:518:GLU:CB	1:K:519:CYS:N	2.74	0.41
1:N:77:VAL:HG22	1:N:510:VAL:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:171:LYS:HE3	1:N:408:GLU:OE1	2.21	0.41
1:N:240:VAL:HB	1:N:247:LEU:HD22	2.02	0.41
1:A:34:LYS:NZ	1:A:483:GLU:OE2	2.52	0.41
1:B:271:VAL:O	1:B:273:VAL:HG23	2.20	0.41
1:C:223:ALA:HB3	1:C:251:ALA:CA	2.51	0.41
1:D:223:ALA:HB3	1:D:251:ALA:CA	2.51	0.41
1:D:249:ILE:HD11	1:D:262:LEU:HD22	1.87	0.41
1:F:278:ALA:HB2	1:F:289:LEU:HG	2.01	0.41
1:G:271:VAL:O	1:G:273:VAL:HG23	2.20	0.41
1:H:301:ILE:HG23	1:H:307:MET:HB2	2.01	0.41
1:H:309:LEU:HA	1:H:309:LEU:HD23	1.81	0.41
1:I:150:ILE:HD12	1:I:494:LEU:H	1.85	0.41
1:I:446:ALA:O	1:I:450:PRO:HD2	2.20	0.41
1:J:149:THR:HG22	1:J:154:SER:HB3	2.02	0.41
1:K:240:VAL:HB	1:K:247:LEU:HD22	2.02	0.41
1:L:240:VAL:HB	1:L:247:LEU:HD22	2.02	0.41
1:L:301:ILE:HG23	1:L:307:MET:HB2	2.01	0.41
1:M:193:MET:HG2	1:M:372:LEU:HA	2.02	0.41
1:A:73:MET:HG2	1:B:46:ALA:CB	2.51	0.41
1:A:209:GLU:H	1:A:209:GLU:CD	2.24	0.41
1:B:165:ALA:HB2	1:B:187:LEU:HD13	2.02	0.41
1:B:254:VAL:HG12	1:B:259:LEU:HB2	2.03	0.41
1:C:165:ALA:HB2	1:C:187:LEU:HD13	2.02	0.41
1:C:215:LEU:HB3	1:C:246:PRO:HG2	2.02	0.41
1:D:250:ILE:HD13	1:D:292:ILE:HG21	2.02	0.41
1:E:197:ARG:HD3	1:E:197:ARG:HA	2.02	0.41
1:H:233:MET:CE	1:H:249:ILE:HD11	2.42	0.41
1:H:516:THR:O	1:N:37:ASN:HB2	2.20	0.41
1:I:8:PHE:HA	1:I:9:GLY:HA3	1.81	0.41
1:J:31:LEU:HB3	1:J:90:THR:HG21	2.03	0.41
1:J:227:ILE:H	1:J:254:VAL:HG22	1.85	0.41
1:J:446:ALA:O	1:J:450:PRO:HD2	2.20	0.41
1:K:31:LEU:HB3	1:K:90:THR:HG21	2.03	0.41
1:L:321:LYS:HZ3	1:L:334:ASP:CG	2.23	0.41
1:M:37:ASN:HB2	1:N:516:THR:O	2.20	0.41
1:N:149:THR:HG22	1:N:154:SER:HB3	2.02	0.41
1:N:227:ILE:H	1:N:254:VAL:HG22	1.85	0.41
1:A:46:ALA:CB	1:G:73:MET:HG2	2.51	0.41
1:B:236:VAL:CG1	1:B:317:LEU:HD13	2.51	0.41
1:D:165:ALA:HB2	1:D:187:LEU:HD13	2.02	0.41
1:F:236:VAL:CG1	1:F:317:LEU:HD13	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:MET:SD	1:G:295:LEU:CB	3.09	0.41
1:G:236:VAL:CG1	1:G:317:LEU:HD13	2.51	0.41
1:H:225:LYS:HA	1:H:303:GLU:HB2	2.02	0.41
1:J:417:VAL:HG11	1:J:477:GLY:HA3	2.02	0.41
1:M:242:LYS:C	1:N:257:GLU:CA	2.78	0.41
1:M:309:LEU:HD23	1:M:309:LEU:HA	1.81	0.41
1:N:225:LYS:CA	1:N:303:GLU:HB2	2.50	0.41
1:A:250:ILE:HD13	1:A:292:ILE:HG21	2.02	0.41
1:B:144:ILE:HG23	1:B:403:THR:HG23	2.03	0.41
1:B:250:ILE:HD13	1:B:292:ILE:HG21	2.02	0.41
1:C:190:VAL:HB	1:C:334:ASP:HB2	2.01	0.41
1:C:271:VAL:HG12	1:C:273:VAL:HG22	2.02	0.41
1:D:73:MET:HG2	1:E:46:ALA:CB	2.51	0.41
1:D:190:VAL:CG2	1:D:333:ILE:CG2	2.98	0.41
1:D:236:VAL:CG1	1:D:317:LEU:HD13	2.51	0.41
1:E:236:VAL:CG1	1:E:317:LEU:HD13	2.51	0.41
1:E:250:ILE:HD13	1:E:292:ILE:HG21	2.02	0.41
2:E:1525:PO4:P	4:E:1527:ATP:O3G	2.79	0.41
1:G:254:VAL:HG12	1:G:259:LEU:HB2	2.03	0.41
1:H:150:ILE:HD12	1:H:494:LEU:H	1.85	0.41
1:H:240:VAL:HB	1:H:247:LEU:HD22	2.02	0.41
1:I:100:ILE:HD11	1:I:514:MET:HE3	2.03	0.41
1:I:225:LYS:HA	1:I:303:GLU:HB2	2.03	0.41
1:J:150:ILE:HD12	1:J:494:LEU:H	1.85	0.41
1:K:207:LYS:HB3	1:K:208:PRO:HD3	2.03	0.41
1:K:225:LYS:HA	1:K:303:GLU:HB2	2.02	0.41
1:K:239:ALA:CB	1:K:314:LEU:HB3	2.51	0.41
1:K:278:ALA:HB3	1:K:285:ARG:HG2	2.02	0.41
1:K:417:VAL:HG11	1:K:477:GLY:HA3	2.03	0.41
1:L:149:THR:HG22	1:L:154:SER:HB3	2.02	0.41
1:L:193:MET:HG2	1:L:372:LEU:HA	2.02	0.41
1:L:223:ALA:HB2	1:L:309:LEU:HD11	2.03	0.41
1:M:149:THR:HG22	1:M:154:SER:HB3	2.02	0.41
1:M:209:GLU:H	1:M:209:GLU:CD	2.24	0.41
1:N:27:VAL:CG1	1:N:90:THR:HG23	2.47	0.41
1:N:31:LEU:HB3	1:N:90:THR:HG21	2.03	0.41
1:N:38:VAL:HG21	1:N:56:VAL:HG22	2.03	0.41
1:N:161:LEU:HD22	1:N:379:ILE:HG23	2.03	0.41
1:N:242:LYS:HA	1:N:243:ALA:HA	1.12	0.41
1:A:236:VAL:CG1	1:A:317:LEU:HD13	2.51	0.41
1:A:311:LYS:O	1:A:313:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:MET:HG2	1:F:46:ALA:CB	2.51	0.41
1:F:193:MET:CE	1:F:292:ILE:HG23	2.50	0.41
1:F:250:ILE:HD13	1:F:292:ILE:HG21	2.02	0.41
1:G:250:ILE:HD13	1:G:292:ILE:HG21	2.02	0.41
1:K:356:ALA:HB2	1:K:365:LEU:HD12	2.03	0.41
1:L:405:ALA:HB1	1:L:498:LYS:CD	2.51	0.41
1:M:182:GLY:HA2	1:M:183:LEU:HA	1.63	0.41
1:M:239:ALA:CB	1:M:314:LEU:HB3	2.50	0.41
1:A:254:VAL:HG12	1:A:259:LEU:HB2	2.03	0.40
1:C:236:VAL:CG1	1:C:317:LEU:HD13	2.51	0.40
1:F:73:MET:HG2	1:G:46:ALA:CB	2.51	0.40
1:F:311:LYS:O	1:F:313:THR:HG23	2.21	0.40
1:G:200:LEU:HD13	1:G:254:VAL:CG1	2.44	0.40
1:G:311:LYS:O	1:G:313:THR:HG23	2.21	0.40
1:H:38:VAL:HG21	1:H:56:VAL:HG22	2.04	0.40
1:H:50:THR:HG22	1:H:52:ASP:O	2.21	0.40
1:I:50:THR:HG22	1:I:52:ASP:O	2.21	0.40
1:I:225:LYS:CA	1:I:303:GLU:HB2	2.50	0.40
1:M:38:VAL:HG21	1:M:56:VAL:HG22	2.03	0.40
1:N:338:GLU:O	1:N:342:ILE:HG13	2.22	0.40
1:N:356:ALA:HB2	1:N:365:LEU:HD12	2.04	0.40
1:B:73:MET:HG2	1:C:46:ALA:CB	2.51	0.40
1:D:201:SER:HA	1:D:202:PRO:HD3	1.98	0.40
1:D:203:TYR:N	1:D:203:TYR:CD1	2.90	0.40
1:D:311:LYS:O	1:D:313:THR:HG23	2.21	0.40
1:E:225:LYS:HB2	1:E:307:MET:O	2.22	0.40
1:G:225:LYS:HB2	1:G:307:MET:O	2.22	0.40
1:J:493:ILE:HD13	4:J:1527:ATP:C6	2.57	0.40
1:M:206:ASN:HB3	1:M:208:PRO:HD2	2.03	0.40
1:M:223:ALA:HB2	1:M:309:LEU:HD11	2.03	0.40
1:M:356:ALA:HB2	1:M:365:LEU:HD12	2.04	0.40
1:A:271:VAL:O	1:A:273:VAL:HG23	2.20	0.40
1:B:223:ALA:HB3	1:B:251:ALA:CA	2.51	0.40
1:C:194:GLN:HG3	1:C:329:THR:HG21	2.03	0.40
2:C:1525:PO4:P	4:C:1527:ATP:O3G	2.79	0.40
1:F:223:ALA:HB3	1:F:251:ALA:CA	2.51	0.40
1:J:193:MET:HG2	1:J:372:LEU:HA	2.02	0.40
1:J:207:LYS:HE2	1:J:207:LYS:HA	2.04	0.40
1:J:209:GLU:CD	1:J:209:GLU:H	2.25	0.40
1:K:149:THR:HG22	1:K:154:SER:HB3	2.02	0.40
1:K:338:GLU:O	1:K:342:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:446:ALA:O	1:K:450:PRO:HD2	2.20	0.40
1:M:80:LYS:HD3	1:M:80:LYS:HA	1.98	0.40
1:A:223:ALA:HB3	1:A:251:ALA:CA	2.51	0.40
1:C:203:TYR:N	1:C:203:TYR:CD1	2.90	0.40
1:C:311:LYS:O	1:C:313:THR:HG23	2.21	0.40
1:D:223:ALA:HB1	1:D:227:ILE:HG12	2.03	0.40
1:E:311:LYS:O	1:E:313:THR:HG23	2.21	0.40
1:H:356:ALA:HB2	1:H:365:LEU:HD12	2.04	0.40
1:J:356:ALA:HB2	1:J:365:LEU:HD12	2.04	0.40
1:K:62:LEU:HD23	1:K:62:LEU:HA	2.02	0.40
1:L:150:ILE:HD12	1:L:494:LEU:H	1.85	0.40
1:L:338:GLU:O	1:L:342:ILE:HG13	2.22	0.40
1:C:201:SER:HA	1:C:202:PRO:HD3	1.84	0.40
1:C:252:GLU:HA	1:C:289:LEU:CD1	2.52	0.40
1:D:225:LYS:HB2	1:D:307:MET:O	2.22	0.40
1:E:203:TYR:N	1:E:203:TYR:CD1	2.90	0.40
1:E:223:ALA:HB1	1:E:227:ILE:HG12	2.03	0.40
1:F:225:LYS:HB2	1:F:307:MET:O	2.22	0.40
1:H:169:VAL:HB	1:H:173:GLY:CA	2.51	0.40
1:H:338:GLU:O	1:H:342:ILE:HG13	2.22	0.40
1:H:405:ALA:HB1	1:H:498:LYS:CD	2.51	0.40
1:J:38:VAL:HG21	1:J:56:VAL:HG22	2.04	0.40
1:J:278:ALA:HA	1:J:279:PRO:HD3	1.86	0.40
1:K:161:LEU:HD21	1:K:185:ASP:HB3	2.03	0.40
1:K:213:VAL:CG1	1:K:325:ILE:HG12	2.51	0.40
1:K:405:ALA:HB1	1:K:498:LYS:CD	2.52	0.40
1:L:493:ILE:HD13	4:L:1527:ATP:C6	2.57	0.40
1:M:206:ASN:HB2	1:M:213:VAL:HG23	2.02	0.40
1:M:227:ILE:H	1:M:254:VAL:HG22	1.85	0.40
1:M:242:LYS:HA	1:M:243:ALA:HA	1.13	0.40
1:M:493:ILE:HD13	4:M:1527:ATP:C6	2.57	0.40
1:N:493:ILE:HD13	4:N:1527:ATP:C6	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/548 (95%)	498 (95%)	21 (4%)	3 (1%)	25	66
1	B	522/548 (95%)	497 (95%)	23 (4%)	2 (0%)	34	72
1	C	522/548 (95%)	497 (95%)	22 (4%)	3 (1%)	25	66
1	D	522/548 (95%)	497 (95%)	22 (4%)	3 (1%)	25	66
1	E	522/548 (95%)	497 (95%)	21 (4%)	4 (1%)	19	60
1	F	522/548 (95%)	497 (95%)	21 (4%)	4 (1%)	19	60
1	G	522/548 (95%)	495 (95%)	24 (5%)	3 (1%)	25	66
1	H	522/548 (95%)	516 (99%)	6 (1%)	0	100	100
1	I	522/548 (95%)	516 (99%)	6 (1%)	0	100	100
1	J	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	K	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	L	522/548 (95%)	513 (98%)	9 (2%)	0	100	100
1	M	522/548 (95%)	515 (99%)	7 (1%)	0	100	100
1	N	522/548 (95%)	515 (99%)	5 (1%)	2 (0%)	34	72
All	All	7308/7672 (95%)	7087 (97%)	197 (3%)	24 (0%)	44	77

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	199	TYR
1	N	207	LYS
1	N	208	PRO
1	A	384	ALA
1	B	384	ALA
1	C	199	TYR
1	C	384	ALA
1	D	384	ALA
1	E	199	TYR
1	E	384	ALA
1	F	199	TYR
1	F	384	ALA
1	G	384	ALA
1	A	271	VAL
1	B	271	VAL

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Mol	Chain	Res	Type
1	C	271	VAL
1	D	208	PRO
1	D	271	VAL
1	E	271	VAL
1	F	271	VAL
1	G	271	VAL
1	A	199	TYR
1	E	208	PRO
1	F	208	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	402/414 (97%)	367 (91%)	35 (9%)	10 31
1	B	402/414 (97%)	366 (91%)	36 (9%)	9 30
1	C	402/414 (97%)	367 (91%)	35 (9%)	10 31
1	D	402/414 (97%)	369 (92%)	33 (8%)	11 34
1	E	402/414 (97%)	368 (92%)	34 (8%)	10 33
1	F	402/414 (97%)	367 (91%)	35 (9%)	10 31
1	G	402/414 (97%)	367 (91%)	35 (9%)	10 31
1	H	402/414 (97%)	359 (89%)	43 (11%)	6 23
1	I	402/414 (97%)	361 (90%)	41 (10%)	7 25
1	J	402/414 (97%)	361 (90%)	41 (10%)	7 25
1	K	402/414 (97%)	358 (89%)	44 (11%)	6 23
1	L	402/414 (97%)	364 (90%)	38 (10%)	8 27
1	M	402/414 (97%)	358 (89%)	44 (11%)	6 23
1	N	402/414 (97%)	360 (90%)	42 (10%)	7 24
All	All	5628/5796 (97%)	5092 (90%)	536 (10%)	12 27

All (536) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	18	ARG
1	A	25	ASP
1	A	34	LYS
1	A	36	ARG
1	A	37	ASN
1	A	171	LYS
1	A	172	GLU
1	A	177	VAL
1	A	183	LEU
1	A	190	VAL
1	A	196	ASP
1	A	197	ARG
1	A	199	TYR
1	A	207	LYS
1	A	213	VAL
1	A	226	LYS
1	A	242	LYS
1	A	252	GLU
1	A	272	LYS
1	A	295	LEU
1	A	300	VAL
1	A	309	LEU
1	A	311	LYS
1	A	316	ASP
1	A	325	ILE
1	A	326	ASN
1	A	327	LYS
1	A	334	ASP
1	A	404	ARG
1	A	428	ASP
1	A	435	ASP
1	A	453	GLN
1	A	484	GLU
1	A	522	THR
1	B	10	ASN
1	B	18	ARG
1	B	25	ASP
1	B	34	LYS
1	B	36	ARG
1	B	37	ASN
1	B	171	LYS
1	B	172	GLU

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Mol	Chain	Res	Type
1	B	177	VAL
1	B	183	LEU
1	B	190	VAL
1	B	195	PHE
1	B	197	ARG
1	B	199	TYR
1	B	207	LYS
1	B	210	THR
1	B	213	VAL
1	B	226	LYS
1	B	242	LYS
1	B	252	GLU
1	B	272	LYS
1	B	295	LEU
1	B	300	VAL
1	B	309	LEU
1	B	311	LYS
1	B	316	ASP
1	B	325	ILE
1	B	326	ASN
1	B	327	LYS
1	B	334	ASP
1	B	404	ARG
1	B	428	ASP
1	B	435	ASP
1	B	453	GLN
1	B	484	GLU
1	B	522	THR
1	C	10	ASN
1	C	18	ARG
1	C	25	ASP
1	C	34	LYS
1	C	36	ARG
1	C	37	ASN
1	C	171	LYS
1	C	172	GLU
1	C	177	VAL
1	C	183	LEU
1	C	190	VAL
1	C	193	MET
1	C	197	ARG
1	C	199	TYR

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Mol	Chain	Res	Type
1	C	207	LYS
1	C	213	VAL
1	C	226	LYS
1	C	242	LYS
1	C	252	GLU
1	C	272	LYS
1	C	295	LEU
1	C	300	VAL
1	C	309	LEU
1	C	311	LYS
1	C	316	ASP
1	C	325	ILE
1	C	326	ASN
1	C	327	LYS
1	C	334	ASP
1	C	404	ARG
1	C	428	ASP
1	C	435	ASP
1	C	453	GLN
1	C	484	GLU
1	C	522	THR
1	D	10	ASN
1	D	18	ARG
1	D	25	ASP
1	D	34	LYS
1	D	36	ARG
1	D	37	ASN
1	D	153	ASN
1	D	171	LYS
1	D	172	GLU
1	D	177	VAL
1	D	183	LEU
1	D	190	VAL
1	D	197	ARG
1	D	213	VAL
1	D	226	LYS
1	D	242	LYS
1	D	252	GLU
1	D	272	LYS
1	D	295	LEU
1	D	300	VAL
1	D	309	LEU

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Mol	Chain	Res	Type
1	D	311	LYS
1	D	316	ASP
1	D	325	ILE
1	D	326	ASN
1	D	327	LYS
1	D	334	ASP
1	D	404	ARG
1	D	428	ASP
1	D	435	ASP
1	D	453	GLN
1	D	484	GLU
1	D	522	THR
1	E	10	ASN
1	E	18	ARG
1	E	25	ASP
1	E	34	LYS
1	E	36	ARG
1	E	37	ASN
1	E	171	LYS
1	E	172	GLU
1	E	177	VAL
1	E	183	LEU
1	E	190	VAL
1	E	197	ARG
1	E	199	TYR
1	E	207	LYS
1	E	213	VAL
1	E	226	LYS
1	E	242	LYS
1	E	252	GLU
1	E	272	LYS
1	E	295	LEU
1	E	300	VAL
1	E	309	LEU
1	E	311	LYS
1	E	316	ASP
1	E	325	ILE
1	E	326	ASN
1	E	327	LYS
1	E	334	ASP
1	E	404	ARG
1	E	428	ASP

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Mol	Chain	Res	Type
1	E	435	ASP
1	E	453	GLN
1	E	484	GLU
1	E	522	THR
1	F	10	ASN
1	F	18	ARG
1	F	25	ASP
1	F	34	LYS
1	F	36	ARG
1	F	37	ASN
1	F	153	ASN
1	F	171	LYS
1	F	172	GLU
1	F	177	VAL
1	F	183	LEU
1	F	190	VAL
1	F	197	ARG
1	F	199	TYR
1	F	207	LYS
1	F	213	VAL
1	F	226	LYS
1	F	242	LYS
1	F	252	GLU
1	F	272	LYS
1	F	295	LEU
1	F	300	VAL
1	F	309	LEU
1	F	311	LYS
1	F	316	ASP
1	F	325	ILE
1	F	326	ASN
1	F	327	LYS
1	F	334	ASP
1	F	404	ARG
1	F	428	ASP
1	F	435	ASP
1	F	453	GLN
1	F	484	GLU
1	F	522	THR
1	G	10	ASN
1	G	18	ARG
1	G	25	ASP

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Mol	Chain	Res	Type
1	G	34	LYS
1	G	36	ARG
1	G	37	ASN
1	G	171	LYS
1	G	172	GLU
1	G	177	VAL
1	G	183	LEU
1	G	190	VAL
1	G	197	ARG
1	G	199	TYR
1	G	201	SER
1	G	207	LYS
1	G	213	VAL
1	G	226	LYS
1	G	242	LYS
1	G	252	GLU
1	G	272	LYS
1	G	295	LEU
1	G	300	VAL
1	G	309	LEU
1	G	311	LYS
1	G	316	ASP
1	G	325	ILE
1	G	326	ASN
1	G	327	LYS
1	G	334	ASP
1	G	404	ARG
1	G	428	ASP
1	G	435	ASP
1	G	453	GLN
1	G	484	GLU
1	G	522	THR
1	H	18	ARG
1	H	31	LEU
1	H	36	ARG
1	H	37	ASN
1	H	48	THR
1	H	54	VAL
1	H	63	GLU
1	H	155	ASP
1	H	166	MET
1	H	183	LEU

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Mol	Chain	Res	Type
1	H	188	ASP
1	H	191	GLU
1	H	193	MET
1	H	195	PHE
1	H	197	ARG
1	H	207	LYS
1	H	213	VAL
1	H	225	LYS
1	H	226	LYS
1	H	229	ASN
1	H	231	ARG
1	H	236	VAL
1	H	238	GLU
1	H	253	ASP
1	H	257	GLU
1	H	272	LYS
1	H	289	LEU
1	H	290	GLN
1	H	321	LYS
1	H	325	ILE
1	H	343	GLN
1	H	358	SER
1	H	389	MET
1	H	391	GLU
1	H	404	ARG
1	H	408	GLU
1	H	430	ARG
1	H	435	ASP
1	H	453	GLN
1	H	460	GLU
1	H	484	GLU
1	H	518	GLU
1	H	523	ASP
1	I	18	ARG
1	I	31	LEU
1	I	36	ARG
1	I	37	ASN
1	I	48	THR
1	I	54	VAL
1	I	63	GLU
1	I	155	ASP
1	I	166	MET

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Mol	Chain	Res	Type
1	I	188	ASP
1	I	191	GLU
1	I	193	MET
1	I	195	PHE
1	I	196	ASP
1	I	197	ARG
1	I	199	TYR
1	I	207	LYS
1	I	213	VAL
1	I	225	LYS
1	I	226	LYS
1	I	236	VAL
1	I	238	GLU
1	I	253	ASP
1	I	257	GLU
1	I	272	LYS
1	I	289	LEU
1	I	321	LYS
1	I	325	ILE
1	I	343	GLN
1	I	358	SER
1	I	389	MET
1	I	391	GLU
1	I	404	ARG
1	I	408	GLU
1	I	430	ARG
1	I	435	ASP
1	I	453	GLN
1	I	460	GLU
1	I	484	GLU
1	I	518	GLU
1	I	523	ASP
1	J	18	ARG
1	J	31	LEU
1	J	36	ARG
1	J	37	ASN
1	J	48	THR
1	J	54	VAL
1	J	63	GLU
1	J	155	ASP
1	J	166	MET
1	J	188	ASP

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Mol	Chain	Res	Type
1	J	191	GLU
1	J	193	MET
1	J	195	PHE
1	J	197	ARG
1	J	199	TYR
1	J	207	LYS
1	J	213	VAL
1	J	225	LYS
1	J	226	LYS
1	J	229	ASN
1	J	236	VAL
1	J	238	GLU
1	J	253	ASP
1	J	257	GLU
1	J	272	LYS
1	J	289	LEU
1	J	321	LYS
1	J	325	ILE
1	J	343	GLN
1	J	358	SER
1	J	389	MET
1	J	391	GLU
1	J	404	ARG
1	J	408	GLU
1	J	430	ARG
1	J	435	ASP
1	J	453	GLN
1	J	460	GLU
1	J	484	GLU
1	J	518	GLU
1	J	523	ASP
1	K	18	ARG
1	K	31	LEU
1	K	36	ARG
1	K	37	ASN
1	K	48	THR
1	K	54	VAL
1	K	63	GLU
1	K	155	ASP
1	K	166	MET
1	K	185	ASP
1	K	188	ASP

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Mol	Chain	Res	Type
1	K	191	GLU
1	K	193	MET
1	K	195	PHE
1	K	197	ARG
1	K	199	TYR
1	K	207	LYS
1	K	213	VAL
1	K	225	LYS
1	K	226	LYS
1	K	229	ASN
1	K	231	ARG
1	K	236	VAL
1	K	238	GLU
1	K	253	ASP
1	K	257	GLU
1	K	272	LYS
1	K	289	LEU
1	K	290	GLN
1	K	321	LYS
1	K	325	ILE
1	K	343	GLN
1	K	358	SER
1	K	389	MET
1	K	391	GLU
1	K	404	ARG
1	K	408	GLU
1	K	430	ARG
1	K	435	ASP
1	K	453	GLN
1	K	460	GLU
1	K	484	GLU
1	K	518	GLU
1	K	523	ASP
1	L	18	ARG
1	L	31	LEU
1	L	36	ARG
1	L	37	ASN
1	L	48	THR
1	L	54	VAL
1	L	63	GLU
1	L	155	ASP
1	L	166	MET

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Mol	Chain	Res	Type
1	L	174	VAL
1	L	188	ASP
1	L	193	MET
1	L	195	PHE
1	L	197	ARG
1	L	199	TYR
1	L	207	LYS
1	L	213	VAL
1	L	225	LYS
1	L	226	LYS
1	L	236	VAL
1	L	253	ASP
1	L	272	LYS
1	L	289	LEU
1	L	321	LYS
1	L	325	ILE
1	L	343	GLN
1	L	358	SER
1	L	389	MET
1	L	391	GLU
1	L	404	ARG
1	L	408	GLU
1	L	430	ARG
1	L	435	ASP
1	L	453	GLN
1	L	460	GLU
1	L	484	GLU
1	L	518	GLU
1	L	523	ASP
1	M	18	ARG
1	M	31	LEU
1	M	36	ARG
1	M	37	ASN
1	M	48	THR
1	M	54	VAL
1	M	63	GLU
1	M	155	ASP
1	M	166	MET
1	M	172	GLU
1	M	188	ASP
1	M	191	GLU
1	M	193	MET

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Mol	Chain	Res	Type
1	M	195	PHE
1	M	197	ARG
1	M	199	TYR
1	M	207	LYS
1	M	213	VAL
1	M	225	LYS
1	M	226	LYS
1	M	228	SER
1	M	229	ASN
1	M	231	ARG
1	M	232	GLU
1	M	236	VAL
1	M	253	ASP
1	M	257	GLU
1	M	272	LYS
1	M	289	LEU
1	M	321	LYS
1	M	325	ILE
1	M	343	GLN
1	M	358	SER
1	M	389	MET
1	M	391	GLU
1	M	404	ARG
1	M	408	GLU
1	M	430	ARG
1	M	435	ASP
1	M	453	GLN
1	M	460	GLU
1	M	484	GLU
1	M	518	GLU
1	M	523	ASP
1	N	18	ARG
1	N	31	LEU
1	N	36	ARG
1	N	37	ASN
1	N	48	THR
1	N	54	VAL
1	N	63	GLU
1	N	155	ASP
1	N	166	MET
1	N	171	LYS
1	N	188	ASP

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Mol	Chain	Res	Type
1	N	191	GLU
1	N	193	MET
1	N	195	PHE
1	N	197	ARG
1	N	199	TYR
1	N	207	LYS
1	N	213	VAL
1	N	225	LYS
1	N	226	LYS
1	N	231	ARG
1	N	236	VAL
1	N	238	GLU
1	N	253	ASP
1	N	257	GLU
1	N	272	LYS
1	N	289	LEU
1	N	321	LYS
1	N	325	ILE
1	N	343	GLN
1	N	358	SER
1	N	389	MET
1	N	391	GLU
1	N	404	ARG
1	N	408	GLU
1	N	430	ARG
1	N	435	ASP
1	N	453	GLN
1	N	460	GLU
1	N	484	GLU
1	N	518	GLU
1	N	523	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	475	ASN
1	B	351	GLN
1	B	475	ASN
1	C	351	GLN
1	C	475	ASN
1	D	351	GLN
1	D	475	ASN

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Mol	Chain	Res	Type
1	E	475	ASN
1	F	475	ASN
1	G	351	GLN
1	G	475	ASN
1	H	401	HIS
1	I	401	HIS
1	J	401	HIS
1	K	401	HIS
1	L	401	HIS
1	M	401	HIS
1	N	401	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 42 ligands modelled in this entry, 14 are modelled with single atom and 14 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ATP	D	1527	3	26,33,33	0.70	0	31,52,52	1.56	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ATP	B	1527	3	26,33,33	0.71	0	31,52,52	1.59	4 (12%)
4	ATP	M	1527	3	26,33,33	0.82	0	31,52,52	1.60	4 (12%)
4	ATP	F	1527	3	26,33,33	0.70	0	31,52,52	1.56	4 (12%)
4	ATP	I	1527	3	26,33,33	0.82	0	31,52,52	1.60	4 (12%)
4	ATP	N	1527	3	26,33,33	0.83	1 (3%)	31,52,52	1.60	4 (12%)
4	ATP	L	1527	3	26,33,33	0.82	1 (3%)	31,52,52	1.60	4 (12%)
4	ATP	J	1527	3	26,33,33	0.82	0	31,52,52	1.60	4 (12%)
4	ATP	A	1527	3	26,33,33	0.74	0	31,52,52	1.69	3 (9%)
4	ATP	H	1527	3	26,33,33	0.82	0	31,52,52	1.60	4 (12%)
4	ATP	C	1527	3	26,33,33	0.74	0	31,52,52	1.69	3 (9%)
4	ATP	K	1527	3	26,33,33	0.82	1 (3%)	31,52,52	1.60	4 (12%)
4	ATP	G	1527	3	26,33,33	0.74	0	31,52,52	1.69	3 (9%)
4	ATP	E	1527	3	26,33,33	0.74	0	31,52,52	1.69	3 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	D	1527	3	-	5/18/38/38	0/3/3/3
4	ATP	B	1527	3	-	5/18/38/38	0/3/3/3
4	ATP	M	1527	3	-	1/18/38/38	0/3/3/3
4	ATP	F	1527	3	-	5/18/38/38	0/3/3/3
4	ATP	I	1527	3	-	1/18/38/38	0/3/3/3
4	ATP	N	1527	3	-	1/18/38/38	0/3/3/3
4	ATP	L	1527	3	-	1/18/38/38	0/3/3/3
4	ATP	J	1527	3	-	1/18/38/38	0/3/3/3
4	ATP	A	1527	3	-	3/18/38/38	0/3/3/3
4	ATP	H	1527	3	-	1/18/38/38	0/3/3/3
4	ATP	C	1527	3	-	3/18/38/38	0/3/3/3
4	ATP	K	1527	3	-	1/18/38/38	0/3/3/3
4	ATP	G	1527	3	-	3/18/38/38	0/3/3/3
4	ATP	E	1527	3	-	3/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	1527	ATP	C2'-C1'	-2.05	1.50	1.53
4	L	1527	ATP	C2'-C1'	-2.01	1.50	1.53
4	K	1527	ATP	C2'-C1'	-2.00	1.50	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1527	ATP	PB-O3B-PG	-5.80	112.94	132.83
4	C	1527	ATP	PB-O3B-PG	-5.79	112.95	132.83
4	A	1527	ATP	PB-O3B-PG	-5.79	112.96	132.83
4	G	1527	ATP	PB-O3B-PG	-5.79	112.96	132.83
4	M	1527	ATP	PA-O3A-PB	-5.42	114.23	132.83
4	H	1527	ATP	PA-O3A-PB	-5.41	114.25	132.83
4	I	1527	ATP	PA-O3A-PB	-5.41	114.25	132.83
4	K	1527	ATP	PA-O3A-PB	-5.41	114.26	132.83
4	J	1527	ATP	PA-O3A-PB	-5.40	114.28	132.83
4	L	1527	ATP	PA-O3A-PB	-5.40	114.29	132.83
4	N	1527	ATP	PA-O3A-PB	-5.40	114.30	132.83
4	B	1527	ATP	PB-O3B-PG	-5.17	115.09	132.83
4	F	1527	ATP	PB-O3B-PG	-5.06	115.47	132.83
4	D	1527	ATP	PB-O3B-PG	-5.06	115.48	132.83
4	A	1527	ATP	PA-O3A-PB	-4.96	115.80	132.83
4	E	1527	ATP	PA-O3A-PB	-4.96	115.80	132.83
4	G	1527	ATP	PA-O3A-PB	-4.96	115.81	132.83
4	C	1527	ATP	PA-O3A-PB	-4.95	115.83	132.83
4	B	1527	ATP	PA-O3A-PB	-4.95	115.85	132.83
4	D	1527	ATP	PA-O3A-PB	-4.65	116.87	132.83
4	F	1527	ATP	PA-O3A-PB	-4.64	116.92	132.83
4	H	1527	ATP	PB-O3B-PG	-4.28	118.13	132.83
4	L	1527	ATP	PB-O3B-PG	-4.28	118.14	132.83
4	K	1527	ATP	PB-O3B-PG	-4.28	118.15	132.83
4	N	1527	ATP	PB-O3B-PG	-4.27	118.16	132.83
4	M	1527	ATP	PB-O3B-PG	-4.27	118.16	132.83
4	J	1527	ATP	PB-O3B-PG	-4.27	118.17	132.83
4	I	1527	ATP	PB-O3B-PG	-4.27	118.17	132.83
4	F	1527	ATP	C5-C6-N6	2.53	124.20	120.35
4	D	1527	ATP	C5-C6-N6	2.50	124.15	120.35
4	J	1527	ATP	C5-C6-N6	2.48	124.12	120.35
4	K	1527	ATP	C5-C6-N6	2.48	124.11	120.35
4	N	1527	ATP	C5-C6-N6	2.46	124.09	120.35
4	L	1527	ATP	C5-C6-N6	2.46	124.08	120.35
4	H	1527	ATP	C5-C6-N6	2.45	124.07	120.35
4	I	1527	ATP	C5-C6-N6	2.45	124.07	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	1527	ATP	C5-C6-N6	2.44	124.06	120.35
4	B	1527	ATP	C5-C6-N6	2.42	124.02	120.35
4	C	1527	ATP	C5-C6-N6	2.28	123.82	120.35
4	A	1527	ATP	C5-C6-N6	2.27	123.81	120.35
4	E	1527	ATP	C5-C6-N6	2.26	123.79	120.35
4	G	1527	ATP	C5-C6-N6	2.25	123.77	120.35
4	F	1527	ATP	O5'-C5'-C4'	2.17	116.48	108.99
4	H	1527	ATP	O3G-PG-O2G	2.17	115.93	107.64
4	L	1527	ATP	O3G-PG-O2G	2.17	115.93	107.64
4	D	1527	ATP	O5'-C5'-C4'	2.17	116.45	108.99
4	I	1527	ATP	O3G-PG-O2G	2.17	115.92	107.64
4	N	1527	ATP	O3G-PG-O2G	2.17	115.91	107.64
4	M	1527	ATP	O3G-PG-O2G	2.16	115.91	107.64
4	K	1527	ATP	O3G-PG-O2G	2.16	115.90	107.64
4	J	1527	ATP	O3G-PG-O2G	2.16	115.89	107.64
4	B	1527	ATP	O5'-C5'-C4'	2.15	116.39	108.99

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1527	ATP	C3'-C4'-C5'-O5'
4	B	1527	ATP	C5'-O5'-PA-O3A
4	C	1527	ATP	C3'-C4'-C5'-O5'
4	D	1527	ATP	C5'-O5'-PA-O3A
4	E	1527	ATP	C3'-C4'-C5'-O5'
4	F	1527	ATP	C5'-O5'-PA-O3A
4	G	1527	ATP	C3'-C4'-C5'-O5'
4	A	1527	ATP	O4'-C4'-C5'-O5'
4	C	1527	ATP	O4'-C4'-C5'-O5'
4	E	1527	ATP	O4'-C4'-C5'-O5'
4	G	1527	ATP	O4'-C4'-C5'-O5'
4	H	1527	ATP	C4'-C5'-O5'-PA
4	I	1527	ATP	C4'-C5'-O5'-PA
4	J	1527	ATP	C4'-C5'-O5'-PA
4	K	1527	ATP	C4'-C5'-O5'-PA
4	L	1527	ATP	C4'-C5'-O5'-PA
4	M	1527	ATP	C4'-C5'-O5'-PA
4	N	1527	ATP	C4'-C5'-O5'-PA
4	B	1527	ATP	C5'-O5'-PA-O1A
4	B	1527	ATP	C5'-O5'-PA-O2A
4	D	1527	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	D	1527	ATP	C5'-O5'-PA-O2A
4	F	1527	ATP	C5'-O5'-PA-O1A
4	F	1527	ATP	C5'-O5'-PA-O2A
4	B	1527	ATP	PG-O3B-PB-O1B
4	A	1527	ATP	PB-O3A-PA-O1A
4	B	1527	ATP	PG-O3B-PB-O2B
4	C	1527	ATP	PB-O3A-PA-O1A
4	D	1527	ATP	PG-O3B-PB-O1B
4	D	1527	ATP	PG-O3B-PB-O2B
4	E	1527	ATP	PB-O3A-PA-O1A
4	F	1527	ATP	PG-O3B-PB-O1B
4	F	1527	ATP	PG-O3B-PB-O2B
4	G	1527	ATP	PB-O3A-PA-O1A

There are no ring outliers.

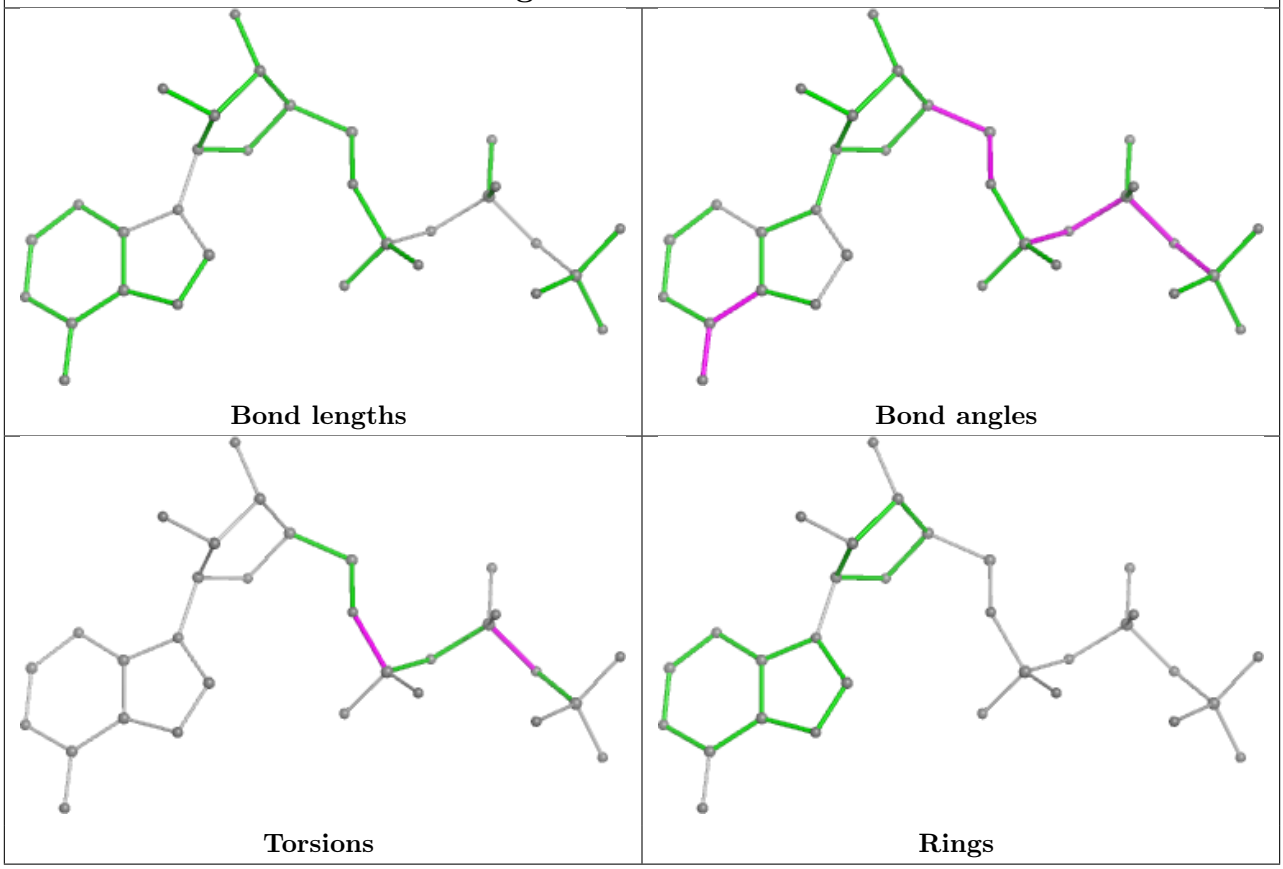
14 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1527	ATP	2	0
4	B	1527	ATP	2	0
4	M	1527	ATP	5	0
4	F	1527	ATP	2	0
4	I	1527	ATP	4	0
4	N	1527	ATP	5	0
4	L	1527	ATP	5	0
4	J	1527	ATP	5	0
4	A	1527	ATP	2	0
4	H	1527	ATP	4	0
4	C	1527	ATP	3	0
4	K	1527	ATP	4	0
4	G	1527	ATP	2	0
4	E	1527	ATP	3	0

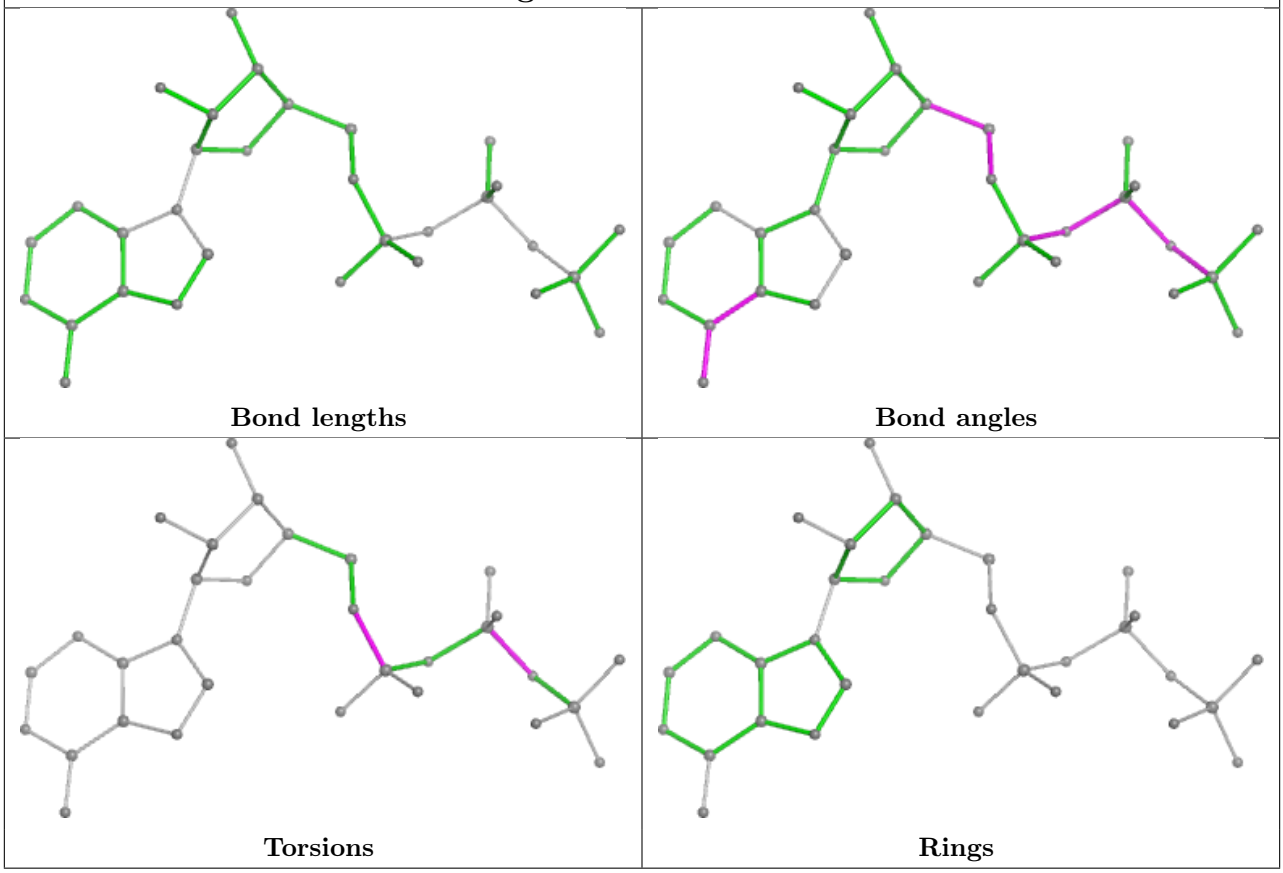
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

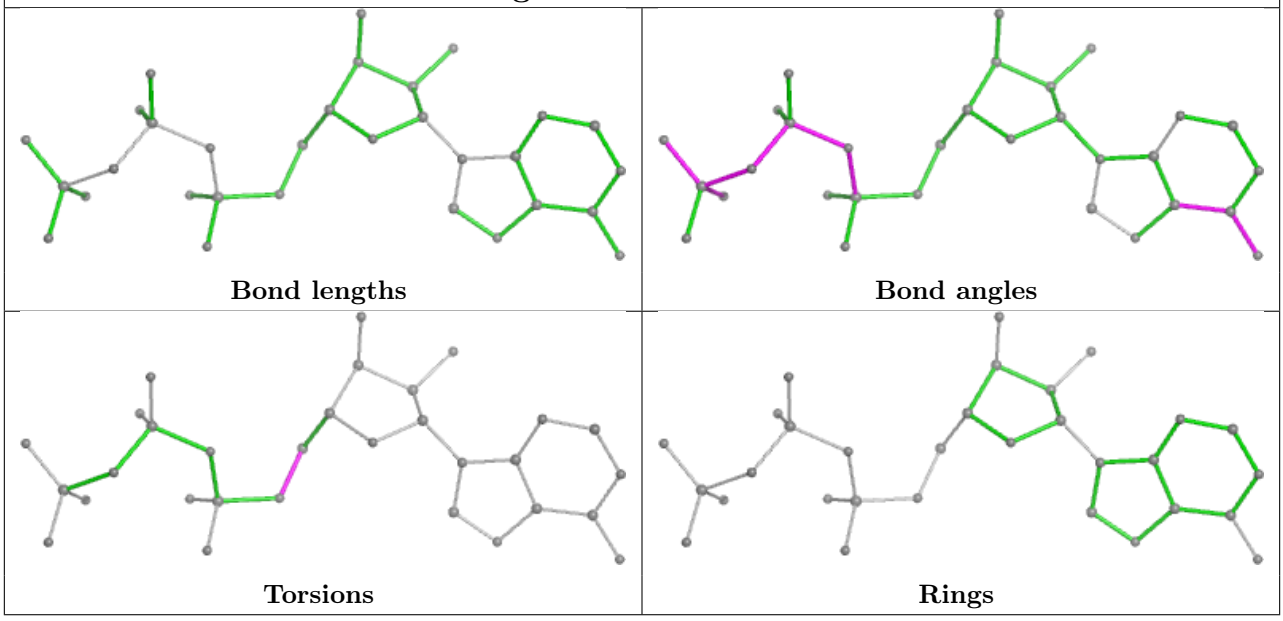
Ligand ATP D 1527



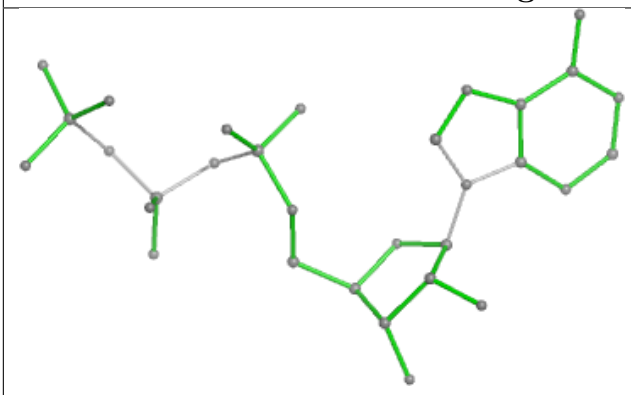
Ligand ATP B 1527



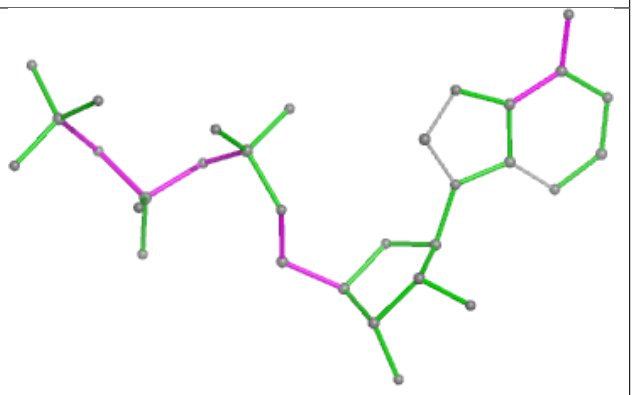
Ligand ATP M 1527



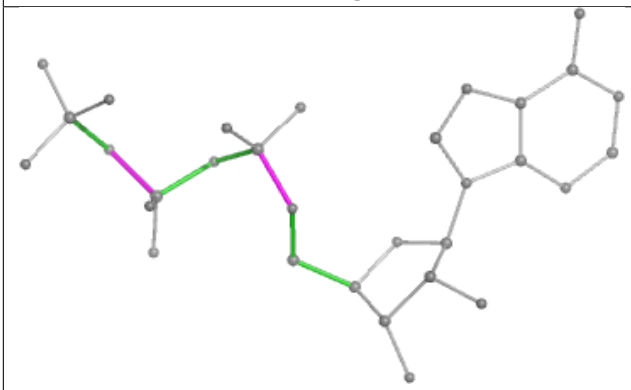
Ligand ATP F 1527



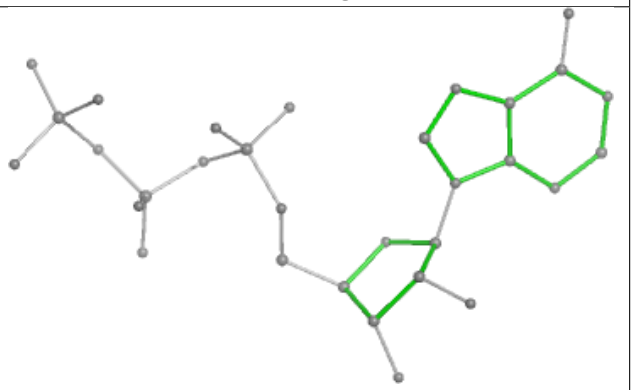
Bond lengths



Bond angles

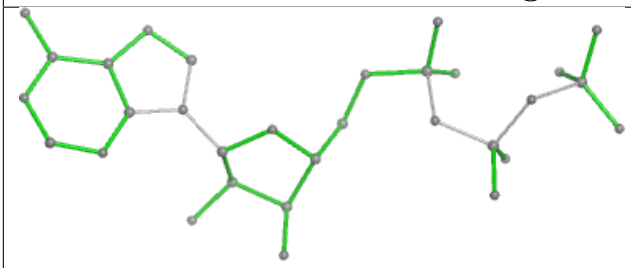


Torsions

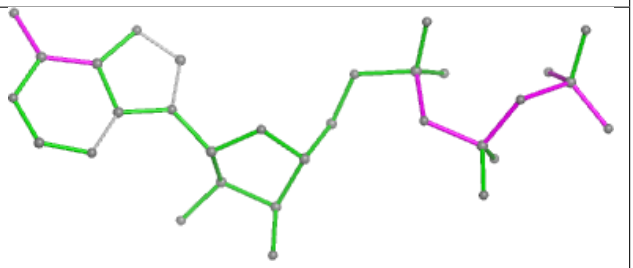


Rings

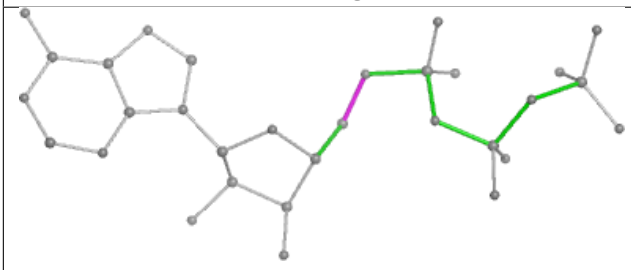
Ligand ATP I 1527



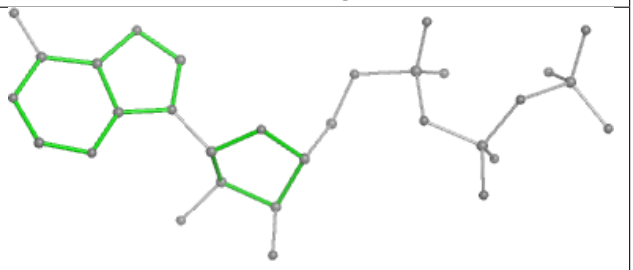
Bond lengths



Bond angles

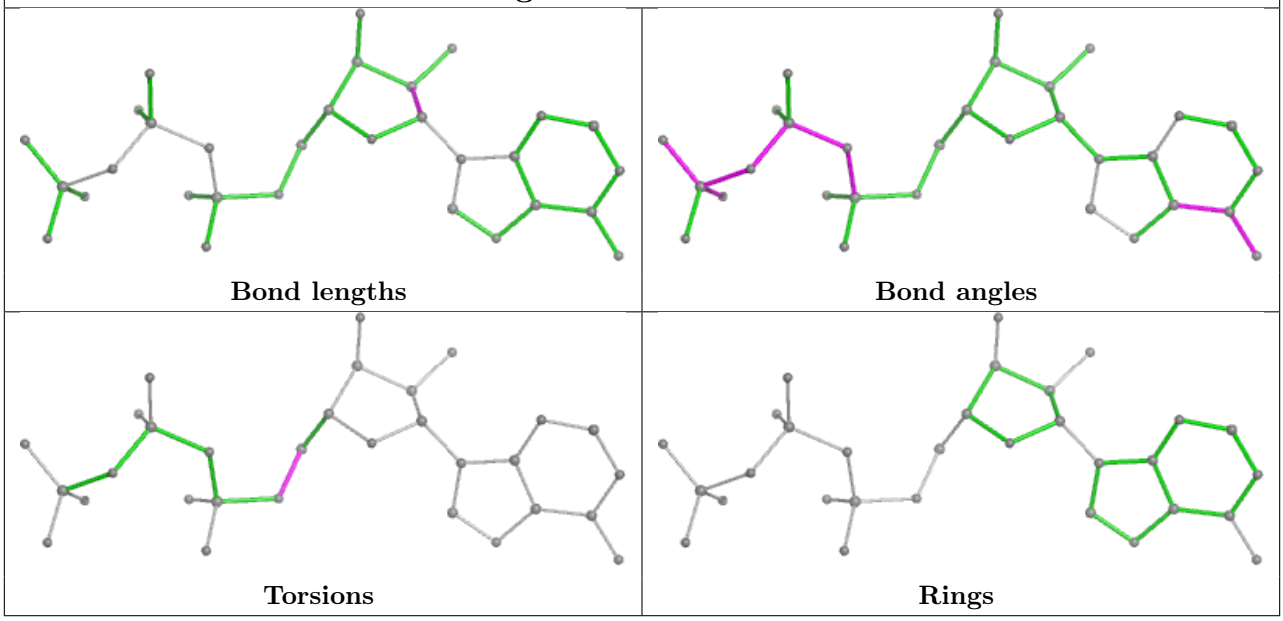


Torsions

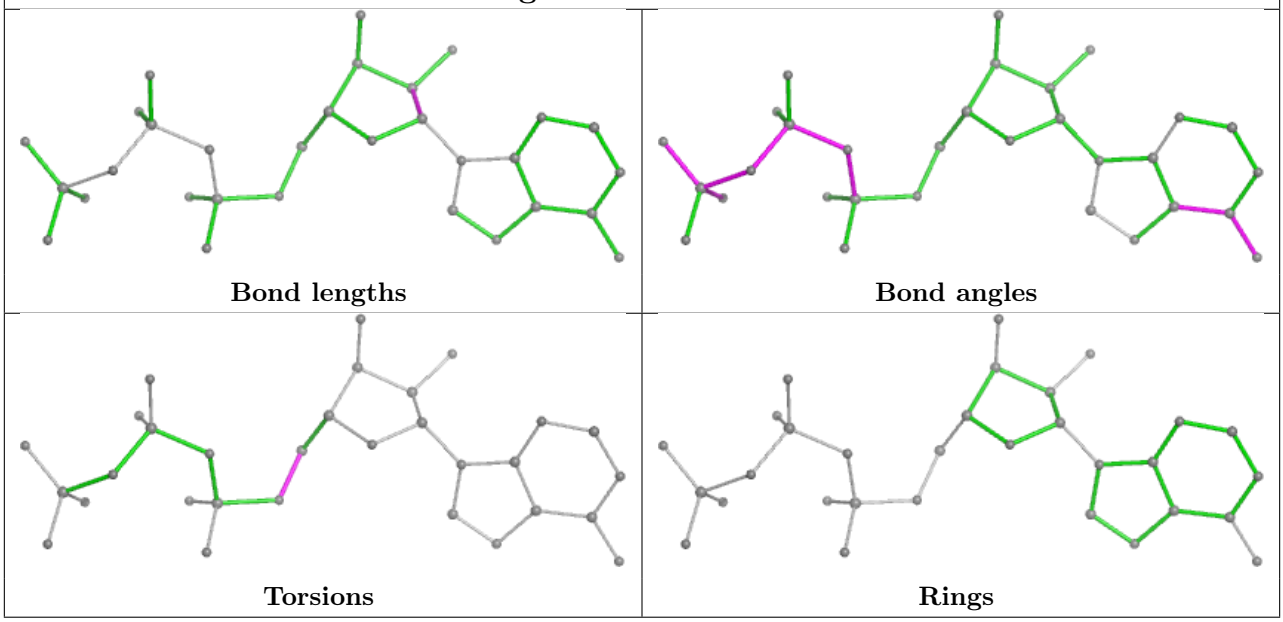


Rings

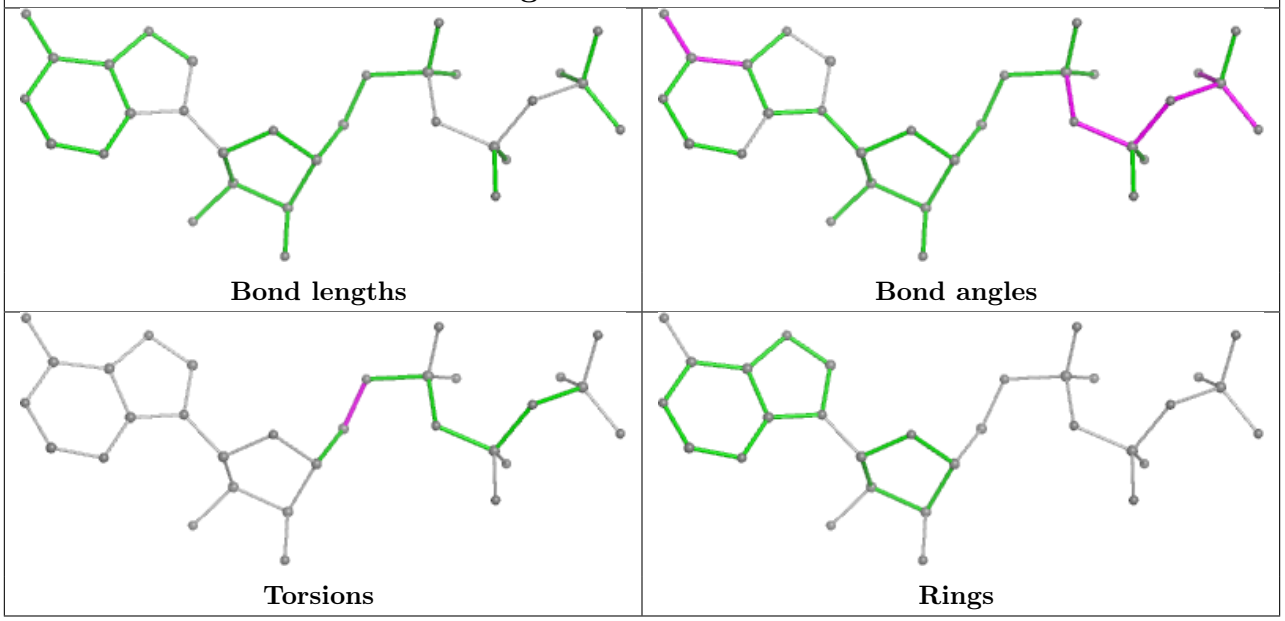
Ligand ATP N 1527



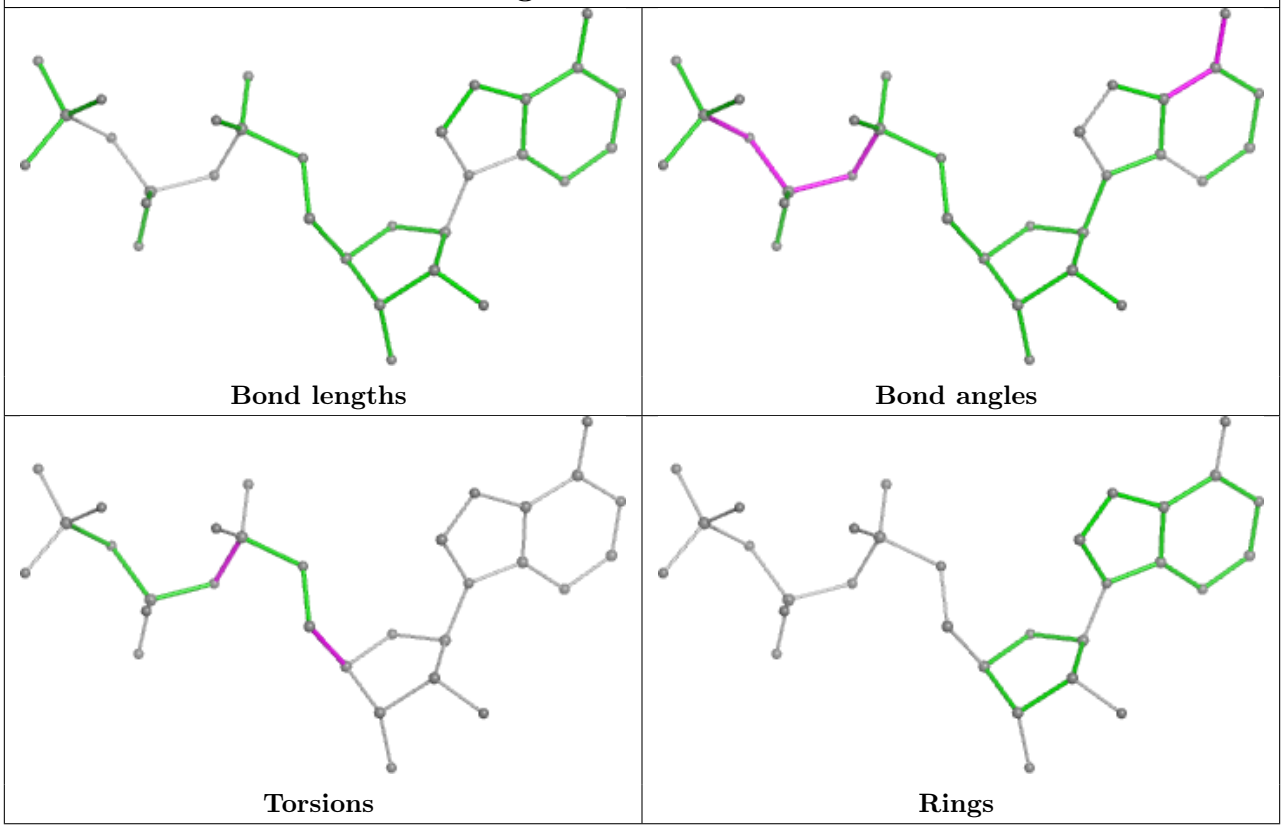
Ligand ATP L 1527



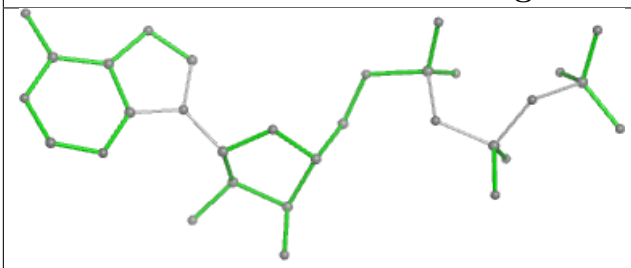
Ligand ATP J 1527



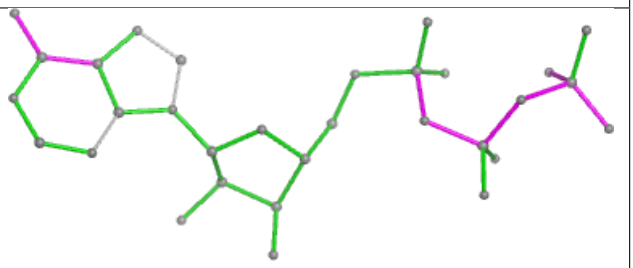
Ligand ATP A 1527



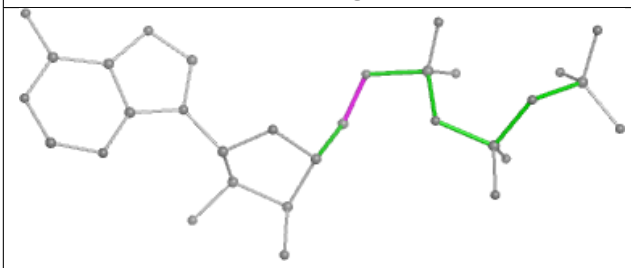
Ligand ATP H 1527



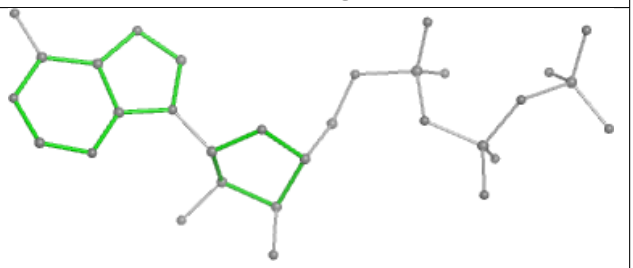
Bond lengths



Bond angles

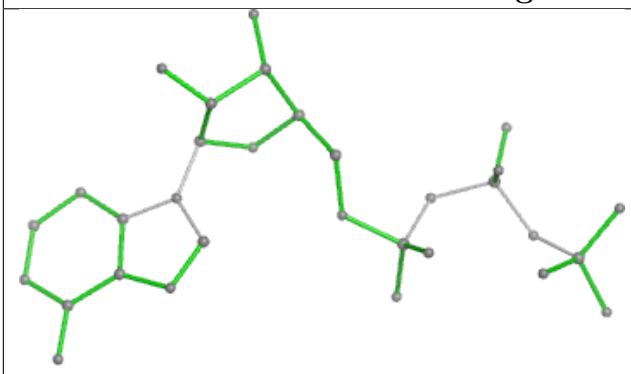


Torsions

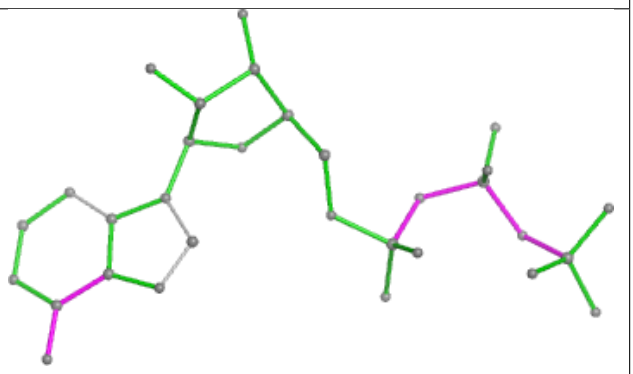


Rings

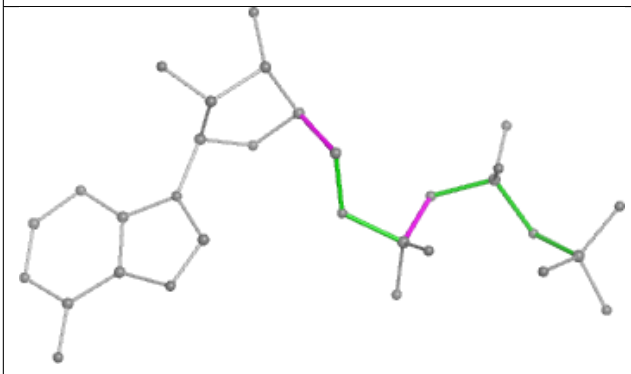
Ligand ATP C 1527



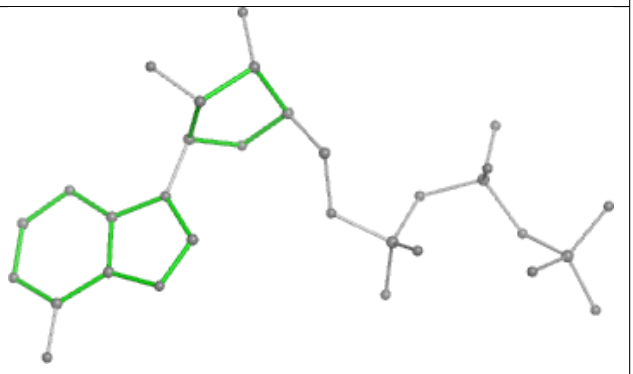
Bond lengths



Bond angles

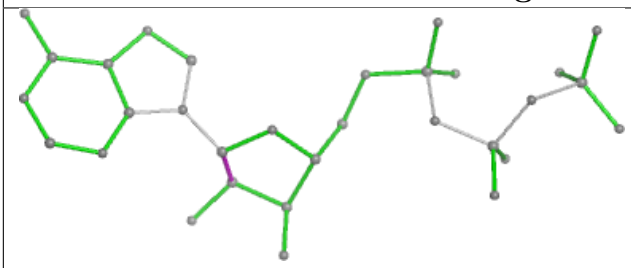


Torsions

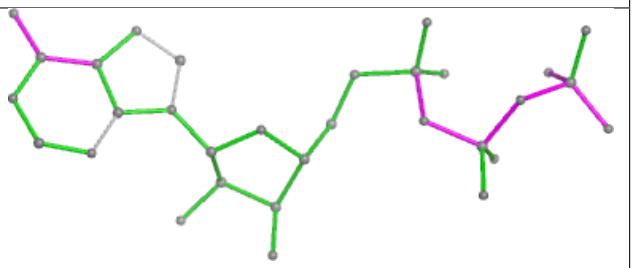


Rings

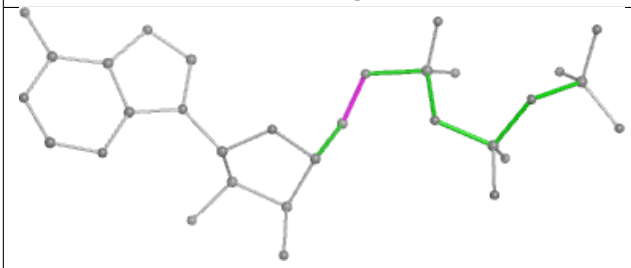
Ligand ATP K 1527



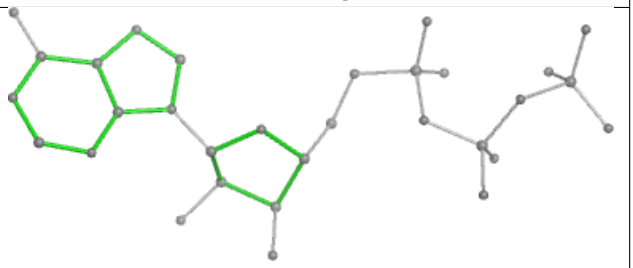
Bond lengths



Bond angles

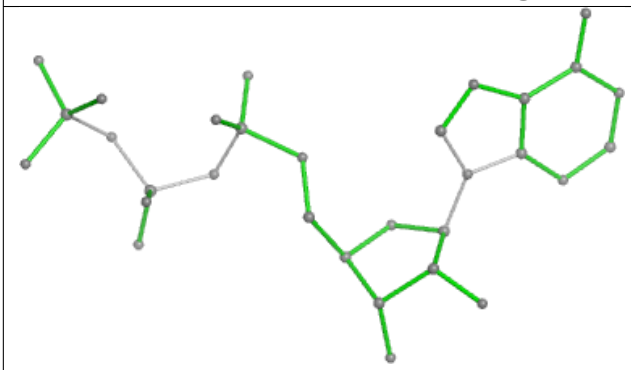


Torsions

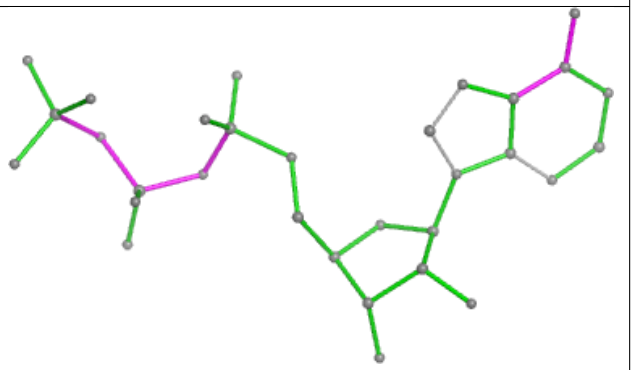


Rings

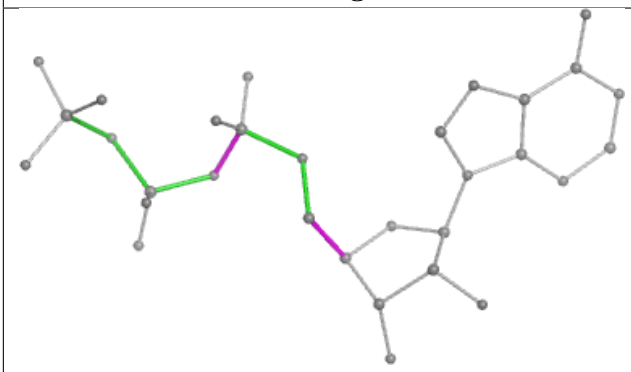
Ligand ATP G 1527



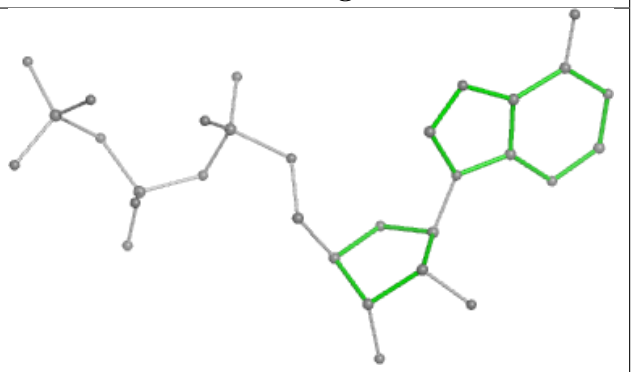
Bond lengths



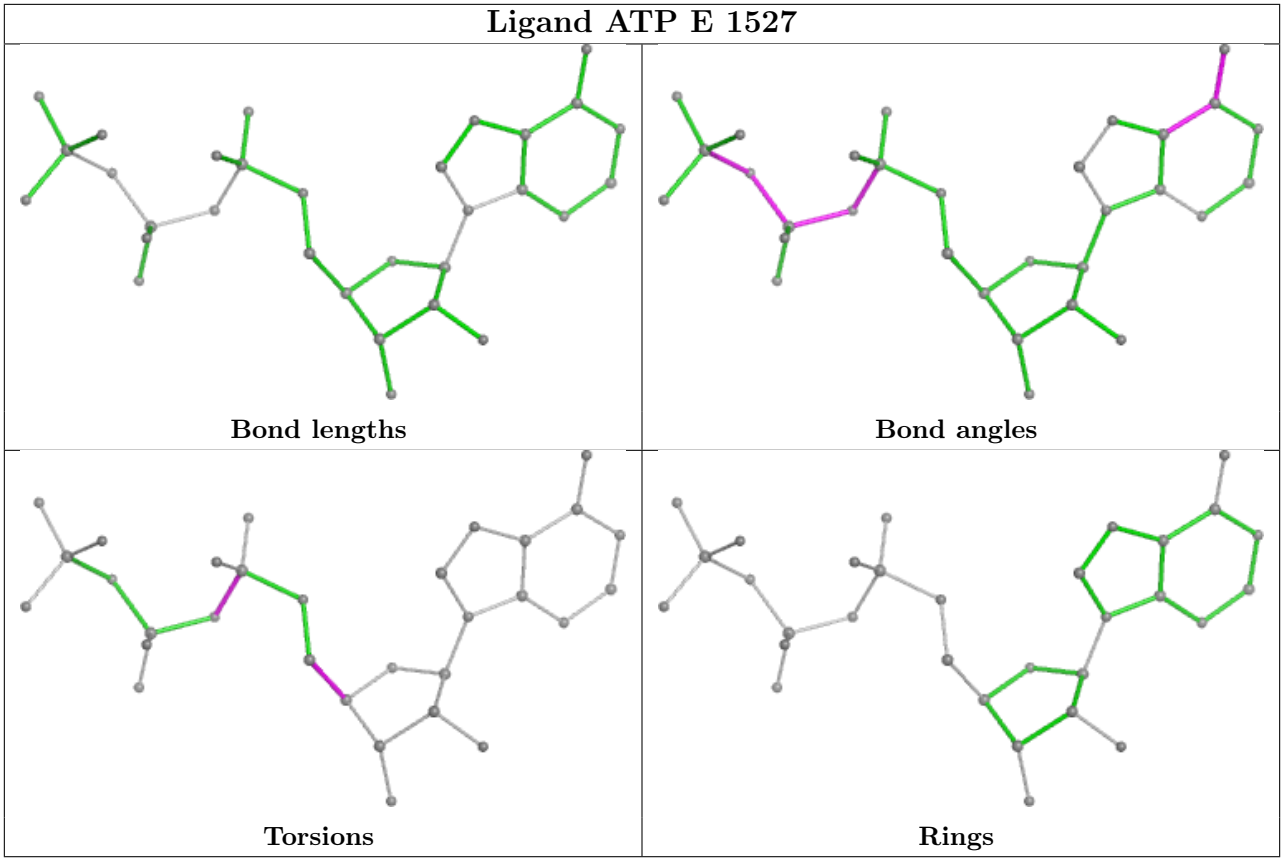
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	5
1	C	5
1	D	5
1	E	5
1	F	5
1	G	5
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	52:ASP	C	53:GLY	N	1.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	52:ASP	C	53:GLY	N	1.20
1	C	52:ASP	C	53:GLY	N	1.20
1	D	52:ASP	C	53:GLY	N	1.20
1	E	52:ASP	C	53:GLY	N	1.20
1	F	52:ASP	C	53:GLY	N	1.20
1	G	52:ASP	C	53:GLY	N	1.20
1	A	518:GLU	C	519:CYS	N	1.19
1	B	518:GLU	C	519:CYS	N	1.19
1	C	518:GLU	C	519:CYS	N	1.19
1	D	513:LEU	C	514:MET	N	1.19
1	D	518:GLU	C	519:CYS	N	1.19
1	E	518:GLU	C	519:CYS	N	1.19
1	F	518:GLU	C	519:CYS	N	1.19
1	G	518:GLU	C	519:CYS	N	1.19
1	A	513:LEU	C	514:MET	N	1.18
1	B	513:LEU	C	514:MET	N	1.18
1	C	513:LEU	C	514:MET	N	1.18
1	E	513:LEU	C	514:MET	N	1.18
1	F	513:LEU	C	514:MET	N	1.18
1	G	513:LEU	C	514:MET	N	1.18
1	B	213:VAL	C	214:GLU	N	1.08
1	C	213:VAL	C	214:GLU	N	1.08
1	D	213:VAL	C	214:GLU	N	1.08
1	E	213:VAL	C	214:GLU	N	1.08
1	F	213:VAL	C	214:GLU	N	1.08
1	G	213:VAL	C	214:GLU	N	1.08
1	A	7:LYS	C	8:PHE	N	1.07
1	B	7:LYS	C	8:PHE	N	1.07
1	C	7:LYS	C	8:PHE	N	1.07
1	D	7:LYS	C	8:PHE	N	1.07
1	E	7:LYS	C	8:PHE	N	1.07
1	F	7:LYS	C	8:PHE	N	1.07
1	G	7:LYS	C	8:PHE	N	1.07

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2003. These allow visual inspection of the internal detail of the map and identification of artifacts.

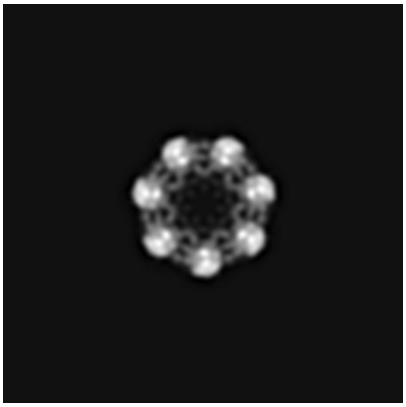
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map

X

Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 96

Y Index: 96

Z Index: 96

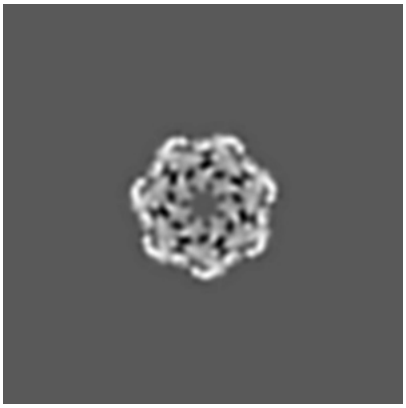
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 119

Y Index: 76

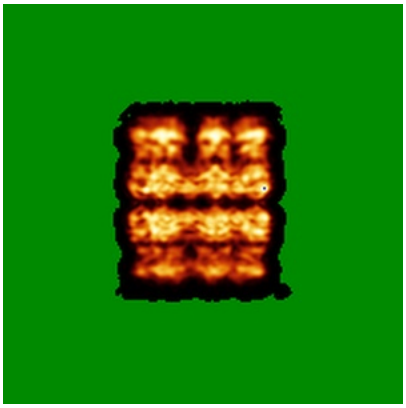


Z Index: 89

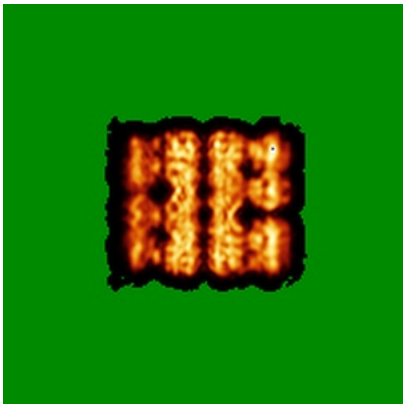
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

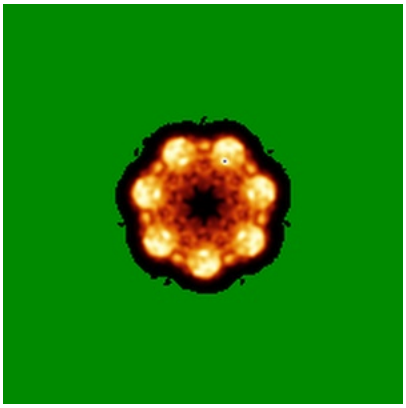
6.4.1 Primary map



X



Y

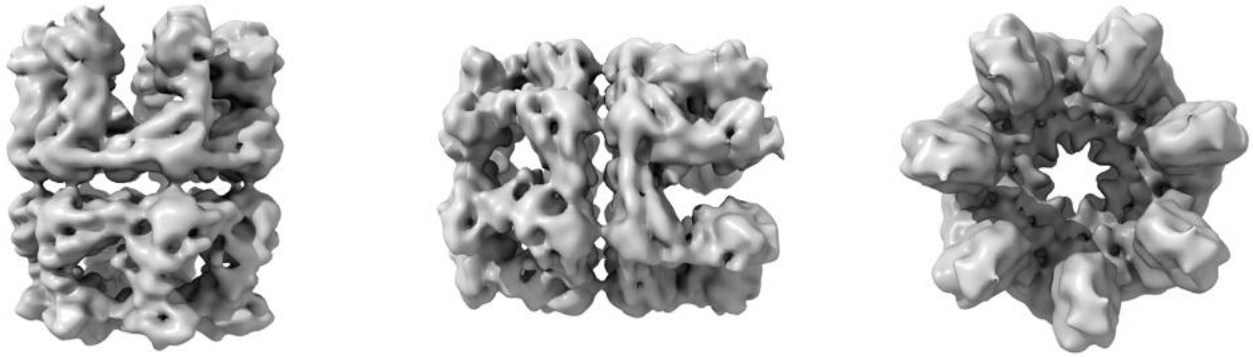


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

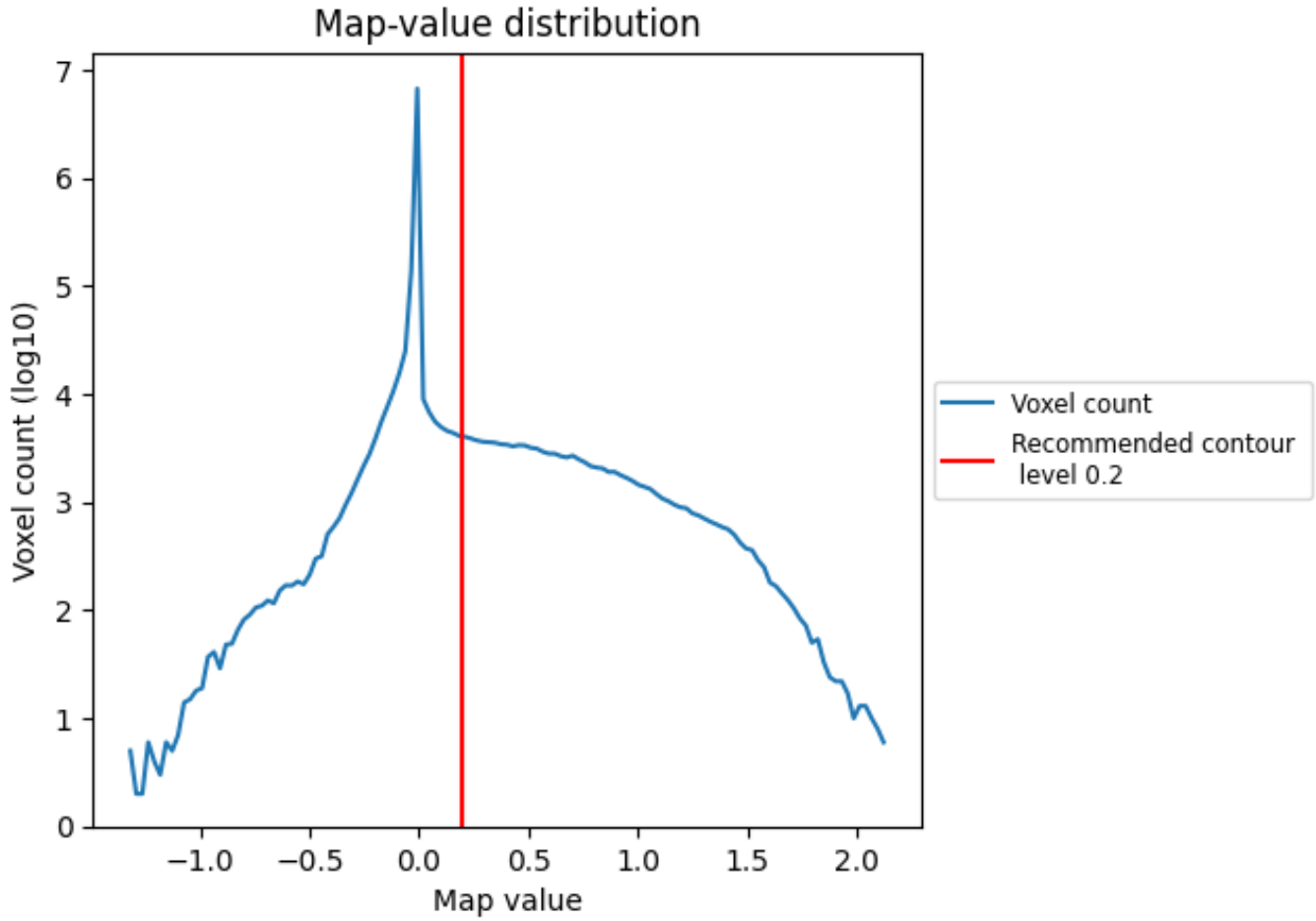
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

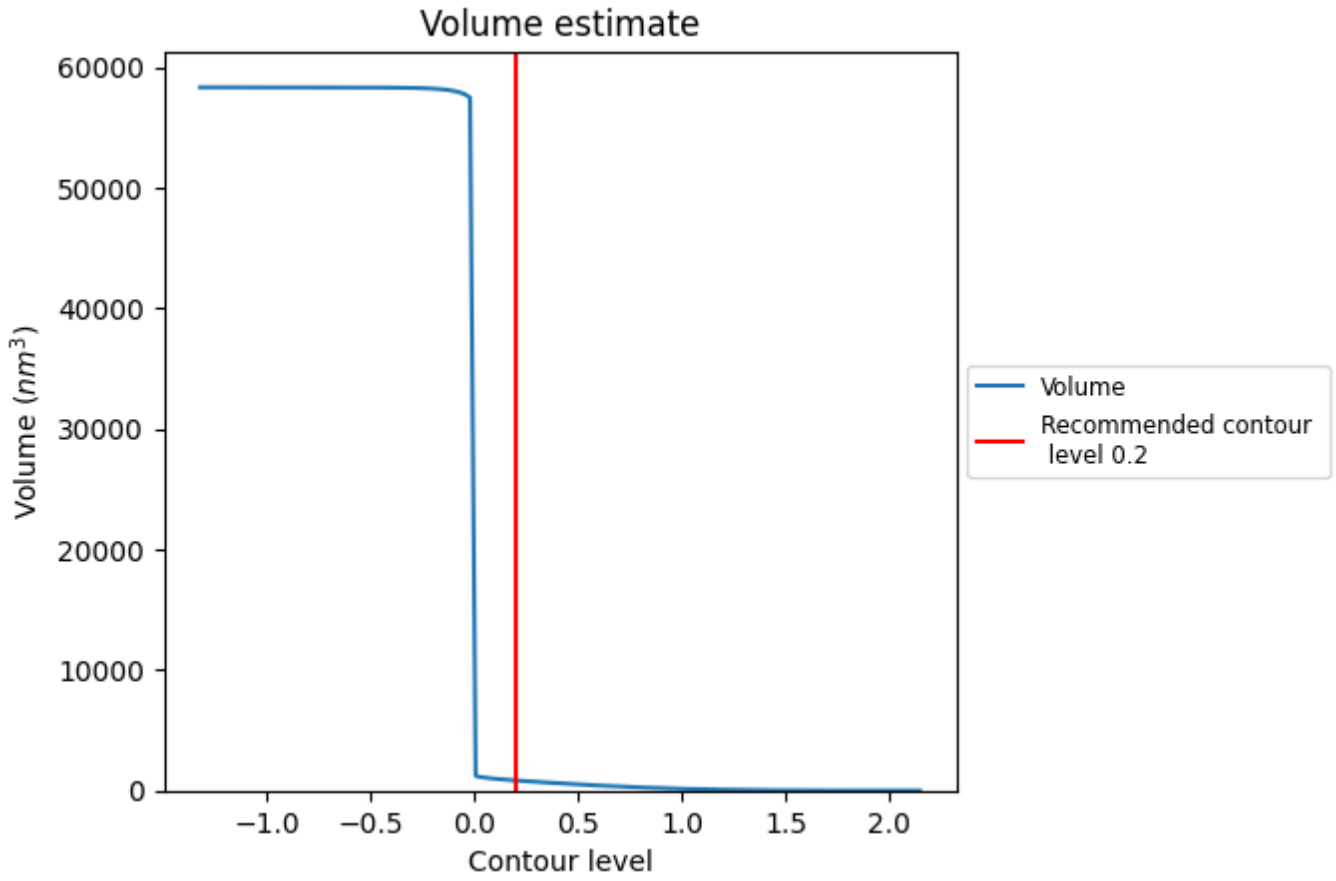
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

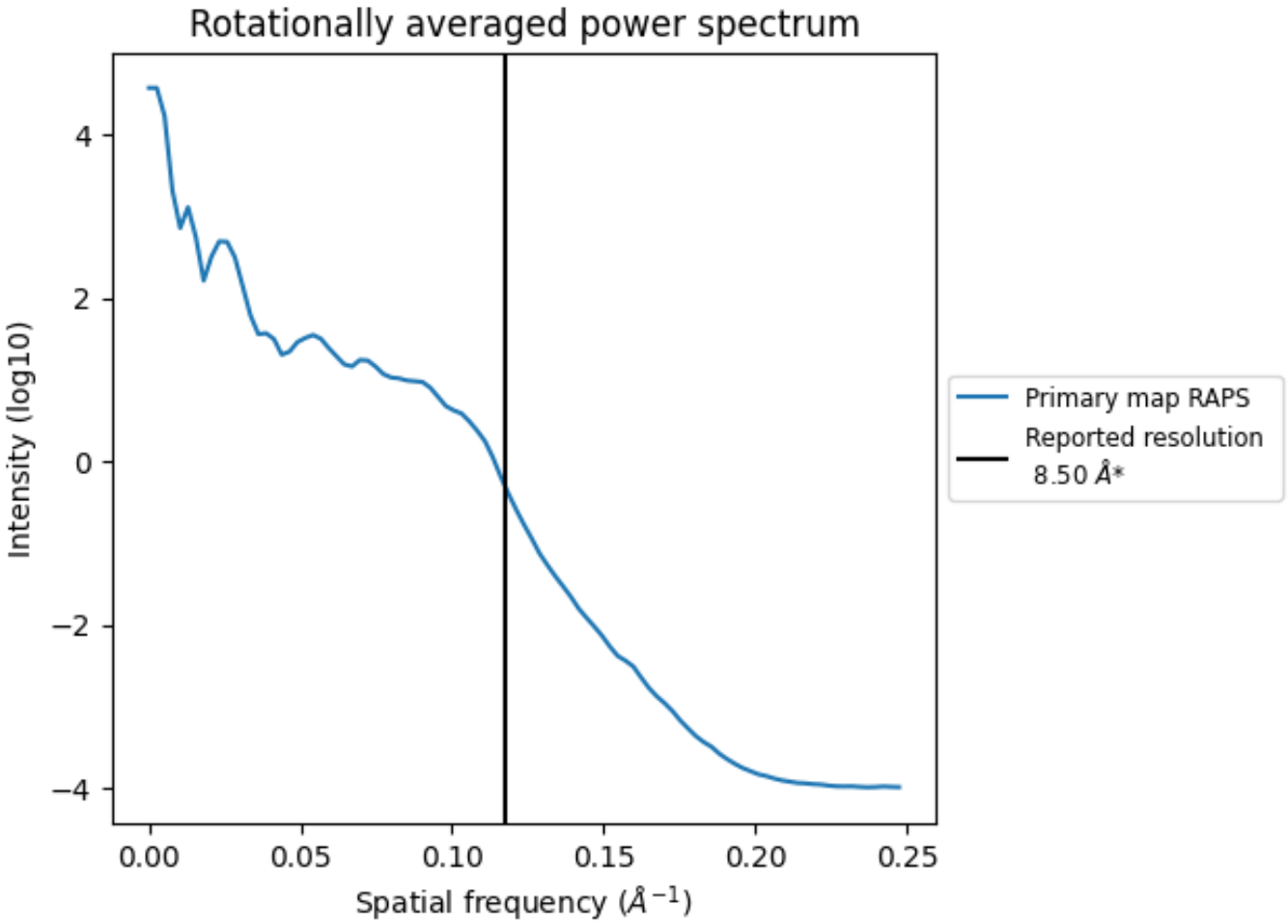
7.2 Volume estimate



The volume at the recommended contour level is 840 nm^3; this corresponds to an approximate mass of 759 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.118 Å^{-1}

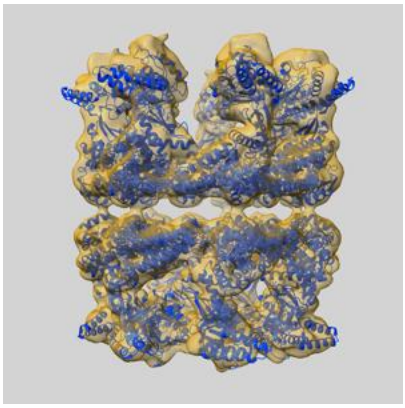
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

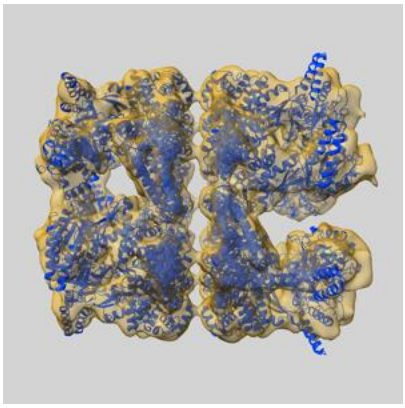
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2003 and PDB model 4AB3. Per-residue inclusion information can be found in section 3 on page 9.

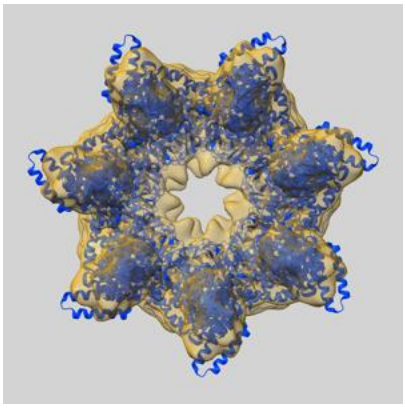
9.1 Map-model overlay



X



Y



Z

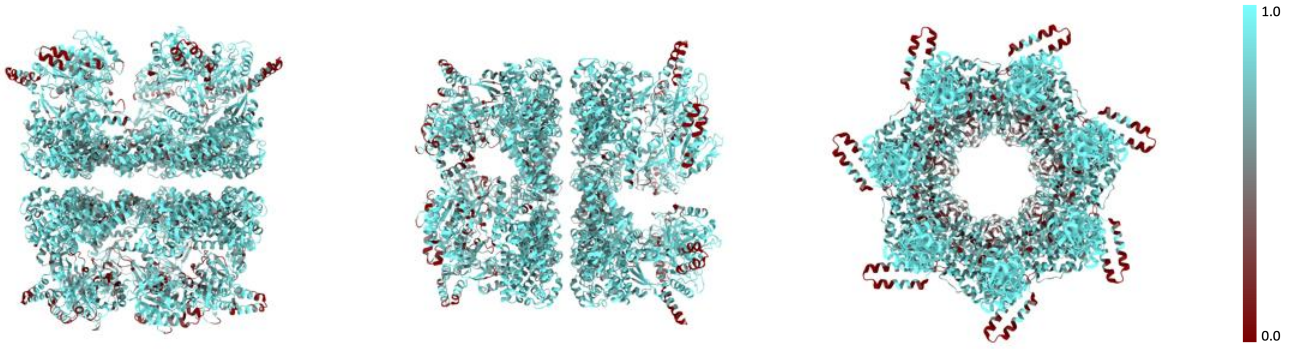
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

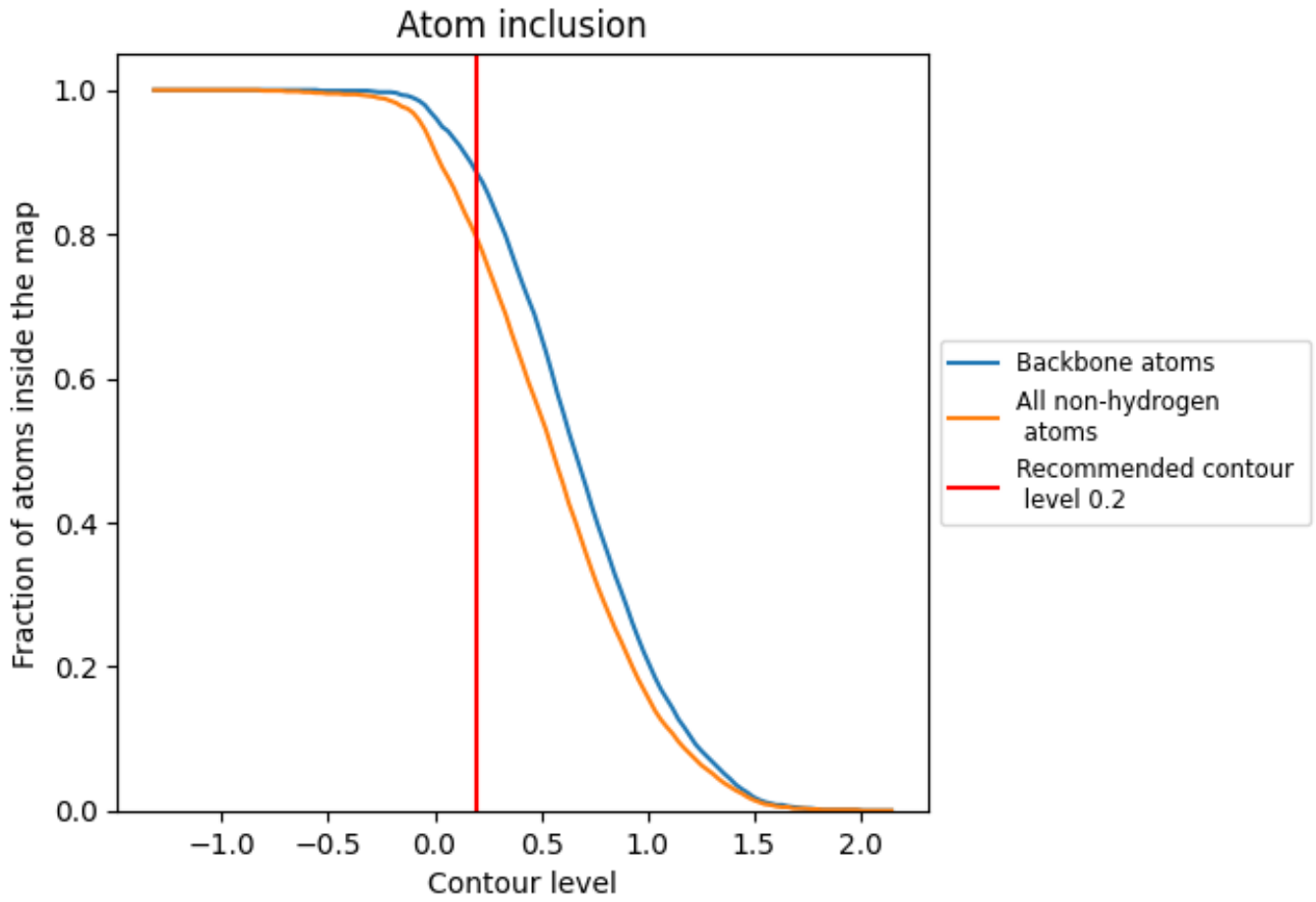
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7930	0.0910
A	0.8040	0.0820
B	0.8030	0.0830
C	0.8030	0.0840
D	0.8030	0.0850
E	0.8040	0.0860
F	0.8030	0.0840
G	0.8030	0.0840
H	0.7810	0.0970
I	0.7830	0.0980
J	0.7830	0.0980
K	0.7820	0.0980
L	0.7840	0.0980
M	0.7830	0.0990
N	0.7820	0.0980