Full wwPDB EM Validation Report ⓘ

May 29, 2024 – 04:53 PM EDT

PDB ID	:	1TUB
Title	:	TUBULIN ALPHA-BETA DIMER, ELECTRON DIFFRACTION
Authors	:	Nogales, E.; Downing, K.H.
Deposited on	:	1997-09-23
Resolution	:	3.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB 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:

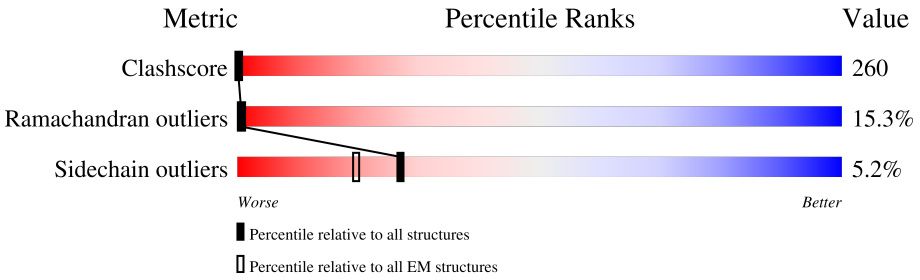
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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%

Mol	Chain	Length	Quality of chain
1	A	440	8% 50% 27% 15%
2	B	427	5% 49% 29% 17%

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
3	GTP	A	500	-	-	X	-
4	GDP	B	500	-	-	X	-
5	TXL	B	501	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6907 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 TUBULIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	440	3430	2168	583	657	22	0	0

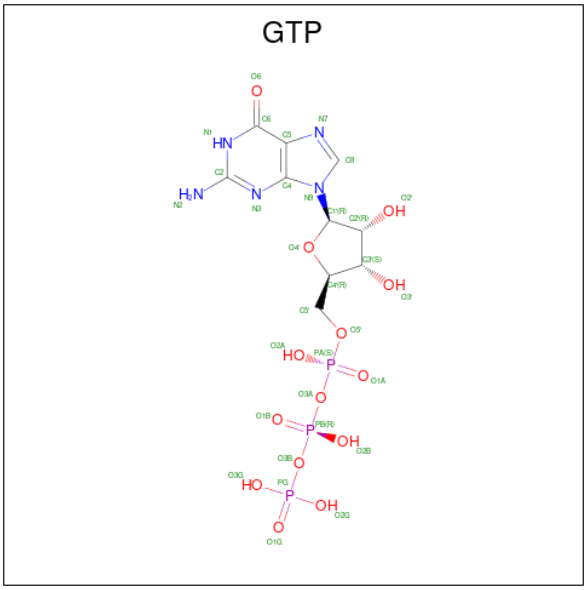
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	conflict	UNP P02550

- Molecule 2 is a protein called TUBULIN.

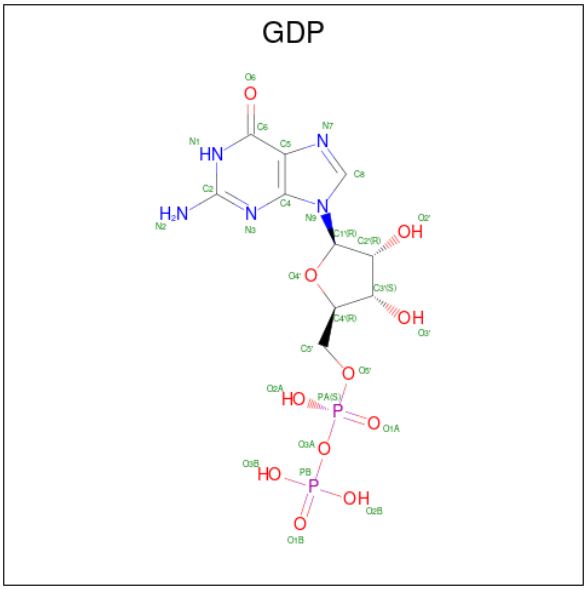
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	427	3359	2110	576	647	26	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



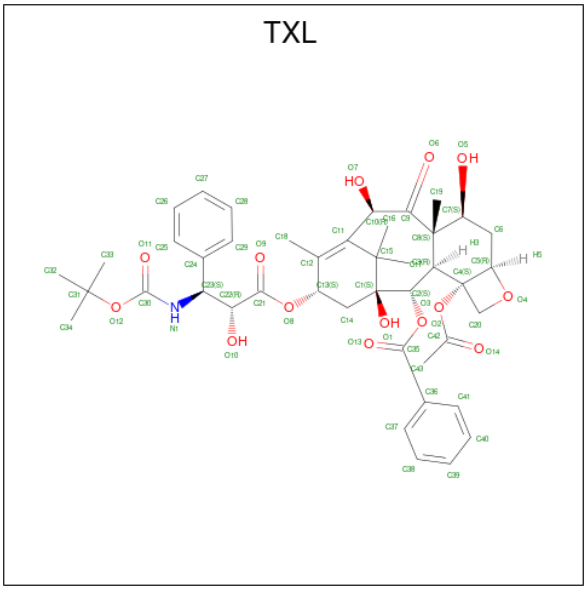
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 5 is TAXOTERE (three-letter code: TXL) (formula: $C_{43}H_{53}NO_{14}$).



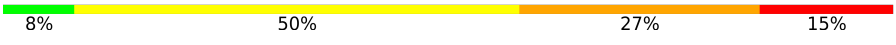
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			58	43	1	14	

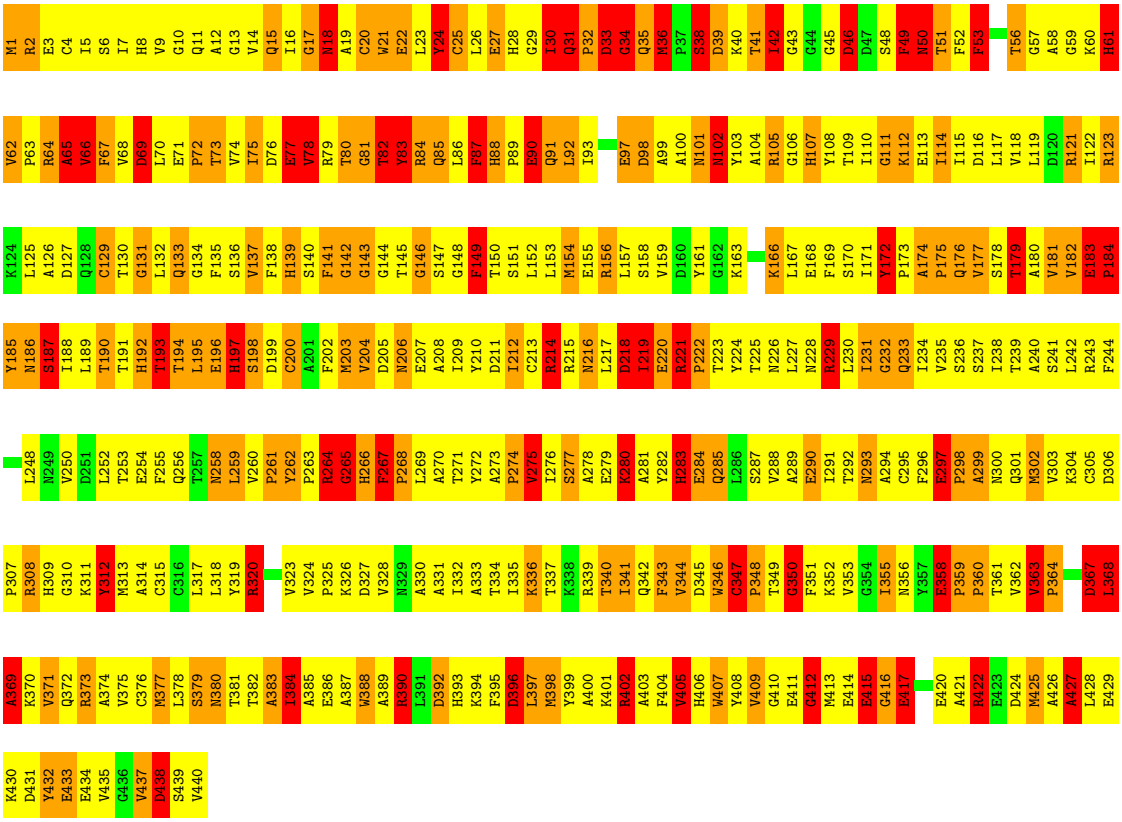
3 Residue-property plots (i)

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. 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. 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: TUBULIN

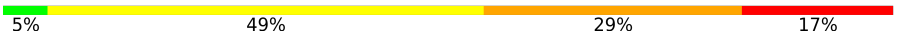
Chain A:

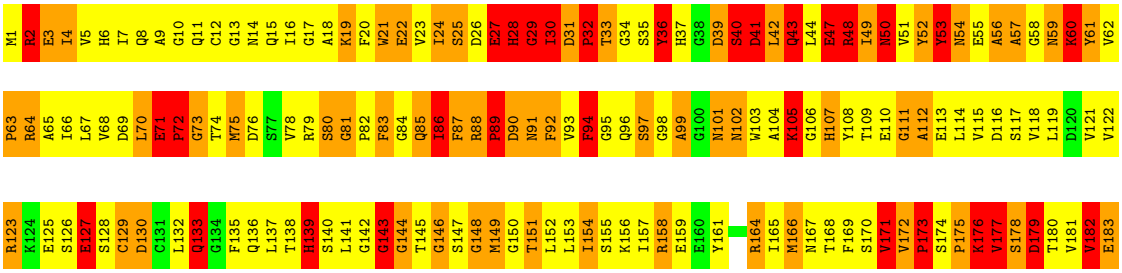


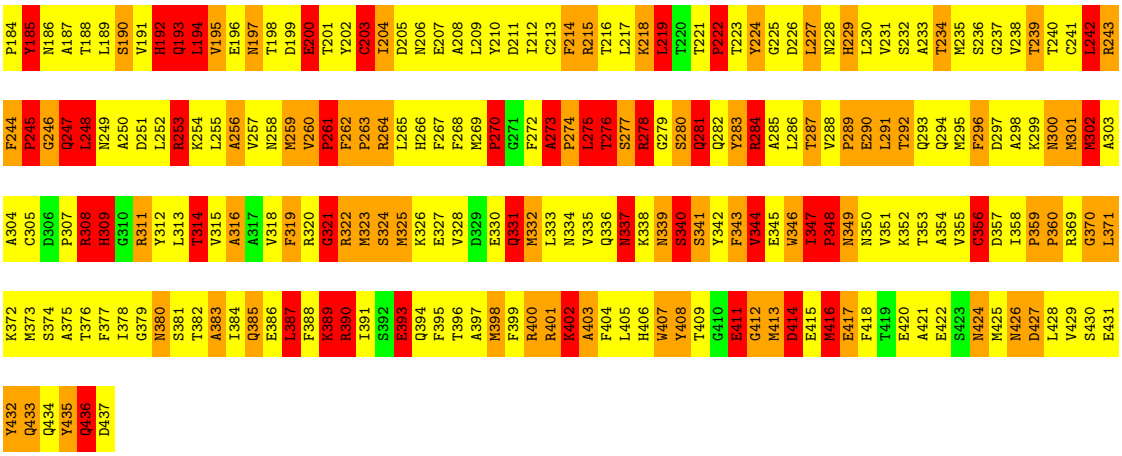


- Molecule 2: TUBULIN

Chain B:






P184 V185 N186 A187 T188 L189 S190 V191 H192 Q193 L194 V195 E196 N197 T198 D199 E200 T201 Y202 C203 I204 D205 N206 E207 A208 L209 Y210 D211 I212 C213 F214 R215 T216 L217 K218 L219 T220 T221 P222 T223 Y224 G225 D226 L227 N228 H229 L230 V231 S232 A233 T234 M235 S236 G237 V238 T239 T240 C241 L242 R243
F244 P245 G246 Q247 L248 N249 A250 D251 L252 R253 K254 L255 A256 V257 N258 M259 V260 P261 F262 P263 R264 L265 H266 F267 F268 M269 P270 G271 F272 A273 P274 L275 T276 S277 R278 G279 S280 Q281 Q282 Y283 R284 A285 L286 T287 V288 P289 E290 L291 T292 Q293 Q294 M295 F296 D297 A298 K299 N300 M301 M302 A303
A304 C305 D306 P307 R308 H309 G310 R311 Y312 L313 T314 V315 A316 A317 V318 F319 R320 G321 R322 M323 S324 M325 K326 E327 V328 D329 E330 Q331 M332 L333 N334 V335 Q336 N337 K338 N339 S340 S341 Y342 F343 V344 E345 W346 I347 P348 N349 N350 V351 K352 T353 A354 V355 C356 D357 I358 P359 P360 R369 G370 L371
K372 M373 S374 A375 T376 F377 I378 G379 N380 S381 T382 A383 I384 Q385 E386 L387 F388 K389 R390 I391 S392 E393 Q394 F395 T396 A397 M398 F399 R400 R401 K402 A403 F404 L405 H406 W407 Y408 T409 G410 E411 G412 M413 D414 E415 M416 E417 F418 T419 E420 A421 E422 S423 N424 M425 N426 D427 L428 V429 S430 E431
Y432 Q433 Q434 Y435 Q436 D437

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.00Å 92.00Å 90.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.70 92.00 – 3.48	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.70) 78.6 (92.00-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) 0.548 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	144.0	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 407.5	EDS
L-test for twinning[1]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.006 for h,-k,-l	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	6907	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2123e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GTP, TXL, GDP

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	2.34	110/3508 (3.1%)	2.76	214/4762 (4.5%)
2	B	2.47	111/3434 (3.2%)	3.07	266/4652 (5.7%)
All	All	2.41	221/6942 (3.2%)	2.92	480/9414 (5.1%)

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	56
2	B	0	59
All	All	0	115

All (221) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	278	ARG	CA-CB	34.96	2.30	1.53
2	B	105	LYS	C-N	-29.38	0.80	1.33
2	B	73	GLY	C-N	-28.00	0.69	1.34
1	A	38	SER	C-N	-27.48	0.70	1.34
1	A	347	CYS	C-N	-23.43	0.89	1.34
1	A	218	ASP	C-N	-21.36	0.84	1.34
2	B	321	GLY	C-N	-19.80	0.88	1.34
1	A	219	ILE	CB-CG2	19.43	2.13	1.52
1	A	358	GLU	C-N	-19.18	0.97	1.34
2	B	200	GLU	C-N	-19.10	0.90	1.34
2	B	182	VAL	C-N	-19.09	0.90	1.34
1	A	53	PHE	C-N	-19.01	0.90	1.34
2	B	197	ASN	C-N	-18.84	0.90	1.34
2	B	340	SER	C-N	-18.05	0.92	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	309	HIS	C-N	-17.98	1.00	1.33
1	A	219	ILE	CB-CG1	-17.61	1.04	1.54
1	A	416	GLY	C-N	-17.00	0.94	1.34
1	A	193	THR	C-N	-16.85	0.95	1.34
1	A	350	GLY	C-N	-16.79	0.95	1.34
1	A	415	GLU	C-N	-16.60	1.03	1.33
2	B	247	GLN	C-N	-16.27	0.96	1.34
2	B	417	GLU	C-N	-15.50	0.98	1.34
2	B	346	TRP	C-N	-15.06	0.99	1.34
2	B	71	GLU	C-N	-14.76	1.06	1.34
1	A	31	GLN	C-N	-14.60	1.06	1.34
1	A	409	VAL	C-N	14.54	1.59	1.33
1	A	34	GLY	N-CA	-14.49	1.24	1.46
2	B	270	PRO	C-N	14.03	1.58	1.33
2	B	203	CYS	C-N	-13.92	1.02	1.34
1	A	220	GLU	CB-CG	13.85	1.78	1.52
2	B	275	LEU	C-N	-13.73	1.02	1.34
1	A	221	ARG	C-N	-13.63	1.08	1.34
1	A	371	VAL	C-N	-13.56	1.02	1.34
1	A	69	ASP	C-N	-13.49	1.03	1.34
1	A	405	VAL	C-N	-13.45	1.03	1.34
2	B	387	LEU	C-N	12.82	1.63	1.34
2	B	380	ASN	C-N	-12.74	1.04	1.34
2	B	400	ARG	C-N	-12.40	1.05	1.34
2	B	127	GLU	C-N	-12.24	1.05	1.34
1	A	33	ASP	C-N	-11.67	1.12	1.33
2	B	331	GLN	C-N	-11.59	1.07	1.34
2	B	22	GLU	C-N	-11.56	1.07	1.34
1	A	32	PRO	N-CD	-11.49	1.31	1.47
1	A	190	THR	C-N	-11.42	1.07	1.34
2	B	273	ALA	C-N	-11.36	1.12	1.34
1	A	221	ARG	CB-CG	-11.14	1.22	1.52
1	A	405	VAL	CB-CG2	11.14	1.76	1.52
1	A	216	ASN	C-N	-10.86	1.09	1.34
1	A	402	ARG	C-N	-10.86	1.09	1.34
2	B	344	VAL	C-N	-10.55	1.09	1.34
1	A	21	TRP	C-O	10.21	1.42	1.23
2	B	60	LYS	C-N	-10.18	1.10	1.34
2	B	179	ASP	C-N	-10.18	1.10	1.34
2	B	371	LEU	C-N	-10.10	1.10	1.34
2	B	334	ASN	C-N	-9.98	1.11	1.34
2	B	287	THR	C-N	9.95	1.56	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	PHE	C-N	-9.88	1.11	1.34
2	B	414	ASP	C-N	-9.82	1.11	1.34
1	A	43	GLY	C-N	9.81	1.50	1.33
2	B	64	ARG	C-N	-9.77	1.11	1.34
1	A	280	LYS	C-N	-9.37	1.12	1.34
1	A	405	VAL	CB-CG1	-9.26	1.33	1.52
2	B	292	THR	C-N	-9.07	1.13	1.34
2	B	193	GLN	C-O	9.03	1.40	1.23
2	B	54	ASN	N-CA	-8.99	1.28	1.46
1	A	187	SER	C-N	8.97	1.54	1.34
2	B	71	GLU	C-O	-8.96	1.06	1.23
1	A	90	GLU	C-N	-8.92	1.13	1.34
2	B	143	GLY	CA-C	-8.82	1.37	1.51
1	A	222	PRO	N-CD	8.60	1.59	1.47
2	B	146	GLY	C-N	8.50	1.53	1.34
2	B	436	GLN	C-N	-8.44	1.14	1.34
2	B	151	THR	C-N	-8.41	1.14	1.34
1	A	231	ILE	C-O	8.38	1.39	1.23
1	A	379	SER	C-N	-8.17	1.15	1.34
1	A	438	ASP	C-O	8.16	1.38	1.23
2	B	173	PRO	C-N	-8.07	1.15	1.34
1	A	24	TYR	C-N	-8.06	1.15	1.34
2	B	244	PHE	C-N	-8.06	1.19	1.34
1	A	229	ARG	NE-CZ	-8.04	1.22	1.33
2	B	154	ILE	C-N	-7.99	1.15	1.34
2	B	337	ASN	C-N	-7.98	1.15	1.34
2	B	347	ILE	C-N	-7.81	1.19	1.34
1	A	233	GLN	C-N	-7.77	1.16	1.34
2	B	89	PRO	C-N	-7.70	1.16	1.34
1	A	43	GLY	C-O	-7.68	1.11	1.23
2	B	70	LEU	C-N	-7.66	1.16	1.34
2	B	291	LEU	N-CA	-7.64	1.31	1.46
2	B	278	ARG	CD-NE	-7.56	1.33	1.46
2	B	171	VAL	C-N	-7.55	1.16	1.34
2	B	72	PRO	C-N	-7.55	1.19	1.33
1	A	204	VAL	C-N	-7.55	1.16	1.34
1	A	229	ARG	CA-CB	-7.55	1.37	1.53
2	B	243	ARG	C-N	-7.51	1.16	1.34
1	A	274	PRO	C-N	-7.49	1.16	1.34
1	A	367	ASP	C-N	-7.42	1.17	1.34
2	B	218	LYS	C-N	7.38	1.51	1.34
1	A	346	TRP	C-N	-7.36	1.17	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	299	LYS	C-N	-7.28	1.17	1.34
1	A	222	PRO	CB-CG	7.23	1.86	1.50
2	B	53	TYR	C-N	-7.22	1.17	1.34
2	B	245	PRO	N-CD	-7.22	1.37	1.47
1	A	259	LEU	C-N	-7.18	1.17	1.34
2	B	192	HIS	C-O	7.03	1.36	1.23
1	A	2	ARG	N-CA	6.98	1.60	1.46
1	A	184	PRO	CA-CB	-6.95	1.39	1.53
1	A	433	GLU	C-N	-6.76	1.18	1.34
2	B	130	ASP	C-N	-6.75	1.18	1.34
2	B	190	SER	C-N	6.71	1.49	1.34
1	A	34	GLY	C-N	-6.66	1.18	1.34
1	A	80	THR	C-N	-6.66	1.21	1.33
1	A	265	GLY	CA-C	-6.65	1.41	1.51
2	B	143	GLY	C-N	-6.64	1.21	1.33
1	A	176	GLN	C-N	6.54	1.49	1.34
1	A	172	TYR	CB-CG	6.52	1.61	1.51
1	A	140	SER	C-N	-6.50	1.19	1.34
1	A	137	VAL	C-N	-6.48	1.19	1.34
2	B	193	GLN	C-N	-6.47	1.19	1.34
1	A	183	GLU	C-N	-6.45	1.22	1.34
1	A	36	MET	C-N	-6.44	1.22	1.34
2	B	348	PRO	C-N	-6.42	1.19	1.34
1	A	146	GLY	C-N	-6.40	1.19	1.34
1	A	43	GLY	CA-C	6.34	1.61	1.51
2	B	244	PHE	N-CA	-6.31	1.33	1.46
1	A	22	GLU	C-O	6.29	1.35	1.23
1	A	111	GLY	C-N	-6.27	1.19	1.34
2	B	111	GLY	C-N	-6.27	1.19	1.34
2	B	234	THR	C-N	-6.26	1.19	1.34
1	A	383	ALA	C-N	-6.24	1.19	1.34
2	B	194	LEU	C-N	-6.23	1.19	1.34
1	A	149	PHE	C-N	-6.22	1.19	1.34
2	B	259	MET	C-N	-6.20	1.19	1.34
2	B	1	MET	CA-C	-6.19	1.36	1.52
2	B	178	SER	C-N	-6.19	1.19	1.34
2	B	412	GLY	C-N	6.16	1.48	1.34
1	A	384	ILE	C-O	-6.16	1.11	1.23
2	B	149	MET	C-N	-6.15	1.22	1.33
1	A	377	MET	C-N	-6.13	1.20	1.34
1	A	1	MET	CA-C	-6.12	1.37	1.52
2	B	393	GLU	C-O	-6.12	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	GLU	C-N	6.09	1.48	1.34
1	A	91	GLN	C-N	6.07	1.48	1.34
1	A	437	VAL	C-N	-6.05	1.20	1.34
2	B	349	ASN	N-CA	-6.04	1.34	1.46
1	A	363	VAL	C-N	6.01	1.45	1.34
1	A	283	HIS	C-N	-6.01	1.20	1.34
1	A	388	TRP	NE1-CE2	-6.00	1.29	1.37
2	B	407	TRP	CA-CB	-5.97	1.40	1.53
2	B	52	TYR	C-N	-5.96	1.20	1.34
1	A	380	ASN	C-N	-5.96	1.20	1.34
2	B	40	SER	N-CA	-5.94	1.34	1.46
1	A	181	VAL	C-N	5.93	1.47	1.34
2	B	167	ASN	C-N	5.90	1.47	1.34
1	A	17	GLY	C-N	5.87	1.47	1.34
2	B	346	TRP	N-CA	-5.84	1.34	1.46
2	B	139	HIS	C-N	5.82	1.47	1.34
1	A	183	GLU	C-O	-5.80	1.12	1.23
1	A	107	HIS	C-O	5.78	1.34	1.23
2	B	107	HIS	C-O	5.78	1.34	1.23
2	B	133	GLN	C-N	-5.77	1.22	1.33
1	A	78	VAL	C-N	-5.77	1.20	1.34
2	B	76	ASP	C-O	5.75	1.34	1.23
2	B	168	THR	C-N	5.72	1.47	1.34
1	A	285	GLN	C-N	-5.71	1.21	1.34
2	B	86	ILE	C-N	5.70	1.47	1.34
1	A	46	ASP	C-N	5.70	1.47	1.34
1	A	232	GLY	CA-C	-5.70	1.42	1.51
1	A	196	GLU	C-N	-5.69	1.21	1.34
1	A	141	PHE	N-CA	-5.68	1.34	1.46
1	A	1	MET	C-N	5.65	1.47	1.34
1	A	166	LYS	C-N	-5.63	1.21	1.34
1	A	258	ASN	C-N	-5.59	1.21	1.34
2	B	52	TYR	N-CA	-5.59	1.35	1.46
2	B	51	VAL	C-N	-5.58	1.21	1.34
2	B	92	PHE	C-N	-5.58	1.21	1.34
1	A	72	PRO	N-CD	-5.57	1.40	1.47
2	B	356	CYS	C-N	-5.56	1.21	1.34
2	B	222	PRO	CA-C	-5.54	1.41	1.52
1	A	163	LYS	C-N	-5.53	1.21	1.34
1	A	200	CYS	C-N	-5.52	1.21	1.34
2	B	298	ALA	C-N	5.49	1.46	1.34
2	B	2	ARG	CA-C	-5.49	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	GLU	C-N	5.48	1.46	1.34
1	A	360	PRO	N-CD	-5.48	1.40	1.47
2	B	242	LEU	C-N	-5.47	1.21	1.34
2	B	383	ALA	C-N	-5.45	1.21	1.34
2	B	2	ARG	C-N	-5.44	1.21	1.34
2	B	21	TRP	NE1-CE2	-5.43	1.30	1.37
1	A	20	CYS	C-N	5.42	1.46	1.34
2	B	53	TYR	CG-CD2	-5.41	1.32	1.39
2	B	296	PHE	C-N	-5.41	1.21	1.34
2	B	221	THR	N-CA	5.40	1.57	1.46
2	B	27	GLU	C-N	-5.39	1.21	1.34
2	B	248	LEU	C-N	-5.39	1.21	1.34
1	A	114	ILE	C-N	-5.38	1.21	1.34
1	A	184	PRO	CA-C	-5.35	1.42	1.52
1	A	355	ILE	C-N	-5.33	1.21	1.34
2	B	28	HIS	C-O	-5.33	1.13	1.23
1	A	229	ARG	CD-NE	-5.31	1.37	1.46
1	A	21	TRP	NE1-CE2	-5.29	1.30	1.37
1	A	266	HIS	N-CA	-5.27	1.35	1.46
2	B	278	ARG	NE-CZ	-5.27	1.26	1.33
1	A	339	ARG	CA-C	-5.24	1.39	1.52
1	A	407	TRP	CA-CB	-5.21	1.42	1.53
2	B	3	GLU	N-CA	-5.20	1.35	1.46
2	B	261	PRO	CA-C	-5.19	1.42	1.52
2	B	435	TYR	CB-CG	-5.17	1.43	1.51
1	A	33	ASP	CA-C	-5.16	1.39	1.52
2	B	164	ARG	C-N	5.14	1.45	1.34
1	A	406	HIS	C-N	-5.13	1.22	1.34
2	B	276	THR	C-O	5.13	1.33	1.23
1	A	102	ASN	C-N	-5.12	1.22	1.34
1	A	66	VAL	N-CA	5.09	1.56	1.46
1	A	41	THR	C-N	-5.08	1.22	1.34
1	A	88	HIS	C-N	-5.08	1.24	1.34
2	B	53	TYR	N-CA	-5.06	1.36	1.46
2	B	290	GLU	C-O	-5.05	1.13	1.23
2	B	222	PRO	C-N	-5.04	1.22	1.34
2	B	261	PRO	N-CD	-5.02	1.40	1.47
1	A	277	SER	C-N	-5.00	1.22	1.34
2	B	85	GLN	C-N	5.00	1.45	1.34

All (480) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	368	LEU	O-C-N	-54.19	36.00	122.70
1	A	363	VAL	C-N-CD	-48.68	13.51	120.60
2	B	273	ALA	C-N-CD	-46.48	18.35	120.60
2	B	105	LYS	O-C-N	-44.51	47.53	123.20
2	B	88	ARG	C-N-CD	-44.07	23.65	120.60
1	A	283	HIS	O-C-N	-34.61	67.32	122.70
1	A	369	ALA	O-C-N	-32.92	70.03	122.70
2	B	73	GLY	O-C-N	-28.94	76.40	122.70
1	A	402	ARG	O-C-N	-27.79	78.24	122.70
2	B	275	LEU	O-C-N	-27.14	79.28	122.70
1	A	1	MET	O-C-N	26.24	164.69	122.70
1	A	358	GLU	C-N-CD	-26.03	63.33	120.60
2	B	143	GLY	O-C-N	-25.67	79.56	123.20
2	B	105	LYS	CA-C-N	25.12	166.45	116.20
2	B	321	GLY	O-C-N	-24.39	83.67	122.70
2	B	179	ASP	O-C-N	-22.43	86.81	122.70
2	B	194	LEU	O-C-N	-21.92	87.62	122.70
1	A	53	PHE	O-C-N	-21.60	88.14	122.70
2	B	85	GLN	O-C-N	21.52	157.13	122.70
2	B	278	ARG	N-CA-CB	21.31	148.96	110.60
2	B	344	VAL	O-C-N	-21.09	88.95	122.70
2	B	73	GLY	CA-C-N	21.07	163.55	117.20
2	B	1	MET	O-C-N	20.97	156.25	122.70
1	A	24	TYR	O-C-N	-20.67	89.62	122.70
2	B	86	ILE	O-C-N	19.91	154.55	122.70
2	B	321	GLY	C-N-CA	19.67	170.87	121.70
2	B	348	PRO	O-C-N	19.55	153.98	122.70
2	B	60	LYS	C-N-CA	18.98	169.14	121.70
2	B	52	TYR	O-C-N	18.59	152.45	122.70
1	A	367	ASP	O-C-N	-18.36	93.33	122.70
2	B	402	LYS	C-N-CA	18.24	167.30	121.70
1	A	218	ASP	O-C-N	-18.23	93.52	122.70
1	A	405	VAL	CA-CB-CG1	18.19	138.19	110.90
2	B	275	LEU	CA-C-N	18.09	156.99	117.20
2	B	411	GLU	C-N-CA	17.57	159.19	122.30
1	A	267	PHE	C-N-CD	-17.45	82.21	120.60
2	B	247	GLN	O-C-N	-17.23	95.13	122.70
2	B	203	CYS	C-N-CA	17.08	164.40	121.70
1	A	34	GLY	O-C-N	-16.93	95.61	122.70
2	B	194	LEU	C-N-CA	16.89	163.94	121.70
2	B	60	LYS	O-C-N	-16.82	95.79	122.70
2	B	127	GLU	O-C-N	-16.73	95.93	122.70
2	B	21	TRP	O-C-N	-16.69	95.99	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	MET	CB-CA-C	16.64	143.67	110.40
1	A	1	MET	CA-C-N	-16.28	81.38	117.20
1	A	402	ARG	CA-C-N	16.19	152.81	117.20
1	A	172	TYR	CB-CG-CD1	15.91	130.54	121.00
2	B	179	ASP	C-N-CA	15.83	161.27	121.70
2	B	53	TYR	O-C-N	15.74	147.88	122.70
1	A	87	PHE	O-C-N	-15.69	97.59	122.70
2	B	321	GLY	CA-C-N	15.31	150.88	117.20
2	B	1	MET	CB-CA-C	15.12	140.65	110.40
2	B	194	LEU	CA-C-N	14.98	150.16	117.20
2	B	30	ILE	CB-CA-C	14.96	141.52	111.60
2	B	1	MET	N-CA-C	-14.80	71.04	111.00
2	B	343	PHE	O-C-N	14.77	146.33	122.70
2	B	1	MET	CA-C-N	-14.75	84.74	117.20
2	B	331	GLN	O-C-N	-14.70	99.19	122.70
2	B	86	ILE	CA-C-N	-14.49	85.32	117.20
2	B	247	GLN	CA-C-N	14.41	148.90	117.20
1	A	405	VAL	C-N-CA	14.38	157.65	121.70
2	B	253	ARG	CD-NE-CZ	14.37	143.72	123.60
1	A	50	ASN	O-C-N	-14.11	100.12	122.70
2	B	344	VAL	C-N-CA	14.08	156.91	121.70
1	A	218	ASP	CA-C-N	13.52	146.95	117.20
2	B	85	GLN	CA-C-N	-13.50	87.51	117.20
1	A	283	HIS	C-N-CA	13.47	155.38	121.70
1	A	347	CYS	C-N-CD	-13.35	91.24	120.60
2	B	400	ARG	O-C-N	-13.28	101.45	122.70
2	B	402	LYS	O-C-N	-13.27	101.47	122.70
1	A	38	SER	C-N-CA	13.22	154.75	121.70
2	B	370	GLY	O-C-N	-13.13	101.69	122.70
1	A	266	HIS	O-C-N	13.12	143.70	122.70
1	A	367	ASP	CA-C-N	13.09	146.00	117.20
1	A	1	MET	N-CA-C	-13.02	75.86	111.00
1	A	21	TRP	CA-CB-CG	-12.96	89.08	113.70
2	B	411	GLU	O-C-N	-12.89	101.29	123.20
2	B	73	GLY	C-N-CA	12.88	153.90	121.70
1	A	38	SER	O-C-N	-12.86	102.12	122.70
2	B	182	VAL	C-N-CA	12.69	153.43	121.70
2	B	247	GLN	C-N-CA	12.56	153.09	121.70
2	B	359	PRO	O-C-N	12.54	144.93	121.10
1	A	347	CYS	O-C-N	-12.43	97.48	121.10
2	B	344	VAL	CA-C-N	12.34	144.34	117.20
2	B	348	PRO	CA-C-N	-12.32	90.09	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	183	GLU	O-C-N	-12.29	97.76	121.10
1	A	38	SER	CA-C-N	12.14	143.92	117.20
2	B	89	PRO	O-C-N	-12.05	103.42	122.70
2	B	203	CYS	O-C-N	-12.01	103.48	122.70
1	A	184	PRO	O-C-N	12.00	141.89	122.70
1	A	32	PRO	CA-N-CD	11.99	128.48	111.70
1	A	219	ILE	CA-CB-CG2	-11.97	86.96	110.90
1	A	30	ILE	C-N-CA	11.89	151.43	121.70
2	B	105	LYS	C-N-CA	11.83	147.15	122.30
1	A	41	THR	O-C-N	11.83	141.63	122.70
2	B	52	TYR	CA-C-N	-11.80	91.24	117.20
2	B	179	ASP	CA-C-N	11.78	143.10	117.20
1	A	24	TYR	CA-C-N	11.75	143.04	117.20
2	B	53	TYR	CB-CG-CD2	-11.65	114.01	121.00
1	A	218	ASP	C-N-CA	11.58	150.66	121.70
1	A	280	LYS	O-C-N	-11.55	104.22	122.70
2	B	143	GLY	CA-C-N	11.49	139.18	116.20
1	A	87	PHE	C-N-CA	11.45	150.33	121.70
2	B	53	TYR	CA-C-N	-11.43	92.05	117.20
2	B	30	ILE	O-C-N	-11.36	104.52	122.70
1	A	415	GLU	O-C-N	-11.34	103.92	123.20
1	A	53	PHE	CA-C-N	11.29	142.03	117.20
2	B	53	TYR	CB-CG-CD1	11.22	127.73	121.00
1	A	179	THR	O-C-N	-11.22	104.75	122.70
2	B	224	TYR	O-C-N	-11.12	104.29	123.20
1	A	1	MET	C-N-CA	11.11	149.48	121.70
2	B	400	ARG	C-N-CA	11.10	149.46	121.70
1	A	396	ASP	O-C-N	-11.04	105.03	122.70
1	A	415	GLU	C-N-CA	11.04	145.47	122.30
2	B	347	ILE	C-N-CD	-10.96	96.50	120.60
2	B	47	GLU	C-N-CA	10.95	149.06	121.70
2	B	284	ARG	NE-CZ-NH2	10.87	125.73	120.30
2	B	269	MET	C-N-CD	-10.82	96.80	120.60
2	B	203	CYS	CA-C-N	10.72	140.78	117.20
2	B	192	HIS	O-C-N	-10.64	105.67	122.70
1	A	69	ASP	O-C-N	-10.60	105.74	122.70
1	A	34	GLY	CA-C-N	10.59	140.49	117.20
1	A	415	GLU	CA-C-N	10.51	137.22	116.20
2	B	171	VAL	O-C-N	-10.42	106.02	122.70
2	B	343	PHE	CA-C-N	-10.36	94.40	117.20
1	A	221	ARG	O-C-N	-10.23	101.67	121.10
1	A	280	LYS	C-N-CA	10.22	147.26	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	264	ARG	NE-CZ-NH2	10.19	125.40	120.30
2	B	127	GLU	CA-C-N	10.18	139.60	117.20
1	A	107	HIS	O-C-N	-10.14	106.47	122.70
2	B	107	HIS	O-C-N	-10.14	106.47	122.70
1	A	87	PHE	CA-C-N	10.12	139.47	117.20
1	A	405	VAL	O-C-N	-10.03	106.65	122.70
2	B	289	PRO	O-C-N	10.02	138.73	122.70
1	A	49	PHE	C-N-CA	10.01	146.72	121.70
1	A	172	TYR	CA-CB-CG	9.96	132.32	113.40
1	A	266	HIS	CA-C-N	-9.94	95.33	117.20
2	B	182	VAL	O-C-N	-9.92	106.83	122.70
2	B	21	TRP	CA-C-N	9.91	139.00	117.20
1	A	229	ARG	NE-CZ-NH2	9.89	125.25	120.30
2	B	311	ARG	NE-CZ-NH2	9.85	125.23	120.30
2	B	29	GLY	O-C-N	9.70	138.22	122.70
2	B	158	ARG	NE-CZ-NH2	9.68	125.14	120.30
2	B	435	TYR	CB-CG-CD1	-9.64	115.22	121.00
2	B	219	LEU	O-C-N	-9.63	107.29	122.70
1	A	90	GLU	O-C-N	-9.57	107.38	122.70
1	A	61	HIS	CB-CA-C	9.57	129.54	110.40
1	A	193	THR	O-C-N	-9.57	107.39	122.70
2	B	356	CYS	O-C-N	-9.55	107.42	122.70
1	A	121	ARG	NE-CZ-NH2	9.55	125.08	120.30
2	B	49	ILE	O-C-N	-9.52	107.47	122.70
2	B	85	GLN	C-N-CA	9.51	145.48	121.70
2	B	52	TYR	C-N-CA	9.48	145.40	121.70
1	A	2	ARG	NE-CZ-NH2	9.40	125.00	120.30
2	B	127	GLU	C-N-CA	9.39	145.17	121.70
1	A	229	ARG	NE-CZ-NH1	-9.38	115.61	120.30
2	B	275	LEU	C-N-CA	9.34	145.04	121.70
2	B	193	GLN	O-C-N	-9.33	107.77	122.70
2	B	414	ASP	C-N-CA	9.33	145.03	121.70
1	A	416	GLY	C-N-CA	9.33	145.03	121.70
2	B	322	ARG	NE-CZ-NH2	9.32	124.96	120.30
2	B	370	GLY	CA-C-N	9.29	137.63	117.20
1	A	320	ARG	NE-CZ-NH2	9.27	124.93	120.30
1	A	65	ALA	CB-CA-C	-9.19	96.32	110.10
2	B	185	TYR	CA-CB-CG	9.18	130.85	113.40
1	A	409	VAL	O-C-N	9.07	138.62	123.20
2	B	48	ARG	NE-CZ-NH2	9.06	124.83	120.30
1	A	172	TYR	CB-CG-CD2	-9.04	115.58	121.00
1	A	367	ASP	C-N-CA	8.98	144.15	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	200	GLU	O-C-N	-8.96	108.37	122.70
2	B	49	ILE	C-N-CA	8.95	144.07	121.70
1	A	21	TRP	O-C-N	-8.92	108.43	122.70
1	A	347	CYS	CA-C-N	8.86	141.91	117.10
2	B	278	ARG	CB-CA-C	-8.85	92.71	110.40
2	B	94	PHE	CB-CG-CD1	-8.78	114.66	120.80
1	A	219	ILE	CG1-CB-CG2	-8.77	92.11	111.40
1	A	139	HIS	CA-CB-CG	8.72	128.43	113.60
1	A	32	PRO	N-CA-CB	-8.69	92.87	103.30
1	A	183	GLU	CA-C-N	8.64	141.30	117.10
1	A	31	GLN	C-N-CD	-8.63	101.62	120.60
1	A	42	ILE	CA-C-N	8.62	133.44	116.20
1	A	222	PRO	N-CA-CB	8.61	113.63	103.30
1	A	56	THR	C-N-CA	-8.58	104.28	122.30
2	B	414	ASP	O-C-N	-8.56	109.01	122.70
2	B	29	GLY	C-N-CA	8.51	142.97	121.70
1	A	412	GLY	O-C-N	-8.48	109.12	122.70
1	A	24	TYR	C-N-CA	8.48	142.89	121.70
2	B	400	ARG	CA-C-N	8.46	135.81	117.20
2	B	436	GLN	C-N-CA	8.45	142.82	121.70
2	B	24	ILE	O-C-N	-8.44	109.19	122.70
2	B	47	GLU	O-C-N	-8.39	109.27	122.70
2	B	229	HIS	O-C-N	-8.37	109.31	122.70
1	A	190	THR	O-C-N	-8.32	109.39	122.70
2	B	400	ARG	NE-CZ-NH2	8.31	124.46	120.30
2	B	92	PHE	CA-CB-CG	-8.28	94.02	113.90
2	B	177	VAL	CA-C-O	8.28	137.49	120.10
1	A	297	GLU	O-C-N	8.28	136.83	121.10
2	B	200	GLU	C-N-CA	8.27	142.37	121.70
2	B	53	TYR	N-CA-CB	8.26	125.47	110.60
2	B	309	HIS	O-C-N	-8.18	109.30	123.20
2	B	411	GLU	CA-C-N	8.13	132.47	116.20
1	A	369	ALA	C-N-CA	8.11	141.97	121.70
2	B	406	HIS	CA-CB-CG	-8.11	99.82	113.60
1	A	184	PRO	CA-C-N	-8.09	99.41	117.20
2	B	402	LYS	CA-C-N	8.07	134.96	117.20
2	B	215	ARG	NE-CZ-NH2	8.07	124.33	120.30
1	A	215	ARG	NE-CZ-NH2	8.05	124.32	120.30
1	A	221	ARG	CA-C-N	8.04	139.61	117.10
1	A	422	ARG	NE-CZ-NH2	8.03	124.31	120.30
1	A	43	GLY	CA-C-N	-7.96	100.27	116.20
2	B	89	PRO	C-N-CA	7.96	141.61	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	65	ALA	N-CA-C	7.96	132.48	111.00
1	A	113	GLU	O-C-N	-7.95	109.98	122.70
2	B	370	GLY	C-N-CA	7.92	141.51	121.70
2	B	245	PRO	CA-N-CD	7.91	122.78	111.70
1	A	190	THR	CA-C-N	7.91	134.60	117.20
2	B	59	ASN	C-N-CA	7.89	141.43	121.70
2	B	289	PRO	CA-C-N	-7.88	99.87	117.20
2	B	299	LYS	O-C-N	7.86	135.27	122.70
2	B	302	MET	CG-SD-CE	7.84	112.74	100.20
2	B	164	ARG	NE-CZ-NH2	7.82	124.21	120.30
2	B	171	VAL	CA-C-N	7.77	134.30	117.20
1	A	33	ASP	C-N-CA	-7.72	106.09	122.30
2	B	359	PRO	CA-C-N	-7.71	95.51	117.10
2	B	21	TRP	C-N-CA	-7.71	102.44	121.70
2	B	182	VAL	CA-C-N	7.71	134.15	117.20
1	A	221	ARG	C-N-CD	-7.70	103.65	120.60
2	B	356	CYS	CA-C-N	7.67	134.08	117.20
1	A	298	PRO	O-C-N	-7.67	110.43	122.70
1	A	340	THR	O-C-N	7.65	134.93	122.70
2	B	412	GLY	O-C-N	-7.63	110.49	122.70
1	A	67	PHE	CA-CB-CG	-7.63	95.59	113.90
2	B	50	ASN	CA-C-N	-7.61	100.45	117.20
1	A	405	VAL	CA-C-N	7.61	133.94	117.20
2	B	185	TYR	CB-CG-CD1	7.55	125.53	121.00
2	B	407	TRP	CA-CB-CG	-7.55	99.35	113.70
1	A	15	GLN	O-C-N	7.54	134.77	122.70
1	A	31	GLN	N-CA-C	7.54	131.35	111.00
1	A	373	ARG	CD-NE-CZ	7.51	134.11	123.60
1	A	392	ASP	CA-C-O	-7.49	104.37	120.10
2	B	64	ARG	NE-CZ-NH2	7.47	124.04	120.30
2	B	253	ARG	NE-CZ-NH2	7.47	124.03	120.30
1	A	18	ASN	O-C-N	7.46	134.64	122.70
2	B	151	THR	O-C-N	-7.42	110.82	122.70
2	B	346	TRP	CA-C-N	-7.42	100.87	117.20
1	A	417	GLU	O-C-N	7.41	134.55	122.70
1	A	339	ARG	O-C-N	7.37	134.50	122.70
2	B	2	ARG	O-C-N	7.35	134.45	122.70
2	B	29	GLY	CA-C-N	-7.31	101.12	117.20
1	A	264	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	34	GLY	C-N-CA	7.30	139.94	121.70
1	A	377	MET	CG-SD-CE	7.29	111.87	100.20
2	B	143	GLY	C-N-CA	7.24	137.51	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	308	ARG	NE-CZ-NH2	7.23	123.92	120.30
2	B	19	LYS	CD-CE-NZ	7.20	128.26	111.70
1	A	50	ASN	CA-C-N	7.19	133.03	117.20
2	B	200	GLU	CA-C-N	7.18	133.01	117.20
1	A	416	GLY	O-C-N	-7.18	111.21	122.70
1	A	32	PRO	N-CD-CG	-7.18	92.43	103.20
2	B	264	ARG	NH1-CZ-NH2	-7.15	111.54	119.40
2	B	290	GLU	O-C-N	7.12	134.10	122.70
1	A	302	MET	CG-SD-CE	7.12	111.60	100.20
2	B	387	LEU	C-N-CA	-7.08	104.00	121.70
2	B	24	ILE	C-N-CA	-7.04	104.09	121.70
1	A	340	THR	CA-C-N	-7.02	101.77	117.20
2	B	331	GLN	CA-C-N	7.00	132.60	117.20
1	A	197	HIS	CA-C-N	-6.94	101.94	117.20
2	B	89	PRO	CA-C-N	6.93	132.44	117.20
1	A	2	ARG	CB-CA-C	-6.92	96.56	110.40
2	B	149	MET	CG-SD-CE	6.90	111.25	100.20
2	B	276	THR	C-N-CA	6.90	138.95	121.70
1	A	61	HIS	CA-CB-CG	6.90	125.33	113.60
1	A	17	GLY	O-C-N	6.88	133.71	122.70
1	A	203	MET	O-C-N	6.87	133.69	122.70
2	B	349	ASN	CB-CA-C	6.86	124.12	110.40
2	B	412	GLY	C-N-CA	6.86	138.86	121.70
2	B	269	MET	CG-SD-CE	6.86	111.18	100.20
2	B	32	PRO	O-C-N	6.86	133.67	122.70
2	B	340	SER	C-N-CA	-6.84	104.59	121.70
2	B	30	ILE	CA-C-N	6.83	132.23	117.20
1	A	355	ILE	CA-C-O	-6.79	105.83	120.10
1	A	368	LEU	C-N-CA	6.79	138.68	121.70
2	B	193	GLN	C-N-CA	6.79	138.67	121.70
1	A	72	PRO	O-C-N	6.76	133.51	122.70
2	B	346	TRP	CD1-CG-CD2	6.75	111.70	106.30
2	B	151	THR	CA-C-N	6.75	132.04	117.20
2	B	436	GLN	O-C-N	-6.72	111.94	122.70
1	A	409	VAL	CA-C-N	-6.71	102.77	116.20
2	B	1	MET	C-N-CA	6.67	138.38	121.70
1	A	290	GLU	O-C-N	6.67	133.37	122.70
1	A	425	MET	CG-SD-CE	6.66	110.86	100.20
2	B	398	MET	CG-SD-CE	6.66	110.86	100.20
2	B	281	GLN	O-C-N	-6.65	112.06	122.70
2	B	91	ASN	CA-CB-CG	6.65	128.03	113.40
1	A	85	GLN	O-C-N	-6.65	112.07	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	224	TYR	CA-C-N	6.63	129.46	116.20
1	A	384	ILE	CA-C-N	-6.62	102.65	117.20
1	A	203	MET	CG-SD-CE	6.59	110.75	100.20
2	B	166	MET	CG-SD-CE	6.59	110.74	100.20
1	A	78	VAL	O-C-N	-6.59	112.16	122.70
1	A	113	GLU	CA-C-O	6.57	133.91	120.10
2	B	113	GLU	CA-C-O	6.57	133.91	120.10
2	B	348	PRO	C-N-CA	6.57	138.13	121.70
1	A	197	HIS	O-C-N	6.57	133.21	122.70
1	A	369	ALA	CA-C-N	-6.56	102.77	117.20
1	A	221	ARG	C-N-CA	6.55	149.49	122.00
2	B	263	PRO	N-CA-C	6.55	129.12	112.10
2	B	219	LEU	CB-CA-C	-6.54	97.78	110.20
2	B	413	MET	CG-SD-CE	6.54	110.66	100.20
1	A	83	TYR	CA-CB-CG	-6.52	101.01	113.40
1	A	49	PHE	O-C-N	-6.50	112.31	122.70
1	A	398	MET	CG-SD-CE	6.49	110.58	100.20
1	A	275	VAL	O-C-N	6.47	133.06	122.70
1	A	396	ASP	CA-C-N	6.47	131.43	117.20
1	A	140	SER	O-C-N	6.46	133.04	122.70
2	B	243	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	A	297	GLU	CA-C-N	-6.45	99.04	117.10
2	B	60	LYS	CA-C-N	6.45	131.39	117.20
2	B	36	TYR	O-C-N	-6.41	112.45	122.70
2	B	290	GLU	CA-C-N	-6.40	103.13	117.20
2	B	332	MET	CG-SD-CE	6.39	110.43	100.20
1	A	111	GLY	CA-C-O	-6.38	109.12	120.60
2	B	111	GLY	CA-C-O	-6.38	109.12	120.60
1	A	407	TRP	CA-CB-CG	-6.37	101.59	113.70
1	A	402	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	A	262	TYR	CB-CG-CD2	6.35	124.81	121.00
1	A	290	GLU	CA-C-N	-6.34	103.26	117.20
1	A	371	VAL	O-C-N	6.33	132.82	122.70
1	A	312	TYR	CB-CG-CD1	-6.28	117.23	121.00
2	B	346	TRP	N-CA-CB	6.27	121.88	110.60
1	A	105	ARG	CD-NE-CZ	6.25	132.35	123.60
1	A	187	SER	CA-C-N	-6.25	103.46	117.20
1	A	280	LYS	CA-C-N	6.24	130.94	117.20
1	A	214	ARG	NE-CZ-NH2	6.24	123.42	120.30
2	B	59	ASN	O-C-N	-6.24	112.72	122.70
2	B	243	ARG	O-C-N	6.21	132.63	122.70
1	A	111	GLY	CA-C-N	6.20	130.84	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	111	GLY	CA-C-N	6.20	130.84	117.20
1	A	412	GLY	C-N-CA	6.18	137.15	121.70
1	A	43	GLY	O-C-N	6.17	133.68	123.20
2	B	177	VAL	O-C-N	-6.16	112.85	122.70
1	A	156	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	A	274	PRO	O-C-N	-6.12	112.92	122.70
2	B	390	ARG	NE-CZ-NH2	6.11	123.36	120.30
2	B	323	MET	CG-SD-CE	6.09	109.95	100.20
1	A	172	TYR	CB-CA-C	6.09	122.58	110.40
1	A	390	ARG	NE-CZ-NH2	6.09	123.34	120.30
2	B	154	ILE	C-N-CA	6.07	136.88	121.70
2	B	314	THR	N-CA-CB	6.04	121.77	110.30
2	B	390	ARG	NE-CZ-NH1	6.03	123.32	120.30
2	B	331	GLN	C-N-CA	5.99	136.67	121.70
2	B	433	GLN	CA-C-N	-5.98	104.04	117.20
1	A	42	ILE	C-N-CA	5.98	134.86	122.30
2	B	308	ARG	NH1-CZ-NH2	-5.96	112.84	119.40
1	A	41	THR	CA-C-N	-5.96	104.10	117.20
2	B	234	THR	CA-C-N	5.96	130.30	117.20
2	B	301	MET	CG-SD-CE	5.95	109.72	100.20
2	B	324	SER	O-C-N	5.95	132.22	122.70
2	B	407	TRP	CD1-CG-CD2	5.95	111.06	106.30
2	B	185	TYR	CB-CG-CD2	-5.94	117.44	121.00
2	B	433	GLN	O-C-N	5.94	132.20	122.70
2	B	52	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	A	1	MET	CG-SD-CE	5.91	109.65	100.20
2	B	412	GLY	CA-C-N	5.90	130.18	117.20
1	A	82	THR	C-N-CA	5.89	136.44	121.70
2	B	308	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	B	416	MET	CG-SD-CE	5.87	109.59	100.20
1	A	82	THR	O-C-N	5.87	132.09	122.70
2	B	244	PHE	CB-CA-C	5.87	122.13	110.40
2	B	278	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	90	GLU	CA-C-N	5.85	130.07	117.20
2	B	171	VAL	C-N-CA	5.84	136.30	121.70
2	B	72	PRO	CA-C-N	5.83	127.87	116.20
2	B	123	ARG	NE-CZ-NH2	5.82	123.21	120.30
2	B	283	TYR	C-N-CA	5.81	136.22	121.70
2	B	36	TYR	CA-C-N	5.80	129.96	117.20
2	B	259	MET	CG-SD-CE	5.79	109.47	100.20
2	B	167	ASN	C-N-CA	-5.78	107.26	121.70
2	B	324	SER	CA-C-N	-5.77	104.51	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	182	VAL	CA-C-N	5.74	129.83	117.20
1	A	50	ASN	C-N-CA	5.74	136.04	121.70
2	B	2	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	B	219	LEU	C-N-CA	-5.70	107.45	121.70
2	B	414	ASP	CA-C-N	5.68	129.70	117.20
1	A	297	GLU	C-N-CD	5.68	140.33	128.40
2	B	417	GLU	C-N-CA	5.66	135.86	121.70
2	B	284	ARG	NH1-CZ-NH2	-5.64	113.19	119.40
1	A	274	PRO	CA-C-N	5.62	129.57	117.20
2	B	219	LEU	CA-C-N	5.62	129.57	117.20
2	B	325	MET	CG-SD-CE	5.61	109.18	100.20
1	A	92	LEU	C-N-CA	5.61	135.72	121.70
1	A	379	SER	CA-C-N	-5.61	104.86	117.20
2	B	28	HIS	CA-C-N	-5.60	105.00	116.20
2	B	113	GLU	O-C-N	-5.60	113.75	122.70
2	B	50	ASN	CA-C-O	5.59	131.84	120.10
1	A	343	PHE	O-C-N	5.59	131.65	122.70
1	A	413	MET	CG-SD-CE	5.59	109.14	100.20
2	B	43	GLN	O-C-N	5.59	131.64	122.70
2	B	192	HIS	CA-C-N	5.58	129.48	117.20
1	A	90	GLU	C-N-CA	5.58	135.64	121.70
1	A	154	MET	CG-SD-CE	5.57	109.11	100.20
2	B	389	LYS	CB-CA-C	5.55	121.51	110.40
2	B	349	ASN	N-CA-C	-5.54	96.03	111.00
2	B	390	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
1	A	139	HIS	N-CA-CB	-5.53	100.64	110.60
2	B	346	TRP	O-C-N	5.52	131.54	122.70
2	B	264	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	B	154	ILE	O-C-N	-5.52	113.87	122.70
2	B	178	SER	CA-C-O	-5.51	108.52	120.10
2	B	299	LYS	C-N-CA	-5.50	107.95	121.70
2	B	71	GLU	O-C-N	-5.50	110.65	121.10
1	A	339	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	A	390	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	B	245	PRO	N-CA-CB	-5.45	96.61	102.60
2	B	253	ARG	NH1-CZ-NH2	-5.44	113.41	119.40
1	A	262	TYR	CA-CB-CG	5.43	123.73	113.40
1	A	297	GLU	C-N-CA	-5.43	99.17	122.00
1	A	221	ARG	CA-CB-CG	5.43	125.35	113.40
1	A	222	PRO	CA-CB-CG	-5.42	93.70	104.00
2	B	86	ILE	C-N-CA	5.41	135.22	121.70
1	A	65	ALA	O-C-N	-5.40	114.06	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	84	ARG	NE-CZ-NH2	5.38	122.99	120.30
2	B	72	PRO	O-C-N	-5.37	114.07	123.20
1	A	62	VAL	O-C-N	5.35	131.27	121.10
2	B	32	PRO	CA-C-N	-5.35	105.43	117.20
1	A	379	SER	O-C-N	5.35	131.26	122.70
2	B	4	ILE	O-C-N	5.34	131.25	122.70
2	B	49	ILE	CA-C-N	5.33	128.94	117.20
1	A	336	LYS	O-C-N	5.32	131.21	122.70
1	A	360	PRO	C-N-CA	-5.31	108.43	121.70
1	A	17	GLY	CA-C-N	-5.29	105.56	117.20
1	A	186	ASN	C-N-CA	5.29	134.92	121.70
1	A	97	GLU	O-C-N	5.28	131.16	122.70
1	A	390	ARG	NH1-CZ-NH2	-5.27	113.60	119.40
2	B	256	ALA	CA-C-N	5.27	128.80	117.20
1	A	407	TRP	CD1-CG-CD2	5.25	110.50	106.30
2	B	185	TYR	N-CA-CB	-5.25	101.14	110.60
2	B	193	GLN	CA-C-N	5.25	128.75	117.20
1	A	36	MET	C-N-CD	-5.24	109.06	120.60
1	A	141	PHE	CB-CG-CD2	-5.24	117.13	120.80
1	A	123	ARG	NE-CZ-NH2	5.24	122.92	120.30
2	B	41	ASP	O-C-N	5.23	131.07	122.70
1	A	195	LEU	CA-C-O	-5.23	109.12	120.10
2	B	173	PRO	O-C-N	-5.22	114.34	122.70
1	A	42	ILE	CA-C-O	-5.22	109.14	120.10
2	B	176	LYS	O-C-N	-5.21	114.36	122.70
2	B	278	ARG	CA-CB-CG	5.21	124.86	113.40
2	B	214	PHE	CB-CG-CD2	-5.21	117.16	120.80
2	B	48	ARG	NH1-CZ-NH2	-5.20	113.67	119.40
2	B	2	ARG	CA-C-N	-5.19	105.79	117.20
2	B	264	ARG	CB-CA-C	5.17	120.73	110.40
2	B	433	GLN	C-N-CA	-5.17	108.79	121.70
1	A	69	ASP	CA-C-N	5.16	128.55	117.20
1	A	405	VAL	N-CA-CB	-5.16	100.15	111.50
1	A	221	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	B	60	LYS	CA-C-O	5.14	130.90	120.10
1	A	31	GLN	O-C-N	5.14	130.87	121.10
1	A	412	GLY	CA-C-N	5.14	128.51	117.20
1	A	298	PRO	CA-C-N	5.14	128.50	117.20
1	A	299	ALA	CA-C-N	5.14	128.50	117.20
2	B	435	TYR	CD1-CG-CD2	5.14	123.55	117.90
2	B	322	ARG	NH1-CZ-NH2	-5.12	113.77	119.40
2	B	289	PRO	C-N-CA	-5.09	108.97	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	408	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	A	17	GLY	C-N-CA	-5.09	108.98	121.70
2	B	172	VAL	C-N-CD	-5.07	109.44	120.60
1	A	427	ALA	O-C-N	5.06	130.80	122.70
2	B	246	GLY	N-CA-C	5.06	125.75	113.10
2	B	346	TRP	CE2-CD2-CG	-5.06	103.25	107.30
1	A	308	ARG	NE-CZ-NH2	5.05	122.83	120.30
2	B	1	MET	CG-SD-CE	5.05	108.28	100.20
1	A	438	ASP	CA-C-N	5.05	128.31	117.20
1	A	203	MET	CA-C-N	-5.05	106.10	117.20
2	B	337	ASN	O-C-N	-5.04	114.63	122.70
1	A	56	THR	O-C-N	5.03	131.75	123.20
2	B	53	TYR	C-N-CA	5.03	134.28	121.70
1	A	105	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	B	139	HIS	N-CA-CB	-5.01	101.58	110.60
1	A	392	ASP	CA-C-N	5.01	128.22	117.20
2	B	260	VAL	C-N-CD	-5.00	109.59	120.60

There are no chirality outliers.

All (115) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	LYS	Mainchain
1	A	143	GLY	Mainchain
1	A	149	PHE	Mainchain
1	A	179	THR	Peptide,Mainchain
1	A	18	ASN	Mainchain
1	A	187	SER	Mainchain
1	A	193	THR	Mainchain
1	A	218	ASP	Peptide
1	A	221	ARG	Peptide,Mainchain
1	A	24	TYR	Peptide,Mainchain
1	A	267	PHE	Mainchain
1	A	280	LYS	Peptide,Mainchain
1	A	283	HIS	Peptide,Mainchain
1	A	297	GLU	Mainchain
1	A	30	ILE	Peptide,Mainchain
1	A	34	GLY	Peptide
1	A	347	CYS	Mainchain
1	A	350	GLY	Mainchain
1	A	358	GLU	Peptide
1	A	36	MET	Mainchain

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Mol	Chain	Res	Type	Group
1	A	363	VAL	Mainchain
1	A	367	ASP	Mainchain
1	A	368	LEU	Peptide,Mainchain
1	A	369	ALA	Peptide,Mainchain
1	A	38	SER	Peptide,Mainchain
1	A	384	ILE	Mainchain
1	A	392	ASP	Mainchain
1	A	397	LEU	Mainchain
1	A	402	ARG	Peptide,Mainchain
1	A	405	VAL	Peptide
1	A	412	GLY	Peptide
1	A	415	GLU	Peptide,Mainchain
1	A	438	ASP	Mainchain
1	A	49	PHE	Peptide,Mainchain
1	A	50	ASN	Peptide,Mainchain
1	A	53	PHE	Mainchain
1	A	64	ARG	Peptide
1	A	69	ASP	Mainchain
1	A	75	ILE	Mainchain
1	A	77	GLU	Mainchain
1	A	78	VAL	Mainchain
1	A	87	PHE	Peptide
1	A	90	GLU	Mainchain
2	B	105	LYS	Mainchain
2	B	112	ALA	Mainchain
2	B	127	GLU	Peptide,Mainchain
2	B	133	GLN	Mainchain
2	B	143	GLY	Peptide,Mainchain
2	B	148	GLY	Mainchain
2	B	171	VAL	Peptide,Mainchain
2	B	173	PRO	Mainchain
2	B	179	ASP	Peptide,Mainchain
2	B	182	VAL	Peptide,Mainchain
2	B	185	TYR	Sidechain
2	B	187	ALA	Mainchain
2	B	193	GLN	Mainchain
2	B	194	LEU	Mainchain
2	B	200	GLU	Mainchain
2	B	203	CYS	Peptide
2	B	239	THR	Mainchain
2	B	242	LEU	Mainchain
2	B	247	GLN	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
2	B	273	ALA	Peptide
2	B	275	LEU	Peptide,Mainchain
2	B	281	GLN	Mainchain
2	B	284	ARG	Mainchain
2	B	309	HIS	Mainchain
2	B	316	ALA	Mainchain
2	B	321	GLY	Mainchain
2	B	331	GLN	Mainchain
2	B	337	ASN	Mainchain
2	B	340	SER	Mainchain
2	B	344	VAL	Peptide,Mainchain
2	B	347	ILE	Peptide,Mainchain
2	B	356	CYS	Peptide,Mainchain
2	B	393	GLU	Mainchain
2	B	402	LYS	Peptide,Mainchain
2	B	411	GLU	Peptide,Mainchain
2	B	414	ASP	Peptide,Mainchain
2	B	436	GLN	Peptide,Mainchain
2	B	47	GLU	Peptide,Mainchain
2	B	56	ALA	Mainchain
2	B	60	LYS	Peptide,Mainchain
2	B	71	GLU	Peptide
2	B	89	PRO	Peptide,Mainchain

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	3430	0	3257	1656	34
2	B	3359	0	3172	1914	15
3	A	32	0	11	29	0
4	B	28	0	12	14	0
5	B	58	0	51	55	0
All	All	6907	0	6503	3472	35

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 260.

All (3472) 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)
2:B:229:HIS:CE1	5:B:501:TXL:H343	1.28	1.68
2:B:346:TRP:CE3	2:B:347:ILE:HG13	1.25	1.66
1:A:212:ILE:HD11	1:A:230:LEU:CD2	1.25	1.65
2:B:151:THR:CB	2:B:192:HIS:CD2	1.75	1.62
1:A:115:ILE:CD1	1:A:152:LEU:HG	1.15	1.62
2:B:405:LEU:HD22	2:B:418:PHE:CZ	1.17	1.62
2:B:147:SER:HB3	2:B:189:LEU:CD1	1.19	1.62
2:B:287:THR:HB	2:B:290:GLU:CB	1.26	1.62
2:B:158:ARG:CB	2:B:197:ASN:CB	1.76	1.61
2:B:184:PRO:HG2	2:B:399:PHE:CE2	1.12	1.60
1:A:210:TYR:CE1	2:B:326:LYS:CG	1.78	1.60
1:A:407:TRP:CH2	2:B:165:ILE:CD1	1.81	1.59
2:B:158:ARG:HB2	2:B:197:ASN:CB	1.14	1.59
1:A:217:LEU:HD13	1:A:368:LEU:CD1	1.25	1.59
1:A:53:PHE:N	1:A:88:HIS:CE1	1.68	1.58
1:A:220:GLU:CB	1:A:220:GLU:CG	1.78	1.58
1:A:405:VAL:CG2	1:A:405:VAL:CB	1.76	1.58
2:B:151:THR:HG22	2:B:192:HIS:CE1	1.39	1.57
2:B:181:VAL:HG13	2:B:399:PHE:CZ	1.40	1.57
1:A:204:VAL:CG1	1:A:209:ILE:HD11	1.17	1.57
2:B:6:HIS:CE1	2:B:30:ILE:HD12	1.39	1.56
2:B:346:TRP:CZ3	2:B:347:ILE:HD11	1.34	1.56
2:B:405:LEU:CD1	2:B:408:TYR:CB	1.76	1.56
2:B:70:LEU:HD12	2:B:94:PHE:CD2	1.40	1.56
2:B:151:THR:CA	2:B:192:HIS:CD2	1.89	1.55
1:A:115:ILE:HD12	1:A:152:LEU:CG	1.26	1.55
1:A:296:PHE:CE1	1:A:335:ILE:HD13	1.38	1.55
1:A:31:GLN:HE22	1:A:243:ARG:CG	1.15	1.54
2:B:158:ARG:CD	2:B:197:ASN:HB2	1.30	1.54
1:A:407:TRP:HH2	2:B:165:ILE:CD1	1.07	1.53
2:B:405:LEU:CD2	2:B:418:PHE:CZ	1.91	1.53
2:B:181:VAL:CG1	2:B:399:PHE:HZ	1.18	1.53
2:B:399:PHE:CE1	2:B:408:TYR:HE2	1.22	1.53
2:B:295:MET:CE	2:B:375:ALA:HB1	1.08	1.53
2:B:158:ARG:CG	2:B:197:ASN:HB2	1.13	1.52
1:A:210:TYR:CD1	2:B:326:LYS:HG2	1.43	1.52
1:A:103:TYR:CE2	1:A:189:LEU:HD23	1.41	1.52
2:B:158:ARG:CA	2:B:197:ASN:HD22	0.89	1.52
1:A:62:VAL:CG1	1:A:63:PRO:HD2	1.39	1.51
1:A:407:TRP:CH2	2:B:165:ILE:HD11	1.39	1.51
2:B:184:PRO:CG	2:B:399:PHE:CG	1.92	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD12	1:A:145:THR:CG2	1.07	1.51
1:A:100:ALA:CB	1:A:105:ARG:HD3	1.38	1.51
1:A:158:SER:CB	1:A:197:HIS:CB	1.84	1.51
1:A:103:TYR:CD2	1:A:189:LEU:HD23	1.44	1.50
2:B:151:THR:HG22	2:B:192:HIS:ND1	1.24	1.50
1:A:64:ARG:HH22	1:A:132:LEU:CD2	1.22	1.50
1:A:210:TYR:CE2	1:A:227:LEU:HD22	1.45	1.50
2:B:169:PHE:CE1	2:B:235:MET:HG2	1.46	1.50
2:B:346:TRP:CE3	2:B:347:ILE:CG1	1.90	1.49
2:B:192:HIS:CA	2:B:196:GLU:HG3	1.42	1.48
1:A:272:TYR:CE1	1:A:274:PRO:O	1.64	1.48
2:B:107:HIS:C	2:B:152:LEU:HD11	1.35	1.47
1:A:107:HIS:HB2	1:A:148:GLY:CA	1.42	1.46
2:B:405:LEU:HD13	2:B:408:TYR:CD2	1.48	1.46
2:B:19:LYS:CB	2:B:228:ASN:HB3	1.45	1.46
2:B:259:MET:HB3	2:B:268:PHE:CE1	1.47	1.46
1:A:31:GLN:CD	1:A:243:ARG:HD2	1.08	1.45
2:B:399:PHE:HE1	2:B:408:TYR:CE2	1.30	1.45
1:A:31:GLN:N	1:A:32:PRO:CD	1.76	1.44
1:A:70:LEU:CD1	1:A:145:THR:HG22	0.98	1.44
2:B:70:LEU:CD1	2:B:94:PHE:CD2	1.99	1.44
1:A:107:HIS:CB	1:A:148:GLY:HA3	1.47	1.44
2:B:87:PHE:CE1	2:B:89:PRO:HG2	1.52	1.44
2:B:135:PHE:HB3	2:B:166:MET:CE	1.47	1.44
2:B:147:SER:CB	2:B:189:LEU:CD1	1.79	1.44
2:B:158:ARG:HD2	2:B:197:ASN:CA	1.44	1.44
2:B:239:THR:O	2:B:243:ARG:CD	1.65	1.44
2:B:405:LEU:CD1	2:B:408:TYR:HB2	0.96	1.44
1:A:250:VAL:HG13	1:A:254:GLU:CB	1.48	1.43
1:A:212:ILE:CD1	1:A:230:LEU:HD21	1.45	1.43
2:B:172:VAL:CG1	2:B:173:PRO:HD2	1.46	1.43
2:B:405:LEU:CD2	2:B:418:PHE:CE2	1.99	1.43
1:A:172:TYR:OH	1:A:387:ALA:CB	1.64	1.43
2:B:286:LEU:CD1	2:B:372:LYS:HB2	1.47	1.43
1:A:397:LEU:CD2	1:A:401:LYS:HD2	1.47	1.42
2:B:295:MET:CE	2:B:375:ALA:CB	1.93	1.42
2:B:405:LEU:HD11	2:B:408:TYR:CB	1.34	1.42
2:B:147:SER:CB	2:B:189:LEU:HD11	0.95	1.41
2:B:19:LYS:HG3	2:B:228:ASN:CB	1.46	1.41
2:B:103:TRP:CZ3	2:B:413:MET:HE2	1.56	1.41
2:B:151:THR:CA	2:B:192:HIS:NE2	1.82	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:PRO:HG2	2:B:399:PHE:CG	1.55	1.40
1:A:53:PHE:CA	1:A:88:HIS:CE1	2.01	1.40
2:B:7:ILE:HB	2:B:137:LEU:CD2	1.51	1.40
2:B:158:ARG:CG	2:B:197:ASN:CB	1.95	1.40
2:B:151:THR:HB	2:B:192:HIS:CD2	1.39	1.40
1:A:64:ARG:NH2	1:A:132:LEU:HD22	1.31	1.40
1:A:222:PRO:CB	1:A:222:PRO:CG	1.86	1.40
1:A:277:SER:OG	1:A:280:LYS:CG	1.68	1.40
2:B:175:PRO:O	2:B:176:LYS:CE	1.70	1.40
1:A:210:TYR:CE1	2:B:326:LYS:HG2	0.86	1.39
2:B:57:ALA:HA	2:B:64:ARG:CB	1.52	1.39
2:B:399:PHE:CE1	2:B:408:TYR:CE2	2.03	1.39
1:A:103:TYR:CD2	1:A:147:SER:HB2	1.50	1.39
2:B:151:THR:HA	2:B:192:HIS:CD2	1.49	1.39
1:A:176:GLN:O	1:A:177:VAL:CG2	1.70	1.38
2:B:19:LYS:CG	2:B:228:ASN:HB3	1.50	1.38
2:B:184:PRO:CB	2:B:399:PHE:CD2	2.05	1.38
2:B:435:TYR:O	2:B:436:GLN:CG	1.72	1.38
1:A:250:VAL:HG13	1:A:254:GLU:CG	1.53	1.37
2:B:103:TRP:CD1	2:B:189:LEU:HD23	1.57	1.37
2:B:75:MET:HE1	2:B:79:ARG:CD	1.53	1.37
2:B:405:LEU:HD22	2:B:418:PHE:CE2	1.56	1.37
1:A:210:TYR:HE1	2:B:326:LYS:CG	1.20	1.37
2:B:20:PHE:HE2	2:B:235:MET:CB	1.24	1.37
2:B:20:PHE:CE2	2:B:235:MET:HB3	1.50	1.36
2:B:87:PHE:CD1	2:B:88:ARG:O	1.76	1.36
1:A:204:VAL:CG2	1:A:231:ILE:HG23	1.50	1.36
1:A:68:VAL:HG11	1:A:149:PHE:CZ	1.57	1.36
2:B:175:PRO:O	2:B:176:LYS:CD	1.74	1.36
1:A:288:VAL:CG2	1:A:373:ARG:HD3	1.52	1.35
2:B:192:HIS:HA	2:B:196:GLU:CG	1.55	1.35
2:B:184:PRO:CD	2:B:399:PHE:CD2	2.08	1.35
1:A:212:ILE:CD1	1:A:230:LEU:CD2	2.02	1.35
2:B:311:ARG:HG2	2:B:341:SER:O	1.21	1.35
1:A:369:ALA:CB	1:A:371:VAL:HG23	1.56	1.34
2:B:151:THR:HA	2:B:192:HIS:NE2	1.04	1.34
2:B:158:ARG:HA	2:B:197:ASN:ND2	1.04	1.34
1:A:217:LEU:CD1	1:A:368:LEU:HD11	1.55	1.34
2:B:19:LYS:CG	2:B:228:ASN:CB	2.02	1.34
1:A:108:TYR:O	1:A:112:LYS:CD	1.76	1.34
1:A:182:VAL:HG13	1:A:186:ASN:ND2	1.40	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:LEU:HD23	2:B:85:GLN:CG	1.34	1.34
2:B:24:ILE:O	2:B:26:ASP:N	1.60	1.33
2:B:405:LEU:CD1	2:B:408:TYR:CD2	2.06	1.33
2:B:97:SER:HB2	2:B:110:GLU:OE1	1.19	1.33
2:B:12:CYS:O	2:B:16:ILE:HG12	1.25	1.33
1:A:184:PRO:HG3	1:A:395:PHE:CB	1.57	1.33
2:B:32:PRO:CB	2:B:59:ASN:HD22	1.25	1.33
2:B:96:GLN:O	2:B:98:GLY:N	1.59	1.33
2:B:229:HIS:CD2	5:B:501:TXL:H38	1.54	1.33
2:B:305:CYS:SG	2:B:384:ILE:HD13	1.67	1.33
2:B:22:GLU:HG2	2:B:83:PHE:CD2	1.63	1.32
2:B:435:TYR:C	2:B:436:GLN:HG3	1.17	1.32
1:A:272:TYR:CZ	1:A:274:PRO:HG2	1.62	1.32
2:B:183:GLU:HB2	2:B:184:PRO:CD	1.59	1.32
2:B:294:GLN:CG	2:B:300:ASN:OD1	1.77	1.32
1:A:30:ILE:O	1:A:32:PRO:HG2	1.27	1.32
2:B:201:THR:CG2	2:B:265:LEU:HD21	1.58	1.32
2:B:346:TRP:CZ3	2:B:347:ILE:CD1	2.10	1.32
1:A:30:ILE:O	1:A:32:PRO:CG	1.78	1.31
1:A:250:VAL:CG2	1:A:352:LYS:HE2	1.60	1.31
1:A:306:ASP:OD1	1:A:308:ARG:CG	1.76	1.31
2:B:335:VAL:O	2:B:339:ASN:ND2	1.60	1.31
1:A:31:GLN:NE2	1:A:243:ARG:CG	1.93	1.31
1:A:179:THR:HG22	1:A:181:VAL:N	1.42	1.31
1:A:31:GLN:NE2	1:A:243:ARG:CD	1.92	1.31
2:B:114:LEU:HD12	2:B:117:SER:OG	1.24	1.31
2:B:435:TYR:O	2:B:436:GLN:HG3	1.20	1.31
2:B:175:PRO:O	2:B:176:LYS:HE2	1.22	1.31
1:A:179:THR:CG2	1:A:181:VAL:H	1.42	1.31
1:A:250:VAL:CG1	1:A:254:GLU:HB3	1.61	1.30
1:A:53:PHE:N	1:A:88:HIS:NE2	1.75	1.30
2:B:20:PHE:CE2	2:B:235:MET:CB	2.00	1.30
2:B:75:MET:CE	2:B:79:ARG:HD2	1.60	1.30
2:B:145:THR:O	2:B:149:MET:HB3	1.19	1.30
2:B:158:ARG:HD2	2:B:197:ASN:CB	1.59	1.30
1:A:103:TYR:CD2	1:A:189:LEU:CD2	2.13	1.30
1:A:277:SER:CB	1:A:280:LYS:HG2	1.59	1.30
1:A:31:GLN:CD	1:A:243:ARG:CD	1.99	1.30
1:A:115:ILE:CD1	1:A:152:LEU:CG	1.92	1.30
1:A:225:THR:CG2	2:B:247:GLN:HE22	1.43	1.30
2:B:151:THR:HG22	2:B:192:HIS:CG	1.67	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:THR:O	2:B:398:MET:CE	1.78	1.29
2:B:229:HIS:CG	5:B:501:TXL:H38	1.67	1.29
2:B:244:PHE:CD2	2:B:245:PRO:HD2	1.65	1.29
2:B:319:PHE:CE1	2:B:353:THR:HG23	1.67	1.29
2:B:201:THR:HG21	2:B:265:LEU:CD2	1.60	1.29
2:B:268:PHE:CE1	2:B:380:ASN:ND2	1.99	1.29
2:B:32:PRO:CB	2:B:59:ASN:ND2	1.80	1.28
2:B:69:ASP:OD2	2:B:74:THR:HB	1.32	1.28
1:A:291:ILE:HG22	1:A:375:VAL:CG2	1.62	1.28
2:B:107:HIS:CA	2:B:152:LEU:HD11	1.63	1.28
1:A:184:PRO:CG	1:A:395:PHE:CD2	2.17	1.28
2:B:4:ILE:HD12	2:B:30:ILE:C	1.53	1.28
2:B:107:HIS:CD2	2:B:152:LEU:HG	1.66	1.28
2:B:181:VAL:CG1	2:B:399:PHE:CZ	2.03	1.28
2:B:295:MET:HE3	2:B:375:ALA:CB	1.55	1.28
1:A:172:TYR:OH	1:A:387:ALA:HB3	1.11	1.28
2:B:142:GLY:C	2:B:185:TYR:CE1	2.07	1.28
2:B:158:ARG:CB	2:B:197:ASN:HB2	1.44	1.28
2:B:192:HIS:O	2:B:196:GLU:HB2	1.17	1.28
1:A:38:SER:O	1:A:39:ASP:N	1.58	1.27
1:A:266:HIS:CD2	1:A:432:TYR:HE1	1.50	1.27
1:A:101:ASN:O	1:A:102:ASN:CG	1.72	1.27
2:B:192:HIS:CA	2:B:196:GLU:CG	2.12	1.27
2:B:192:HIS:O	2:B:196:GLU:CB	1.80	1.27
2:B:287:THR:O	2:B:291:LEU:CG	1.81	1.27
1:A:97:GLU:CB	1:A:110:ILE:HG21	1.65	1.27
2:B:193:GLN:O	2:B:265:LEU:CD2	1.82	1.27
2:B:151:THR:CG2	2:B:192:HIS:CG	2.16	1.27
2:B:259:MET:HE1	2:B:379:GLY:CA	1.64	1.26
2:B:103:TRP:CE3	2:B:413:MET:HE1	1.69	1.26
2:B:92:PHE:CD2	2:B:114:LEU:HD11	1.70	1.26
2:B:312:TYR:HA	2:B:381:SER:CB	1.63	1.26
1:A:2:ARG:CG	1:A:133:GLN:OE1	1.82	1.26
1:A:272:TYR:HE1	1:A:274:PRO:O	0.94	1.26
2:B:94:PHE:HD1	2:B:94:PHE:O	1.16	1.26
2:B:12:CYS:O	2:B:16:ILE:CG1	1.82	1.26
1:A:204:VAL:CG1	1:A:209:ILE:CD1	2.13	1.25
2:B:102:ASN:HD22	2:B:105:LYS:CE	1.49	1.25
2:B:183:GLU:CB	2:B:184:PRO:HD3	1.63	1.25
1:A:219:ILE:CB	1:A:219:ILE:CG2	2.13	1.25
2:B:107:HIS:O	2:B:152:LEU:HD11	1.28	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLU:HA	1:A:80:THR:OG1	1.09	1.25
2:B:103:TRP:CD1	2:B:189:LEU:CD2	2.18	1.25
2:B:111:GLY:O	2:B:115:VAL:HG23	1.32	1.25
2:B:3:GLU:OE1	2:B:130:ASP:CB	1.84	1.25
2:B:287:THR:CG2	2:B:289:PRO:HD2	1.67	1.25
1:A:288:VAL:HG22	1:A:373:ARG:CD	1.65	1.25
2:B:57:ALA:CA	2:B:64:ARG:HB2	1.64	1.25
1:A:108:TYR:CA	1:A:112:LYS:HE3	1.67	1.24
1:A:306:ASP:OD1	1:A:308:ARG:HG3	1.16	1.24
2:B:87:PHE:CE1	2:B:88:ARG:O	1.87	1.24
2:B:312:TYR:O	2:B:344:VAL:CG2	1.84	1.24
1:A:9:VAL:HG11	1:A:150:THR:CG2	1.67	1.24
2:B:4:ILE:HD13	2:B:30:ILE:CG2	1.68	1.24
2:B:107:HIS:HA	2:B:152:LEU:CD1	1.67	1.24
2:B:182:VAL:HG13	2:B:186:ASN:ND2	1.48	1.24
1:A:53:PHE:HA	1:A:88:HIS:CE1	1.64	1.24
2:B:237:GLY:HA2	2:B:241:CYS:SG	1.74	1.24
1:A:433:GLU:O	1:A:437:VAL:HG23	1.32	1.24
2:B:143:GLY:N	2:B:185:TYR:CE1	2.06	1.24
2:B:143:GLY:N	2:B:185:TYR:HE1	1.35	1.24
1:A:38:SER:C	1:A:39:ASP:CA	2.04	1.24
1:A:291:ILE:CG2	1:A:375:VAL:HG23	1.65	1.24
1:A:383:ALA:O	1:A:385:ALA:N	1.69	1.24
1:A:107:HIS:HB2	1:A:148:GLY:C	1.59	1.23
1:A:242:LEU:HD12	1:A:255:PHE:CZ	1.73	1.23
2:B:237:GLY:O	2:B:241:CYS:HB2	1.33	1.23
1:A:20:CYS:O	1:A:24:TYR:CD2	1.91	1.23
1:A:276:ILE:O	1:A:368:LEU:HB3	1.31	1.23
2:B:103:TRP:CE3	2:B:413:MET:CE	2.20	1.23
1:A:4:CYS:HB2	1:A:30:ILE:CG2	1.68	1.23
1:A:30:ILE:CG2	1:A:64:ARG:HG2	1.68	1.23
1:A:206:ASN:ND2	1:A:227:LEU:CD2	2.00	1.23
1:A:210:TYR:CE2	1:A:227:LEU:CD2	2.21	1.23
2:B:35:SER:O	2:B:37:HIS:N	1.71	1.23
1:A:185:TYR:HD2	1:A:408:TYR:OH	0.92	1.23
2:B:87:PHE:HE1	2:B:89:PRO:CG	1.51	1.23
1:A:77:GLU:CA	1:A:80:THR:OG1	1.86	1.23
1:A:360:PRO:CG	1:A:371:VAL:O	1.86	1.23
2:B:287:THR:CB	2:B:290:GLU:HB2	1.67	1.23
1:A:312:TYR:O	1:A:344:VAL:CG2	1.87	1.22
2:B:244:PHE:CE2	2:B:358:ILE:HD12	1.73	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:TYR:O	1:A:112:LYS:CE	1.85	1.22
2:B:184:PRO:CD	2:B:399:PHE:HD2	1.49	1.22
2:B:103:TRP:HD1	2:B:189:LEU:CD2	1.49	1.22
2:B:189:LEU:O	2:B:193:GLN:HG3	1.31	1.22
2:B:319:PHE:HE1	2:B:353:THR:CG2	1.50	1.22
2:B:405:LEU:CD1	2:B:408:TYR:CG	2.20	1.22
1:A:3:GLU:HA	1:A:31:GLN:CB	1.70	1.22
1:A:28:HIS:CE1	1:A:29:GLY:O	1.93	1.22
1:A:93:ILE:CD1	1:A:118:VAL:HG22	1.70	1.22
1:A:16:ILE:HD13	1:A:138:PHE:CD1	1.75	1.22
1:A:108:TYR:O	1:A:112:LYS:HE3	1.40	1.22
1:A:206:ASN:ND2	1:A:227:LEU:HD21	1.51	1.22
1:A:78:VAL:CG1	1:A:87:PHE:HE1	1.53	1.21
2:B:97:SER:CB	2:B:110:GLU:OE1	1.89	1.21
1:A:31:GLN:OE1	1:A:243:ARG:CD	1.85	1.21
1:A:48:SER:O	1:A:56:THR:CG2	1.87	1.21
1:A:158:SER:CB	1:A:197:HIS:HB3	1.49	1.21
1:A:220:GLU:O	1:A:222:PRO:CD	1.89	1.21
1:A:259:LEU:O	1:A:261:PRO:HD3	1.38	1.21
2:B:175:PRO:O	2:B:176:LYS:CG	1.88	1.21
1:A:220:GLU:C	1:A:222:PRO:HD3	1.61	1.21
2:B:319:PHE:CE1	2:B:328:VAL:CG1	2.24	1.21
1:A:344:VAL:HB	1:A:347:CYS:SG	1.80	1.21
1:A:396:ASP:O	1:A:401:LYS:HB2	1.40	1.21
1:A:2:ARG:HG2	1:A:133:GLN:OE1	1.05	1.21
1:A:26:LEU:HD11	1:A:361:THR:CG2	1.69	1.21
1:A:108:TYR:C	1:A:112:LYS:HE3	1.59	1.21
1:A:3:GLU:O	1:A:132:LEU:O	1.59	1.20
1:A:31:GLN:OE1	1:A:243:ARG:HD2	1.02	1.20
2:B:229:HIS:CE1	5:B:501:TXL:C34	2.23	1.20
1:A:183:GLU:HB3	1:A:394:LYS:HB3	1.24	1.20
1:A:272:TYR:CE1	1:A:274:PRO:HG2	1.75	1.20
1:A:343:PHE:CE2	1:A:351:PHE:CZ	2.30	1.20
1:A:31:GLN:N	1:A:32:PRO:HD3	1.05	1.20
1:A:176:GLN:O	1:A:177:VAL:HG23	1.03	1.20
1:A:184:PRO:HG3	1:A:395:PHE:CD2	1.74	1.20
1:A:332:ILE:CD1	1:A:353:VAL:HG21	1.70	1.20
2:B:6:HIS:HE1	2:B:30:ILE:CD1	1.53	1.20
1:A:177:VAL:HG12	1:A:178:SER:H	1.04	1.19
2:B:36:TYR:CE2	2:B:244:PHE:CE1	1.94	1.19
2:B:107:HIS:O	2:B:152:LEU:CD1	1.89	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:PHE:CE1	2:B:235:MET:CG	2.25	1.19
1:A:222:PRO:O	2:B:324:SER:HB2	1.40	1.19
1:A:103:TYR:CD1	1:A:188:ILE:CG2	2.26	1.19
2:B:44:LEU:O	2:B:47:GLU:CG	1.91	1.19
1:A:30:ILE:HB	1:A:64:ARG:HB2	1.24	1.19
1:A:224:TYR:CD2	2:B:325:MET:HB3	1.77	1.19
2:B:151:THR:CG2	2:B:192:HIS:CE1	2.26	1.19
2:B:259:MET:CE	2:B:379:GLY:HA2	1.72	1.19
2:B:312:TYR:HA	2:B:381:SER:CA	1.71	1.19
1:A:48:SER:O	1:A:56:THR:HG21	1.02	1.18
2:B:175:PRO:HD3	2:B:390:ARG:NH2	1.57	1.18
1:A:4:CYS:SG	1:A:252:LEU:HD11	1.83	1.18
2:B:370:GLY:O	5:B:501:TXL:H183	1.43	1.18
1:A:184:PRO:CB	1:A:395:PHE:HD2	1.55	1.18
2:B:135:PHE:CB	2:B:166:MET:CE	2.20	1.18
2:B:250:ALA:HA	2:B:254:LYS:HD2	1.25	1.18
2:B:346:TRP:HE3	2:B:347:ILE:CG1	1.35	1.18
1:A:100:ALA:HB2	1:A:105:ARG:HD3	1.19	1.18
2:B:44:LEU:O	2:B:47:GLU:HG3	1.01	1.18
2:B:174:SER:CB	2:B:207:GLU:HB3	1.73	1.18
1:A:62:VAL:CG1	1:A:63:PRO:CD	2.22	1.17
1:A:437:VAL:O	1:A:438:ASP:OD1	1.62	1.17
2:B:294:GLN:HG2	2:B:300:ASN:OD1	1.01	1.17
1:A:397:LEU:HD22	1:A:401:LYS:HD2	1.27	1.17
1:A:115:ILE:HD13	1:A:156:ARG:CZ	1.74	1.17
1:A:174:ALA:HB1	1:A:175:PRO:CD	1.75	1.17
1:A:100:ALA:CB	1:A:105:ARG:CD	2.23	1.17
1:A:177:VAL:HB	2:B:349:ASN:ND2	1.60	1.17
2:B:382:THR:CG2	2:B:436:GLN:OE1	1.78	1.17
1:A:220:GLU:O	1:A:222:PRO:HD2	1.45	1.16
2:B:7:ILE:CA	2:B:66:ILE:HG23	1.75	1.16
2:B:87:PHE:CE1	2:B:89:PRO:CG	2.23	1.16
2:B:435:TYR:C	2:B:436:GLN:CG	2.06	1.16
1:A:30:ILE:C	1:A:32:PRO:CD	2.11	1.16
2:B:183:GLU:HB2	2:B:398:MET:SD	1.85	1.16
2:B:405:LEU:HD12	2:B:408:TYR:CB	1.56	1.16
1:A:176:GLN:HE21	2:B:333:LEU:CD2	1.58	1.16
1:A:217:LEU:CD1	1:A:368:LEU:CD1	2.14	1.16
2:B:154:ILE:HG21	2:B:198:THR:HG23	1.21	1.16
2:B:183:GLU:CD	2:B:394:GLN:HB3	1.66	1.16
1:A:184:PRO:HG3	1:A:395:PHE:CG	1.80	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:VAL:CG2	2:B:421:ALA:HA	1.75	1.16
2:B:287:THR:HG22	2:B:289:PRO:HD2	1.20	1.16
1:A:59:GLY:O	1:A:62:VAL:O	1.63	1.16
2:B:32:PRO:HB2	2:B:59:ASN:ND2	1.00	1.16
1:A:115:ILE:HD12	1:A:152:LEU:CD2	1.75	1.15
1:A:185:TYR:CD2	1:A:408:TYR:OH	1.85	1.15
1:A:210:TYR:CD1	2:B:326:LYS:CG	2.10	1.15
1:A:103:TYR:HD2	1:A:147:SER:CB	1.59	1.15
1:A:137:VAL:HG21	1:A:154:MET:SD	1.85	1.15
2:B:75:MET:CE	2:B:79:ARG:CD	2.17	1.15
2:B:151:THR:CG2	2:B:192:HIS:CD2	2.27	1.15
1:A:176:GLN:NE2	2:B:333:LEU:HD22	1.60	1.15
1:A:204:VAL:HG21	1:A:231:ILE:CG2	1.47	1.15
2:B:7:ILE:HA	2:B:66:ILE:CG2	1.75	1.15
2:B:175:PRO:C	2:B:176:LYS:HG2	1.54	1.15
2:B:313:LEU:CD2	2:B:344:VAL:HG11	1.75	1.15
2:B:7:ILE:CG1	2:B:66:ILE:HG21	1.77	1.15
1:A:31:GLN:NE2	1:A:243:ARG:HD2	1.51	1.15
2:B:320:ARG:HG2	2:B:374:SER:OG	1.47	1.15
2:B:22:GLU:HB3	2:B:83:PHE:CZ	1.82	1.14
1:A:155:GLU:HG3	1:A:192:HIS:CD2	1.82	1.14
1:A:62:VAL:HG13	1:A:63:PRO:CD	1.77	1.14
2:B:22:GLU:CG	2:B:83:PHE:CD2	2.30	1.14
2:B:103:TRP:CZ3	2:B:413:MET:CE	2.28	1.14
2:B:151:THR:CB	2:B:192:HIS:CG	2.31	1.14
2:B:158:ARG:CB	2:B:197:ASN:HD22	1.60	1.14
2:B:312:TYR:HA	2:B:381:SER:HB3	1.30	1.14
2:B:22:GLU:HB3	2:B:83:PHE:CE2	1.81	1.14
2:B:33:THR:N	2:B:59:ASN:HD22	1.42	1.14
2:B:50:ASN:N	2:B:61:TYR:CD2	2.15	1.14
2:B:172:VAL:CG1	2:B:173:PRO:CD	2.25	1.14
2:B:234:THR:OG1	2:B:302:MET:SD	2.05	1.14
2:B:241:CYS:SG	2:B:320:ARG:NH1	2.20	1.14
2:B:244:PHE:HE2	2:B:358:ILE:CD1	1.60	1.14
1:A:312:TYR:HA	1:A:381:THR:HG22	1.26	1.14
2:B:56:ALA:HB3	2:B:62:VAL:CB	1.78	1.14
2:B:104:ALA:HA	2:B:108:TYR:CD2	1.83	1.14
2:B:151:THR:HB	2:B:192:HIS:CG	1.81	1.14
2:B:234:THR:OG1	2:B:302:MET:CE	1.95	1.14
2:B:296:PHE:CZ	2:B:335:VAL:HG11	1.83	1.14
2:B:193:GLN:O	2:B:265:LEU:HD22	0.96	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ALA:CB	1:A:175:PRO:CD	2.20	1.13
1:A:296:PHE:CE1	1:A:335:ILE:CD1	2.31	1.13
1:A:57:GLY:HA3	1:A:61:HIS:CE1	1.83	1.13
1:A:184:PRO:CG	1:A:395:PHE:HD2	1.56	1.13
1:A:217:LEU:HD13	1:A:368:LEU:HD13	1.21	1.13
1:A:217:LEU:CG	1:A:368:LEU:HD11	1.79	1.13
2:B:48:ARG:HH11	2:B:60:LYS:CA	1.62	1.13
2:B:105:LYS:HE2	2:B:411:GLU:OE2	1.48	1.13
1:A:217:LEU:HG	1:A:218:ASP:H	0.96	1.13
1:A:312:TYR:CE2	1:A:377:MET:CE	2.32	1.13
2:B:107:HIS:CD2	2:B:152:LEU:CG	2.32	1.13
2:B:44:LEU:CD2	2:B:85:GLN:HG3	1.78	1.12
2:B:176:LYS:HE3	2:B:207:GLU:OE2	1.49	1.12
2:B:390:ARG:O	2:B:394:GLN:HG2	1.46	1.13
1:A:100:ALA:HB1	1:A:105:ARG:HD3	1.13	1.12
1:A:182:VAL:CG1	1:A:186:ASN:ND2	2.12	1.12
1:A:266:HIS:CD2	1:A:432:TYR:CE1	2.38	1.12
1:A:312:TYR:CE2	1:A:377:MET:HE1	1.84	1.12
2:B:141:LEU:HD22	2:B:186:ASN:HB3	1.21	1.12
2:B:154:ILE:HG21	2:B:198:THR:CG2	1.79	1.12
1:A:105:ARG:HH21	1:A:110:ILE:HD11	1.03	1.12
2:B:107:HIS:CE1	2:B:152:LEU:HD21	1.84	1.12
1:A:38:SER:CA	1:A:39:ASP:N	2.11	1.12
2:B:102:ASN:HD22	2:B:105:LYS:NZ	1.45	1.12
2:B:158:ARG:CB	2:B:197:ASN:ND2	2.10	1.12
1:A:26:LEU:HD11	1:A:361:THR:HG21	1.23	1.12
2:B:41:ASP:O	2:B:42:LEU:HG	1.45	1.12
2:B:154:ILE:CG2	2:B:198:THR:HG23	1.79	1.12
1:A:48:SER:OG	1:A:56:THR:HB	1.51	1.11
2:B:80:SER:C	2:B:82:PRO:HD2	1.70	1.11
2:B:107:HIS:NE2	2:B:152:LEU:HD23	1.64	1.11
2:B:242:LEU:HD13	2:B:250:ALA:HB3	1.28	1.11
1:A:10:GLY:O	1:A:13:GLY:N	1.83	1.11
1:A:97:GLU:CB	1:A:110:ILE:CG2	2.27	1.11
1:A:407:TRP:CZ2	2:B:256:ALA:HB1	1.84	1.11
2:B:201:THR:CG2	2:B:265:LEU:HD11	1.79	1.11
2:B:209:LEU:HD13	2:B:227:LEU:HG	1.21	1.11
2:B:287:THR:CB	2:B:290:GLU:CB	2.23	1.11
2:B:312:TYR:O	2:B:344:VAL:HG23	1.47	1.11
2:B:313:LEU:HD23	2:B:344:VAL:CG2	1.79	1.11
2:B:385:GLN:CG	2:B:389:LYS:HE3	1.79	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:HIS:O	2:B:196:GLU:CG	1.98	1.11
2:B:287:THR:HB	2:B:290:GLU:HB3	1.21	1.11
2:B:295:MET:HE1	2:B:375:ALA:CB	1.62	1.11
2:B:319:PHE:CD1	2:B:328:VAL:HG11	1.85	1.11
1:A:22:GLU:HG2	1:A:85:GLN:HE22	0.95	1.11
1:A:174:ALA:HB1	1:A:390:ARG:HH22	1.03	1.10
2:B:6:HIS:CE1	2:B:30:ILE:CD1	2.32	1.10
2:B:287:THR:HG22	2:B:289:PRO:CD	1.79	1.10
1:A:103:TYR:CD1	1:A:188:ILE:HG21	1.86	1.10
2:B:70:LEU:CD1	2:B:94:PHE:HD2	1.47	1.10
2:B:184:PRO:CG	2:B:399:PHE:CE2	1.90	1.10
2:B:346:TRP:O	2:B:347:ILE:HB	1.49	1.10
2:B:405:LEU:HD21	2:B:418:PHE:CE2	1.82	1.10
1:A:107:HIS:CB	1:A:148:GLY:CA	2.17	1.10
1:A:169:PHE:CZ	1:A:235:VAL:HG22	1.85	1.10
2:B:107:HIS:CA	2:B:152:LEU:CD1	2.25	1.10
2:B:181:VAL:HG12	2:B:399:PHE:HZ	1.06	1.10
1:A:93:ILE:HD13	1:A:118:VAL:HG22	1.11	1.10
2:B:80:SER:O	2:B:82:PRO:HD2	1.52	1.10
2:B:103:TRP:HZ3	2:B:108:TYR:OH	1.33	1.10
1:A:100:ALA:HB2	1:A:105:ARG:CD	1.80	1.10
1:A:177:VAL:HB	2:B:349:ASN:HD21	1.05	1.10
2:B:3:GLU:HB3	2:B:132:LEU:HD23	1.33	1.10
2:B:66:ILE:HG13	2:B:121:VAL:CG1	1.82	1.10
2:B:94:PHE:O	2:B:94:PHE:CD1	2.05	1.10
2:B:259:MET:CE	2:B:379:GLY:CA	2.29	1.10
2:B:286:LEU:HD11	2:B:372:LYS:HB2	1.12	1.10
2:B:321:GLY:HA3	2:B:373:MET:HG3	1.22	1.10
1:A:174:ALA:HB1	1:A:175:PRO:HD3	1.27	1.09
2:B:48:ARG:HB2	2:B:61:TYR:HA	1.33	1.09
2:B:242:LEU:N	2:B:356:CYS:SG	2.25	1.09
2:B:278:ARG:CA	2:B:278:ARG:CB	2.30	1.09
2:B:385:GLN:HG3	2:B:389:LYS:HE3	1.21	1.09
1:A:45:GLY:O	1:A:46:ASP:CB	1.98	1.09
1:A:176:GLN:C	1:A:177:VAL:HG23	1.71	1.09
1:A:266:HIS:NE2	1:A:432:TYR:HE1	1.48	1.09
2:B:111:GLY:C	2:B:115:VAL:HG23	1.70	1.09
2:B:147:SER:OG	2:B:189:LEU:HD11	1.50	1.09
2:B:175:PRO:CD	2:B:390:ARG:HH21	1.66	1.09
2:B:260:VAL:HG22	2:B:266:HIS:HB2	1.21	1.09
1:A:62:VAL:HG12	1:A:63:PRO:HD2	1.24	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:CG	1:A:145:THR:HG22	1.82	1.09
1:A:210:TYR:CZ	1:A:227:LEU:HD22	1.87	1.09
2:B:4:ILE:CD1	2:B:30:ILE:HA	1.83	1.09
2:B:107:HIS:CD2	2:B:152:LEU:CD2	2.34	1.09
2:B:150:GLY:O	2:B:154:ILE:HG13	1.52	1.09
1:A:237:SER:O	1:A:241:SER:OG	1.69	1.09
1:A:312:TYR:HE2	1:A:377:MET:HE1	1.04	1.09
1:A:407:TRP:HH2	2:B:165:ILE:HD12	1.02	1.09
2:B:7:ILE:HG12	2:B:66:ILE:HD13	1.09	1.09
2:B:56:ALA:HB3	2:B:62:VAL:CG2	1.81	1.09
2:B:97:SER:HB2	2:B:110:GLU:CD	1.71	1.09
1:A:97:GLU:HB3	1:A:110:ILE:CG2	1.81	1.09
2:B:3:GLU:OE1	2:B:130:ASP:HB2	0.91	1.09
2:B:158:ARG:CB	2:B:197:ASN:CG	2.19	1.09
1:A:2:ARG:O	1:A:31:GLN:HG3	1.51	1.08
1:A:191:THR:HG21	1:A:421:ALA:CB	1.81	1.08
2:B:135:PHE:CB	2:B:166:MET:HE3	1.78	1.08
2:B:313:LEU:N	2:B:380:ASN:O	1.86	1.08
1:A:277:SER:OG	1:A:280:LYS:HG2	0.93	1.08
2:B:24:ILE:C	2:B:26:ASP:N	2.01	1.08
2:B:158:ARG:HB2	2:B:197:ASN:CG	1.72	1.08
2:B:313:LEU:CD2	2:B:344:VAL:CG1	2.32	1.08
2:B:3:GLU:HA	2:B:31:ASP:CB	1.83	1.08
2:B:44:LEU:HD23	2:B:85:GLN:HG3	1.12	1.08
2:B:244:PHE:CG	2:B:245:PRO:HD2	1.89	1.08
2:B:313:LEU:HD22	2:B:344:VAL:HG11	1.13	1.08
1:A:252:LEU:HA	1:A:255:PHE:HD2	1.18	1.08
1:A:277:SER:OG	1:A:280:LYS:N	1.87	1.08
1:A:360:PRO:HG3	1:A:371:VAL:O	0.91	1.08
2:B:102:ASN:HB2	2:B:105:LYS:HD2	1.33	1.08
2:B:305:CYS:SG	2:B:384:ILE:CD1	2.41	1.08
1:A:3:GLU:CA	1:A:31:GLN:HB2	1.82	1.08
1:A:171:ILE:N	1:A:203:MET:HE1	1.52	1.08
1:A:204:VAL:HG12	1:A:209:ILE:HD11	1.10	1.08
1:A:332:ILE:HD13	1:A:353:VAL:HG21	1.35	1.08
2:B:180:THR:O	2:B:398:MET:HE3	1.47	1.08
1:A:31:GLN:NE2	1:A:243:ARG:HG3	1.56	1.07
1:A:103:TYR:HD2	1:A:189:LEU:CD2	1.59	1.07
1:A:108:TYR:CE2	1:A:417:GLU:OE2	2.06	1.07
1:A:179:THR:HG21	1:A:181:VAL:HB	1.13	1.07
1:A:217:LEU:HD11	1:A:368:LEU:HD21	1.15	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:HG13	1:A:332:ILE:HD11	1.31	1.07
2:B:19:LYS:CD	2:B:228:ASN:HB2	1.84	1.07
2:B:174:SER:OG	2:B:207:GLU:CB	2.02	1.07
2:B:243:ARG:HH21	2:B:252:LEU:HD21	1.17	1.07
2:B:233:ALA:HB1	2:B:272:PHE:CD2	1.87	1.07
2:B:244:PHE:HE2	2:B:358:ILE:HD12	1.06	1.07
1:A:184:PRO:CG	1:A:395:PHE:HA	1.84	1.07
1:A:397:LEU:HD23	1:A:401:LYS:HD2	1.19	1.07
2:B:33:THR:O	2:B:59:ASN:ND2	1.87	1.07
2:B:192:HIS:C	2:B:196:GLU:HG3	1.73	1.07
1:A:78:VAL:HG11	1:A:87:PHE:HE1	1.19	1.07
2:B:319:PHE:CE1	2:B:328:VAL:HG11	1.87	1.07
2:B:33:THR:H	2:B:59:ASN:ND2	1.47	1.07
2:B:107:HIS:NE2	2:B:152:LEU:CD2	2.18	1.07
2:B:277:SER:HB2	2:B:280:SER:HB2	1.30	1.07
1:A:30:ILE:HG21	1:A:64:ARG:HG2	1.15	1.06
1:A:192:HIS:ND1	1:A:193:THR:N	2.03	1.06
1:A:250:VAL:HG21	1:A:352:LYS:HE2	1.13	1.06
1:A:262:TYR:HB3	1:A:263:PRO:CD	1.84	1.06
2:B:107:HIS:HA	2:B:152:LEU:HD12	1.35	1.06
2:B:44:LEU:HD21	2:B:86:ILE:N	1.67	1.06
1:A:32:PRO:O	1:A:34:GLY:N	1.89	1.06
1:A:224:TYR:H	2:B:325:MET:HB2	1.19	1.06
2:B:36:TYR:CD2	2:B:244:PHE:CE1	2.22	1.06
2:B:382:THR:HG21	2:B:436:GLN:OE1	1.51	1.06
1:A:24:TYR:O	1:A:26:LEU:N	1.87	1.06
2:B:53:TYR:CD1	2:B:87:PHE:CZ	2.44	1.06
2:B:154:ILE:HD12	2:B:192:HIS:CE1	1.90	1.06
2:B:192:HIS:C	2:B:196:GLU:CG	2.24	1.06
1:A:105:ARG:NH2	1:A:110:ILE:HD11	1.67	1.05
1:A:204:VAL:HG11	1:A:209:ILE:HD11	1.10	1.05
1:A:206:ASN:HD22	1:A:227:LEU:HD21	0.97	1.05
1:A:250:VAL:HG13	1:A:254:GLU:HB3	1.08	1.05
1:A:292:THR:HG22	1:A:319:TYR:OH	1.53	1.05
2:B:7:ILE:HG12	2:B:66:ILE:HG21	1.34	1.05
2:B:22:GLU:CB	2:B:83:PHE:CE2	2.39	1.05
2:B:36:TYR:CE2	2:B:244:PHE:HE1	1.46	1.05
2:B:213:CYS:HA	2:B:217:LEU:HD12	1.10	1.05
2:B:275:LEU:HG	2:B:294:GLN:HE22	1.21	1.05
1:A:97:GLU:HB2	1:A:110:ILE:HG21	1.38	1.05
1:A:205:ASP:OD1	1:A:303:VAL:CG2	1.98	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:SER:N	2:B:60:LYS:HE3	1.71	1.05
2:B:70:LEU:HD11	2:B:94:PHE:CD2	1.92	1.05
2:B:141:LEU:CD1	2:B:172:VAL:HA	1.86	1.05
2:B:265:LEU:HD23	2:B:267:PHE:CZ	1.92	1.05
1:A:70:LEU:HD12	1:A:145:THR:CB	1.86	1.05
1:A:174:ALA:CB	1:A:175:PRO:HD2	1.86	1.05
2:B:19:LYS:CG	2:B:228:ASN:HB2	1.86	1.05
2:B:135:PHE:CD2	2:B:166:MET:HE1	1.92	1.05
2:B:158:ARG:HD2	2:B:197:ASN:N	1.70	1.05
2:B:180:THR:O	2:B:398:MET:HE1	1.45	1.05
1:A:31:GLN:HE22	1:A:243:ARG:HG3	0.94	1.05
1:A:103:TYR:CD1	1:A:188:ILE:HG22	1.89	1.05
2:B:103:TRP:NE1	2:B:189:LEU:HD23	1.70	1.05
2:B:141:LEU:HD12	2:B:172:VAL:CA	1.86	1.05
1:A:121:ARG:O	1:A:125:LEU:HG	1.56	1.05
2:B:3:GLU:C	2:B:4:ILE:HG13	1.77	1.05
1:A:217:LEU:HD11	1:A:368:LEU:CD2	1.86	1.04
2:B:41:ASP:C	2:B:42:LEU:HG	1.76	1.04
2:B:69:ASP:CG	2:B:74:THR:HB	1.77	1.04
2:B:308:ARG:HD3	2:B:342:TYR:CE2	1.92	1.04
2:B:384:ILE:C	2:B:386:GLU:H	1.52	1.04
2:B:405:LEU:HD12	2:B:408:TYR:CG	1.88	1.04
1:A:184:PRO:HG3	1:A:395:PHE:HB2	1.33	1.04
1:A:59:GLY:C	1:A:62:VAL:O	1.95	1.04
1:A:103:TYR:OH	1:A:151:SER:CB	2.04	1.04
2:B:7:ILE:CB	2:B:137:LEU:CD2	2.34	1.04
2:B:172:VAL:HG12	2:B:173:PRO:CD	1.88	1.04
2:B:259:MET:CB	2:B:268:PHE:CE1	2.38	1.04
1:A:126:ALA:O	1:A:132:LEU:HD11	1.57	1.04
1:A:312:TYR:CD2	1:A:381:THR:CG2	2.40	1.04
2:B:24:ILE:O	2:B:25:SER:C	1.80	1.04
2:B:69:ASP:OD2	2:B:74:THR:CB	2.06	1.04
2:B:145:THR:O	2:B:149:MET:CB	2.05	1.04
2:B:194:LEU:HA	2:B:265:LEU:CB	1.88	1.04
2:B:200:GLU:OE2	2:B:256:ALA:HA	1.56	1.04
2:B:435:TYR:O	2:B:436:GLN:CD	1.95	1.04
1:A:266:HIS:NE2	1:A:432:TYR:CE1	2.26	1.04
1:A:306:ASP:OD1	1:A:308:ARG:CB	2.05	1.04
2:B:4:ILE:HD12	2:B:30:ILE:O	1.57	1.04
2:B:244:PHE:CD2	2:B:245:PRO:CD	2.39	1.04
1:A:30:ILE:HB	1:A:64:ARG:CB	1.87	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:VAL:HG22	1:A:409:VAL:HG23	1.39	1.03
2:B:56:ALA:O	2:B:59:ASN:O	1.73	1.03
2:B:102:ASN:OD1	2:B:408:TYR:CE1	2.09	1.03
2:B:151:THR:CG2	2:B:192:HIS:ND1	2.14	1.03
2:B:242:LEU:HD22	2:B:250:ALA:H	1.23	1.03
1:A:183:GLU:HB3	1:A:394:LYS:CB	1.87	1.03
2:B:48:ARG:HH11	2:B:60:LYS:HA	1.17	1.03
1:A:16:ILE:HD13	1:A:138:PHE:HD1	0.88	1.03
1:A:45:GLY:O	1:A:46:ASP:CG	1.96	1.03
1:A:155:GLU:CG	1:A:192:HIS:CD2	2.41	1.03
1:A:193:THR:O	1:A:194:THR:O	1.77	1.03
2:B:44:LEU:C	2:B:47:GLU:HG3	1.79	1.03
2:B:56:ALA:HB3	2:B:62:VAL:HB	1.35	1.03
2:B:78:VAL:O	2:B:82:PRO:HG2	1.59	1.03
2:B:311:ARG:CG	2:B:341:SER:O	2.04	1.03
1:A:191:THR:O	1:A:194:THR:HB	1.56	1.03
2:B:4:ILE:CD1	2:B:30:ILE:HG22	1.88	1.03
2:B:102:ASN:HD22	2:B:105:LYS:HE3	1.17	1.03
2:B:107:HIS:C	2:B:152:LEU:CD1	2.27	1.03
2:B:147:SER:CA	2:B:189:LEU:CD1	2.36	1.03
2:B:287:THR:O	2:B:291:LEU:HG	0.85	1.03
2:B:397:ALA:HA	2:B:401:ARG:HD3	1.33	1.03
1:A:179:THR:HG21	1:A:181:VAL:CB	1.87	1.03
1:A:407:TRP:CH2	2:B:165:ILE:HD13	1.91	1.03
2:B:66:ILE:HG13	2:B:121:VAL:HG11	1.04	1.03
2:B:295:MET:HE1	2:B:375:ALA:HB1	1.14	1.03
2:B:44:LEU:CD2	2:B:85:GLN:CG	2.15	1.02
2:B:19:LYS:HD2	2:B:228:ASN:HB2	1.39	1.02
2:B:268:PHE:CD1	2:B:380:ASN:ND2	2.28	1.02
1:A:210:TYR:CD1	2:B:326:LYS:CD	2.43	1.02
1:A:276:ILE:HD12	1:A:371:VAL:HG22	1.41	1.02
2:B:49:ILE:C	2:B:61:TYR:CD2	2.32	1.02
2:B:103:TRP:HD1	2:B:189:LEU:HD21	1.17	1.02
1:A:97:GLU:HB3	1:A:110:ILE:HG21	1.35	1.02
1:A:217:LEU:CD2	1:A:368:LEU:HD11	1.88	1.02
2:B:49:ILE:C	2:B:61:TYR:HD2	1.63	1.02
2:B:70:LEU:HD23	2:B:145:THR:HG22	1.05	1.02
2:B:326:LYS:O	2:B:330:GLU:HG3	1.56	1.02
1:A:30:ILE:O	1:A:32:PRO:CD	2.08	1.02
1:A:70:LEU:CG	1:A:145:THR:CG2	2.36	1.01
1:A:204:VAL:HG23	1:A:231:ILE:HG23	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:O	1:A:210:TYR:HD2	1.41	1.01
2:B:80:SER:O	2:B:82:PRO:CD	2.07	1.01
2:B:107:HIS:CE1	2:B:152:LEU:CD2	2.42	1.01
2:B:172:VAL:HG13	2:B:173:PRO:HD2	1.05	1.01
2:B:190:SER:O	2:B:193:GLN:N	1.93	1.01
2:B:275:LEU:HG	2:B:294:GLN:NE2	1.73	1.01
2:B:287:THR:CG2	2:B:289:PRO:CD	2.38	1.01
1:A:4:CYS:HB2	1:A:30:ILE:HG23	1.03	1.01
2:B:422:GLU:O	2:B:426:ASN:HB2	1.60	1.01
1:A:62:VAL:HG13	1:A:63:PRO:HD2	1.07	1.01
1:A:73:THR:HG21	2:B:249:ASN:ND2	1.74	1.01
1:A:115:ILE:HD11	1:A:152:LEU:HG	1.40	1.01
1:A:224:TYR:HD2	2:B:325:MET:HB3	0.87	1.01
1:A:225:THR:CG2	2:B:247:GLN:NE2	2.23	1.01
2:B:296:PHE:CE1	2:B:335:VAL:HG11	1.96	1.01
2:B:370:GLY:C	5:B:501:TXL:H183	1.81	1.01
2:B:384:ILE:O	2:B:386:GLU:N	1.93	1.01
2:B:405:LEU:CD1	2:B:408:TYR:HD2	1.53	1.01
1:A:103:TYR:CE1	1:A:188:ILE:HG22	1.96	1.01
2:B:286:LEU:CD1	2:B:372:LYS:CB	2.39	1.01
1:A:296:PHE:HE1	1:A:335:ILE:CD1	1.67	1.00
2:B:103:TRP:NE1	2:B:148:GLY:HA2	1.75	1.00
2:B:192:HIS:CB	2:B:196:GLU:HG3	1.90	1.00
2:B:279:GLY:C	2:B:281:GLN:H	1.63	1.00
1:A:88:HIS:CG	1:A:89:PRO:HD2	1.95	1.00
1:A:103:TYR:CD2	1:A:147:SER:CB	2.36	1.00
1:A:184:PRO:CD	1:A:395:PHE:HA	1.91	1.00
1:A:296:PHE:CZ	1:A:335:ILE:HG21	1.95	1.00
1:A:328:VAL:HG13	1:A:332:ILE:CD1	1.90	1.00
2:B:262:PHE:HB3	2:B:263:PRO:HD2	1.43	1.00
1:A:174:ALA:CB	1:A:390:ARG:HH22	1.75	1.00
2:B:33:THR:N	2:B:59:ASN:ND2	2.04	1.00
2:B:191:VAL:HG21	2:B:421:ALA:HA	1.42	1.00
2:B:201:THR:HG23	2:B:265:LEU:CD1	1.91	1.00
2:B:260:VAL:CG1	2:B:262:PHE:O	2.08	1.00
2:B:396:THR:OG1	2:B:422:GLU:OE2	1.79	1.00
1:A:103:TYR:CE2	1:A:189:LEU:CD2	2.38	1.00
1:A:108:TYR:O	1:A:112:LYS:HD2	1.61	1.00
1:A:256:GLN:O	1:A:260:VAL:HG23	1.61	1.00
2:B:384:ILE:C	2:B:386:GLU:N	2.11	1.00
2:B:405:LEU:HD12	2:B:408:TYR:HB2	1.03	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ALA:HA	1:A:108:TYR:CD2	1.97	1.00
1:A:145:THR:O	1:A:149:PHE:HB3	1.62	1.00
2:B:184:PRO:CD	2:B:399:PHE:CE2	2.37	1.00
2:B:343:PHE:HB3	2:B:350:ASN:HD22	1.26	1.00
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.42	1.00
2:B:102:ASN:HB2	2:B:105:LYS:CD	1.92	1.00
2:B:111:GLY:O	2:B:115:VAL:N	1.95	1.00
1:A:143:GLY:O	1:A:146:GLY:N	1.95	1.00
2:B:24:ILE:C	2:B:26:ASP:H	1.55	1.00
1:A:51:THR:HG22	1:A:52:PHE:N	1.74	0.99
2:B:173:PRO:CG	2:B:391:ILE:HD11	1.92	0.99
1:A:204:VAL:HG21	1:A:231:ILE:HG23	1.07	0.99
2:B:44:LEU:CD2	2:B:86:ILE:H	1.61	0.99
2:B:147:SER:HB3	2:B:189:LEU:CG	1.77	0.99
1:A:269:LEU:O	1:A:378:LEU:HA	1.61	0.99
1:A:397:LEU:CD2	1:A:401:LYS:CD	2.40	0.99
2:B:158:ARG:CA	2:B:197:ASN:ND2	1.74	0.99
1:A:312:TYR:O	1:A:344:VAL:HG23	1.58	0.99
2:B:181:VAL:HG13	2:B:399:PHE:CE1	1.97	0.99
2:B:243:ARG:NH2	2:B:252:LEU:HD11	1.77	0.99
1:A:36:MET:SD	1:A:61:HIS:N	2.33	0.99
1:A:407:TRP:CH2	2:B:256:ALA:HB3	1.96	0.99
2:B:260:VAL:HG13	2:B:266:HIS:ND1	1.78	0.99
2:B:313:LEU:HA	2:B:344:VAL:HG21	1.43	0.99
1:A:324:VAL:HB	1:A:327:ASP:CG	1.82	0.99
1:A:77:GLU:HA	1:A:80:THR:HG1	1.16	0.99
1:A:433:GLU:O	1:A:437:VAL:CG2	2.10	0.99
2:B:181:VAL:HG22	2:B:404:PHE:CE2	1.97	0.99
1:A:103:TYR:CE2	1:A:189:LEU:HA	1.98	0.98
1:A:115:ILE:HG21	1:A:152:LEU:HD21	1.45	0.98
1:A:222:PRO:HG2	2:B:326:LYS:CD	1.93	0.98
1:A:250:VAL:HG13	1:A:254:GLU:HG2	1.44	0.98
1:A:422:ARG:O	1:A:426:ALA:HB2	1.63	0.98
2:B:155:SER:O	2:B:159:GLU:HG3	1.63	0.98
2:B:174:SER:OG	2:B:207:GLU:HB2	1.63	0.98
2:B:286:LEU:HD11	2:B:371:LEU:O	1.62	0.98
2:B:405:LEU:HD11	2:B:408:TYR:HB3	1.44	0.98
1:A:45:GLY:O	1:A:46:ASP:HB2	1.61	0.98
2:B:173:PRO:HG3	2:B:391:ILE:HD11	1.45	0.98
1:A:171:ILE:N	1:A:203:MET:CE	2.24	0.98
1:A:343:PHE:CZ	1:A:351:PHE:CZ	2.50	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:LEU:HA	2:B:265:LEU:HB3	1.44	0.98
2:B:320:ARG:HG2	2:B:374:SER:HG	1.24	0.98
2:B:405:LEU:HD22	2:B:418:PHE:CE1	1.98	0.98
1:A:219:ILE:CG2	1:A:219:ILE:CG1	2.40	0.98
2:B:23:VAL:HG22	5:B:501:TXL:H333	1.41	0.98
1:A:174:ALA:HB3	1:A:175:PRO:HD2	1.44	0.98
1:A:184:PRO:CB	1:A:395:PHE:CD2	2.45	0.98
1:A:76:ASP:O	1:A:80:THR:N	1.97	0.98
1:A:194:THR:HG22	1:A:195:LEU:HG	1.43	0.98
2:B:275:LEU:HD11	2:B:300:ASN:ND2	1.78	0.98
1:A:72:PRO:O	1:A:76:ASP:N	1.96	0.98
1:A:242:LEU:HB3	1:A:250:VAL:O	1.63	0.98
1:A:270:ALA:O	1:A:302:MET:HG2	1.63	0.98
2:B:199:ASP:OD2	2:B:256:ALA:HB2	1.62	0.98
1:A:68:VAL:CG1	1:A:149:PHE:CZ	2.47	0.98
2:B:275:LEU:CD1	2:B:294:GLN:HE21	1.74	0.98
1:A:141:PHE:O	1:A:186:ASN:ND2	1.58	0.98
2:B:7:ILE:HB	2:B:137:LEU:HD23	1.01	0.98
1:A:22:GLU:HG2	1:A:85:GLN:NE2	1.78	0.98
1:A:158:SER:HB3	1:A:197:HIS:CB	1.34	0.98
2:B:36:TYR:CD2	2:B:244:PHE:HE1	1.43	0.98
2:B:70:LEU:HD23	2:B:145:THR:CG2	1.93	0.98
1:A:217:LEU:HD13	1:A:368:LEU:HD11	1.02	0.97
1:A:313:MET:HE3	1:A:346:TRP:CH2	1.98	0.97
1:A:429:GLU:O	1:A:433:GLU:HG3	1.64	0.97
2:B:111:GLY:O	2:B:115:VAL:CG2	2.12	0.97
2:B:343:PHE:HD1	2:B:350:ASN:ND2	1.62	0.97
2:B:142:GLY:CA	2:B:182:VAL:HG22	1.94	0.97
1:A:15:GLN:HA	1:A:18:ASN:HD22	1.30	0.97
1:A:172:TYR:OH	1:A:387:ALA:HB1	1.58	0.97
1:A:205:ASP:CB	1:A:303:VAL:HA	1.92	0.97
1:A:397:LEU:HD22	1:A:401:LYS:CD	1.93	0.97
2:B:102:ASN:ND2	2:B:105:LYS:NZ	2.12	0.97
2:B:243:ARG:HH21	2:B:252:LEU:CD2	1.78	0.97
1:A:78:VAL:CG1	1:A:87:PHE:CE1	2.46	0.97
1:A:312:TYR:O	1:A:344:VAL:HG22	1.62	0.97
1:A:369:ALA:HB2	1:A:371:VAL:HG23	1.46	0.97
2:B:385:GLN:CG	2:B:389:LYS:CE	2.37	0.97
1:A:177:VAL:HG12	1:A:178:SER:N	1.79	0.97
2:B:287:THR:HG22	2:B:290:GLU:H	1.29	0.97
1:A:100:ALA:HB1	1:A:105:ARG:CD	1.91	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLN:O	1:A:373:ARG:HG3	1.65	0.97
2:B:44:LEU:HD11	2:B:86:ILE:O	1.63	0.97
2:B:175:PRO:O	2:B:176:LYS:HG2	1.49	0.97
2:B:284:ARG:HD2	2:B:290:GLU:OE1	1.62	0.97
2:B:154:ILE:CG2	2:B:198:THR:CG2	2.40	0.97
1:A:42:ILE:O	1:A:42:ILE:HG22	1.60	0.97
1:A:78:VAL:HG11	1:A:87:PHE:CE1	2.00	0.97
1:A:217:LEU:CD1	1:A:368:LEU:HD21	1.95	0.97
2:B:19:LYS:HB2	2:B:228:ASN:HB3	1.42	0.97
1:A:241:SER:HB2	1:A:356:ASN:ND2	1.78	0.97
2:B:3:GLU:HA	2:B:31:ASP:HB3	1.47	0.97
2:B:53:TYR:HE1	2:B:89:PRO:HG3	1.29	0.97
2:B:103:TRP:CD1	2:B:148:GLY:CA	2.47	0.97
2:B:147:SER:HA	2:B:189:LEU:HD13	1.47	0.97
2:B:206:ASN:O	2:B:210:TYR:CE2	2.18	0.97
1:A:119:LEU:O	1:A:122:ILE:HG22	1.65	0.96
1:A:310:GLY:O	1:A:342:GLN:OE1	1.82	0.96
2:B:151:THR:HG22	2:B:192:HIS:CD2	1.96	0.96
1:A:9:VAL:CG1	1:A:150:THR:CG2	2.42	0.96
1:A:313:MET:CE	1:A:346:TRP:CH2	2.47	0.96
2:B:206:ASN:O	2:B:210:TYR:CD2	2.18	0.96
2:B:343:PHE:HD1	2:B:350:ASN:CG	1.67	0.96
1:A:16:ILE:CD1	1:A:138:PHE:HD1	1.78	0.96
1:A:206:ASN:ND2	1:A:227:LEU:HD23	1.79	0.96
1:A:407:TRP:CH2	2:B:256:ALA:CB	2.48	0.96
2:B:7:ILE:CA	2:B:66:ILE:CG2	2.38	0.96
2:B:201:THR:HG23	2:B:265:LEU:HD11	0.97	0.96
2:B:346:TRP:O	2:B:347:ILE:CB	2.09	0.96
2:B:3:GLU:HG2	2:B:4:ILE:H	1.27	0.96
2:B:6:HIS:HB2	2:B:65:ALA:HA	1.46	0.96
1:A:115:ILE:HD13	1:A:156:ARG:NE	1.80	0.96
2:B:4:ILE:CD1	2:B:30:ILE:O	2.14	0.96
1:A:224:TYR:HD2	2:B:325:MET:CB	1.78	0.96
1:A:309:HIS:CG	1:A:386:GLU:OE2	2.19	0.96
2:B:208:ALA:CB	2:B:303:ALA:O	2.13	0.96
2:B:229:HIS:CD2	5:B:501:TXL:H37	1.98	0.96
1:A:53:PHE:CA	1:A:88:HIS:NE2	2.20	0.96
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.46	0.96
1:A:241:SER:HB2	1:A:356:ASN:HD22	1.27	0.95
2:B:70:LEU:HD11	2:B:94:PHE:CE2	2.01	0.95
2:B:104:ALA:HA	2:B:108:TYR:HD2	1.20	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:O	1:A:102:ASN:ND2	1.97	0.95
2:B:39:ASP:O	2:B:40:SER:OG	1.82	0.95
2:B:312:TYR:HA	2:B:381:SER:HA	1.43	0.95
1:A:2:ARG:HG2	1:A:133:GLN:CD	1.85	0.95
1:A:217:LEU:HD22	1:A:368:LEU:HD11	1.47	0.95
2:B:20:PHE:HE2	2:B:235:MET:HB3	0.80	0.95
2:B:79:ARG:O	2:B:80:SER:CB	2.10	0.95
1:A:31:GLN:N	1:A:32:PRO:HD2	1.81	0.95
1:A:141:PHE:O	1:A:182:VAL:HG13	1.66	0.95
1:A:158:SER:HB2	1:A:197:HIS:CB	1.67	0.95
1:A:314:ALA:HB3	1:A:380:ASN:HD22	1.31	0.95
2:B:97:SER:O	2:B:110:GLU:OE2	1.84	0.95
1:A:68:VAL:HG11	1:A:149:PHE:CE1	2.01	0.95
1:A:397:LEU:HA	1:A:401:LYS:CB	1.96	0.95
2:B:433:GLN:HG2	2:B:437:ASP:OD2	1.65	0.95
1:A:20:CYS:O	1:A:24:TYR:HD2	1.46	0.95
1:A:103:TYR:HE2	1:A:189:LEU:HD23	1.29	0.95
1:A:221:ARG:O	2:B:324:SER:HB3	1.67	0.95
2:B:398:MET:O	2:B:401:ARG:HB3	1.66	0.95
1:A:229:ARG:O	1:A:233:GLN:HG3	1.66	0.94
1:A:333:ALA:O	1:A:337:THR:HG23	1.66	0.94
1:A:212:ILE:HD13	1:A:230:LEU:HD21	1.49	0.94
1:A:250:VAL:CG2	1:A:352:LYS:CE	2.43	0.94
1:A:294:ALA:O	1:A:300:ASN:ND2	1.99	0.94
2:B:7:ILE:CB	2:B:137:LEU:HD23	1.96	0.94
2:B:22:GLU:CD	2:B:83:PHE:CG	2.39	0.94
2:B:287:THR:HG21	2:B:289:PRO:HG2	1.49	0.94
1:A:108:TYR:HA	1:A:112:LYS:HE3	1.47	0.94
1:A:183:GLU:OE2	1:A:394:LYS:NZ	1.76	0.94
1:A:250:VAL:HG22	1:A:352:LYS:HE2	1.49	0.94
2:B:158:ARG:CD	2:B:197:ASN:CA	2.39	0.94
2:B:181:VAL:O	2:B:399:PHE:CE2	2.19	0.94
2:B:382:THR:HG23	2:B:436:GLN:OE1	1.64	0.94
1:A:405:VAL:CG2	1:A:405:VAL:CG1	2.44	0.94
2:B:79:ARG:O	2:B:80:SER:HB3	1.66	0.94
2:B:142:GLY:HA2	2:B:182:VAL:HG22	1.50	0.94
1:A:36:MET:SD	1:A:61:HIS:CA	2.56	0.94
2:B:229:HIS:HD2	5:B:501:TXL:C38	1.47	0.94
2:B:319:PHE:HE1	2:B:353:THR:HG23	0.78	0.94
1:A:210:TYR:HE1	2:B:326:LYS:HG3	1.28	0.94
1:A:250:VAL:HG13	1:A:352:LYS:HZ3	1.12	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:ASN:O	2:B:102:ASN:CG	2.05	0.94
1:A:212:ILE:HD11	1:A:230:LEU:HD22	0.96	0.94
2:B:48:ARG:NH1	2:B:60:LYS:CA	2.31	0.94
2:B:229:HIS:NE2	5:B:501:TXL:H343	1.82	0.94
2:B:259:MET:HB3	2:B:268:PHE:CZ	2.02	0.94
1:A:30:ILE:C	1:A:32:PRO:HD3	1.81	0.94
1:A:59:GLY:CA	1:A:62:VAL:O	2.15	0.94
1:A:107:HIS:HD2	1:A:148:GLY:O	1.51	0.94
1:A:191:THR:O	1:A:194:THR:CB	2.14	0.94
1:A:225:THR:HG22	2:B:247:GLN:HE22	1.32	0.94
1:A:252:LEU:HA	1:A:255:PHE:CD2	2.02	0.94
2:B:172:VAL:HG12	2:B:173:PRO:HD2	1.43	0.94
1:A:250:VAL:HG22	1:A:254:GLU:HG2	1.50	0.94
2:B:44:LEU:HD21	2:B:86:ILE:H	1.00	0.94
1:A:65:ALA:CB	1:A:91:GLN:OE1	2.16	0.94
2:B:182:VAL:CG1	2:B:186:ASN:ND2	2.30	0.94
2:B:295:MET:CE	2:B:375:ALA:CA	2.45	0.94
2:B:346:TRP:CZ3	2:B:347:ILE:CG1	2.45	0.94
1:A:204:VAL:CG2	1:A:231:ILE:CG2	2.24	0.93
2:B:71:GLU:O	2:B:73:GLY:N	2.01	0.93
2:B:275:LEU:HD12	2:B:294:GLN:HE21	1.29	0.93
2:B:39:ASP:O	2:B:40:SER:CB	2.16	0.93
2:B:274:PRO:HB3	2:B:371:LEU:HD21	1.50	0.93
2:B:274:PRO:O	2:B:276:THR:HG23	1.67	0.93
2:B:142:GLY:HA2	2:B:185:TYR:CD1	2.03	0.93
1:A:51:THR:HG22	1:A:52:PHE:H	1.26	0.93
1:A:181:VAL:O	1:A:184:PRO:O	1.87	0.93
1:A:217:LEU:HG	1:A:218:ASP:N	1.77	0.93
2:B:154:ILE:HD12	2:B:192:HIS:NE2	1.83	0.93
2:B:241:CYS:SG	2:B:320:ARG:HD3	2.08	0.93
1:A:426:ALA:O	1:A:429:GLU:N	2.00	0.93
2:B:56:ALA:HB1	2:B:60:LYS:O	1.68	0.93
1:A:343:PHE:HE2	1:A:351:PHE:HZ	1.08	0.93
2:B:181:VAL:O	2:B:399:PHE:HE2	1.50	0.93
2:B:386:GLU:O	2:B:388:PHE:N	2.01	0.93
1:A:31:GLN:HE22	1:A:243:ARG:CB	1.81	0.93
1:A:184:PRO:CG	1:A:395:PHE:CB	2.45	0.93
1:A:272:TYR:CD1	1:A:274:PRO:O	2.22	0.93
2:B:435:TYR:N	2:B:435:TYR:HD1	1.66	0.93
2:B:86:ILE:HD12	2:B:91:ASN:HD21	1.33	0.93
2:B:275:LEU:CG	2:B:294:GLN:NE2	2.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:TRP:CE3	2:B:347:ILE:CD1	2.43	0.93
1:A:15:GLN:HA	1:A:18:ASN:ND2	1.83	0.93
1:A:405:VAL:CG2	1:A:409:VAL:HG23	1.98	0.93
1:A:184:PRO:CG	1:A:395:PHE:CA	2.47	0.93
1:A:250:VAL:CG1	1:A:254:GLU:CG	2.46	0.93
2:B:49:ILE:CA	2:B:61:TYR:HD2	1.82	0.93
2:B:343:PHE:HB3	2:B:350:ASN:ND2	1.83	0.93
1:A:83:TYR:CD2	1:A:83:TYR:O	2.22	0.92
1:A:119:LEU:HD11	1:A:156:ARG:HD3	1.48	0.92
1:A:225:THR:HG22	2:B:247:GLN:NE2	1.84	0.92
1:A:277:SER:H	1:A:280:LYS:CG	1.82	0.92
1:A:64:ARG:NH2	1:A:132:LEU:CD2	2.05	0.92
2:B:107:HIS:ND1	2:B:152:LEU:HD21	1.85	0.92
2:B:184:PRO:CD	2:B:398:MET:SD	2.57	0.92
1:A:177:VAL:CG1	1:A:178:SER:H	1.78	0.92
1:A:204:VAL:HG12	1:A:209:ILE:CD1	1.87	0.92
2:B:435:TYR:N	2:B:435:TYR:CD1	2.32	0.92
1:A:68:VAL:HG11	1:A:149:PHE:HZ	1.30	0.92
1:A:158:SER:HB3	1:A:197:HIS:HB2	1.51	0.92
1:A:217:LEU:CD1	1:A:368:LEU:CD2	2.46	0.92
2:B:343:PHE:CD1	2:B:350:ASN:ND2	2.37	0.92
1:A:332:ILE:HD13	1:A:353:VAL:CG2	1.99	0.92
2:B:103:TRP:CD1	2:B:148:GLY:HA2	2.05	0.92
2:B:184:PRO:CB	2:B:399:PHE:CG	2.41	0.92
2:B:241:CYS:O	2:B:242:LEU:HB2	1.69	0.92
2:B:426:ASN:O	2:B:429:VAL:N	2.00	0.92
2:B:151:THR:HG22	2:B:192:HIS:NE2	1.83	0.92
1:A:103:TYR:HE2	1:A:189:LEU:HA	1.32	0.92
2:B:346:TRP:HE3	2:B:347:ILE:HG12	1.33	0.92
1:A:103:TYR:H	1:A:408:TYR:HE1	0.96	0.92
1:A:176:GLN:HE21	2:B:333:LEU:HD22	0.76	0.92
1:A:231:ILE:HD13	1:A:302:MET:HE1	1.52	0.92
1:A:256:GLN:O	1:A:260:VAL:CG2	2.16	0.92
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.52	0.92
2:B:126:SER:HA	2:B:132:LEU:HD12	1.50	0.92
1:A:250:VAL:HG22	1:A:352:LYS:CE	2.00	0.92
1:A:383:ALA:O	1:A:384:ILE:C	2.07	0.92
1:A:64:ARG:HH22	1:A:132:LEU:HD22	0.76	0.91
1:A:155:GLU:HG2	1:A:196:GLU:HG3	1.51	0.91
1:A:258:ASN:OD1	1:A:352:LYS:HD2	1.69	0.91
1:A:277:SER:H	1:A:280:LYS:HG3	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ASN:ND2	2:B:105:LYS:CE	2.33	0.91
2:B:229:HIS:CB	5:B:501:TXL:H38	2.01	0.91
1:A:5:ILE:HG21	1:A:135:PHE:HE1	1.35	0.91
1:A:105:ARG:NH1	2:B:253:ARG:CZ	2.33	0.91
2:B:192:HIS:HA	2:B:196:GLU:HG2	1.53	0.91
2:B:405:LEU:CD2	2:B:418:PHE:HZ	1.84	0.91
1:A:262:TYR:HB3	1:A:263:PRO:HD2	1.49	0.91
1:A:312:TYR:CA	1:A:381:THR:HG22	1.99	0.91
2:B:48:ARG:NH1	2:B:60:LYS:HA	1.83	0.91
1:A:108:TYR:O	1:A:112:LYS:CG	2.17	0.91
1:A:210:TYR:CE1	2:B:326:LYS:CD	2.54	0.91
2:B:126:SER:HA	2:B:132:LEU:CD1	2.01	0.91
2:B:313:LEU:HD23	2:B:344:VAL:HG21	1.52	0.91
1:A:3:GLU:HA	1:A:31:GLN:HB2	0.94	0.91
1:A:3:GLU:O	1:A:132:LEU:C	2.09	0.91
1:A:103:TYR:CG	1:A:188:ILE:CG2	2.54	0.91
1:A:369:ALA:HB3	1:A:371:VAL:HG23	1.50	0.91
1:A:428:LEU:O	1:A:432:TYR:HB2	1.70	0.91
2:B:87:PHE:HD1	2:B:88:ARG:O	1.47	0.91
2:B:101:ASN:O	2:B:102:ASN:CB	2.17	0.91
1:A:59:GLY:HA2	1:A:62:VAL:O	1.70	0.91
1:A:382:THR:O	1:A:385:ALA:HB3	1.71	0.91
2:B:4:ILE:HD13	2:B:30:ILE:HG22	0.93	0.91
2:B:158:ARG:HD2	2:B:197:ASN:HA	1.51	0.91
2:B:24:ILE:O	2:B:27:GLU:N	2.04	0.91
2:B:189:LEU:O	2:B:193:GLN:CG	2.19	0.91
1:A:288:VAL:HG22	1:A:373:ARG:HD3	0.93	0.91
1:A:405:VAL:HG22	1:A:409:VAL:CG2	2.01	0.91
2:B:151:THR:HB	2:B:192:HIS:HD2	1.31	0.91
2:B:268:PHE:HE1	2:B:380:ASN:ND2	1.65	0.91
1:A:328:VAL:CG1	1:A:332:ILE:CD1	2.49	0.90
1:A:328:VAL:CG1	1:A:353:VAL:HG11	2.00	0.90
2:B:158:ARG:CG	2:B:197:ASN:CG	2.38	0.90
1:A:26:LEU:CD1	1:A:361:THR:OG1	2.19	0.90
1:A:107:HIS:CD2	1:A:148:GLY:O	2.23	0.90
1:A:107:HIS:HB2	1:A:148:GLY:HA3	1.01	0.90
1:A:222:PRO:CG	2:B:326:LYS:HD2	2.01	0.90
2:B:11:GLN:HB3	4:B:500:GDP:PA	2.11	0.90
2:B:102:ASN:ND2	2:B:105:LYS:HE3	1.85	0.90
2:B:405:LEU:HD12	2:B:408:TYR:CD2	2.00	0.90
2:B:80:SER:O	2:B:82:PRO:N	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:PHE:HD2	2:B:114:LEU:HD11	1.04	0.90
2:B:94:PHE:CD1	2:B:97:SER:HB3	2.06	0.90
2:B:278:ARG:O	2:B:281:GLN:HB3	1.71	0.90
2:B:312:TYR:CA	2:B:381:SER:HB3	2.02	0.90
1:A:31:GLN:HE22	1:A:243:ARG:CD	1.67	0.90
1:A:107:HIS:CG	1:A:148:GLY:CA	2.54	0.90
1:A:220:GLU:C	1:A:222:PRO:CD	2.37	0.90
1:A:407:TRP:CZ2	2:B:256:ALA:CB	2.54	0.90
2:B:20:PHE:CE2	2:B:235:MET:HB2	2.06	0.90
2:B:259:MET:CB	2:B:268:PHE:CZ	2.55	0.90
1:A:106:GLY:O	1:A:111:GLY:HA3	1.70	0.90
2:B:14:ASN:HB3	2:B:74:THR:CG2	2.01	0.90
2:B:75:MET:CE	2:B:79:ARG:HD3	1.99	0.90
2:B:106:GLY:O	2:B:111:GLY:HA3	1.70	0.90
2:B:118:VAL:HG11	2:B:153:LEU:HD22	1.54	0.90
2:B:275:LEU:CD1	2:B:294:GLN:NE2	2.35	0.90
2:B:312:TYR:CA	2:B:381:SER:CB	2.49	0.90
2:B:4:ILE:CD1	2:B:30:ILE:C	2.40	0.90
1:A:312:TYR:CD2	1:A:381:THR:HG21	2.06	0.90
2:B:70:LEU:CD1	2:B:94:PHE:CE2	2.53	0.90
2:B:260:VAL:HG12	2:B:262:PHE:O	1.69	0.90
1:A:205:ASP:OD1	1:A:303:VAL:HG22	1.18	0.90
1:A:238:ILE:HG23	1:A:255:PHE:CE1	2.05	0.90
1:A:328:VAL:HG12	1:A:332:ILE:HD12	1.53	0.90
2:B:11:GLN:CB	4:B:500:GDP:O2A	2.20	0.90
1:A:107:HIS:CB	1:A:148:GLY:C	2.36	0.90
1:A:166:LYS:O	1:A:199:ASP:HB2	1.72	0.90
1:A:250:VAL:HG13	1:A:352:LYS:NZ	1.86	0.90
2:B:78:VAL:C	2:B:82:PRO:HG2	1.91	0.90
2:B:319:PHE:CZ	2:B:328:VAL:CG1	2.54	0.90
2:B:70:LEU:CD2	2:B:145:THR:HG22	1.98	0.89
2:B:183:GLU:CD	2:B:394:GLN:CB	2.41	0.89
1:A:72:PRO:O	1:A:75:ILE:CG2	2.19	0.89
2:B:25:SER:O	2:B:27:GLU:HG3	1.73	0.89
2:B:239:THR:O	2:B:243:ARG:HD2	0.72	0.89
2:B:302:MET:O	2:B:302:MET:HG2	1.72	0.89
2:B:151:THR:CG2	2:B:192:HIS:NE2	2.35	0.89
1:A:53:PHE:N	1:A:88:HIS:HE1	1.41	0.89
1:A:276:ILE:HG21	1:A:282:TYR:CD1	2.08	0.89
2:B:98:GLY:O	2:B:99:ALA:O	1.91	0.89
2:B:229:HIS:HE1	5:B:501:TXL:H343	1.30	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLU:O	1:A:159:VAL:HG23	1.72	0.89
1:A:72:PRO:HA	1:A:75:ILE:CG2	2.03	0.89
1:A:291:ILE:CD1	1:A:373:ARG:HB3	2.03	0.89
2:B:158:ARG:HA	2:B:197:ASN:HD21	1.35	0.89
2:B:104:ALA:CA	2:B:108:TYR:HD2	1.85	0.89
2:B:135:PHE:CG	2:B:166:MET:HE1	2.07	0.89
2:B:56:ALA:HB3	2:B:62:VAL:HG23	1.54	0.89
2:B:103:TRP:HE3	2:B:413:MET:HE1	1.33	0.89
2:B:184:PRO:HD2	2:B:399:PHE:CE2	2.06	0.89
2:B:87:PHE:HE1	2:B:89:PRO:HG2	0.84	0.89
2:B:182:VAL:HG13	2:B:186:ASN:HD22	1.29	0.89
1:A:258:ASN:CG	1:A:352:LYS:HD2	1.93	0.89
2:B:8:GLN:HE21	2:B:21:TRP:HE1	1.21	0.89
2:B:158:ARG:HG3	2:B:197:ASN:CG	1.93	0.89
1:A:184:PRO:HB3	1:A:395:PHE:HD2	1.33	0.88
1:A:231:ILE:HD13	1:A:302:MET:CE	2.03	0.88
2:B:173:PRO:HG3	2:B:391:ILE:CD1	2.03	0.88
2:B:183:GLU:HB2	2:B:184:PRO:HD3	0.90	0.88
1:A:239:THR:HG23	1:A:243:ARG:HG3	1.54	0.88
1:A:191:THR:CG2	1:A:421:ALA:HB1	2.03	0.88
2:B:7:ILE:HD12	2:B:137:LEU:HD21	1.55	0.88
2:B:44:LEU:CG	2:B:85:GLN:HG3	2.02	0.88
2:B:66:ILE:CG1	2:B:121:VAL:HG11	1.99	0.88
1:A:425:MET:O	1:A:428:LEU:HB3	1.74	0.88
2:B:158:ARG:CD	2:B:197:ASN:CB	2.09	0.88
1:A:59:GLY:O	1:A:62:VAL:C	2.12	0.88
1:A:65:ALA:HB1	1:A:91:GLN:OE1	1.73	0.88
1:A:67:PHE:HB2	1:A:92:LEU:HD23	1.53	0.88
1:A:206:ASN:O	1:A:210:TYR:CD2	2.25	0.88
1:A:222:PRO:O	2:B:326:LYS:HB2	1.73	0.88
1:A:328:VAL:CG1	1:A:332:ILE:HD12	2.03	0.88
2:B:22:GLU:OE2	2:B:83:PHE:HB2	1.74	0.88
2:B:275:LEU:CG	2:B:294:GLN:HE22	1.85	0.88
1:A:9:VAL:HG11	1:A:150:THR:HG21	1.53	0.88
1:A:93:ILE:HD13	1:A:118:VAL:CG2	2.01	0.88
2:B:19:LYS:HG3	2:B:228:ASN:CG	1.92	0.88
2:B:53:TYR:CE1	2:B:87:PHE:CE1	2.62	0.88
2:B:142:GLY:HA3	2:B:182:VAL:CG2	2.04	0.88
2:B:243:ARG:NH2	2:B:252:LEU:HD21	1.86	0.88
1:A:183:GLU:CB	1:A:394:LYS:HB3	2.04	0.88
2:B:42:LEU:O	2:B:43:GLN:HG3	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:GLU:OE1	2:B:394:GLN:CB	2.21	0.88
2:B:385:GLN:NE2	2:B:433:GLN:OE1	2.07	0.88
2:B:405:LEU:HD13	2:B:408:TYR:HD2	0.74	0.88
1:A:23:LEU:CD2	1:A:236:SER:HB3	2.04	0.88
2:B:4:ILE:HD12	2:B:30:ILE:CA	2.03	0.88
2:B:284:ARG:CD	2:B:290:GLU:OE1	2.22	0.88
2:B:405:LEU:CD1	2:B:418:PHE:HZ	1.85	0.88
1:A:88:HIS:ND1	1:A:89:PRO:HD2	1.88	0.88
1:A:193:THR:O	1:A:194:THR:C	2.05	0.88
2:B:57:ALA:CA	2:B:64:ARG:CB	2.38	0.88
2:B:184:PRO:HD3	2:B:398:MET:SD	2.14	0.88
1:A:305:CYS:O	1:A:307:PRO:HD3	1.71	0.87
2:B:49:ILE:CA	2:B:61:TYR:CD2	2.57	0.87
2:B:53:TYR:CE1	2:B:87:PHE:CZ	2.62	0.87
2:B:311:ARG:O	2:B:382:THR:N	2.05	0.87
2:B:6:HIS:CD2	2:B:21:TRP:HH2	1.92	0.87
2:B:185:TYR:O	2:B:189:LEU:HG	1.72	0.87
1:A:133:GLN:O	1:A:252:LEU:HD12	1.73	0.87
1:A:276:ILE:O	1:A:368:LEU:CB	2.21	0.87
2:B:48:ARG:HD2	2:B:60:LYS:HA	1.55	0.87
2:B:68:VAL:HG11	2:B:149:MET:HE2	1.56	0.87
2:B:172:VAL:HG12	2:B:173:PRO:N	1.89	0.87
2:B:274:PRO:CB	2:B:371:LEU:HD21	2.04	0.87
2:B:194:LEU:CD2	2:B:267:PHE:CE2	2.58	0.87
1:A:277:SER:HA	1:A:368:LEU:HD22	1.56	0.87
1:A:311:LYS:HB3	1:A:342:GLN:O	1.74	0.87
1:A:382:THR:O	1:A:385:ALA:CB	2.22	0.87
2:B:174:SER:OG	2:B:207:GLU:HB3	1.65	0.87
2:B:433:GLN:HG2	2:B:437:ASP:CG	1.95	0.87
1:A:196:GLU:O	1:A:197:HIS:ND1	2.08	0.87
2:B:19:LYS:HG3	2:B:228:ASN:HB2	1.43	0.87
2:B:200:GLU:HB3	2:B:268:PHE:HE2	1.37	0.87
1:A:115:ILE:CD1	1:A:152:LEU:CD2	2.45	0.87
1:A:210:TYR:HD1	2:B:326:LYS:CG	1.87	0.87
1:A:208:ALA:O	1:A:212:ILE:HG23	1.75	0.87
1:A:222:PRO:HG2	2:B:326:LYS:HD2	1.56	0.87
1:A:277:SER:HB3	1:A:280:LYS:HE2	1.56	0.87
2:B:184:PRO:HG3	2:B:399:PHE:CG	1.84	0.87
2:B:279:GLY:O	2:B:281:GLN:N	2.08	0.87
2:B:320:ARG:CG	2:B:374:SER:OG	2.23	0.87
1:A:194:THR:HG22	1:A:195:LEU:H	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ILE:HD13	2:B:198:THR:HG21	1.56	0.86
2:B:172:VAL:HG11	2:B:387:LEU:HD11	1.54	0.86
1:A:76:ASP:O	1:A:80:THR:OG1	1.91	0.86
1:A:174:ALA:HB1	1:A:390:ARG:NH2	1.81	0.86
2:B:29:GLY:O	2:B:58:GLY:C	2.14	0.86
2:B:200:GLU:OE2	2:B:256:ALA:CA	2.15	0.86
2:B:276:THR:OG1	5:B:501:TXL:H62	1.74	0.86
2:B:384:ILE:CG2	2:B:388:PHE:HE2	1.88	0.86
2:B:33:THR:H	2:B:59:ASN:HD22	0.93	0.86
5:B:501:TXL:H173	5:B:501:TXL:H13	1.57	0.86
1:A:191:THR:CG2	1:A:421:ALA:CB	2.53	0.86
1:A:303:VAL:CG1	1:A:305:CYS:SG	2.64	0.86
2:B:7:ILE:HA	2:B:66:ILE:HG23	0.89	0.86
2:B:244:PHE:CG	2:B:245:PRO:CD	2.56	0.86
1:A:104:ALA:HA	1:A:108:TYR:HD2	1.39	0.86
2:B:7:ILE:HG13	2:B:66:ILE:HG21	1.58	0.86
2:B:33:THR:C	2:B:59:ASN:HD21	1.76	0.86
2:B:169:PHE:CE1	2:B:235:MET:SD	2.67	0.86
2:B:327:GLU:O	2:B:331:GLN:HG2	1.75	0.86
1:A:100:ALA:HB1	1:A:105:ARG:HB3	1.55	0.86
1:A:204:VAL:HG13	1:A:302:MET:HE2	1.57	0.86
1:A:204:VAL:HG13	1:A:209:ILE:HD11	1.56	0.86
2:B:178:SER:HB3	4:B:500:GDP:O3'	1.74	0.86
2:B:405:LEU:HD21	2:B:418:PHE:HE2	1.41	0.86
1:A:115:ILE:HD13	1:A:152:LEU:CG	2.02	0.86
1:A:313:MET:HB2	1:A:380:ASN:O	1.75	0.86
2:B:181:VAL:HA	2:B:398:MET:CE	2.06	0.86
2:B:184:PRO:CG	2:B:399:PHE:CD2	0.91	0.86
2:B:273:ALA:N	2:B:274:PRO:HD2	1.45	0.86
1:A:108:TYR:HA	1:A:112:LYS:CE	2.05	0.86
2:B:107:HIS:CG	2:B:152:LEU:HD21	2.11	0.86
1:A:276:ILE:HD13	1:A:282:TYR:CD1	2.11	0.86
2:B:144:GLY:N	2:B:185:TYR:CE1	2.44	0.86
2:B:313:LEU:HD23	2:B:344:VAL:HG22	1.58	0.86
1:A:4:CYS:CB	1:A:30:ILE:HG23	1.99	0.86
1:A:109:THR:HG21	1:A:411:GLU:OE1	1.75	0.86
1:A:175:PRO:HD3	1:A:390:ARG:NH2	1.91	0.86
1:A:179:THR:CG2	1:A:181:VAL:HB	2.04	0.86
1:A:224:TYR:HE1	3:A:500:GTP:N3	1.73	0.86
1:A:282:TYR:CD2	1:A:285:GLN:HA	2.11	0.86
1:A:397:LEU:HA	1:A:401:LYS:HB2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:SER:CA	2:B:189:LEU:HD13	2.04	0.86
2:B:241:CYS:HG	2:B:320:ARG:NH1	1.72	0.86
2:B:254:LYS:O	2:B:258:ASN:OD1	1.94	0.86
1:A:271:THR:OG1	1:A:377:MET:HB3	1.76	0.85
2:B:13:GLY:CA	2:B:138:THR:OG1	2.24	0.85
1:A:154:MET:HB2	1:A:192:HIS:CE1	2.11	0.85
1:A:306:ASP:OD2	1:A:308:ARG:HD2	1.76	0.85
2:B:135:PHE:HB3	2:B:166:MET:HE3	0.87	0.85
2:B:158:ARG:CB	2:B:197:ASN:HB3	1.71	0.85
2:B:174:SER:CB	2:B:207:GLU:CB	2.52	0.85
1:A:250:VAL:HG12	1:A:254:GLU:HB3	1.55	0.85
2:B:312:TYR:CA	2:B:381:SER:HA	2.06	0.85
1:A:23:LEU:HD23	1:A:236:SER:HB3	1.57	0.85
1:A:103:TYR:HA	1:A:147:SER:OG	1.77	0.85
3:A:500:GTP:PA	2:B:248:LEU:CD1	2.64	0.85
2:B:169:PHE:HE1	2:B:235:MET:HG2	0.82	0.85
2:B:239:THR:C	2:B:243:ARG:HD2	1.95	0.85
1:A:83:TYR:O	1:A:84:ARG:HG3	1.76	0.85
1:A:158:SER:HB2	1:A:197:HIS:HB3	0.87	0.85
2:B:41:ASP:O	2:B:42:LEU:CG	2.25	0.85
2:B:401:ARG:HG3	2:B:402:LYS:H	1.41	0.85
2:B:430:SER:O	2:B:434:GLN:HG3	1.76	0.85
1:A:1:MET:O	1:A:130:THR:O	1.94	0.85
1:A:184:PRO:HG3	1:A:395:PHE:CA	2.06	0.85
2:B:53:TYR:CD1	2:B:87:PHE:CE1	2.63	0.85
2:B:275:LEU:HD12	2:B:294:GLN:NE2	1.92	0.85
1:A:115:ILE:O	1:A:119:LEU:HG	1.75	0.85
1:A:276:ILE:HD12	1:A:371:VAL:CG2	2.06	0.85
2:B:339:ASN:O	2:B:342:TYR:N	2.09	0.85
1:A:88:HIS:CE1	1:A:89:PRO:HD2	2.12	0.85
1:A:407:TRP:CZ2	2:B:165:ILE:CD1	2.58	0.85
2:B:184:PRO:HG3	2:B:399:PHE:CB	2.07	0.85
2:B:127:GLU:O	2:B:129:CYS:N	2.09	0.85
2:B:151:THR:CA	2:B:192:HIS:HD2	1.82	0.85
2:B:114:LEU:CD1	2:B:117:SER:OG	2.19	0.84
1:A:41:THR:O	1:A:42:ILE:HB	1.73	0.84
2:B:287:THR:HB	2:B:290:GLU:HB2	0.86	0.84
1:A:108:TYR:CA	1:A:112:LYS:CE	2.54	0.84
1:A:221:ARG:O	2:B:324:SER:CB	2.26	0.84
2:B:19:LYS:CB	2:B:228:ASN:CB	2.41	0.84
2:B:385:GLN:HE22	2:B:433:GLN:CD	1.79	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:ASP:OD1	5:B:501:TXL:C39	2.25	0.84
2:B:4:ILE:HD12	2:B:30:ILE:HA	1.48	0.84
2:B:14:ASN:HB3	2:B:74:THR:HG21	1.59	0.84
2:B:233:ALA:HB1	2:B:272:PHE:CG	2.12	0.84
2:B:288:VAL:N	2:B:289:PRO:HD2	1.92	0.84
2:B:428:LEU:O	2:B:432:TYR:HB2	1.77	0.84
1:A:48:SER:HG	1:A:56:THR:HB	1.43	0.84
2:B:175:PRO:HD3	2:B:390:ARG:HH21	0.74	0.84
1:A:184:PRO:HB2	1:A:399:TYR:CD2	2.12	0.84
1:A:217:LEU:CG	1:A:218:ASP:H	1.86	0.84
1:A:220:GLU:O	1:A:222:PRO:HD3	1.60	0.84
2:B:174:SER:HB2	2:B:175:PRO:HD2	1.59	0.84
2:B:405:LEU:CG	2:B:408:TYR:HB2	2.07	0.84
1:A:292:THR:HG22	1:A:319:TYR:CZ	2.12	0.84
2:B:229:HIS:CG	5:B:501:TXL:C38	2.41	0.84
2:B:433:GLN:HG2	2:B:437:ASP:OD1	1.78	0.84
1:A:193:THR:O	1:A:197:HIS:O	1.94	0.84
1:A:217:LEU:HD22	1:A:368:LEU:CD1	2.08	0.84
1:A:272:TYR:CZ	1:A:274:PRO:CG	2.56	0.84
1:A:277:SER:OG	1:A:280:LYS:CB	2.25	0.84
2:B:87:PHE:CD1	2:B:89:PRO:HG2	2.03	0.84
2:B:102:ASN:HA	2:B:408:TYR:HE1	1.42	0.84
2:B:158:ARG:HB2	2:B:197:ASN:HB3	0.85	0.84
1:A:272:TYR:CE1	1:A:274:PRO:CG	2.59	0.83
1:A:273:ALA:HB1	1:A:294:ALA:CB	2.07	0.83
2:B:183:GLU:CB	2:B:398:MET:SD	2.65	0.83
2:B:388:PHE:C	2:B:390:ARG:H	1.80	0.83
1:A:9:VAL:HG11	1:A:150:THR:HG22	1.57	0.83
1:A:18:ASN:O	1:A:22:GLU:HG3	1.78	0.83
1:A:206:ASN:HD21	1:A:227:LEU:CD2	1.87	0.83
1:A:273:ALA:HB1	1:A:294:ALA:HB3	1.60	0.83
1:A:64:ARG:HH22	1:A:132:LEU:HD23	1.41	0.83
1:A:313:MET:HA	1:A:344:VAL:HG21	1.60	0.83
2:B:182:VAL:HG13	2:B:186:ASN:HD21	1.41	0.83
2:B:199:ASP:OD2	2:B:256:ALA:CB	2.26	0.83
1:A:264:ARG:O	1:A:266:HIS:CE1	2.32	0.83
2:B:48:ARG:NH1	2:B:60:LYS:CG	2.42	0.83
1:A:258:ASN:OD1	1:A:352:LYS:NZ	2.10	0.83
2:B:229:HIS:NE2	5:B:501:TXL:C37	2.40	0.83
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.58	0.83
1:A:72:PRO:C	1:A:75:ILE:HG22	1.99	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:VAL:HG11	1:A:209:ILE:CD1	1.92	0.83
2:B:6:HIS:NE2	2:B:21:TRP:HH2	1.77	0.83
2:B:49:ILE:N	2:B:61:TYR:HD2	1.75	0.83
2:B:53:TYR:CD1	2:B:87:PHE:HZ	1.96	0.83
2:B:241:CYS:O	2:B:242:LEU:CB	2.27	0.83
2:B:289:PRO:O	2:B:293:GLN:HB2	1.78	0.83
1:A:73:THR:CG2	2:B:249:ASN:ND2	2.42	0.83
1:A:320:ARG:HG2	1:A:374:ALA:HB3	1.60	0.83
2:B:226:ASP:OD2	5:B:501:TXL:H40	1.77	0.83
1:A:70:LEU:CD1	1:A:145:THR:CG2	1.89	0.83
1:A:81:GLY:O	1:A:82:THR:C	2.18	0.83
2:B:234:THR:OG1	2:B:302:MET:HE1	1.78	0.83
1:A:77:GLU:HA	1:A:80:THR:CB	2.08	0.82
1:A:202:PHE:CE1	1:A:378:LEU:HD13	2.14	0.82
1:A:222:PRO:CB	2:B:326:LYS:HD2	2.08	0.82
1:A:288:VAL:HG22	1:A:373:ARG:CG	2.08	0.82
1:A:332:ILE:CD1	1:A:353:VAL:CG2	2.54	0.82
2:B:250:ALA:CA	2:B:254:LYS:HD2	2.09	0.82
2:B:405:LEU:O	2:B:405:LEU:HG	1.75	0.82
1:A:33:ASP:OD2	1:A:244:PHE:HD2	1.62	0.82
1:A:76:ASP:O	1:A:80:THR:CA	2.27	0.82
2:B:23:VAL:CG2	5:B:501:TXL:H333	2.09	0.82
2:B:339:ASN:O	2:B:342:TYR:HB2	1.79	0.82
2:B:385:GLN:HG2	2:B:389:LYS:HD2	1.59	0.82
1:A:107:HIS:HB3	1:A:148:GLY:HA3	1.59	0.82
1:A:51:THR:CG2	1:A:52:PHE:H	1.92	0.82
1:A:407:TRP:CD2	2:B:257:VAL:HG22	2.15	0.82
2:B:48:ARG:NH1	2:B:60:LYS:HG2	1.95	0.82
2:B:68:VAL:CG1	2:B:149:MET:CE	2.58	0.82
2:B:96:GLN:C	2:B:98:GLY:N	2.31	0.82
1:A:107:HIS:CG	1:A:148:GLY:HA3	2.13	0.82
2:B:13:GLY:HA2	2:B:138:THR:HB	1.62	0.82
2:B:35:SER:N	2:B:60:LYS:CE	2.42	0.82
2:B:143:GLY:N	2:B:147:SER:OG	2.12	0.82
1:A:219:ILE:CG2	1:A:219:ILE:CA	2.57	0.82
2:B:287:THR:CG2	2:B:290:GLU:H	1.92	0.82
2:B:319:PHE:CE1	2:B:353:THR:CG2	2.42	0.82
1:A:179:THR:CG2	1:A:181:VAL:CB	2.58	0.82
2:B:105:LYS:HG2	2:B:411:GLU:CG	2.09	0.82
2:B:222:PRO:O	2:B:223:THR:HG23	1.79	0.82
2:B:14:ASN:CB	2:B:74:THR:OG1	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:THR:CA	2:B:192:HIS:HE2	1.68	0.82
2:B:169:PHE:CZ	2:B:235:MET:SD	2.73	0.82
1:A:30:ILE:CG2	1:A:64:ARG:CG	2.55	0.81
1:A:108:TYR:O	1:A:112:LYS:HG3	1.80	0.81
2:B:7:ILE:CG1	2:B:66:ILE:CG2	2.58	0.81
2:B:201:THR:OG1	2:B:267:PHE:HA	1.78	0.81
1:A:312:TYR:HA	1:A:381:THR:CG2	2.09	0.81
1:A:407:TRP:CZ2	2:B:165:ILE:HD13	2.15	0.81
2:B:6:HIS:CD2	2:B:21:TRP:CH2	2.68	0.81
2:B:10:GLY:O	2:B:14:ASN:ND2	2.14	0.81
2:B:135:PHE:HB3	2:B:166:MET:HE1	1.62	0.81
2:B:165:ILE:HD13	2:B:199:ASP:OD2	1.79	0.81
2:B:287:THR:CB	2:B:290:GLU:HB3	1.99	0.81
1:A:13:GLY:O	1:A:16:ILE:HG22	1.80	0.81
1:A:30:ILE:C	1:A:32:PRO:HD2	1.98	0.81
1:A:194:THR:HG22	1:A:195:LEU:N	1.95	0.81
1:A:209:ILE:CD1	1:A:227:LEU:HD11	1.93	0.81
1:A:212:ILE:CD1	1:A:230:LEU:HD22	1.89	0.81
1:A:250:VAL:CG1	1:A:352:LYS:NZ	2.43	0.81
2:B:22:GLU:OE2	2:B:83:PHE:CB	2.27	0.81
2:B:287:THR:HG22	2:B:288:VAL:N	1.95	0.81
2:B:346:TRP:CE3	2:B:347:ILE:HG12	2.06	0.81
2:B:4:ILE:CD1	2:B:30:ILE:CA	2.58	0.81
2:B:226:ASP:CG	5:B:501:TXL:C39	2.49	0.81
1:A:2:ARG:CB	1:A:133:GLN:OE1	2.27	0.81
2:B:7:ILE:HB	2:B:137:LEU:HD21	1.62	0.81
2:B:174:SER:HB2	2:B:207:GLU:HB3	1.59	0.81
2:B:30:ILE:CG2	2:B:243:ARG:NH1	2.44	0.81
2:B:226:ASP:CG	5:B:501:TXL:H39	2.00	0.81
2:B:286:LEU:HD13	2:B:373:MET:N	1.96	0.81
1:A:407:TRP:CZ3	2:B:165:ILE:HD11	2.13	0.81
2:B:80:SER:C	2:B:82:PRO:CD	2.48	0.81
2:B:194:LEU:HD23	2:B:265:LEU:HB3	1.62	0.81
1:A:106:GLY:O	1:A:111:GLY:CA	2.29	0.81
3:A:500:GTP:O1A	2:B:248:LEU:HD11	1.80	0.81
2:B:13:GLY:HA2	2:B:138:THR:CB	2.10	0.81
2:B:75:MET:HE2	2:B:79:ARG:CD	2.11	0.81
2:B:106:GLY:O	2:B:111:GLY:CA	2.29	0.81
1:A:70:LEU:HB2	1:A:145:THR:HG21	1.62	0.81
2:B:184:PRO:HB3	2:B:395:PHE:CE1	2.16	0.81
2:B:385:GLN:HG2	2:B:389:LYS:CE	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLY:HA2	1:A:185:TYR:OH	1.81	0.81
2:B:105:LYS:CE	2:B:411:GLU:OE2	2.27	0.81
2:B:166:MET:HB2	2:B:198:THR:HA	1.61	0.81
1:A:101:ASN:HA	3:A:500:GTP:O2G	1.81	0.80
1:A:177:VAL:CB	2:B:349:ASN:HD21	1.91	0.80
1:A:184:PRO:CD	1:A:395:PHE:CA	2.58	0.80
2:B:95:GLY:O	2:B:96:GLN:HB2	1.81	0.80
1:A:15:GLN:O	1:A:18:ASN:N	2.14	0.80
2:B:14:ASN:CG	2:B:69:ASP:OD1	2.20	0.80
2:B:103:TRP:CZ3	2:B:108:TYR:OH	2.18	0.80
2:B:178:SER:CB	4:B:500:GDP:HO3'	1.92	0.80
2:B:385:GLN:HG2	2:B:389:LYS:CD	2.11	0.80
1:A:72:PRO:O	1:A:75:ILE:HG23	1.82	0.80
1:A:271:THR:OG1	1:A:377:MET:CB	2.30	0.80
2:B:64:ARG:NH2	2:B:125:GLU:O	2.13	0.80
2:B:194:LEU:HA	2:B:265:LEU:HB2	1.60	0.80
2:B:218:LYS:O	2:B:219:LEU:O	2.00	0.80
2:B:229:HIS:CG	5:B:501:TXL:C37	2.62	0.80
1:A:20:CYS:O	1:A:24:TYR:CE2	2.33	0.80
1:A:32:PRO:C	1:A:34:GLY:N	2.32	0.80
1:A:97:GLU:HB3	1:A:110:ILE:HG23	1.61	0.80
1:A:103:TYR:CG	1:A:188:ILE:HG22	2.16	0.80
1:A:276:ILE:HG21	1:A:282:TYR:HD1	1.44	0.80
2:B:319:PHE:CD1	2:B:328:VAL:CG1	2.58	0.80
1:A:9:VAL:CG1	1:A:150:THR:HG22	2.08	0.80
1:A:206:ASN:HD21	1:A:227:LEU:HD23	1.42	0.80
1:A:210:TYR:HD1	2:B:326:LYS:HD3	1.46	0.80
1:A:223:THR:HG22	2:B:324:SER:HA	1.62	0.80
2:B:11:GLN:HB3	4:B:500:GDP:O2A	1.79	0.80
2:B:35:SER:HA	2:B:60:LYS:HE2	1.62	0.80
2:B:119:LEU:O	2:B:123:ARG:HG3	1.80	0.80
2:B:142:GLY:CA	2:B:185:TYR:CD1	2.65	0.80
2:B:311:ARG:O	2:B:381:SER:HB2	1.80	0.80
1:A:3:GLU:HA	1:A:31:GLN:CG	2.11	0.80
1:A:17:GLY:O	1:A:21:TRP:N	2.11	0.80
1:A:291:ILE:HG22	1:A:375:VAL:HG23	0.84	0.80
1:A:343:PHE:HZ	1:A:351:PHE:CE2	1.99	0.80
1:A:105:ARG:HH21	1:A:110:ILE:CD1	1.92	0.80
1:A:119:LEU:O	1:A:122:ILE:CG2	2.29	0.80
2:B:102:ASN:OD1	2:B:408:TYR:HE1	1.62	0.80
1:A:88:HIS:CG	1:A:89:PRO:CD	2.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:TYR:N	2:B:325:MET:HB2	1.96	0.80
1:A:306:ASP:OD1	1:A:308:ARG:HB2	1.79	0.80
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.62	0.80
1:A:4:CYS:CB	1:A:30:ILE:CG2	2.57	0.80
1:A:108:TYR:HE2	1:A:417:GLU:OE2	1.63	0.80
1:A:191:THR:HG21	1:A:421:ALA:HB2	1.63	0.80
2:B:12:CYS:O	2:B:16:ILE:CB	2.29	0.80
1:A:64:ARG:CZ	1:A:132:LEU:HD22	2.10	0.79
1:A:343:PHE:CZ	1:A:351:PHE:CE2	2.69	0.79
2:B:70:LEU:HD12	2:B:94:PHE:HD2	0.68	0.79
2:B:142:GLY:C	2:B:185:TYR:CZ	2.56	0.79
2:B:244:PHE:CB	2:B:245:PRO:HD2	2.05	0.79
2:B:313:LEU:HD23	2:B:344:VAL:CG1	2.08	0.79
1:A:309:HIS:CD2	1:A:386:GLU:OE2	2.36	0.79
1:A:361:THR:HG22	1:A:362:VAL:N	1.97	0.79
2:B:102:ASN:HB3	2:B:408:TYR:HD1	1.45	0.79
2:B:142:GLY:CA	2:B:185:TYR:CE1	2.64	0.79
1:A:154:MET:CE	1:A:166:LYS:HD3	2.11	0.79
2:B:53:TYR:CE1	2:B:89:PRO:HG3	2.17	0.79
2:B:265:LEU:HD23	2:B:267:PHE:CE1	2.18	0.79
1:A:115:ILE:CG2	1:A:152:LEU:HD21	2.12	0.79
1:A:301:GLN:NE2	1:A:305:CYS:O	2.12	0.79
2:B:4:ILE:HG21	2:B:30:ILE:CG2	2.12	0.79
2:B:96:GLN:O	2:B:97:SER:C	2.21	0.79
2:B:175:PRO:HB2	2:B:176:LYS:HE2	1.65	0.79
2:B:35:SER:CA	2:B:60:LYS:CE	2.60	0.79
2:B:56:ALA:CB	2:B:62:VAL:HB	2.11	0.79
2:B:141:LEU:HD22	2:B:186:ASN:CB	2.09	0.79
1:A:6:SER:HA	1:A:136:SER:OG	1.81	0.79
1:A:258:ASN:OD1	1:A:352:LYS:CD	2.30	0.79
1:A:409:VAL:HG22	1:A:414:GLU:HG2	1.64	0.79
2:B:158:ARG:HG3	2:B:197:ASN:CB	2.08	0.79
2:B:190:SER:O	2:B:192:HIS:N	2.14	0.79
2:B:192:HIS:CA	2:B:196:GLU:HG2	2.11	0.79
2:B:259:MET:HE2	2:B:379:GLY:N	1.97	0.79
1:A:16:ILE:CD1	1:A:138:PHE:CD1	2.59	0.79
1:A:176:GLN:O	1:A:177:VAL:HG22	1.78	0.79
1:A:383:ALA:C	1:A:385:ALA:N	2.23	0.79
2:B:181:VAL:HA	2:B:398:MET:HE2	1.64	0.79
2:B:287:THR:CG2	2:B:289:PRO:HG2	2.12	0.79
2:B:34:GLY:O	2:B:35:SER:OG	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:OE2	1:A:129:CYS:HB3	1.82	0.79
1:A:116:ASP:O	1:A:119:LEU:N	2.15	0.79
1:A:221:ARG:N	1:A:222:PRO:HD3	1.97	0.79
2:B:4:ILE:HD13	2:B:30:ILE:CB	2.13	0.79
2:B:19:LYS:HB3	2:B:228:ASN:HB3	1.61	0.79
2:B:105:LYS:HE2	2:B:411:GLU:CD	2.03	0.79
2:B:107:HIS:HD2	2:B:152:LEU:HG	1.48	0.79
2:B:135:PHE:CG	2:B:166:MET:CE	2.63	0.79
2:B:305:CYS:SG	2:B:387:LEU:HB2	2.23	0.79
1:A:5:ILE:HG21	1:A:135:PHE:CE1	2.18	0.78
1:A:152:LEU:HD11	1:A:156:ARG:CZ	2.13	0.78
1:A:172:TYR:CE2	1:A:388:TRP:CZ3	2.70	0.78
2:B:69:ASP:OD2	2:B:74:THR:CG2	2.31	0.78
2:B:295:MET:HE3	2:B:375:ALA:HB1	0.79	0.78
1:A:80:THR:O	1:A:81:GLY:C	2.19	0.78
2:B:48:ARG:CD	2:B:60:LYS:HA	2.13	0.78
2:B:102:ASN:HA	2:B:408:TYR:CE1	2.18	0.78
2:B:323:MET:HG2	2:B:324:SER:N	1.98	0.78
2:B:405:LEU:HD21	2:B:418:PHE:CZ	2.03	0.78
1:A:51:THR:CG2	1:A:52:PHE:N	2.45	0.78
1:A:396:ASP:OD2	1:A:422:ARG:NH1	2.15	0.78
1:A:407:TRP:HZ2	2:B:256:ALA:HB1	1.43	0.78
2:B:300:ASN:ND2	2:B:300:ASN:O	2.16	0.78
1:A:109:THR:CG2	1:A:411:GLU:HB3	2.12	0.78
1:A:303:VAL:HG11	1:A:305:CYS:SG	2.22	0.78
2:B:19:LYS:CD	2:B:228:ASN:CB	2.53	0.78
2:B:128:SER:O	2:B:129:CYS:HB2	1.84	0.78
2:B:184:PRO:HG3	2:B:399:PHE:CD2	1.33	0.78
1:A:65:ALA:O	1:A:66:VAL:HG23	1.83	0.78
1:A:155:GLU:HG3	1:A:192:HIS:NE2	1.98	0.78
1:A:173:PRO:HG3	1:A:182:VAL:HG12	1.66	0.78
1:A:210:TYR:HD1	2:B:326:LYS:CD	1.94	0.78
2:B:49:ILE:N	2:B:61:TYR:CD2	2.51	0.78
2:B:107:HIS:CG	2:B:152:LEU:HG	2.19	0.78
1:A:196:GLU:O	1:A:197:HIS:CB	2.31	0.78
2:B:48:ARG:NH1	2:B:60:LYS:N	2.32	0.78
2:B:194:LEU:HD23	2:B:267:PHE:CZ	2.19	0.78
2:B:213:CYS:HB3	2:B:219:LEU:HD11	1.64	0.78
2:B:405:LEU:HD13	2:B:418:PHE:HZ	1.47	0.78
1:A:155:GLU:OE2	1:A:192:HIS:HD2	1.65	0.78
2:B:30:ILE:HG21	2:B:136:GLN:HE22	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:SER:CB	2:B:280:SER:HB2	2.13	0.78
1:A:206:ASN:HD21	3:A:500:GTP:N2	1.82	0.78
1:A:210:TYR:CZ	1:A:227:LEU:CD2	2.60	0.78
1:A:383:ALA:C	1:A:385:ALA:H	1.84	0.78
2:B:104:ALA:HA	2:B:108:TYR:CE2	2.19	0.78
2:B:105:LYS:CG	2:B:411:GLU:HG3	2.14	0.78
2:B:169:PHE:CZ	2:B:235:MET:HG2	2.17	0.78
2:B:401:ARG:HG3	2:B:402:LYS:N	1.99	0.78
1:A:217:LEU:HD13	1:A:368:LEU:CG	2.12	0.78
2:B:242:LEU:CD1	2:B:250:ALA:HB3	2.11	0.78
2:B:286:LEU:CD1	2:B:371:LEU:O	2.32	0.78
2:B:286:LEU:HD12	2:B:372:LYS:HB2	1.61	0.78
2:B:399:PHE:CZ	2:B:408:TYR:OH	2.37	0.78
1:A:105:ARG:HH12	2:B:253:ARG:CZ	1.94	0.78
2:B:244:PHE:CD2	2:B:358:ILE:HD12	2.18	0.78
2:B:320:ARG:NH2	5:B:501:TXL:H27	1.98	0.78
2:B:346:TRP:CD2	2:B:347:ILE:HG13	2.14	0.78
1:A:105:ARG:NH2	1:A:110:ILE:CD1	2.46	0.77
1:A:72:PRO:O	1:A:75:ILE:HG22	1.83	0.77
1:A:277:SER:OG	1:A:280:LYS:CA	2.32	0.77
2:B:229:HIS:ND1	5:B:501:TXL:O11	2.18	0.77
2:B:343:PHE:CD1	2:B:350:ASN:CG	2.55	0.77
1:A:153:LEU:O	1:A:157:LEU:HG	1.84	0.77
1:A:155:GLU:OE2	1:A:192:HIS:CD2	2.37	0.77
2:B:86:ILE:HD12	2:B:91:ASN:ND2	1.99	0.77
2:B:176:LYS:CE	2:B:207:GLU:OE2	2.29	0.77
2:B:222:PRO:O	2:B:223:THR:CG2	2.32	0.77
1:A:227:LEU:HB2	2:B:326:LYS:HE2	1.64	0.77
1:A:296:PHE:HE1	1:A:335:ILE:HD13	0.98	0.77
2:B:273:ALA:HB1	2:B:294:GLN:OE1	1.83	0.77
2:B:425:MET:O	2:B:428:LEU:HB3	1.84	0.77
2:B:7:ILE:CD1	2:B:137:LEU:HD21	2.14	0.77
2:B:8:GLN:NE2	2:B:21:TRP:NE1	2.31	0.77
1:A:103:TYR:O	1:A:107:HIS:HB3	1.85	0.77
2:B:383:ALA:O	2:B:386:GLU:HG3	1.84	0.77
1:A:97:GLU:O	1:A:98:ASP:HB3	1.85	0.77
1:A:115:ILE:CD1	1:A:152:LEU:CD1	2.63	0.77
2:B:191:VAL:CG2	2:B:421:ALA:CA	2.61	0.77
1:A:70:LEU:HB2	1:A:145:THR:CG2	2.14	0.77
1:A:148:GLY:HA2	1:A:151:SER:OG	1.85	0.77
1:A:369:ALA:CB	1:A:371:VAL:CG2	2.51	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ILE:HG22	2:B:196:GLU:O	1.85	0.77
1:A:83:TYR:C	1:A:84:ARG:HG3	2.05	0.77
1:A:151:SER:HB2	1:A:192:HIS:CB	2.15	0.77
1:A:158:SER:OG	1:A:196:GLU:O	2.02	0.77
1:A:192:HIS:O	1:A:196:GLU:HG2	1.85	0.77
1:A:312:TYR:CE2	1:A:377:MET:HE3	2.19	0.77
2:B:66:ILE:HB	2:B:125:GLU:OE2	1.84	0.77
2:B:107:HIS:CG	2:B:152:LEU:CD2	2.67	0.77
2:B:184:PRO:HD2	2:B:399:PHE:HE2	1.47	0.77
2:B:208:ALA:HB1	2:B:303:ALA:O	1.82	0.77
1:A:88:HIS:CD2	1:A:89:PRO:HD2	2.20	0.76
2:B:92:PHE:CE2	2:B:114:LEU:HD11	2.20	0.76
2:B:107:HIS:O	2:B:152:LEU:HD13	1.82	0.76
2:B:144:GLY:N	2:B:185:TYR:CZ	2.52	0.76
2:B:319:PHE:CZ	2:B:328:VAL:HG13	2.19	0.76
1:A:313:MET:CB	1:A:380:ASN:O	2.34	0.76
5:B:501:TXL:C9	5:B:501:TXL:H162	2.15	0.76
2:B:194:LEU:CD2	2:B:267:PHE:HE2	1.93	0.76
2:B:249:ASN:O	2:B:254:LYS:NZ	2.16	0.76
2:B:384:ILE:CG2	2:B:388:PHE:CE2	2.69	0.76
1:A:93:ILE:HD11	1:A:121:ARG:HD2	1.66	0.76
1:A:288:VAL:HG23	1:A:373:ARG:HD3	1.62	0.76
1:A:383:ALA:O	1:A:386:GLU:N	2.18	0.76
2:B:7:ILE:HG12	2:B:66:ILE:CD1	2.04	0.76
2:B:103:TRP:CZ3	2:B:108:TYR:CZ	2.73	0.76
2:B:107:HIS:CG	2:B:152:LEU:CG	2.69	0.76
1:A:70:LEU:CG	1:A:145:THR:HG21	2.14	0.76
1:A:252:LEU:HD23	1:A:255:PHE:CE2	2.19	0.76
2:B:262:PHE:HB3	2:B:263:PRO:CD	2.14	0.76
2:B:308:ARG:HD3	2:B:342:TYR:CZ	2.21	0.76
2:B:319:PHE:CE1	2:B:328:VAL:HG12	2.18	0.76
2:B:102:ASN:CG	2:B:408:TYR:CD1	2.59	0.76
2:B:105:LYS:HG2	2:B:411:GLU:CD	2.06	0.76
2:B:141:LEU:CD1	2:B:173:PRO:HD3	2.16	0.76
2:B:229:HIS:CE1	5:B:501:TXL:O11	2.38	0.76
1:A:97:GLU:CG	1:A:110:ILE:CG2	2.63	0.76
1:A:369:ALA:HB1	1:A:371:VAL:HG23	1.67	0.76
2:B:12:CYS:SG	4:B:500:GDP:C4	2.79	0.76
2:B:184:PRO:CG	2:B:399:PHE:HD2	0.66	0.76
2:B:259:MET:HE2	2:B:378:ILE:HG22	1.65	0.76
1:A:97:GLU:HG3	1:A:110:ILE:CG2	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASP:CG	1:A:308:ARG:HB2	2.06	0.76
1:A:311:LYS:CB	1:A:342:GLN:O	2.34	0.76
2:B:183:GLU:OE1	2:B:394:GLN:HB3	1.83	0.76
2:B:399:PHE:O	2:B:403:ALA:HA	1.86	0.76
2:B:400:ARG:HD3	2:B:422:GLU:OE1	1.85	0.76
1:A:344:VAL:CB	1:A:347:CYS:SG	2.69	0.76
2:B:147:SER:CB	2:B:189:LEU:HD13	2.08	0.76
2:B:27:GLU:O	2:B:36:TYR:HB3	1.86	0.76
2:B:105:LYS:HG2	2:B:411:GLU:HG3	1.67	0.76
2:B:135:PHE:CB	2:B:166:MET:SD	2.74	0.76
2:B:147:SER:OG	2:B:189:LEU:CD1	2.21	0.76
2:B:201:THR:CG2	2:B:265:LEU:CD1	2.59	0.76
2:B:213:CYS:HB3	2:B:219:LEU:CD1	2.16	0.76
1:A:179:THR:CG2	1:A:181:VAL:N	2.21	0.75
2:B:48:ARG:HH11	2:B:60:LYS:CG	1.97	0.75
1:A:101:ASN:OD1	2:B:254:LYS:HG2	1.86	0.75
1:A:179:THR:HG22	1:A:180:ALA:N	1.95	0.75
2:B:7:ILE:CG1	2:B:66:ILE:HD13	2.05	0.75
2:B:35:SER:CA	2:B:60:LYS:HE3	2.16	0.75
2:B:243:ARG:HH21	2:B:252:LEU:CD1	1.98	0.75
2:B:252:LEU:O	2:B:255:LEU:HB2	1.85	0.75
2:B:268:PHE:CD1	2:B:380:ASN:CG	2.59	0.75
2:B:313:LEU:HD22	2:B:344:VAL:CG1	1.98	0.75
1:A:179:THR:HG22	1:A:181:VAL:H	0.63	0.75
1:A:209:ILE:HG12	1:A:302:MET:HE3	1.69	0.75
2:B:102:ASN:ND2	2:B:105:LYS:HZ2	1.85	0.75
2:B:275:LEU:HD11	2:B:300:ASN:HD21	1.49	0.75
2:B:343:PHE:CB	2:B:350:ASN:ND2	2.50	0.75
1:A:38:SER:C	1:A:39:ASP:N	0.70	0.75
1:A:53:PHE:HA	1:A:88:HIS:NE2	1.92	0.75
1:A:183:GLU:HB2	1:A:398:MET:SD	2.26	0.75
1:A:262:TYR:HB3	1:A:263:PRO:HD3	1.65	0.75
1:A:313:MET:CE	1:A:346:TRP:CZ2	2.70	0.75
2:B:42:LEU:C	2:B:43:GLN:HG3	2.07	0.75
2:B:200:GLU:HB3	2:B:268:PHE:CE2	2.21	0.75
2:B:399:PHE:HZ	2:B:408:TYR:OH	1.68	0.75
1:A:66:VAL:CG2	1:A:125:LEU:CD1	2.64	0.75
2:B:170:SER:OG	2:B:203:CYS:HA	1.86	0.75
2:B:184:PRO:HG2	2:B:399:PHE:CD2	0.29	0.75
2:B:398:MET:HG2	2:B:399:PHE:N	2.00	0.75
1:A:26:LEU:HD11	1:A:361:THR:CB	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CD1	2:B:326:LYS:HD3	2.15	0.75
1:A:228:ASN:ND2	3:A:500:GTP:HN1	1.84	0.75
2:B:6:HIS:NE2	2:B:21:TRP:CH2	2.55	0.75
2:B:87:PHE:CD1	2:B:89:PRO:HD2	2.20	0.75
2:B:188:THR:HG22	2:B:417:GLU:O	1.87	0.75
2:B:259:MET:HE1	2:B:379:GLY:HA2	0.83	0.75
1:A:219:ILE:CG2	1:A:219:ILE:HG12	2.16	0.75
2:B:154:ILE:HD13	2:B:198:THR:CG2	2.17	0.75
1:A:115:ILE:HD13	1:A:152:LEU:CD1	2.16	0.75
1:A:287:SER:OG	1:A:290:GLU:HB2	1.87	0.75
1:A:326:LYS:O	1:A:330:ALA:HB3	1.87	0.75
2:B:89:PRO:O	2:B:90:ASP:OD1	2.05	0.75
2:B:296:PHE:CE2	2:B:335:VAL:HG11	2.22	0.75
1:A:88:HIS:CD2	1:A:89:PRO:CD	2.70	0.74
1:A:184:PRO:HD3	1:A:395:PHE:N	2.01	0.74
2:B:53:TYR:HE1	2:B:89:PRO:CG	1.98	0.74
2:B:123:ARG:O	2:B:127:GLU:HG3	1.87	0.74
2:B:181:VAL:CG2	2:B:404:PHE:CE2	2.70	0.74
2:B:184:PRO:HA	2:B:395:PHE:HD1	1.52	0.74
2:B:192:HIS:HA	2:B:196:GLU:CD	2.08	0.74
2:B:259:MET:HB3	2:B:268:PHE:HE1	1.45	0.74
1:A:57:GLY:HA3	1:A:61:HIS:NE2	2.01	0.74
1:A:184:PRO:HB3	1:A:395:PHE:CD2	2.19	0.74
2:B:6:HIS:CG	2:B:21:TRP:HZ2	2.05	0.74
2:B:9:ALA:HA	2:B:68:VAL:O	1.86	0.74
1:A:42:ILE:O	1:A:42:ILE:CG2	2.30	0.74
2:B:22:GLU:HG2	2:B:83:PHE:HD2	1.47	0.74
2:B:102:ASN:CG	2:B:408:TYR:CE1	2.60	0.74
1:A:33:ASP:OD2	1:A:244:PHE:CD2	2.39	0.74
2:B:287:THR:CG2	2:B:289:PRO:CG	2.65	0.74
1:A:62:VAL:HG12	1:A:63:PRO:CD	2.06	0.74
1:A:196:GLU:O	1:A:197:HIS:HB3	1.87	0.74
1:A:222:PRO:CG	2:B:326:LYS:CD	2.61	0.74
2:B:213:CYS:SG	2:B:227:LEU:CD1	2.75	0.74
2:B:405:LEU:HD11	2:B:408:TYR:HB2	0.78	0.74
1:A:30:ILE:CB	1:A:64:ARG:CB	2.66	0.74
1:A:80:THR:O	1:A:83:TYR:N	2.19	0.74
1:A:172:TYR:CZ	1:A:387:ALA:HB1	2.22	0.74
1:A:273:ALA:CB	1:A:294:ALA:HB3	2.16	0.74
1:A:313:MET:HE1	1:A:346:TRP:CZ2	2.23	0.74
1:A:224:TYR:CE1	3:A:500:GTP:N3	2.55	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:THR:O	1:A:362:VAL:HG23	1.87	0.74
2:B:35:SER:H	2:B:60:LYS:HE3	1.53	0.74
2:B:181:VAL:HG12	2:B:399:PHE:CZ	1.95	0.74
2:B:226:ASP:OD1	5:B:501:TXL:H39	1.87	0.74
2:B:243:ARG:HH21	2:B:252:LEU:HD11	1.47	0.74
2:B:22:GLU:CG	2:B:83:PHE:CE2	2.70	0.74
2:B:229:HIS:NE2	5:B:501:TXL:H37	2.02	0.74
1:A:206:ASN:ND2	3:A:500:GTP:HN22	1.85	0.74
2:B:92:PHE:CE1	2:B:121:VAL:HG21	2.23	0.74
1:A:210:TYR:CD2	1:A:227:LEU:HD22	2.20	0.74
1:A:282:TYR:HD2	1:A:285:GLN:CA	2.01	0.73
2:B:259:MET:CE	2:B:379:GLY:N	2.51	0.73
2:B:284:ARG:HD2	2:B:290:GLU:CD	2.08	0.73
2:B:336:GLN:NE2	2:B:351:VAL:HB	2.03	0.73
1:A:3:GLU:HB3	1:A:64:ARG:CZ	2.18	0.73
1:A:103:TYR:OH	1:A:151:SER:HB3	1.87	0.73
1:A:154:MET:HE3	1:A:166:LYS:HD3	1.70	0.73
1:A:179:THR:HG23	1:A:181:VAL:HG23	1.70	0.73
2:B:105:LYS:HE2	2:B:411:GLU:CG	2.18	0.73
1:A:65:ALA:HB2	1:A:91:GLN:OE1	1.87	0.73
1:A:137:VAL:HB	1:A:168:GLU:HG2	1.70	0.73
1:A:397:LEU:HD23	1:A:401:LYS:CD	2.11	0.73
2:B:169:PHE:HE1	2:B:235:MET:CG	1.76	0.73
2:B:239:THR:HA	2:B:243:ARG:CZ	2.18	0.73
2:B:346:TRP:HZ3	2:B:347:ILE:HD11	0.95	0.73
2:B:397:ALA:O	2:B:401:ARG:HG2	1.87	0.73
1:A:6:SER:HB3	1:A:30:ILE:CD1	2.19	0.73
1:A:319:TYR:O	1:A:355:ILE:HA	1.87	0.73
2:B:8:GLN:NE2	2:B:21:TRP:CD1	2.56	0.73
2:B:244:PHE:CE2	2:B:358:ILE:CD1	2.48	0.73
2:B:3:GLU:CB	2:B:132:LEU:HD23	2.14	0.73
2:B:75:MET:HA	2:B:75:MET:HE3	1.69	0.73
2:B:101:ASN:O	2:B:102:ASN:HB2	1.88	0.73
2:B:141:LEU:HD12	2:B:172:VAL:HA	0.91	0.73
2:B:143:GLY:O	4:B:500:GDP:PB	2.41	0.73
1:A:152:LEU:HD11	1:A:156:ARG:NE	2.04	0.73
1:A:184:PRO:HD3	1:A:395:PHE:CA	2.19	0.73
1:A:405:VAL:CG2	1:A:409:VAL:CG2	2.65	0.73
1:A:431:ASP:O	1:A:435:VAL:HG23	1.88	0.73
2:B:229:HIS:HB2	5:B:501:TXL:H38	1.68	0.73
1:A:97:GLU:O	1:A:110:ILE:HD13	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:HIS:CD2	1:A:148:GLY:CA	2.71	0.73
1:A:142:GLY:C	1:A:185:TYR:CE1	2.62	0.73
1:A:341:ILE:CG2	1:A:343:PHE:CE2	2.72	0.73
2:B:44:LEU:HD11	2:B:86:ILE:C	2.09	0.73
2:B:56:ALA:CB	2:B:62:VAL:HG23	2.18	0.73
2:B:128:SER:O	2:B:129:CYS:CB	2.37	0.73
1:A:103:TYR:HD2	1:A:189:LEU:CG	2.00	0.73
2:B:286:LEU:HB3	2:B:373:MET:HB3	1.71	0.73
1:A:179:THR:CG2	1:A:181:VAL:HG23	2.18	0.73
1:A:209:ILE:HG23	1:A:230:LEU:CD2	2.17	0.73
1:A:314:ALA:O	1:A:379:SER:HA	1.89	0.73
2:B:75:MET:HE2	2:B:79:ARG:HB3	1.70	0.73
2:B:237:GLY:O	2:B:241:CYS:CB	2.26	0.73
2:B:313:LEU:CD2	2:B:344:VAL:HG13	2.17	0.73
1:A:13:GLY:HA2	1:A:16:ILE:CG2	2.18	0.73
1:A:70:LEU:CB	1:A:145:THR:CG2	2.65	0.72
1:A:153:LEU:O	1:A:157:LEU:CD1	2.37	0.72
1:A:250:VAL:HG21	1:A:352:LYS:CE	2.07	0.72
1:A:277:SER:HB2	1:A:279:GLU:H	1.53	0.72
2:B:226:ASP:OD2	5:B:501:TXL:C40	2.37	0.72
2:B:259:MET:HB2	2:B:268:PHE:CZ	2.23	0.72
2:B:265:LEU:CD2	2:B:267:PHE:CE1	2.71	0.72
1:A:262:TYR:CB	1:A:263:PRO:CD	2.57	0.72
2:B:6:HIS:CG	2:B:21:TRP:CZ2	2.77	0.72
2:B:68:VAL:CG1	2:B:149:MET:HE2	2.19	0.72
2:B:244:PHE:HD2	2:B:245:PRO:HD2	1.45	0.72
1:A:154:MET:HE3	1:A:166:LYS:CD	2.19	0.72
1:A:277:SER:CA	1:A:280:LYS:HG2	2.18	0.72
1:A:404:PHE:HZ	2:B:257:VAL:O	1.73	0.72
1:A:407:TRP:CE3	2:B:257:VAL:CG2	2.72	0.72
2:B:103:TRP:CZ3	2:B:108:TYR:CE2	2.75	0.72
1:A:36:MET:SD	1:A:60:LYS:HB2	2.29	0.72
1:A:158:SER:H	1:A:166:LYS:NZ	1.86	0.72
1:A:206:ASN:HD21	3:A:500:GTP:HN22	1.35	0.72
1:A:222:PRO:O	2:B:324:SER:CB	2.29	0.72
2:B:242:LEU:HD22	2:B:250:ALA:N	2.01	0.72
2:B:288:VAL:H	2:B:289:PRO:HD2	1.53	0.72
2:B:295:MET:HE1	2:B:375:ALA:CA	2.15	0.72
2:B:326:LYS:O	2:B:330:GLU:CG	2.35	0.72
1:A:70:LEU:CB	1:A:145:THR:HG21	2.20	0.72
1:A:144:GLY:N	3:A:500:GTP:O2G	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ALA:C	1:A:300:ASN:ND2	2.43	0.72
2:B:7:ILE:CG2	2:B:137:LEU:HD22	2.19	0.72
2:B:14:ASN:HB2	2:B:74:THR:OG1	1.89	0.72
2:B:194:LEU:HD21	2:B:267:PHE:CE2	2.23	0.72
2:B:204:ILE:O	2:B:204:ILE:HG22	1.90	0.72
2:B:265:LEU:O	2:B:267:PHE:CE2	2.41	0.72
1:A:100:ALA:HB2	1:A:105:ARG:NE	2.04	0.72
1:A:292:THR:HG22	1:A:319:TYR:CE2	2.25	0.72
1:A:336:LYS:HG2	1:A:336:LYS:O	1.88	0.72
2:B:35:SER:H	2:B:60:LYS:CE	2.02	0.72
2:B:75:MET:HE2	2:B:79:ARG:CB	2.19	0.72
1:A:225:THR:HG23	2:B:247:GLN:HE22	1.52	0.72
1:A:250:VAL:CG2	1:A:254:GLU:HG2	2.19	0.72
1:A:289:ALA:HB1	1:A:331:ALA:CB	2.20	0.72
1:A:184:PRO:CB	1:A:399:TYR:CD2	2.73	0.72
1:A:184:PRO:HG2	1:A:395:PHE:CD2	2.20	0.72
2:B:102:ASN:CB	2:B:408:TYR:CD1	2.73	0.72
2:B:280:SER:O	2:B:282:GLN:N	2.21	0.72
2:B:284:ARG:HB3	2:B:287:THR:OG1	1.90	0.72
2:B:383:ALA:O	2:B:386:GLU:CG	2.37	0.72
2:B:68:VAL:CG1	2:B:149:MET:HE1	2.20	0.72
2:B:192:HIS:C	2:B:196:GLU:HG2	2.09	0.72
2:B:360:PRO:CD	2:B:374:SER:HB3	2.20	0.72
2:B:405:LEU:HD13	2:B:418:PHE:CZ	2.25	0.72
1:A:5:ILE:CD1	1:A:135:PHE:CE1	2.73	0.71
1:A:184:PRO:HG2	1:A:395:PHE:HA	1.72	0.71
1:A:210:TYR:HE2	1:A:227:LEU:CD2	2.01	0.71
1:A:253:THR:O	1:A:253:THR:HG22	1.90	0.71
1:A:397:LEU:HD22	1:A:401:LYS:CE	2.20	0.71
2:B:20:PHE:CZ	2:B:235:MET:HB3	2.22	0.71
2:B:288:VAL:O	2:B:292:THR:N	2.19	0.71
1:A:225:THR:HG21	2:B:247:GLN:HE22	1.47	0.71
1:A:266:HIS:HD2	1:A:432:TYR:CE1	2.04	0.71
1:A:291:ILE:C	1:A:375:VAL:HG21	2.10	0.71
2:B:133:GLN:NE2	2:B:253:ARG:NH1	2.38	0.71
2:B:142:GLY:HA3	2:B:182:VAL:HG21	1.71	0.71
1:A:4:CYS:SG	1:A:252:LEU:CD1	2.72	0.71
1:A:152:LEU:HD11	1:A:156:ARG:NH2	2.05	0.71
2:B:2:ARG:CG	2:B:2:ARG:O	2.36	0.71
2:B:184:PRO:HG3	2:B:399:PHE:HB2	1.70	0.71
1:A:9:VAL:HB	1:A:138:PHE:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:GLU:HG2	2:B:4:ILE:N	2.04	0.71
2:B:111:GLY:CA	2:B:115:VAL:HG23	2.20	0.71
2:B:340:SER:HG	2:B:341:SER:N	1.85	0.71
1:A:241:SER:CB	1:A:356:ASN:HD22	2.04	0.71
2:B:7:ILE:CG2	2:B:137:LEU:CD2	2.69	0.71
2:B:95:GLY:O	2:B:96:GLN:CB	2.39	0.71
1:A:30:ILE:HD12	1:A:64:ARG:HB3	1.72	0.71
1:A:119:LEU:C	1:A:122:ILE:HG22	2.11	0.71
2:B:237:GLY:CA	2:B:241:CYS:SG	2.68	0.71
2:B:259:MET:SD	2:B:378:ILE:HG22	2.31	0.71
2:B:272:PHE:CD1	2:B:274:PRO:HG2	2.24	0.71
2:B:311:ARG:C	2:B:381:SER:HB2	2.11	0.71
2:B:390:ARG:O	2:B:394:GLN:CG	2.33	0.71
2:B:397:ALA:CA	2:B:401:ARG:HD3	2.19	0.71
1:A:234:ILE:HD12	1:A:270:ALA:HB1	1.71	0.71
1:A:319:TYR:CE2	1:A:375:VAL:HG22	2.26	0.71
2:B:312:TYR:O	2:B:344:VAL:HG22	1.84	0.71
1:A:101:ASN:O	1:A:102:ASN:OD1	2.07	0.71
2:B:15:GLN:CD	4:B:500:GDP:O6	2.29	0.71
1:A:202:PHE:HE1	1:A:378:LEU:HD13	1.55	0.71
1:A:222:PRO:HG2	2:B:326:LYS:HD3	1.72	0.71
2:B:104:ALA:CA	2:B:108:TYR:CD2	2.63	0.71
2:B:254:LYS:O	2:B:258:ASN:CG	2.28	0.71
1:A:155:GLU:HG2	1:A:196:GLU:CG	2.21	0.71
1:A:291:ILE:HD11	1:A:373:ARG:HB3	1.72	0.71
1:A:312:TYR:CD2	1:A:381:THR:HG22	2.23	0.71
1:A:312:TYR:CB	1:A:381:THR:HG22	2.21	0.71
2:B:75:MET:CE	2:B:75:MET:HA	2.21	0.71
1:A:16:ILE:HG21	1:A:138:PHE:CD1	2.26	0.70
1:A:228:ASN:ND2	3:A:500:GTP:O6	2.23	0.70
1:A:407:TRP:CG	2:B:257:VAL:HG22	2.26	0.70
2:B:213:CYS:SG	2:B:227:LEU:HD12	2.31	0.70
2:B:222:PRO:C	2:B:223:THR:HG23	2.11	0.70
1:A:30:ILE:HG22	1:A:64:ARG:HG2	1.70	0.70
1:A:231:ILE:CD1	1:A:302:MET:CE	2.69	0.70
2:B:143:GLY:CA	2:B:185:TYR:HE1	2.03	0.70
2:B:286:LEU:HD13	2:B:372:LYS:HB2	1.68	0.70
5:B:501:TXL:H181	5:B:501:TXL:C21	2.20	0.70
1:A:104:ALA:HA	1:A:108:TYR:CE2	2.25	0.70
1:A:239:THR:O	1:A:243:ARG:HB2	1.91	0.70
1:A:242:LEU:HD22	1:A:250:VAL:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:TYR:HD1	2:B:87:PHE:CZ	2.05	0.70
2:B:142:GLY:HA3	2:B:182:VAL:HG22	1.65	0.70
2:B:386:GLU:C	2:B:388:PHE:N	2.44	0.70
1:A:36:MET:SD	1:A:61:HIS:HA	2.30	0.70
1:A:100:ALA:O	1:A:144:GLY:HA3	1.90	0.70
2:B:53:TYR:HE1	2:B:87:PHE:CE1	2.08	0.70
1:A:3:GLU:HB2	1:A:132:LEU:HA	1.73	0.70
1:A:100:ALA:HB1	1:A:105:ARG:CB	2.22	0.70
1:A:108:TYR:OH	1:A:417:GLU:HG3	1.91	0.70
2:B:48:ARG:HH11	2:B:60:LYS:CB	2.04	0.70
2:B:165:ILE:CD1	2:B:199:ASP:OD2	2.39	0.70
1:A:103:TYR:CE1	1:A:188:ILE:CG2	2.67	0.70
1:A:313:MET:HE1	1:A:346:TRP:CH2	2.25	0.70
2:B:3:GLU:OE2	2:B:64:ARG:NH1	2.25	0.70
2:B:21:TRP:HA	2:B:24:ILE:HD12	1.71	0.70
2:B:97:SER:OG	2:B:110:GLU:OE1	2.10	0.70
1:A:167:LEU:CD1	1:A:252:LEU:HD22	2.21	0.70
2:B:102:ASN:HB3	2:B:408:TYR:CD1	2.25	0.70
2:B:184:PRO:HG3	2:B:399:PHE:HD2	0.76	0.70
2:B:190:SER:O	2:B:191:VAL:C	2.30	0.70
2:B:53:TYR:CE1	2:B:87:PHE:HZ	2.07	0.70
2:B:242:LEU:CA	2:B:356:CYS:SG	2.79	0.70
2:B:287:THR:CG2	2:B:288:VAL:N	2.55	0.70
1:A:103:TYR:OH	1:A:151:SER:OG	2.08	0.70
1:A:103:TYR:CG	1:A:188:ILE:HG21	2.22	0.70
1:A:220:GLU:CG	1:A:220:GLU:CA	2.67	0.70
1:A:395:PHE:CE1	1:A:422:ARG:HG3	2.26	0.70
2:B:183:GLU:CG	2:B:394:GLN:HB3	2.21	0.70
2:B:194:LEU:CD2	2:B:267:PHE:CZ	2.75	0.70
2:B:338:LYS:O	2:B:339:ASN:CG	2.29	0.70
1:A:76:ASP:C	1:A:80:THR:OG1	2.29	0.69
1:A:158:SER:N	1:A:166:LYS:NZ	2.40	0.69
1:A:271:THR:O	1:A:376:CYS:HA	1.92	0.69
1:A:273:ALA:N	1:A:274:PRO:HD2	2.07	0.69
2:B:132:LEU:HB2	2:B:164:ARG:NH1	2.06	0.69
2:B:141:LEU:CD2	2:B:186:ASN:HB3	2.12	0.69
2:B:259:MET:CE	2:B:378:ILE:HG22	2.22	0.69
2:B:265:LEU:CD2	2:B:267:PHE:CZ	2.71	0.69
2:B:435:TYR:CA	2:B:436:GLN:HG3	2.18	0.69
1:A:72:PRO:CA	1:A:75:ILE:CG2	2.70	0.69
1:A:200:CYS:SG	1:A:259:LEU:HB2	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:LEU:CG	2:B:85:GLN:CG	2.67	0.69
2:B:104:ALA:HA	2:B:413:MET:CE	2.22	0.69
2:B:142:GLY:CA	2:B:182:VAL:CG2	2.65	0.69
2:B:158:ARG:CD	2:B:197:ASN:N	2.51	0.69
2:B:405:LEU:O	2:B:409:THR:OG1	2.07	0.69
1:A:241:SER:CB	1:A:356:ASN:ND2	2.53	0.69
1:A:282:TYR:HD2	1:A:285:GLN:HA	1.52	0.69
2:B:259:MET:HE2	2:B:379:GLY:CA	2.22	0.69
2:B:265:LEU:O	2:B:267:PHE:CD2	2.45	0.69
2:B:369:ARG:O	5:B:501:TXL:C21	2.41	0.69
1:A:291:ILE:HD11	1:A:373:ARG:CB	2.22	0.69
2:B:75:MET:HE1	2:B:79:ARG:HD2	0.74	0.69
1:A:5:ILE:HD12	1:A:135:PHE:CE1	2.28	0.69
1:A:115:ILE:CD1	1:A:156:ARG:HD2	2.23	0.69
2:B:2:ARG:O	2:B:2:ARG:HG2	1.91	0.69
2:B:53:TYR:CE1	2:B:87:PHE:HE1	2.07	0.69
2:B:371:LEU:O	2:B:372:LYS:HB2	1.93	0.69
1:A:28:HIS:CG	1:A:29:GLY:H	2.10	0.69
1:A:115:ILE:CD1	1:A:156:ARG:CZ	2.62	0.69
1:A:122:ILE:CD1	1:A:157:LEU:HD22	2.22	0.69
1:A:200:CYS:SG	1:A:260:VAL:HG23	2.33	0.69
1:A:288:VAL:O	1:A:291:ILE:HG13	1.92	0.69
2:B:229:HIS:CE1	5:B:501:TXL:H37	2.28	0.69
2:B:242:LEU:HD13	2:B:250:ALA:CB	2.15	0.69
2:B:242:LEU:HD23	2:B:356:CYS:SG	2.33	0.69
2:B:416:MET:O	2:B:417:GLU:HB2	1.90	0.69
1:A:17:GLY:O	1:A:21:TRP:HD1	1.76	0.69
1:A:17:GLY:O	1:A:21:TRP:CD1	2.46	0.69
1:A:184:PRO:CG	1:A:399:TYR:HD2	2.05	0.69
1:A:341:ILE:HG21	1:A:343:PHE:CE2	2.27	0.69
1:A:369:ALA:HB2	1:A:371:VAL:CG2	2.21	0.69
1:A:397:LEU:HD22	1:A:401:LYS:NZ	2.08	0.69
2:B:7:ILE:HG12	2:B:66:ILE:CG2	2.16	0.69
2:B:133:GLN:HE21	2:B:253:ARG:HH11	1.39	0.69
2:B:169:PHE:CZ	2:B:235:MET:CG	2.75	0.69
2:B:184:PRO:HD2	2:B:398:MET:SD	2.32	0.69
2:B:407:TRP:N	2:B:407:TRP:CD1	2.58	0.69
1:A:57:GLY:HA3	1:A:61:HIS:ND1	2.08	0.69
2:B:14:ASN:ND2	2:B:69:ASP:OD1	2.25	0.69
2:B:253:ARG:HH11	2:B:253:ARG:HB2	1.58	0.69
2:B:35:SER:CA	2:B:60:LYS:HE2	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:VAL:HG21	2:B:421:ALA:CA	2.21	0.69
1:A:97:GLU:HB3	1:A:110:ILE:HD13	1.74	0.68
1:A:401:LYS:HG2	1:A:402:ARG:HG3	1.75	0.68
2:B:158:ARG:HH11	2:B:197:ASN:H	1.40	0.68
1:A:258:ASN:O	1:A:314:ALA:HB1	1.92	0.68
2:B:44:LEU:O	2:B:44:LEU:HG	1.93	0.68
2:B:320:ARG:HE	2:B:360:PRO:HG3	1.58	0.68
1:A:172:TYR:CZ	1:A:387:ALA:CB	2.74	0.68
1:A:250:VAL:CG1	1:A:254:GLU:HG2	2.15	0.68
1:A:315:CYS:HG	1:A:343:PHE:HE1	1.39	0.68
2:B:35:SER:HB3	2:B:60:LYS:CG	2.22	0.68
2:B:184:PRO:HB2	2:B:399:PHE:CD2	2.22	0.68
2:B:259:MET:O	2:B:261:PRO:HD3	1.93	0.68
2:B:323:MET:HG2	2:B:324:SER:H	1.55	0.68
1:A:66:VAL:HG22	1:A:125:LEU:CD1	2.23	0.68
1:A:158:SER:CB	1:A:196:GLU:O	2.41	0.68
1:A:312:TYR:CG	1:A:381:THR:HG22	2.28	0.68
2:B:92:PHE:CD2	2:B:114:LEU:CD1	2.64	0.68
2:B:339:ASN:O	2:B:342:TYR:CB	2.40	0.68
1:A:13:GLY:HA2	1:A:16:ILE:HG22	1.75	0.68
1:A:296:PHE:CE1	1:A:335:ILE:HG21	2.28	0.68
1:A:395:PHE:CD1	1:A:422:ARG:HG3	2.28	0.68
2:B:244:PHE:O	2:B:245:PRO:O	2.12	0.68
2:B:286:LEU:HD11	2:B:372:LYS:CB	2.07	0.68
1:A:5:ILE:HD12	1:A:135:PHE:CZ	2.28	0.68
1:A:234:ILE:O	1:A:237:SER:OG	2.11	0.68
2:B:44:LEU:HB3	2:B:85:GLN:HG3	1.76	0.68
2:B:194:LEU:HD23	2:B:267:PHE:CE2	2.28	0.68
1:A:5:ILE:HD11	1:A:132:LEU:HD13	1.76	0.68
1:A:26:LEU:HD11	1:A:361:THR:OG1	1.94	0.68
1:A:184:PRO:CG	1:A:395:PHE:HB2	2.19	0.68
1:A:317:LEU:HA	1:A:376:CYS:O	1.94	0.68
1:A:361:THR:O	1:A:362:VAL:CG2	2.41	0.68
2:B:144:GLY:N	2:B:185:TYR:OH	2.27	0.68
2:B:201:THR:HG21	2:B:265:LEU:CG	2.24	0.68
1:A:107:HIS:CD2	1:A:148:GLY:HA2	2.29	0.68
1:A:145:THR:C	1:A:149:PHE:HB3	2.13	0.68
1:A:154:MET:HE1	1:A:166:LYS:HB3	1.76	0.68
1:A:242:LEU:CD1	1:A:255:PHE:CZ	2.67	0.68
1:A:311:LYS:O	1:A:312:TYR:O	2.12	0.68
1:A:315:CYS:SG	1:A:343:PHE:CE1	2.87	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:PRO:O	2:B:176:LYS:HD3	1.88	0.68
2:B:352:LYS:HG2	2:B:353:THR:N	2.09	0.68
1:A:57:GLY:CA	1:A:61:HIS:CE1	2.71	0.68
1:A:66:VAL:CG2	1:A:125:LEU:HD13	2.24	0.68
1:A:275:VAL:O	1:A:275:VAL:HG12	1.94	0.68
2:B:111:GLY:C	2:B:115:VAL:CG2	2.56	0.68
1:A:48:SER:O	1:A:50:ASN:ND2	2.22	0.68
1:A:115:ILE:HD13	1:A:152:LEU:HD11	1.73	0.68
1:A:191:THR:HG21	1:A:421:ALA:CA	2.24	0.67
2:B:44:LEU:HB2	2:B:84:GLY:HA2	1.74	0.67
2:B:289:PRO:HA	2:B:292:THR:OG1	1.93	0.67
1:A:102:ASN:C	1:A:185:TYR:HE2	1.98	0.67
1:A:231:ILE:CD1	1:A:302:MET:HE2	2.23	0.67
2:B:178:SER:HB2	4:B:500:GDP:O3'	1.89	0.67
2:B:183:GLU:CG	2:B:398:MET:SD	2.82	0.67
1:A:83:TYR:O	1:A:84:ARG:CG	2.41	0.67
1:A:153:LEU:O	1:A:157:LEU:CG	2.42	0.67
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.76	0.67
2:B:242:LEU:HD21	2:B:354:ALA:HB1	1.77	0.67
2:B:244:PHE:CB	2:B:245:PRO:CD	2.71	0.67
1:A:75:ILE:HD12	1:A:93:ILE:O	1.95	0.67
1:A:209:ILE:HD13	1:A:227:LEU:CD1	2.24	0.67
1:A:222:PRO:HB2	2:B:326:LYS:HD2	1.75	0.67
1:A:399:TYR:O	1:A:403:ALA:HA	1.94	0.67
1:A:422:ARG:O	1:A:426:ALA:CB	2.41	0.67
2:B:53:TYR:HD1	2:B:87:PHE:CE1	2.11	0.67
2:B:87:PHE:CE1	2:B:89:PRO:HG3	2.28	0.67
2:B:102:ASN:CB	2:B:408:TYR:HD1	2.07	0.67
2:B:151:THR:HA	2:B:192:HIS:HE2	0.84	0.67
2:B:398:MET:HE2	2:B:399:PHE:CE2	2.29	0.67
1:A:58:ALA:HB3	1:A:60:LYS:HG3	1.75	0.67
1:A:239:THR:CG2	1:A:243:ARG:HG3	2.23	0.67
2:B:96:GLN:O	2:B:98:GLY:CA	2.42	0.67
1:A:16:ILE:CG2	1:A:138:PHE:CD1	2.77	0.67
1:A:103:TYR:N	1:A:408:TYR:HE1	1.81	0.67
1:A:277:SER:CA	1:A:368:LEU:HD22	2.24	0.67
2:B:399:PHE:CE1	2:B:408:TYR:CZ	2.80	0.67
1:A:172:TYR:HE2	1:A:388:TRP:CZ3	2.12	0.67
2:B:284:ARG:O	2:B:286:LEU:N	2.28	0.67
2:B:328:VAL:O	2:B:332:MET:HG2	1.93	0.67
2:B:336:GLN:HE21	2:B:351:VAL:HB	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:CG	1:A:89:PRO:N	2.62	0.67
1:A:311:LYS:C	1:A:312:TYR:O	2.31	0.67
2:B:30:ILE:HG23	2:B:243:ARG:NH1	2.08	0.67
2:B:31:ASP:H	2:B:32:PRO:HD3	1.59	0.67
2:B:44:LEU:CB	2:B:85:GLN:HG3	2.24	0.67
1:A:77:GLU:O	1:A:80:THR:HB	1.95	0.67
1:A:176:GLN:NE2	2:B:333:LEU:CD2	2.36	0.67
1:A:312:TYR:HD2	1:A:381:THR:CG2	2.04	0.67
2:B:431:GLU:HA	2:B:434:GLN:CD	2.15	0.67
1:A:65:ALA:O	1:A:66:VAL:CG2	2.42	0.67
1:A:146:GLY:HA2	1:A:150:THR:HG23	1.76	0.67
2:B:107:HIS:CE1	2:B:152:LEU:HD23	2.22	0.67
2:B:181:VAL:CG2	2:B:404:PHE:HE2	2.09	0.67
2:B:197:ASN:OD1	2:B:197:ASN:O	2.13	0.67
1:A:196:GLU:O	1:A:197:HIS:CG	2.48	0.66
1:A:210:TYR:CE1	2:B:326:LYS:HE2	2.30	0.66
2:B:135:PHE:HB2	2:B:166:MET:SD	2.34	0.66
2:B:201:THR:HG21	2:B:265:LEU:HD21	0.74	0.66
1:A:22:GLU:O	1:A:25:CYS:CB	2.43	0.66
1:A:103:TYR:CE2	1:A:189:LEU:CA	2.75	0.66
1:A:220:GLU:H	1:A:220:GLU:HG3	1.58	0.66
1:A:291:ILE:HD12	1:A:373:ARG:HB3	1.77	0.66
1:A:407:TRP:CH2	2:B:256:ALA:HB1	2.21	0.66
2:B:11:GLN:HB2	4:B:500:GDP:O2A	1.95	0.66
2:B:19:LYS:HD2	2:B:228:ASN:CB	2.18	0.66
2:B:107:HIS:CD2	2:B:152:LEU:HD23	2.19	0.66
1:A:72:PRO:C	1:A:75:ILE:CG2	2.64	0.66
1:A:328:VAL:HG13	1:A:353:VAL:HG11	1.77	0.66
2:B:141:LEU:HD12	2:B:173:PRO:HD3	1.77	0.66
2:B:359:PRO:CB	2:B:372:LYS:O	2.43	0.66
1:A:88:HIS:CD2	1:A:89:PRO:N	2.63	0.66
1:A:210:TYR:CE1	2:B:326:LYS:CE	2.78	0.66
1:A:239:THR:O	1:A:243:ARG:CG	2.43	0.66
3:A:500:GTP:O2A	2:B:248:LEU:HD12	1.95	0.66
1:A:14:VAL:HB	1:A:74:VAL:HG21	1.78	0.66
1:A:28:HIS:CG	1:A:29:GLY:N	2.64	0.66
1:A:104:ALA:CA	1:A:108:TYR:HD2	2.08	0.66
1:A:288:VAL:O	1:A:291:ILE:CG1	2.44	0.66
2:B:154:ILE:HG23	2:B:198:THR:CG2	2.26	0.66
2:B:272:PHE:CE1	2:B:274:PRO:HG2	2.30	0.66
2:B:391:ILE:O	2:B:394:GLN:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:TYR:CE1	1:A:435:VAL:HG13	2.31	0.66
2:B:153:LEU:O	2:B:157:ILE:HG13	1.95	0.66
2:B:154:ILE:HD12	2:B:192:HIS:HE2	1.60	0.66
2:B:184:PRO:HB3	2:B:395:PHE:CD1	2.30	0.66
2:B:388:PHE:C	2:B:390:ARG:N	2.49	0.66
1:A:5:ILE:HG13	1:A:64:ARG:HH21	1.61	0.66
2:B:42:LEU:O	2:B:43:GLN:CG	2.42	0.66
2:B:103:TRP:HZ3	2:B:108:TYR:HH	1.00	0.66
1:A:179:THR:CG2	1:A:181:VAL:CG2	2.74	0.66
1:A:437:VAL:C	1:A:438:ASP:OD1	2.33	0.66
1:A:73:THR:CB	2:B:249:ASN:ND2	2.59	0.66
1:A:107:HIS:CD2	1:A:151:SER:OG	2.49	0.66
1:A:109:THR:HG21	1:A:411:GLU:HB3	1.78	0.66
1:A:176:GLN:NE2	2:B:333:LEU:HB2	2.11	0.66
1:A:272:TYR:CE2	1:A:274:PRO:HG2	2.26	0.66
1:A:277:SER:N	1:A:280:LYS:CG	2.58	0.66
1:A:294:ALA:C	1:A:300:ASN:HD22	2.00	0.66
1:A:313:MET:HA	1:A:344:VAL:CG2	2.25	0.66
1:A:210:TYR:CD1	2:B:326:LYS:CB	2.78	0.65
2:B:103:TRP:CD1	2:B:148:GLY:HA3	2.31	0.65
2:B:229:HIS:CG	5:B:501:TXL:H37	2.28	0.65
1:A:172:TYR:HD1	1:A:173:PRO:O	1.79	0.65
1:A:239:THR:O	1:A:243:ARG:CB	2.44	0.65
1:A:291:ILE:CD1	1:A:373:ARG:CB	2.74	0.65
1:A:361:THR:CG2	1:A:362:VAL:N	2.59	0.65
2:B:23:VAL:HG21	2:B:232:SER:CB	2.26	0.65
2:B:133:GLN:NE2	2:B:253:ARG:HH11	1.94	0.65
2:B:268:PHE:CD1	2:B:380:ASN:OD1	2.49	0.65
2:B:422:GLU:O	2:B:426:ASN:CB	2.41	0.65
1:A:5:ILE:HB	1:A:135:PHE:CD1	2.32	0.65
1:A:205:ASP:HB2	1:A:302:MET:O	1.96	0.65
1:A:277:SER:N	1:A:280:LYS:HG2	2.11	0.65
2:B:433:GLN:CG	2:B:437:ASP:OD2	2.43	0.65
1:A:22:GLU:O	1:A:25:CYS:HB3	1.96	0.65
1:A:331:ALA:O	1:A:334:THR:OG1	2.12	0.65
2:B:158:ARG:HA	2:B:197:ASN:HD22	0.52	0.65
1:A:197:HIS:O	1:A:198:SER:CB	2.45	0.65
2:B:184:PRO:HA	2:B:395:PHE:CD1	2.30	0.65
2:B:234:THR:CB	2:B:302:MET:CE	2.75	0.65
2:B:397:ALA:C	2:B:401:ARG:HB2	2.17	0.65
1:A:171:ILE:H	1:A:203:MET:HE1	1.57	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PHE:CD1	1:A:378:LEU:HD22	2.30	0.65
1:A:217:LEU:CD1	1:A:277:SER:HA	2.27	0.65
2:B:22:GLU:CA	2:B:83:PHE:CE2	2.79	0.65
2:B:33:THR:HG22	2:B:34:GLY:N	2.11	0.65
2:B:34:GLY:O	2:B:36:TYR:CD2	2.49	0.65
2:B:313:LEU:CA	2:B:344:VAL:HG21	2.22	0.65
1:A:30:ILE:HG21	1:A:64:ARG:CG	2.09	0.65
1:A:83:TYR:O	1:A:84:ARG:CB	2.44	0.65
2:B:101:ASN:O	2:B:105:LYS:HD2	1.97	0.65
2:B:241:CYS:SG	2:B:320:ARG:CD	2.84	0.65
2:B:165:ILE:HD13	2:B:256:ALA:CB	2.26	0.65
2:B:183:GLU:CD	2:B:394:GLN:CG	2.65	0.65
2:B:405:LEU:O	2:B:409:THR:N	2.26	0.65
1:A:77:GLU:N	1:A:80:THR:OG1	2.30	0.65
2:B:3:GLU:C	2:B:4:ILE:CG1	2.58	0.65
2:B:53:TYR:CE1	2:B:89:PRO:CG	2.78	0.65
2:B:103:TRP:HE1	2:B:189:LEU:HD23	1.59	0.65
2:B:246:GLY:HA2	2:B:357:ASP:CG	2.18	0.65
2:B:426:ASN:C	2:B:428:LEU:N	2.51	0.65
1:A:361:THR:C	1:A:362:VAL:HG23	2.18	0.64
2:B:142:GLY:O	2:B:185:TYR:CZ	2.49	0.64
2:B:296:PHE:CE1	2:B:335:VAL:HG21	2.32	0.64
1:A:13:GLY:CA	1:A:16:ILE:HG22	2.26	0.64
1:A:73:THR:HG21	2:B:249:ASN:HD21	1.59	0.64
1:A:142:GLY:HA2	1:A:185:TYR:CD1	2.32	0.64
2:B:8:GLN:HB2	2:B:67:LEU:HD12	1.78	0.64
2:B:103:TRP:HE3	2:B:413:MET:CE	1.90	0.64
2:B:111:GLY:O	2:B:115:VAL:CB	2.45	0.64
1:A:2:ARG:O	1:A:31:GLN:CG	2.39	0.64
1:A:175:PRO:HD3	1:A:390:ARG:HH22	1.62	0.64
1:A:176:GLN:C	1:A:177:VAL:CG2	2.42	0.64
1:A:224:TYR:HB2	2:B:325:MET:CB	2.28	0.64
1:A:426:ALA:C	1:A:428:LEU:N	2.51	0.64
2:B:103:TRP:CD1	2:B:189:LEU:HD21	2.08	0.64
2:B:183:GLU:HB2	2:B:184:PRO:HD2	1.70	0.64
2:B:319:PHE:CE2	2:B:328:VAL:HG13	2.32	0.64
2:B:401:ARG:CG	2:B:402:LYS:H	2.03	0.64
1:A:13:GLY:C	1:A:16:ILE:HG22	2.18	0.64
1:A:151:SER:HB2	1:A:192:HIS:HB2	1.79	0.64
1:A:219:ILE:CG2	1:A:219:ILE:C	2.65	0.64
1:A:223:THR:H	1:A:226:ASN:HD22	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ALA:O	1:A:302:MET:CG	2.43	0.64
2:B:12:CYS:SG	4:B:500:GDP:O4'	2.55	0.64
2:B:30:ILE:CG2	2:B:136:GLN:HE22	2.09	0.64
2:B:32:PRO:CA	2:B:59:ASN:HD22	2.05	0.64
2:B:92:PHE:CE1	2:B:121:VAL:CG2	2.80	0.64
2:B:94:PHE:CD2	2:B:114:LEU:HD22	2.32	0.64
2:B:342:TYR:C	2:B:343:PHE:CD2	2.71	0.64
1:A:80:THR:O	1:A:82:THR:N	2.30	0.64
2:B:80:SER:O	2:B:81:GLY:C	2.35	0.64
2:B:296:PHE:O	2:B:297:ASP:C	2.34	0.64
1:A:77:GLU:C	1:A:80:THR:H	2.01	0.64
1:A:115:ILE:HD11	1:A:156:ARG:HD2	1.79	0.64
1:A:179:THR:HB	1:A:182:VAL:HG23	1.79	0.64
1:A:287:SER:OG	1:A:290:GLU:CB	2.45	0.64
2:B:11:GLN:HB3	4:B:500:GDP:O1A	1.97	0.64
2:B:12:CYS:SG	4:B:500:GDP:N9	2.71	0.64
2:B:231:VAL:HA	2:B:302:MET:CE	2.28	0.64
1:A:238:ILE:O	1:A:255:PHE:HZ	1.80	0.64
2:B:47:GLU:HG2	2:B:63:PRO:HD3	1.80	0.64
2:B:166:MET:O	2:B:199:ASP:HB3	1.97	0.64
2:B:433:GLN:O	2:B:434:GLN:C	2.34	0.64
1:A:30:ILE:CB	1:A:64:ARG:HB2	2.15	0.64
1:A:48:SER:OG	1:A:56:THR:CB	2.37	0.64
1:A:224:TYR:CE1	3:A:500:GTP:C2	2.86	0.64
1:A:348:PRO:O	1:A:349:THR:OG1	2.13	0.64
2:B:6:HIS:CE1	2:B:21:TRP:CH2	2.86	0.64
2:B:13:GLY:HA3	2:B:138:THR:OG1	1.98	0.64
2:B:173:PRO:HG2	2:B:391:ILE:HD11	1.78	0.64
2:B:175:PRO:C	2:B:176:LYS:HE2	2.12	0.64
1:A:41:THR:O	1:A:41:THR:HG22	1.97	0.64
1:A:191:THR:CG2	1:A:421:ALA:HA	2.28	0.64
1:A:426:ALA:O	1:A:428:LEU:N	2.31	0.64
2:B:30:ILE:HG22	2:B:243:ARG:NH1	2.13	0.64
2:B:272:PHE:CZ	5:B:501:TXL:H28	2.33	0.64
1:A:26:LEU:CD1	1:A:361:THR:HG21	2.15	0.64
1:A:132:LEU:O	1:A:134:GLY:N	2.30	0.64
1:A:397:LEU:HA	1:A:401:LYS:HB3	1.78	0.64
2:B:12:CYS:O	2:B:16:ILE:HB	1.98	0.64
2:B:13:GLY:HA2	2:B:138:THR:OG1	1.95	0.64
2:B:57:ALA:C	2:B:64:ARG:H	2.00	0.64
2:B:181:VAL:CA	2:B:398:MET:HE1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:PRO:HB2	2:B:399:PHE:CG	2.33	0.64
2:B:405:LEU:CG	2:B:418:PHE:CZ	2.77	0.64
1:A:102:ASN:CA	1:A:185:TYR:HE2	2.11	0.63
1:A:303:VAL:HG12	1:A:305:CYS:SG	2.38	0.63
2:B:68:VAL:HG11	2:B:149:MET:CE	2.24	0.63
2:B:101:ASN:ND2	2:B:185:TYR:OH	2.31	0.63
2:B:398:MET:O	2:B:401:ARG:CB	2.45	0.63
1:A:238:ILE:HG23	1:A:255:PHE:CZ	2.32	0.63
1:A:324:VAL:O	1:A:327:ASP:HB2	1.97	0.63
2:B:183:GLU:OE1	2:B:394:GLN:HG3	1.98	0.63
1:A:115:ILE:CD1	1:A:156:ARG:NE	2.59	0.63
1:A:315:CYS:SG	1:A:343:PHE:HE1	2.21	0.63
2:B:92:PHE:HE1	2:B:121:VAL:CG2	2.10	0.63
2:B:229:HIS:NE2	5:B:501:TXL:C34	2.50	0.63
1:A:97:GLU:CB	1:A:110:ILE:HG23	2.21	0.63
1:A:267:PHE:O	1:A:380:ASN:OD1	2.15	0.63
1:A:282:TYR:CE2	1:A:285:GLN:HA	2.33	0.63
1:A:405:VAL:CG2	1:A:405:VAL:HG11	2.25	0.63
2:B:92:PHE:HE1	2:B:121:VAL:HG21	1.62	0.63
2:B:118:VAL:O	2:B:118:VAL:HG12	1.98	0.63
2:B:165:ILE:HD13	2:B:256:ALA:HB1	1.80	0.63
2:B:288:VAL:N	2:B:289:PRO:CD	2.59	0.63
2:B:287:THR:HG22	2:B:289:PRO:N	2.14	0.63
2:B:426:ASN:O	2:B:428:LEU:N	2.32	0.63
1:A:67:PHE:HB2	1:A:92:LEU:CD2	2.28	0.63
1:A:70:LEU:CD1	1:A:145:THR:CB	2.60	0.63
1:A:97:GLU:HA	1:A:97:GLU:OE1	1.97	0.63
2:B:183:GLU:OE2	2:B:394:GLN:CD	2.36	0.63
1:A:107:HIS:CD2	1:A:148:GLY:C	2.72	0.63
1:A:192:HIS:O	1:A:196:GLU:CG	2.46	0.63
1:A:277:SER:CB	1:A:280:LYS:CG	2.51	0.63
1:A:282:TYR:O	1:A:284:GLU:N	2.31	0.63
1:A:296:PHE:CZ	1:A:335:ILE:HD13	2.22	0.63
2:B:5:VAL:HG11	2:B:135:PHE:CE2	2.33	0.63
2:B:250:ALA:HB2	2:B:352:LYS:NZ	2.13	0.63
1:A:14:VAL:HA	1:A:67:PHE:CE1	2.34	0.63
1:A:154:MET:HB2	1:A:192:HIS:NE2	2.14	0.63
2:B:102:ASN:HB2	2:B:105:LYS:CG	2.29	0.63
2:B:301:MET:HE2	2:B:377:PHE:CE1	2.34	0.63
1:A:57:GLY:HA3	1:A:61:HIS:CD2	2.34	0.62
1:A:103:TYR:CD2	1:A:189:LEU:CG	2.78	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLY:O	1:A:111:GLY:N	2.32	0.62
1:A:193:THR:HG1	1:A:194:THR:N	1.96	0.62
1:A:237:SER:HA	1:A:320:ARG:NH1	2.13	0.62
1:A:282:TYR:CE2	1:A:284:GLU:O	2.51	0.62
1:A:317:LEU:O	1:A:353:VAL:HA	1.98	0.62
2:B:200:GLU:CB	2:B:268:PHE:HE2	2.09	0.62
1:A:103:TYR:OH	1:A:151:SER:HB2	1.98	0.62
1:A:155:GLU:CD	1:A:192:HIS:HD2	1.88	0.62
1:A:361:THR:HG22	1:A:362:VAL:H	1.63	0.62
2:B:23:VAL:O	2:B:26:ASP:CB	2.47	0.62
2:B:106:GLY:O	2:B:111:GLY:N	2.33	0.62
2:B:166:MET:CG	2:B:197:ASN:O	2.46	0.62
2:B:223:THR:OG1	2:B:226:ASP:HB2	1.99	0.62
1:A:202:PHE:CE1	1:A:378:LEU:HD22	2.34	0.62
1:A:404:PHE:CD2	1:A:404:PHE:O	2.52	0.62
5:B:501:TXL:H192	5:B:501:TXL:C20	2.29	0.62
1:A:264:ARG:NH1	1:A:424:ASP:O	2.32	0.62
1:A:343:PHE:CE2	1:A:351:PHE:HZ	1.81	0.62
2:B:4:ILE:CD1	2:B:30:ILE:CB	2.77	0.62
2:B:238:VAL:HG13	2:B:255:LEU:CD1	2.30	0.62
2:B:274:PRO:HB2	2:B:371:LEU:HD11	1.81	0.62
2:B:342:TYR:O	2:B:343:PHE:CD2	2.52	0.62
1:A:2:ARG:O	1:A:243:ARG:NH1	2.32	0.62
1:A:139:HIS:HB3	1:A:169:PHE:O	2.00	0.62
1:A:224:TYR:CD1	3:A:500:GTP:C2	2.88	0.62
2:B:35:SER:HB3	2:B:60:LYS:HG3	1.81	0.62
2:B:57:ALA:O	2:B:62:VAL:O	2.16	0.62
2:B:190:SER:C	2:B:192:HIS:N	2.53	0.62
2:B:216:THR:HG21	2:B:275:LEU:CD1	2.29	0.62
1:A:73:THR:CG2	2:B:249:ASN:HD22	2.10	0.62
1:A:103:TYR:CZ	1:A:188:ILE:HG22	2.34	0.62
1:A:115:ILE:HD12	1:A:152:LEU:HG	0.67	0.62
2:B:70:LEU:O	2:B:71:GLU:CG	2.47	0.62
2:B:133:GLN:O	2:B:133:GLN:HG2	1.99	0.62
2:B:246:GLY:CA	2:B:357:ASP:OD2	2.48	0.62
1:A:8:HIS:HE1	1:A:17:GLY:HA3	1.65	0.62
1:A:148:GLY:HA2	1:A:151:SER:HG	1.62	0.62
1:A:341:ILE:HG22	1:A:343:PHE:CE2	2.35	0.62
2:B:22:GLU:HG2	2:B:83:PHE:CE2	2.26	0.62
2:B:183:GLU:OE1	2:B:394:GLN:CG	2.48	0.62
1:A:142:GLY:CA	1:A:185:TYR:CE1	2.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:TYR:CD2	2:B:325:MET:CB	2.64	0.62
2:B:181:VAL:CA	2:B:398:MET:CE	2.77	0.62
2:B:243:ARG:NH2	2:B:252:LEU:CD1	2.52	0.62
1:A:122:ILE:CD1	1:A:157:LEU:CD2	2.77	0.62
1:A:276:ILE:HD13	1:A:282:TYR:CG	2.35	0.62
2:B:141:LEU:HD13	2:B:173:PRO:HD3	1.81	0.62
2:B:246:GLY:HA2	2:B:357:ASP:OD2	2.00	0.62
2:B:250:ALA:CB	2:B:352:LYS:NZ	2.63	0.62
1:A:103:TYR:N	1:A:408:TYR:CE1	2.61	0.61
1:A:143:GLY:O	1:A:144:GLY:C	2.35	0.61
1:A:204:VAL:HG13	1:A:302:MET:CE	2.28	0.61
2:B:169:PHE:HA	2:B:202:TYR:HB2	1.81	0.61
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.35	0.61
1:A:151:SER:CB	1:A:192:HIS:CB	2.75	0.61
1:A:242:LEU:HD12	1:A:255:PHE:CE2	2.34	0.61
1:A:304:LYS:HG2	1:A:304:LYS:O	1.98	0.61
2:B:3:GLU:CG	2:B:4:ILE:H	2.09	0.61
2:B:288:VAL:O	2:B:291:LEU:N	2.33	0.61
2:B:313:LEU:HD13	2:B:435:TYR:HD2	1.65	0.61
2:B:384:ILE:O	2:B:385:GLN:C	2.33	0.61
1:A:64:ARG:HH22	1:A:132:LEU:CG	2.09	0.61
1:A:78:VAL:HG13	1:A:87:PHE:HE1	1.61	0.61
1:A:296:PHE:HD2	1:A:312:TYR:HH	1.48	0.61
2:B:4:ILE:HG21	2:B:30:ILE:HB	1.82	0.61
2:B:40:SER:O	2:B:41:ASP:CG	2.38	0.61
2:B:78:VAL:CA	2:B:82:PRO:HG2	2.30	0.61
2:B:250:ALA:CB	2:B:352:LYS:HZ3	2.13	0.61
1:A:172:TYR:CE1	1:A:387:ALA:HB1	2.34	0.61
1:A:209:ILE:HD11	1:A:231:ILE:CD1	2.17	0.61
2:B:250:ALA:HA	2:B:254:LYS:CD	2.17	0.61
2:B:360:PRO:CG	2:B:374:SER:HB3	2.30	0.61
1:A:3:GLU:CB	1:A:64:ARG:CZ	2.77	0.61
1:A:38:SER:C	1:A:39:ASP:CB	2.68	0.61
1:A:72:PRO:HA	1:A:75:ILE:HG21	1.80	0.61
2:B:22:GLU:HA	2:B:83:PHE:CE2	2.35	0.61
2:B:75:MET:HE2	2:B:79:ARG:HD3	1.75	0.61
2:B:78:VAL:O	2:B:82:PRO:CG	2.43	0.61
1:A:6:SER:OG	1:A:65:ALA:N	2.34	0.61
1:A:45:GLY:C	1:A:46:ASP:CG	2.58	0.61
1:A:209:ILE:CD1	1:A:227:LEU:CD1	2.67	0.61
1:A:269:LEU:HD21	1:A:384:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:O	1:A:291:ILE:HB	2.00	0.61
2:B:201:THR:CG2	2:B:265:LEU:CD2	2.43	0.61
2:B:433:GLN:CG	2:B:437:ASP:OD1	2.48	0.61
1:A:313:MET:CE	1:A:346:TRP:HH2	2.12	0.61
2:B:31:ASP:N	2:B:32:PRO:CD	2.64	0.61
2:B:41:ASP:C	2:B:42:LEU:CG	2.54	0.61
2:B:69:ASP:CG	2:B:74:THR:CB	2.60	0.61
2:B:115:VAL:HG12	2:B:156:LYS:NZ	2.16	0.61
1:A:5:ILE:CG2	1:A:135:PHE:CE1	2.83	0.61
1:A:7:ILE:HG21	1:A:153:LEU:HD21	1.83	0.61
1:A:97:GLU:O	1:A:110:ILE:CD1	2.48	0.61
1:A:194:THR:CG2	1:A:195:LEU:H	2.02	0.61
2:B:216:THR:HG21	2:B:275:LEU:HD12	1.83	0.61
2:B:346:TRP:HZ3	2:B:347:ILE:CD1	1.79	0.61
2:B:386:GLU:C	2:B:388:PHE:H	2.01	0.61
2:B:399:PHE:CZ	2:B:408:TYR:CE2	2.80	0.61
1:A:9:VAL:CG1	1:A:146:GLY:HA2	2.31	0.61
1:A:277:SER:H	1:A:280:LYS:HG2	1.60	0.61
1:A:289:ALA:HB1	1:A:331:ALA:HB2	1.82	0.61
1:A:109:THR:HG23	1:A:411:GLU:HB3	1.81	0.61
1:A:151:SER:HB2	1:A:155:GLU:OE2	2.01	0.61
1:A:259:LEU:HB3	1:A:380:ASN:HD21	1.64	0.61
1:A:14:VAL:HB	1:A:74:VAL:CG2	2.30	0.60
1:A:122:ILE:HD13	1:A:157:LEU:CD2	2.31	0.60
1:A:217:LEU:CD1	1:A:368:LEU:CG	2.75	0.60
1:A:437:VAL:O	1:A:437:VAL:HG12	2.01	0.60
2:B:18:ALA:O	2:B:22:GLU:HG3	2.00	0.60
2:B:398:MET:CG	2:B:399:PHE:H	2.12	0.60
2:B:165:ILE:CD1	2:B:256:ALA:CB	2.79	0.60
1:A:34:GLY:O	1:A:60:LYS:NZ	2.34	0.60
1:A:242:LEU:HD13	1:A:250:VAL:O	2.00	0.60
2:B:15:GLN:O	2:B:18:ALA:HB3	2.00	0.60
2:B:34:GLY:HA2	2:B:37:HIS:CD2	2.36	0.60
2:B:68:VAL:HG13	2:B:149:MET:HE1	1.83	0.60
1:A:83:TYR:O	1:A:83:TYR:CG	2.54	0.60
1:A:158:SER:CB	1:A:197:HIS:HB2	2.14	0.60
1:A:191:THR:O	1:A:194:THR:OG1	2.19	0.60
1:A:228:ASN:ND2	3:A:500:GTP:N1	2.49	0.60
1:A:358:GLU:O	1:A:359:PRO:O	2.19	0.60
2:B:57:ALA:HA	2:B:64:ARG:HB2	0.69	0.60
1:A:219:ILE:HG22	1:A:219:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HB2	2:B:326:LYS:CE	2.31	0.60
1:A:327:ASP:O	1:A:331:ALA:HB3	2.01	0.60
3:A:500:GTP:PA	2:B:248:LEU:HD12	2.41	0.60
2:B:48:ARG:HH11	2:B:60:LYS:HG2	1.60	0.60
2:B:141:LEU:HG	2:B:171:VAL:O	2.01	0.60
2:B:182:VAL:CG1	2:B:186:ASN:HD22	2.01	0.60
2:B:274:PRO:C	2:B:276:THR:HG23	2.21	0.60
2:B:279:GLY:C	2:B:281:GLN:N	2.35	0.60
1:A:85:GLN:O	1:A:86:LEU:C	2.39	0.60
1:A:108:TYR:CZ	1:A:417:GLU:OE2	2.53	0.60
1:A:117:LEU:O	1:A:121:ARG:HG3	2.01	0.60
1:A:153:LEU:O	1:A:157:LEU:HD12	2.01	0.60
1:A:209:ILE:O	1:A:212:ILE:HG12	2.02	0.60
2:B:33:THR:C	2:B:59:ASN:ND2	2.44	0.60
2:B:104:ALA:O	2:B:108:TYR:HB2	2.01	0.60
2:B:219:LEU:CD2	2:B:226:ASP:OD2	2.50	0.60
2:B:226:ASP:CG	5:B:501:TXL:C40	2.70	0.60
2:B:323:MET:CG	2:B:324:SER:H	2.13	0.60
2:B:323:MET:CG	2:B:324:SER:N	2.65	0.60
2:B:397:ALA:O	2:B:401:ARG:CG	2.50	0.60
1:A:98:ASP:OD2	2:B:133:GLN:CD	2.40	0.60
1:A:100:ALA:HB1	1:A:105:ARG:CG	2.31	0.60
2:B:78:VAL:HA	2:B:82:PRO:CG	2.32	0.60
2:B:139:HIS:NE2	2:B:193:GLN:NE2	2.49	0.60
2:B:178:SER:O	2:B:179:ASP:HB2	2.01	0.60
2:B:424:ASN:O	2:B:424:ASN:ND2	2.32	0.60
1:A:237:SER:HB2	1:A:376:CYS:SG	2.41	0.60
2:B:289:PRO:O	2:B:293:GLN:CB	2.48	0.60
2:B:313:LEU:CD2	2:B:344:VAL:HG21	2.28	0.60
1:A:9:VAL:CG1	1:A:150:THR:HG23	2.31	0.60
1:A:14:VAL:HG11	1:A:74:VAL:HG13	1.83	0.60
2:B:79:ARG:O	2:B:80:SER:OG	2.19	0.60
1:A:115:ILE:CD1	1:A:152:LEU:HD21	2.32	0.60
1:A:141:PHE:HB3	1:A:173:PRO:HD3	1.84	0.60
1:A:237:SER:CB	1:A:376:CYS:SG	2.90	0.60
1:A:262:TYR:HE1	1:A:435:VAL:HG13	1.65	0.60
2:B:136:GLN:HE22	2:B:243:ARG:HH12	1.49	0.60
2:B:274:PRO:O	2:B:276:THR:CG2	2.46	0.60
2:B:320:ARG:HG3	2:B:320:ARG:O	2.00	0.60
2:B:339:ASN:O	2:B:342:TYR:CA	2.50	0.60
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:HG13	1:A:63:PRO:HD3	1.79	0.59
1:A:126:ALA:O	1:A:132:LEU:CD1	2.41	0.59
2:B:20:PHE:HZ	2:B:239:THR:HG21	1.67	0.59
2:B:22:GLU:OE1	2:B:83:PHE:CD1	2.55	0.59
2:B:30:ILE:CG2	2:B:243:ARG:HH12	2.13	0.59
2:B:251:ASP:O	2:B:253:ARG:N	2.35	0.59
2:B:274:PRO:CB	2:B:371:LEU:HD11	2.32	0.59
1:A:33:ASP:C	1:A:33:ASP:OD1	2.40	0.59
1:A:122:ILE:O	1:A:126:ALA:N	2.35	0.59
1:A:277:SER:OG	1:A:280:LYS:CD	2.47	0.59
1:A:296:PHE:O	1:A:297:GLU:C	2.31	0.59
2:B:66:ILE:CG1	2:B:121:VAL:CG1	2.69	0.59
1:A:144:GLY:CA	1:A:185:TYR:OH	2.50	0.59
1:A:173:PRO:HG3	1:A:182:VAL:CG1	2.32	0.59
2:B:23:VAL:O	2:B:26:ASP:HB2	2.02	0.59
2:B:27:GLU:HB2	2:B:36:TYR:HB3	1.84	0.59
2:B:198:THR:O	2:B:265:LEU:HD13	2.02	0.59
2:B:431:GLU:HA	2:B:434:GLN:NE2	2.17	0.59
1:A:36:MET:SD	1:A:60:LYS:CB	2.90	0.59
1:A:57:GLY:HA3	1:A:61:HIS:CG	2.37	0.59
1:A:103:TYR:CE2	1:A:147:SER:C	2.76	0.59
1:A:105:ARG:NH1	2:B:253:ARG:NH2	2.51	0.59
1:A:177:VAL:CB	2:B:349:ASN:ND2	2.52	0.59
1:A:191:THR:CG2	1:A:421:ALA:CA	2.79	0.59
2:B:48:ARG:C	2:B:61:TYR:CD2	2.76	0.59
2:B:62:VAL:HG12	2:B:63:PRO:N	2.18	0.59
2:B:103:TRP:O	2:B:107:HIS:HB3	2.02	0.59
2:B:174:SER:HB2	2:B:175:PRO:CD	2.29	0.59
2:B:398:MET:HG2	2:B:399:PHE:H	1.64	0.59
1:A:184:PRO:CB	1:A:399:TYR:HD2	2.15	0.59
2:B:383:ALA:O	2:B:386:GLU:CB	2.51	0.59
1:A:264:ARG:O	1:A:265:GLY:O	2.19	0.59
1:A:362:VAL:HG12	1:A:363:VAL:N	2.18	0.59
2:B:14:ASN:HB3	2:B:74:THR:OG1	2.01	0.59
2:B:19:LYS:HG3	2:B:228:ASN:ND2	2.16	0.59
2:B:175:PRO:CB	2:B:176:LYS:HE2	2.32	0.59
2:B:340:SER:O	2:B:343:PHE:N	2.35	0.59
1:A:288:VAL:CG2	1:A:373:ARG:CD	2.44	0.59
1:A:312:TYR:CE1	1:A:341:ILE:HG23	2.38	0.59
2:B:3:GLU:HA	2:B:31:ASP:CG	2.19	0.59
2:B:4:ILE:HD11	2:B:30:ILE:O	1.98	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:ALA:CB	2:B:62:VAL:CG2	2.69	0.59
2:B:182:VAL:CG1	2:B:186:ASN:HD21	2.05	0.59
1:A:143:GLY:O	1:A:145:THR:N	2.36	0.59
1:A:206:ASN:CG	3:A:500:GTP:HN22	2.06	0.59
1:A:282:TYR:O	1:A:284:GLU:CA	2.50	0.59
2:B:6:HIS:HB2	2:B:65:ALA:CA	2.28	0.59
2:B:295:MET:HE3	2:B:375:ALA:CA	2.21	0.59
2:B:371:LEU:O	2:B:372:LYS:CB	2.50	0.59
2:B:383:ALA:O	2:B:386:GLU:HB2	2.03	0.59
1:A:182:VAL:HG12	1:A:186:ASN:ND2	2.14	0.59
1:A:184:PRO:HG2	1:A:399:TYR:HD2	1.67	0.59
1:A:202:PHE:HA	1:A:268:PRO:HG2	1.85	0.59
1:A:306:ASP:CG	1:A:308:ARG:CG	2.69	0.59
2:B:30:ILE:HG23	2:B:243:ARG:HH11	1.65	0.59
2:B:49:ILE:O	2:B:50:ASN:CG	2.40	0.59
2:B:55:GLU:C	2:B:57:ALA:N	2.56	0.59
2:B:346:TRP:HZ2	2:B:435:TYR:CD2	2.21	0.59
1:A:224:TYR:HB2	2:B:325:MET:HG3	1.84	0.59
1:A:303:VAL:HG12	1:A:304:LYS:N	2.17	0.59
2:B:133:GLN:HE21	2:B:253:ARG:HB2	1.68	0.59
2:B:142:GLY:HA2	2:B:185:TYR:CG	2.37	0.59
2:B:405:LEU:CD1	2:B:418:PHE:CZ	2.71	0.59
1:A:18:ASN:O	1:A:22:GLU:CG	2.50	0.58
1:A:65:ALA:CB	1:A:91:GLN:CD	2.71	0.58
1:A:268:PRO:HA	1:A:379:SER:O	2.03	0.58
1:A:361:THR:CG2	1:A:362:VAL:H	2.15	0.58
1:A:362:VAL:HG13	1:A:367:ASP:HB3	1.83	0.58
2:B:87:PHE:HE1	2:B:89:PRO:HG3	1.58	0.58
2:B:295:MET:CE	2:B:375:ALA:C	2.72	0.58
1:A:70:LEU:HG	1:A:145:THR:CG2	2.32	0.58
1:A:185:TYR:CE1	1:A:189:LEU:HD11	2.39	0.58
1:A:194:THR:CG2	1:A:195:LEU:HG	2.27	0.58
1:A:324:VAL:HB	1:A:327:ASP:OD2	2.03	0.58
1:A:346:TRP:CE3	1:A:346:TRP:O	2.56	0.58
1:A:397:LEU:HA	1:A:401:LYS:CD	2.32	0.58
2:B:272:PHE:CE2	5:B:501:TXL:H28	2.38	0.58
1:A:4:CYS:HB2	1:A:30:ILE:HG21	1.76	0.58
1:A:28:HIS:ND1	1:A:29:GLY:O	2.32	0.58
1:A:196:GLU:C	1:A:197:HIS:ND1	2.56	0.58
1:A:217:LEU:HD13	1:A:368:LEU:CD2	2.27	0.58
1:A:236:SER:O	1:A:240:ALA:HB3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLU:C	1:A:299:ALA:N	2.55	0.58
1:A:324:VAL:CG1	1:A:325:PRO:HD2	2.33	0.58
1:A:332:ILE:HD11	1:A:353:VAL:HG21	1.78	0.58
2:B:29:GLY:O	2:B:58:GLY:CA	2.52	0.58
2:B:191:VAL:HG22	2:B:421:ALA:HA	1.79	0.58
2:B:308:ARG:O	2:B:342:TYR:HE2	1.86	0.58
1:A:100:ALA:CB	1:A:105:ARG:CG	2.81	0.58
1:A:115:ILE:CD1	1:A:156:ARG:CD	2.82	0.58
1:A:313:MET:HE3	1:A:346:TRP:CZ2	2.34	0.58
2:B:22:GLU:C	2:B:24:ILE:H	2.06	0.58
2:B:29:GLY:HA2	2:B:30:ILE:HG12	1.85	0.58
2:B:92:PHE:HD2	2:B:114:LEU:CD1	1.97	0.58
1:A:291:ILE:O	1:A:294:ALA:HB3	2.03	0.58
1:A:310:GLY:HA3	1:A:382:THR:OG1	2.03	0.58
2:B:104:ALA:HB2	2:B:413:MET:SD	2.44	0.58
1:A:3:GLU:CA	1:A:31:GLN:CB	2.61	0.58
1:A:155:GLU:CD	1:A:192:HIS:CD2	2.68	0.58
1:A:2:ARG:HB3	1:A:243:ARG:HH12	1.67	0.58
1:A:89:PRO:O	1:A:90:GLU:HB2	2.04	0.58
1:A:197:HIS:O	1:A:198:SER:HB3	2.03	0.58
1:A:273:ALA:CB	1:A:294:ALA:CB	2.78	0.58
2:B:50:ASN:N	2:B:61:TYR:CE2	2.71	0.58
2:B:55:GLU:C	2:B:57:ALA:H	2.07	0.58
2:B:123:ARG:O	2:B:126:SER:OG	2.20	0.58
2:B:346:TRP:O	2:B:347:ILE:CG1	2.51	0.58
1:A:45:GLY:O	1:A:46:ASP:OD2	2.22	0.58
1:A:65:ALA:HB1	1:A:91:GLN:CD	2.23	0.58
1:A:97:GLU:CG	1:A:110:ILE:HG23	2.33	0.58
1:A:273:ALA:N	1:A:274:PRO:CD	2.66	0.58
2:B:70:LEU:O	2:B:71:GLU:HG3	2.03	0.58
2:B:274:PRO:HB2	2:B:371:LEU:CD1	2.34	0.58
2:B:295:MET:SD	2:B:375:ALA:HB1	2.36	0.58
5:B:501:TXL:C9	5:B:501:TXL:C16	2.79	0.58
1:A:82:THR:C	1:A:84:ARG:H	2.07	0.58
1:A:328:VAL:O	1:A:332:ILE:HG13	2.04	0.58
2:B:105:LYS:CE	2:B:411:GLU:HG3	2.34	0.58
2:B:251:ASP:O	2:B:254:LYS:N	2.33	0.58
1:A:74:VAL:O	1:A:77:GLU:HB2	2.03	0.58
1:A:324:VAL:HB	1:A:327:ASP:OD1	2.03	0.58
1:A:385:ALA:HB2	1:A:432:TYR:HD2	1.68	0.58
2:B:6:HIS:CD2	2:B:64:ARG:O	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:SER:HB2	2:B:207:GLU:CB	2.26	0.58
2:B:338:LYS:O	2:B:339:ASN:OD1	2.22	0.58
1:A:340:THR:O	1:A:341:ILE:HG12	2.04	0.57
1:A:208:ALA:HB2	1:A:303:VAL:HA	1.85	0.57
2:B:64:ARG:HH21	2:B:125:GLU:HB3	1.69	0.57
2:B:192:HIS:ND1	2:B:192:HIS:C	2.57	0.57
2:B:242:LEU:HA	2:B:356:CYS:SG	2.45	0.57
1:A:107:HIS:HB2	1:A:149:PHE:N	2.17	0.57
1:A:108:TYR:CB	1:A:112:LYS:HE3	2.34	0.57
1:A:154:MET:CE	1:A:166:LYS:CD	2.80	0.57
2:B:151:THR:C	2:B:192:HIS:CD2	2.73	0.57
1:A:8:HIS:CE1	1:A:17:GLY:HA3	2.39	0.57
1:A:14:VAL:CG1	1:A:74:VAL:HG22	2.35	0.57
1:A:271:THR:CG2	1:A:377:MET:HB3	2.35	0.57
1:A:407:TRP:CE3	2:B:257:VAL:HG22	2.36	0.57
2:B:4:ILE:HG21	2:B:30:ILE:CB	2.34	0.57
2:B:32:PRO:C	2:B:59:ASN:HD22	2.05	0.57
2:B:241:CYS:SG	2:B:320:ARG:CZ	2.89	0.57
2:B:268:PHE:HA	2:B:380:ASN:OD1	2.03	0.57
2:B:388:PHE:O	2:B:390:ARG:N	2.38	0.57
1:A:23:LEU:CD2	1:A:236:SER:CB	2.81	0.57
1:A:407:TRP:CE3	2:B:257:VAL:HG23	2.39	0.57
2:B:6:HIS:O	2:B:66:ILE:N	2.23	0.57
2:B:158:ARG:CG	2:B:197:ASN:ND2	2.61	0.57
2:B:385:GLN:O	2:B:389:LYS:HG3	2.04	0.57
2:B:427:ASP:O	2:B:431:GLU:N	2.18	0.57
1:A:76:ASP:O	1:A:80:THR:CB	2.51	0.57
2:B:158:ARG:HH11	2:B:197:ASN:N	2.03	0.57
1:A:23:LEU:HD21	1:A:236:SER:CB	2.34	0.57
1:A:77:GLU:O	1:A:83:TYR:HB2	2.05	0.57
1:A:107:HIS:CG	1:A:148:GLY:C	2.77	0.57
1:A:242:LEU:CB	1:A:250:VAL:O	2.47	0.57
1:A:250:VAL:CG1	1:A:254:GLU:CB	2.34	0.57
2:B:274:PRO:CB	2:B:371:LEU:CD2	2.80	0.57
2:B:21:TRP:HA	2:B:24:ILE:CD1	2.34	0.57
2:B:181:VAL:HG22	2:B:404:PHE:HE2	1.60	0.57
2:B:325:MET:HE1	2:B:355:VAL:HB	1.87	0.57
2:B:431:GLU:HA	2:B:434:GLN:HG3	1.87	0.57
1:A:175:PRO:HG2	1:A:207:GLU:HG2	1.86	0.57
1:A:177:VAL:CG1	1:A:178:SER:N	2.49	0.57
1:A:191:THR:HG23	1:A:421:ALA:HB1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ASN:OD1	1:A:352:LYS:CE	2.53	0.57
1:A:267:PHE:CG	1:A:388:TRP:HZ2	2.23	0.57
1:A:335:ILE:C	1:A:337:THR:H	2.06	0.57
1:A:14:VAL:CG2	1:A:69:ASP:OD1	2.52	0.57
1:A:154:MET:HE1	1:A:166:LYS:HD3	1.87	0.57
1:A:222:PRO:HG2	2:B:326:LYS:CB	2.35	0.57
1:A:275:VAL:O	1:A:368:LEU:HD13	2.04	0.57
1:A:327:ASP:O	1:A:331:ALA:CB	2.53	0.57
1:A:341:ILE:HG22	1:A:343:PHE:CD2	2.40	0.57
2:B:71:GLU:O	2:B:72:PRO:C	2.38	0.57
2:B:181:VAL:HG22	2:B:404:PHE:CD2	2.39	0.57
2:B:320:ARG:HH22	5:B:501:TXL:H27	1.70	0.57
2:B:400:ARG:CD	2:B:422:GLU:OE1	2.51	0.57
1:A:23:LEU:HD21	1:A:236:SER:HB3	1.86	0.56
1:A:102:ASN:C	1:A:185:TYR:CE2	2.78	0.56
1:A:106:GLY:HA2	1:A:111:GLY:H	1.69	0.56
1:A:405:VAL:CG2	1:A:405:VAL:CA	2.77	0.56
2:B:158:ARG:NH1	2:B:197:ASN:H	2.03	0.56
1:A:70:LEU:HG	1:A:145:THR:HG21	1.87	0.56
1:A:407:TRP:CH2	2:B:165:ILE:HD12	1.94	0.56
2:B:4:ILE:HD13	2:B:30:ILE:HA	1.66	0.56
2:B:7:ILE:O	2:B:137:LEU:HA	2.04	0.56
1:A:9:VAL:CG2	1:A:138:PHE:O	2.54	0.56
1:A:85:GLN:O	1:A:87:PHE:N	2.37	0.56
1:A:180:ALA:HB1	1:A:398:MET:CE	2.36	0.56
1:A:219:ILE:C	1:A:219:ILE:HG22	2.26	0.56
1:A:239:THR:O	1:A:243:ARG:HG2	2.05	0.56
1:A:254:GLU:OE2	1:A:352:LYS:HE3	2.05	0.56
1:A:267:PHE:CE1	1:A:388:TRP:CZ2	2.93	0.56
2:B:26:ASP:OD1	2:B:26:ASP:O	2.23	0.56
2:B:102:ASN:CB	2:B:408:TYR:CE1	2.88	0.56
2:B:103:TRP:HZ3	2:B:413:MET:HE2	1.17	0.56
2:B:183:GLU:OE2	2:B:394:GLN:CG	2.53	0.56
2:B:209:LEU:HD13	2:B:227:LEU:CG	2.15	0.56
2:B:212:ILE:CD1	2:B:302:MET:HB2	2.36	0.56
2:B:262:PHE:HB2	2:B:266:HIS:HE1	1.71	0.56
2:B:385:GLN:CD	2:B:433:GLN:HB2	2.26	0.56
1:A:10:GLY:O	1:A:13:GLY:CA	2.53	0.56
1:A:13:GLY:HA2	1:A:16:ILE:HG21	1.87	0.56
1:A:25:CYS:O	1:A:26:LEU:HD23	2.06	0.56
1:A:324:VAL:HG13	1:A:325:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ARG:HD3	2:B:290:GLU:OE1	2.04	0.56
2:B:359:PRO:HB2	2:B:372:LYS:O	2.05	0.56
1:A:192:HIS:CG	1:A:193:THR:N	2.73	0.56
1:A:292:THR:O	1:A:295:CYS:HB2	2.05	0.56
1:A:335:ILE:CG2	1:A:341:ILE:HG13	2.35	0.56
2:B:6:HIS:ND1	2:B:21:TRP:CZ2	2.74	0.56
2:B:22:GLU:CD	2:B:83:PHE:CB	2.72	0.56
2:B:223:THR:OG1	2:B:226:ASP:CB	2.54	0.56
2:B:230:LEU:O	2:B:233:ALA:HB3	2.04	0.56
2:B:239:THR:HB	2:B:243:ARG:NH1	2.20	0.56
1:A:28:HIS:ND1	1:A:29:GLY:N	2.54	0.56
1:A:224:TYR:CE1	3:A:500:GTP:C4	2.94	0.56
1:A:335:ILE:HG22	1:A:341:ILE:HG13	1.88	0.56
2:B:53:TYR:HE1	2:B:87:PHE:HE1	1.46	0.56
2:B:78:VAL:HA	2:B:82:PRO:HG2	1.86	0.56
2:B:89:PRO:O	2:B:90:ASP:CG	2.43	0.56
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.86	0.56
1:A:66:VAL:HG21	1:A:125:LEU:HD12	1.87	0.56
2:B:44:LEU:O	2:B:47:GLU:CB	2.54	0.56
2:B:311:ARG:O	2:B:381:SER:CB	2.52	0.56
1:A:2:ARG:HB3	1:A:243:ARG:NH1	2.21	0.56
1:A:141:PHE:HB2	1:A:172:TYR:HA	1.87	0.56
1:A:292:THR:CG2	1:A:319:TYR:OH	2.42	0.56
2:B:3:GLU:CD	2:B:64:ARG:HH12	2.09	0.56
2:B:40:SER:O	2:B:41:ASP:CB	2.54	0.56
2:B:280:SER:C	2:B:282:GLN:H	2.07	0.56
2:B:414:ASP:C	2:B:416:MET:H	2.05	0.56
1:A:33:ASP:OD1	1:A:33:ASP:O	2.23	0.56
1:A:363:VAL:HG12	1:A:364:PRO:CG	2.35	0.56
2:B:191:VAL:HG23	2:B:421:ALA:CB	2.36	0.56
1:A:14:VAL:HG21	1:A:69:ASP:OD1	2.06	0.55
1:A:97:GLU:CB	1:A:110:ILE:HD13	2.35	0.55
1:A:187:SER:O	1:A:191:THR:HG23	2.07	0.55
1:A:288:VAL:HG22	1:A:373:ARG:HG2	1.88	0.55
1:A:314:ALA:HB3	1:A:380:ASN:ND2	2.13	0.55
2:B:229:HIS:O	2:B:230:LEU:C	2.43	0.55
2:B:296:PHE:CD1	2:B:335:VAL:HG11	2.40	0.55
1:A:72:PRO:CA	1:A:75:ILE:HG22	2.33	0.55
1:A:108:TYR:HA	1:A:112:LYS:HE2	1.87	0.55
1:A:230:LEU:HG	1:A:302:MET:CE	2.36	0.55
1:A:288:VAL:O	1:A:291:ILE:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ILE:CB	2:B:137:LEU:HD21	2.28	0.55
2:B:147:SER:HB3	2:B:189:LEU:HD11	0.56	0.55
2:B:154:ILE:HG23	2:B:198:THR:HG22	1.87	0.55
1:A:22:GLU:O	1:A:25:CYS:HB2	2.07	0.55
1:A:137:VAL:CB	1:A:168:GLU:HG2	2.37	0.55
1:A:217:LEU:CB	1:A:368:LEU:HD11	2.35	0.55
1:A:405:VAL:HG11	1:A:405:VAL:HG21	1.87	0.55
2:B:301:MET:HE1	2:B:377:PHE:CD1	2.40	0.55
2:B:302:MET:O	2:B:302:MET:CG	2.47	0.55
2:B:371:LEU:N	5:B:501:TXL:H183	2.20	0.55
1:A:157:LEU:HB2	1:A:166:LYS:NZ	2.21	0.55
2:B:49:ILE:HA	2:B:61:TYR:CE2	2.41	0.55
2:B:234:THR:CB	2:B:302:MET:HE2	2.35	0.55
1:A:4:CYS:HG	1:A:252:LEU:HD11	1.68	0.55
1:A:14:VAL:HG21	1:A:74:VAL:CG1	2.36	0.55
1:A:28:HIS:CD2	1:A:33:ASP:HB3	2.41	0.55
1:A:35:GLN:O	1:A:36:MET:CG	2.54	0.55
1:A:69:ASP:HB3	1:A:71:GLU:O	2.07	0.55
1:A:427:ALA:O	1:A:431:ASP:N	2.19	0.55
2:B:206:ASN:O	2:B:210:TYR:HD2	1.86	0.55
2:B:287:THR:CA	2:B:290:GLU:HB3	2.36	0.55
2:B:311:ARG:CD	2:B:341:SER:O	2.54	0.55
2:B:295:MET:HE3	2:B:375:ALA:C	2.26	0.55
1:A:14:VAL:HG21	1:A:74:VAL:HG13	1.88	0.55
1:A:192:HIS:ND1	1:A:192:HIS:C	2.57	0.55
2:B:14:ASN:HD21	2:B:69:ASP:HA	1.72	0.55
2:B:174:SER:O	2:B:176:LYS:N	2.39	0.55
2:B:176:LYS:C	2:B:177:VAL:HG13	2.25	0.55
2:B:394:GLN:O	2:B:398:MET:CB	2.54	0.55
1:A:313:MET:N	1:A:380:ASN:O	2.40	0.55
2:B:142:GLY:HA2	2:B:185:TYR:CE1	2.37	0.55
2:B:181:VAL:O	2:B:399:PHE:CZ	2.57	0.55
1:A:5:ILE:HD13	1:A:135:PHE:CE1	2.42	0.55
2:B:238:VAL:HG13	2:B:255:LEU:HD13	1.88	0.55
1:A:157:LEU:O	1:A:161:TYR:HB2	2.07	0.54
1:A:242:LEU:HD11	1:A:318:LEU:HD11	1.87	0.54
1:A:267:PHE:CD2	1:A:388:TRP:HZ2	2.25	0.54
2:B:170:SER:O	2:B:204:ILE:HB	2.06	0.54
2:B:316:ALA:O	2:B:378:ILE:N	2.38	0.54
2:B:344:VAL:O	2:B:344:VAL:HG12	2.07	0.54
1:A:141:PHE:O	1:A:182:VAL:CG1	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLN:O	2:B:68:VAL:N	2.41	0.54
2:B:12:CYS:O	2:B:16:ILE:HG13	1.98	0.54
2:B:202:TYR:OH	2:B:238:VAL:HG11	2.08	0.54
1:A:26:LEU:O	1:A:27:GLU:HB2	2.06	0.54
1:A:41:THR:O	1:A:42:ILE:CB	2.43	0.54
1:A:219:ILE:HG21	1:A:219:ILE:HD13	1.87	0.54
2:B:106:GLY:HA2	2:B:111:GLY:H	1.72	0.54
2:B:136:GLN:NE2	2:B:243:ARG:HH12	2.05	0.54
2:B:143:GLY:C	2:B:185:TYR:CE1	2.80	0.54
2:B:242:LEU:HB3	2:B:250:ALA:O	2.08	0.54
2:B:288:VAL:C	2:B:291:LEU:H	2.10	0.54
2:B:313:LEU:N	2:B:381:SER:HA	2.22	0.54
1:A:9:VAL:HG11	1:A:150:THR:HG23	1.78	0.54
1:A:9:VAL:CB	1:A:138:PHE:O	2.55	0.54
1:A:166:LYS:CD	1:A:197:HIS:HD2	2.20	0.54
1:A:191:THR:HG21	1:A:421:ALA:HA	1.88	0.54
1:A:256:GLN:O	1:A:260:VAL:CB	2.55	0.54
2:B:56:ALA:HB1	2:B:62:VAL:H	1.71	0.54
2:B:126:SER:HA	2:B:132:LEU:HD11	1.88	0.54
2:B:143:GLY:C	2:B:185:TYR:HE1	2.11	0.54
2:B:175:PRO:HD2	2:B:207:GLU:HG2	1.88	0.54
2:B:195:VAL:O	2:B:195:VAL:HG12	2.08	0.54
2:B:286:LEU:HD12	2:B:372:LYS:CB	2.29	0.54
1:A:184:PRO:CG	1:A:395:PHE:CG	2.60	0.54
1:A:207:GLU:HG3	1:A:207:GLU:O	2.08	0.54
2:B:6:HIS:HD2	2:B:64:ARG:O	1.90	0.54
1:A:107:HIS:HD2	1:A:151:SER:OG	1.89	0.54
1:A:146:GLY:HA2	1:A:150:THR:CG2	2.37	0.54
1:A:185:TYR:HD2	1:A:408:TYR:HH	0.55	0.54
1:A:220:GLU:CG	1:A:220:GLU:N	2.70	0.54
2:B:201:THR:OG1	2:B:267:PHE:CD1	2.58	0.54
2:B:244:PHE:CG	2:B:245:PRO:HD3	2.40	0.54
1:A:11:GLN:OE1	1:A:74:VAL:HB	2.07	0.54
1:A:100:ALA:CB	1:A:105:ARG:HB3	2.31	0.54
1:A:166:LYS:HD2	1:A:197:HIS:HD2	1.73	0.54
1:A:208:ALA:HB2	1:A:303:VAL:CA	2.36	0.54
1:A:259:LEU:O	1:A:380:ASN:ND2	2.41	0.54
2:B:157:ILE:HG21	2:B:166:MET:HE1	1.90	0.54
2:B:41:ASP:O	2:B:42:LEU:CB	2.56	0.54
1:A:119:LEU:HD11	1:A:156:ARG:CD	2.30	0.54
2:B:102:ASN:ND2	2:B:105:LYS:HZ1	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:CYS:O	2:B:130:ASP:OD1	2.24	0.54
2:B:213:CYS:HA	2:B:217:LEU:CD1	2.06	0.54
1:A:103:TYR:O	1:A:148:GLY:HA3	2.08	0.54
1:A:114:ILE:O	1:A:114:ILE:HG22	2.07	0.54
1:A:148:GLY:O	1:A:152:LEU:N	2.40	0.54
2:B:288:VAL:C	2:B:290:GLU:N	2.57	0.54
1:A:200:CYS:SG	1:A:256:GLN:HA	2.48	0.53
2:B:92:PHE:CE2	2:B:114:LEU:CD1	2.89	0.53
2:B:286:LEU:HD13	2:B:373:MET:H	1.70	0.53
2:B:296:PHE:CE1	2:B:335:VAL:CG1	2.82	0.53
2:B:321:GLY:HA2	2:B:359:PRO:HB3	1.90	0.53
1:A:108:TYR:C	1:A:112:LYS:HG3	2.29	0.53
1:A:169:PHE:HZ	1:A:235:VAL:HG22	1.61	0.53
1:A:289:ALA:HB1	1:A:331:ALA:HB1	1.89	0.53
2:B:49:ILE:O	2:B:50:ASN:ND2	2.40	0.53
2:B:118:VAL:O	2:B:122:VAL:HG23	2.07	0.53
2:B:172:VAL:HG21	2:B:205:ASP:OD1	2.09	0.53
2:B:319:PHE:HZ	2:B:332:MET:SD	2.31	0.53
1:A:3:GLU:CA	1:A:31:GLN:CG	2.86	0.53
1:A:212:ILE:HD13	1:A:230:LEU:CD2	2.15	0.53
1:A:219:ILE:O	1:A:222:PRO:HD3	2.09	0.53
2:B:135:PHE:CG	2:B:166:MET:SD	3.02	0.53
2:B:309:HIS:HB3	2:B:386:GLU:OE2	2.07	0.53
2:B:319:PHE:CZ	2:B:328:VAL:HG12	2.36	0.53
2:B:431:GLU:HA	2:B:434:GLN:CG	2.39	0.53
2:B:23:VAL:O	2:B:26:ASP:HB3	2.08	0.53
2:B:94:PHE:HZ	2:B:110:GLU:O	1.92	0.53
2:B:141:LEU:HB3	2:B:186:ASN:ND2	1.87	0.53
2:B:190:SER:OG	2:B:191:VAL:N	2.41	0.53
2:B:192:HIS:HA	2:B:196:GLU:OE2	2.08	0.53
1:A:40:LYS:C	1:A:42:ILE:H	2.08	0.53
1:A:167:LEU:HD11	1:A:252:LEU:HD22	1.90	0.53
2:B:141:LEU:HD12	2:B:173:PRO:CD	2.37	0.53
2:B:293:GLN:O	2:B:297:ASP:OD1	2.27	0.53
2:B:294:GLN:CD	2:B:300:ASN:OD1	2.45	0.53
1:A:174:ALA:CB	1:A:390:ARG:NH2	2.52	0.53
1:A:407:TRP:CD2	2:B:257:VAL:CG2	2.88	0.53
1:A:2:ARG:HG2	1:A:133:GLN:NE2	2.23	0.53
1:A:81:GLY:O	1:A:83:TYR:N	2.41	0.53
1:A:237:SER:HA	1:A:320:ARG:HH11	1.73	0.53
1:A:416:GLY:O	1:A:417:GLU:CB	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:GLU:OE1	2:B:36:TYR:HA	2.09	0.53
2:B:107:HIS:CD2	2:B:151:THR:OG1	2.62	0.53
2:B:158:ARG:HG3	2:B:197:ASN:ND2	2.22	0.53
2:B:339:ASN:HB3	2:B:342:TYR:HB2	1.90	0.53
1:A:21:TRP:N	1:A:21:TRP:CD1	2.76	0.53
1:A:191:THR:HG22	1:A:421:ALA:HA	1.91	0.53
1:A:219:ILE:CG2	1:A:219:ILE:CD1	2.86	0.53
1:A:301:GLN:NE2	1:A:305:CYS:HB2	2.24	0.53
2:B:57:ALA:O	2:B:64:ARG:N	2.42	0.53
2:B:135:PHE:CD2	2:B:157:ILE:HG21	2.44	0.53
2:B:192:HIS:CG	2:B:196:GLU:HG3	2.44	0.53
2:B:208:ALA:HB2	2:B:303:ALA:O	2.05	0.53
1:A:205:ASP:HB2	1:A:303:VAL:CA	2.32	0.53
1:A:282:TYR:CD2	1:A:285:GLN:CA	2.81	0.53
1:A:313:MET:CG	1:A:380:ASN:O	2.57	0.53
2:B:32:PRO:HB2	2:B:59:ASN:HD22	0.60	0.53
2:B:42:LEU:O	2:B:43:GLN:CB	2.56	0.53
2:B:346:TRP:HE3	2:B:347:ILE:HG13	0.87	0.53
1:A:34:GLY:C	1:A:35:GLN:HG3	2.29	0.53
1:A:204:VAL:CG1	1:A:209:ILE:CG1	2.86	0.53
2:B:8:GLN:O	2:B:68:VAL:HB	2.08	0.53
2:B:22:GLU:HA	2:B:83:PHE:HE2	1.73	0.53
2:B:339:ASN:HA	2:B:342:TYR:HD1	1.73	0.53
1:A:53:PHE:HA	1:A:88:HIS:ND1	2.16	0.52
1:A:119:LEU:CA	1:A:122:ILE:HG22	2.38	0.52
1:A:224:TYR:HB2	2:B:325:MET:HB2	1.91	0.52
1:A:386:GLU:O	1:A:389:ALA:HB3	2.09	0.52
2:B:181:VAL:C	2:B:399:PHE:HE2	2.12	0.52
1:A:17:GLY:C	1:A:21:TRP:HD1	2.13	0.52
1:A:179:THR:CG2	1:A:180:ALA:N	2.67	0.52
2:B:40:SER:C	2:B:41:ASP:CG	2.67	0.52
2:B:312:TYR:O	2:B:344:VAL:HG21	2.00	0.52
2:B:319:PHE:CZ	2:B:332:MET:SD	3.03	0.52
2:B:342:TYR:O	2:B:343:PHE:CG	2.62	0.52
2:B:360:PRO:HG2	2:B:374:SER:HB3	1.90	0.52
1:A:83:TYR:O	1:A:84:ARG:HB2	2.09	0.52
1:A:142:GLY:HA2	1:A:185:TYR:CE1	2.43	0.52
1:A:209:ILE:HD12	1:A:227:LEU:HD21	1.90	0.52
1:A:219:ILE:CG2	1:A:219:ILE:HD13	2.39	0.52
1:A:362:VAL:CG1	1:A:363:VAL:N	2.73	0.52
2:B:141:LEU:C	2:B:186:ASN:ND2	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ILE:HD11	2:B:302:MET:HA	1.91	0.52
2:B:339:ASN:HA	2:B:342:TYR:CD1	2.43	0.52
1:A:101:ASN:ND2	3:A:500:GTP:O2G	2.42	0.52
1:A:196:GLU:C	1:A:197:HIS:CG	2.83	0.52
2:B:6:HIS:CE1	2:B:21:TRP:CZ2	2.97	0.52
2:B:64:ARG:HH21	2:B:125:GLU:C	2.13	0.52
2:B:105:LYS:CE	2:B:411:GLU:CG	2.86	0.52
2:B:399:PHE:CZ	2:B:408:TYR:CZ	2.96	0.52
1:A:13:GLY:O	1:A:16:ILE:CG2	2.56	0.52
1:A:228:ASN:ND2	3:A:500:GTP:C6	2.72	0.52
2:B:212:ILE:HD11	2:B:302:MET:CA	2.40	0.52
1:A:5:ILE:CD1	1:A:135:PHE:CZ	2.93	0.52
2:B:259:MET:CE	2:B:379:GLY:C	2.78	0.52
2:B:343:PHE:CG	2:B:350:ASN:ND2	2.78	0.52
1:A:142:GLY:O	1:A:185:TYR:CE1	2.63	0.52
1:A:205:ASP:HB2	1:A:208:ALA:HB3	1.91	0.52
2:B:7:ILE:HG13	2:B:66:ILE:CG2	2.36	0.52
2:B:31:ASP:H	2:B:32:PRO:CD	2.20	0.52
2:B:33:THR:CG2	2:B:34:GLY:N	2.73	0.52
2:B:49:ILE:CA	2:B:61:TYR:CE2	2.93	0.52
1:A:7:ILE:HG22	1:A:8:HIS:O	2.10	0.52
1:A:223:THR:O	2:B:326:LYS:HE3	2.10	0.52
2:B:33:THR:HG22	2:B:34:GLY:H	1.73	0.52
2:B:233:ALA:CB	2:B:272:PHE:CD2	2.79	0.52
2:B:259:MET:CE	2:B:268:PHE:CD1	2.93	0.52
2:B:259:MET:HE3	2:B:268:PHE:CD1	2.44	0.52
2:B:319:PHE:CD1	2:B:319:PHE:N	2.78	0.52
2:B:384:ILE:HG23	2:B:388:PHE:CE2	2.45	0.52
1:A:63:PRO:HB2	1:A:65:ALA:HB2	1.92	0.52
1:A:78:VAL:O	1:A:78:VAL:HG12	2.10	0.52
1:A:224:TYR:HE1	3:A:500:GTP:C2	2.27	0.52
2:B:6:HIS:ND1	2:B:21:TRP:HZ2	2.07	0.52
2:B:28:HIS:CD2	2:B:240:THR:HA	2.45	0.52
1:A:101:ASN:C	1:A:102:ASN:CG	2.59	0.51
1:A:180:ALA:HB1	1:A:398:MET:HE2	1.92	0.51
2:B:135:PHE:CD2	2:B:157:ILE:HD13	2.45	0.51
2:B:140:SER:OG	2:B:143:GLY:HA3	2.10	0.51
2:B:141:LEU:C	2:B:186:ASN:HD21	2.13	0.51
2:B:229:HIS:ND1	5:B:501:TXL:H432	2.25	0.51
2:B:360:PRO:HD3	2:B:374:SER:HB3	1.91	0.51
1:A:30:ILE:O	1:A:32:PRO:HG3	1.95	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:VAL:HG13	2:B:377:PHE:CE2	2.45	0.51
2:B:339:ASN:O	2:B:340:SER:O	2.29	0.51
1:A:181:VAL:HG13	1:A:399:TYR:OH	2.11	0.51
1:A:224:TYR:HB2	2:B:325:MET:CG	2.41	0.51
1:A:382:THR:O	1:A:385:ALA:N	2.43	0.51
2:B:9:ALA:O	2:B:13:GLY:HA3	2.10	0.51
2:B:104:ALA:HA	2:B:413:MET:HE1	1.91	0.51
2:B:151:THR:C	2:B:192:HIS:HD2	2.12	0.51
2:B:241:CYS:C	2:B:242:LEU:HG	2.31	0.51
2:B:389:LYS:O	2:B:393:GLU:HG2	2.09	0.51
1:A:154:MET:HE3	1:A:166:LYS:HD2	1.90	0.51
2:B:4:ILE:HD13	2:B:30:ILE:CA	2.35	0.51
2:B:184:PRO:CG	2:B:399:PHE:CB	2.69	0.51
2:B:369:ARG:O	5:B:501:TXL:C22	2.59	0.51
5:B:501:TXL:H192	5:B:501:TXL:C5	2.39	0.51
1:A:41:THR:O	1:A:41:THR:CG2	2.59	0.51
1:A:152:LEU:HD11	1:A:156:ARG:HE	1.75	0.51
1:A:183:GLU:OE1	1:A:183:GLU:HA	2.10	0.51
1:A:209:ILE:CG2	1:A:230:LEU:HD23	2.29	0.51
2:B:35:SER:HB3	2:B:60:LYS:CE	2.40	0.51
2:B:378:ILE:HG22	2:B:379:GLY:N	2.24	0.51
1:A:6:SER:HB3	1:A:30:ILE:HD12	1.92	0.51
1:A:66:VAL:HG21	1:A:125:LEU:CD1	2.40	0.51
1:A:97:GLU:O	1:A:98:ASP:CB	2.57	0.51
1:A:253:THR:O	1:A:253:THR:CG2	2.57	0.51
1:A:396:ASP:O	1:A:401:LYS:CB	2.34	0.51
1:A:405:VAL:HG23	1:A:409:VAL:HG23	1.89	0.51
1:A:105:ARG:NH2	2:B:253:ARG:NH2	2.59	0.51
1:A:150:THR:O	1:A:154:MET:HG2	2.11	0.51
1:A:340:THR:O	1:A:341:ILE:HD13	2.11	0.51
2:B:64:ARG:HH22	2:B:132:LEU:HD11	1.76	0.51
2:B:94:PHE:CE2	2:B:114:LEU:HB2	2.46	0.51
2:B:103:TRP:HE1	2:B:148:GLY:HA2	1.72	0.51
2:B:114:LEU:O	2:B:117:SER:N	2.44	0.51
1:A:155:GLU:CG	1:A:196:GLU:HG3	2.34	0.51
2:B:7:ILE:HG21	2:B:137:LEU:HD22	1.91	0.51
2:B:40:SER:C	2:B:41:ASP:OD1	2.49	0.51
2:B:278:ARG:CB	2:B:278:ARG:C	2.79	0.51
2:B:385:GLN:HG3	2:B:389:LYS:CE	2.04	0.51
2:B:404:PHE:CD2	2:B:404:PHE:O	2.64	0.51
1:A:267:PHE:CD1	1:A:388:TRP:CZ2	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ASP:O	2:B:40:SER:HB3	2.08	0.51
2:B:184:PRO:CB	2:B:399:PHE:CE2	2.69	0.51
2:B:197:ASN:CG	2:B:197:ASN:O	2.50	0.51
2:B:398:MET:CE	2:B:399:PHE:CE2	2.93	0.51
1:A:158:SER:HB2	1:A:196:GLU:O	2.11	0.51
2:B:154:ILE:CG2	2:B:198:THR:HG22	2.37	0.51
2:B:234:THR:HB	2:B:302:MET:HE2	1.93	0.51
2:B:312:TYR:CG	2:B:381:SER:HB3	2.46	0.51
5:B:501:TXL:H173	5:B:501:TXL:C13	2.37	0.51
5:B:501:TXL:C17	5:B:501:TXL:C13	2.89	0.51
1:A:25:CYS:O	1:A:25:CYS:SG	2.69	0.50
1:A:68:VAL:CG1	1:A:149:PHE:HZ	2.07	0.50
1:A:396:ASP:OD2	1:A:422:ARG:CZ	2.59	0.50
1:A:205:ASP:O	1:A:209:ILE:HG13	2.11	0.50
1:A:221:ARG:N	1:A:222:PRO:CD	2.65	0.50
1:A:306:ASP:CG	1:A:308:ARG:HD2	2.32	0.50
1:A:340:THR:O	1:A:341:ILE:CG1	2.59	0.50
2:B:231:VAL:O	2:B:232:SER:C	2.46	0.50
2:B:259:MET:HG3	2:B:378:ILE:HG21	1.92	0.50
1:A:178:SER:O	1:A:179:THR:HB	2.10	0.50
1:A:344:VAL:HB	1:A:347:CYS:HG	1.72	0.50
2:B:287:THR:CG2	2:B:290:GLU:N	2.68	0.50
1:A:241:SER:HB2	1:A:356:ASN:CB	2.42	0.50
1:A:269:LEU:O	1:A:377:MET:O	2.29	0.50
1:A:306:ASP:OD1	1:A:308:ARG:CD	2.55	0.50
2:B:184:PRO:CA	2:B:395:PHE:HD1	2.22	0.50
2:B:226:ASP:OD1	2:B:226:ASP:O	2.30	0.50
2:B:251:ASP:O	2:B:252:LEU:C	2.49	0.50
2:B:287:THR:CG2	2:B:290:GLU:HB2	2.39	0.50
2:B:308:ARG:CD	2:B:342:TYR:CZ	2.93	0.50
1:A:119:LEU:HA	1:A:122:ILE:HG22	1.93	0.50
1:A:267:PHE:CZ	1:A:388:TRP:CZ2	2.99	0.50
2:B:47:GLU:OE2	2:B:85:GLN:OE1	2.30	0.50
2:B:229:HIS:HD1	5:B:501:TXL:H432	1.75	0.50
2:B:384:ILE:HG22	2:B:388:PHE:CE2	2.45	0.50
2:B:29:GLY:O	2:B:58:GLY:O	2.30	0.50
2:B:30:ILE:HG21	2:B:136:GLN:NE2	2.23	0.50
2:B:63:PRO:CG	2:B:86:ILE:O	2.60	0.50
2:B:217:LEU:HD23	2:B:275:LEU:O	2.10	0.50
2:B:230:LEU:HD21	2:B:302:MET:HB2	1.94	0.50
1:A:88:HIS:NE2	1:A:89:PRO:HD2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLN:HE21	1:A:305:CYS:HB2	1.76	0.50
2:B:33:THR:CA	2:B:59:ASN:ND2	2.72	0.50
2:B:34:GLY:HA2	2:B:37:HIS:NE2	2.26	0.50
2:B:70:LEU:HA	2:B:94:PHE:HB2	1.94	0.50
2:B:101:ASN:O	2:B:102:ASN:ND2	2.43	0.50
2:B:273:ALA:HB1	2:B:294:GLN:CD	2.32	0.50
2:B:273:ALA:CB	2:B:294:GLN:CD	2.80	0.50
2:B:332:MET:O	2:B:336:GLN:HG3	2.11	0.50
5:B:501:TXL:O11	5:B:501:TXL:H332	2.12	0.50
1:A:105:ARG:HG3	1:A:411:GLU:CD	2.32	0.50
1:A:155:GLU:HA	1:A:196:GLU:HB3	1.94	0.50
1:A:209:ILE:HD13	1:A:231:ILE:HG12	1.94	0.50
1:A:252:LEU:CA	1:A:255:PHE:HD2	2.07	0.50
2:B:259:MET:HB3	2:B:268:PHE:CD1	2.30	0.50
2:B:270:PRO:HB3	2:B:378:ILE:HD13	1.94	0.50
2:B:416:MET:N	2:B:416:MET:SD	2.85	0.50
1:A:33:ASP:O	1:A:33:ASP:CG	2.49	0.49
1:A:66:VAL:HG22	1:A:125:LEU:HD13	1.92	0.49
1:A:108:TYR:CZ	1:A:417:GLU:CD	2.85	0.49
1:A:170:SER:OG	1:A:203:MET:CG	1.65	0.49
1:A:205:ASP:HB2	1:A:208:ALA:CB	2.42	0.49
1:A:390:ARG:O	1:A:394:LYS:HG3	2.12	0.49
2:B:12:CYS:SG	4:B:500:GDP:C1'	3.00	0.49
2:B:151:THR:CB	2:B:192:HIS:NE2	2.28	0.49
2:B:389:LYS:HG2	2:B:429:VAL:HG21	1.93	0.49
2:B:434:GLN:C	2:B:435:TYR:HD1	2.14	0.49
1:A:166:LYS:CE	1:A:197:HIS:CD2	2.63	0.49
1:A:222:PRO:O	2:B:326:LYS:CB	2.56	0.49
2:B:135:PHE:CE2	2:B:157:ILE:HD13	2.47	0.49
1:A:101:ASN:ND2	3:A:500:GTP:PG	2.85	0.49
1:A:141:PHE:CB	1:A:173:PRO:HD3	2.41	0.49
1:A:179:THR:CG2	1:A:181:VAL:CA	2.88	0.49
1:A:261:PRO:HB2	1:A:346:TRP:HH2	1.77	0.49
1:A:274:PRO:C	1:A:275:VAL:HG23	2.33	0.49
2:B:23:VAL:HG22	5:B:501:TXL:C33	2.30	0.49
2:B:192:HIS:O	2:B:196:GLU:HG2	2.05	0.49
1:A:70:LEU:HD12	1:A:145:THR:CA	2.40	0.49
1:A:212:ILE:HD12	1:A:230:LEU:HD21	1.75	0.49
1:A:420:GLU:OE1	1:A:420:GLU:HA	2.13	0.49
2:B:35:SER:H	2:B:60:LYS:NZ	2.09	0.49
2:B:213:CYS:HB3	2:B:219:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:VAL:HB	2:B:289:PRO:CD	2.42	0.49
2:B:359:PRO:O	2:B:360:PRO:C	2.49	0.49
2:B:433:GLN:O	2:B:435:TYR:N	2.46	0.49
1:A:11:GLN:HG2	3:A:500:GTP:O2A	2.12	0.49
1:A:14:VAL:HB	1:A:74:VAL:CG1	2.43	0.49
1:A:369:ALA:O	1:A:370:LYS:HG3	2.12	0.49
2:B:213:CYS:CB	2:B:219:LEU:HD11	2.30	0.49
2:B:13:GLY:CA	2:B:138:THR:CB	2.85	0.49
2:B:44:LEU:CD1	2:B:63:PRO:HG3	2.42	0.49
2:B:62:VAL:CG1	2:B:63:PRO:N	2.76	0.49
2:B:121:VAL:O	2:B:125:GLU:HG3	2.12	0.49
2:B:181:VAL:C	2:B:398:MET:HE1	2.33	0.49
2:B:183:GLU:OE1	2:B:183:GLU:HA	2.13	0.49
2:B:191:VAL:CG2	2:B:421:ALA:CB	2.90	0.49
2:B:400:ARG:NH1	2:B:422:GLU:OE1	2.37	0.49
1:A:108:TYR:OH	1:A:417:GLU:CG	2.59	0.49
1:A:152:LEU:CD1	1:A:156:ARG:NE	2.75	0.49
1:A:220:GLU:HG3	1:A:220:GLU:N	2.28	0.49
1:A:277:SER:CB	1:A:279:GLU:H	2.23	0.49
1:A:306:ASP:OD1	1:A:308:ARG:N	2.46	0.49
2:B:14:ASN:OD1	2:B:69:ASP:OD1	2.29	0.49
2:B:57:ALA:CA	2:B:64:ARG:HB3	2.35	0.49
2:B:79:ARG:HB2	2:B:86:ILE:HD11	1.95	0.49
2:B:180:THR:C	2:B:398:MET:HE1	2.25	0.49
1:A:186:ASN:O	1:A:190:THR:N	2.44	0.49
1:A:264:ARG:O	1:A:266:HIS:ND1	2.45	0.49
1:A:346:TRP:HZ2	1:A:435:VAL:HG12	1.77	0.49
2:B:4:ILE:HG21	2:B:30:ILE:HG21	1.93	0.49
2:B:115:VAL:HG12	2:B:156:LYS:HZ2	1.77	0.49
2:B:194:LEU:CD2	2:B:265:LEU:HB3	2.38	0.49
2:B:206:ASN:O	2:B:210:TYR:HE2	1.85	0.49
1:A:14:VAL:HG12	1:A:74:VAL:HG22	1.95	0.49
1:A:97:GLU:HG3	1:A:110:ILE:HG22	1.92	0.49
1:A:99:ALA:HB3	2:B:251:ASP:OD2	2.13	0.49
1:A:134:GLY:HA3	1:A:252:LEU:CD1	2.43	0.49
1:A:142:GLY:O	1:A:185:TYR:CZ	2.66	0.49
2:B:102:ASN:CB	2:B:105:LYS:CD	2.79	0.49
2:B:246:GLY:N	2:B:357:ASP:OD2	2.45	0.49
1:A:3:GLU:HB3	1:A:64:ARG:NH1	2.28	0.49
1:A:14:VAL:HB	1:A:74:VAL:HG11	1.94	0.49
1:A:78:VAL:HG13	1:A:87:PHE:CE1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:CZ	1:A:151:SER:OG	2.59	0.49
1:A:104:ALA:O	1:A:108:TYR:HD2	1.96	0.49
1:A:176:GLN:NE2	2:B:333:LEU:CB	2.74	0.49
2:B:52:TYR:N	2:B:52:TYR:CD1	2.81	0.49
2:B:108:TYR:OH	2:B:417:GLU:HG3	2.13	0.49
1:A:158:SER:N	1:A:166:LYS:CE	2.76	0.48
1:A:276:ILE:CD1	1:A:371:VAL:CG2	2.87	0.48
1:A:312:TYR:CE1	1:A:341:ILE:HD12	2.47	0.48
2:B:61:TYR:O	2:B:61:TYR:CD1	2.66	0.48
2:B:192:HIS:CE1	2:B:193:GLN:HG2	2.48	0.48
1:A:34:GLY:O	1:A:35:GLN:HG3	2.13	0.48
1:A:291:ILE:HD13	1:A:373:ARG:C	2.33	0.48
1:A:326:LYS:O	1:A:326:LYS:HG2	2.12	0.48
2:B:44:LEU:CD1	2:B:86:ILE:O	2.49	0.48
2:B:324:SER:CB	2:B:327:GLU:H	2.25	0.48
2:B:394:GLN:OE1	2:B:394:GLN:HA	2.12	0.48
1:A:220:GLU:CG	1:A:220:GLU:H	2.20	0.48
1:A:233:GLN:O	1:A:234:ILE:C	2.49	0.48
2:B:25:SER:O	2:B:27:GLU:CG	2.55	0.48
2:B:102:ASN:CB	2:B:105:LYS:HG3	2.43	0.48
2:B:308:ARG:HD3	2:B:342:TYR:HE2	1.66	0.48
2:B:385:GLN:O	2:B:389:LYS:CG	2.62	0.48
1:A:206:ASN:HD22	1:A:206:ASN:HA	1.46	0.48
1:A:224:TYR:HD1	3:A:500:GTP:C2	2.31	0.48
1:A:292:THR:N	1:A:375:VAL:HG21	2.28	0.48
1:A:397:LEU:CA	1:A:401:LYS:HB2	2.37	0.48
2:B:102:ASN:CA	2:B:408:TYR:CE1	2.91	0.48
1:A:16:ILE:HG23	1:A:138:PHE:CD1	2.48	0.48
1:A:180:ALA:CB	1:A:398:MET:CE	2.91	0.48
1:A:200:CYS:SG	1:A:260:VAL:CG2	3.00	0.48
1:A:359:PRO:HB2	1:A:360:PRO:HD2	1.94	0.48
1:A:9:VAL:HG11	1:A:146:GLY:HA2	1.95	0.48
1:A:42:ILE:HD13	1:A:61:HIS:O	2.13	0.48
1:A:73:THR:HB	2:B:249:ASN:ND2	2.27	0.48
1:A:230:LEU:CD2	1:A:302:MET:HE3	2.42	0.48
1:A:291:ILE:O	1:A:375:VAL:HG21	2.13	0.48
3:A:500:GTP:O1A	2:B:248:LEU:CD1	2.51	0.48
2:B:35:SER:HA	2:B:60:LYS:CE	2.30	0.48
2:B:98:GLY:C	2:B:99:ALA:O	2.52	0.48
2:B:239:THR:O	2:B:243:ARG:CG	2.51	0.48
1:A:126:ALA:C	1:A:132:LEU:HD11	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:CD1	1:A:173:PRO:O	2.64	0.48
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.13	0.48
1:A:217:LEU:CD2	1:A:368:LEU:CD1	2.70	0.48
1:A:256:GLN:O	1:A:260:VAL:HB	2.13	0.48
2:B:50:ASN:HD22	2:B:61:TYR:HB2	1.78	0.48
2:B:114:LEU:HA	2:B:117:SER:OG	2.14	0.48
2:B:118:VAL:O	2:B:118:VAL:CG1	2.62	0.48
2:B:213:CYS:SG	2:B:227:LEU:HD11	2.52	0.48
2:B:244:PHE:O	2:B:245:PRO:C	2.51	0.48
2:B:311:ARG:O	2:B:381:SER:CA	2.62	0.48
1:A:15:GLN:O	1:A:18:ASN:HB2	2.13	0.48
1:A:137:VAL:HB	1:A:168:GLU:CG	2.40	0.48
1:A:175:PRO:HD3	1:A:390:ARG:CZ	2.44	0.48
1:A:276:ILE:HB	1:A:369:ALA:HB2	1.95	0.48
1:A:400:ALA:O	1:A:401:LYS:C	2.52	0.48
2:B:2:ARG:NH2	2:B:243:ARG:O	2.46	0.48
2:B:23:VAL:O	2:B:23:VAL:HG12	2.14	0.48
2:B:102:ASN:CA	2:B:408:TYR:HE1	2.18	0.48
2:B:268:PHE:HD1	2:B:380:ASN:CG	2.13	0.48
1:A:122:ILE:HG23	1:A:123:ARG:N	2.29	0.48
1:A:242:LEU:HD13	1:A:250:VAL:HB	1.94	0.48
2:B:188:THR:CG2	2:B:417:GLU:O	2.59	0.48
2:B:209:LEU:HB3	2:B:227:LEU:HD21	1.96	0.48
2:B:241:CYS:O	2:B:242:LEU:HG	2.14	0.48
2:B:394:GLN:O	2:B:398:MET:HB2	2.14	0.48
1:A:73:THR:CB	2:B:249:ASN:HD21	2.27	0.48
1:A:175:PRO:HG3	1:A:304:LYS:NZ	2.29	0.48
1:A:209:ILE:HG12	1:A:302:MET:CE	2.42	0.48
1:A:275:VAL:O	1:A:275:VAL:CG1	2.62	0.48
2:B:109:THR:CG2	2:B:411:GLU:O	2.62	0.48
2:B:238:VAL:HG13	2:B:255:LEU:HD11	1.94	0.48
2:B:295:MET:HE1	2:B:375:ALA:HA	1.93	0.48
2:B:311:ARG:H	2:B:382:THR:HB	1.79	0.48
2:B:435:TYR:O	2:B:436:GLN:OE1	2.29	0.48
1:A:209:ILE:CD1	1:A:231:ILE:CG1	2.90	0.47
2:B:62:VAL:HG12	2:B:63:PRO:O	2.14	0.47
2:B:87:PHE:CD1	2:B:88:ARG:N	2.82	0.47
2:B:119:LEU:HD21	2:B:156:LYS:HD3	1.96	0.47
2:B:139:HIS:C	2:B:139:HIS:ND1	2.67	0.47
2:B:143:GLY:O	2:B:185:TYR:OH	2.31	0.47
2:B:230:LEU:HG	2:B:302:MET:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:VAL:HG12	2:B:353:THR:HG21	1.96	0.47
1:A:3:GLU:OE1	1:A:132:LEU:CD2	2.62	0.47
1:A:9:VAL:HG13	1:A:150:THR:HG22	1.95	0.47
1:A:346:TRP:N	1:A:346:TRP:CD1	2.82	0.47
1:A:404:PHE:CZ	2:B:257:VAL:O	2.61	0.47
2:B:3:GLU:HA	2:B:31:ASP:HB2	1.86	0.47
1:A:250:VAL:CB	1:A:254:GLU:HG2	2.43	0.47
2:B:3:GLU:O	2:B:4:ILE:HG13	2.11	0.47
2:B:42:LEU:C	2:B:43:GLN:CG	2.75	0.47
1:A:196:GLU:HB3	1:A:197:HIS:CE1	2.50	0.47
1:A:287:SER:O	1:A:291:ILE:HG13	2.13	0.47
1:A:296:PHE:O	1:A:298:PRO:N	2.47	0.47
1:A:311:LYS:O	1:A:312:TYR:C	2.51	0.47
2:B:180:THR:C	2:B:398:MET:CE	2.73	0.47
2:B:347:ILE:N	2:B:348:PRO:HD3	2.27	0.47
1:A:3:GLU:OE1	1:A:132:LEU:HD23	2.14	0.47
1:A:6:SER:O	1:A:66:VAL:N	2.47	0.47
1:A:115:ILE:CB	1:A:152:LEU:HD21	2.43	0.47
1:A:272:TYR:HD1	1:A:275:VAL:CG2	2.28	0.47
1:A:387:ALA:O	1:A:390:ARG:HB2	2.15	0.47
1:A:389:ALA:O	1:A:393:HIS:ND1	2.47	0.47
1:A:426:ALA:C	1:A:428:LEU:H	2.14	0.47
2:B:23:VAL:HG21	2:B:232:SER:HB2	1.95	0.47
2:B:201:THR:CG2	2:B:265:LEU:CG	2.87	0.47
2:B:272:PHE:O	2:B:275:LEU:HD21	2.13	0.47
2:B:416:MET:O	2:B:417:GLU:CB	2.55	0.47
1:A:121:ARG:O	1:A:125:LEU:CG	2.44	0.47
1:A:282:TYR:O	1:A:284:GLU:C	2.53	0.47
1:A:7:ILE:HG21	1:A:153:LEU:CD2	2.43	0.47
1:A:35:GLN:O	1:A:36:MET:HG2	2.13	0.47
1:A:105:ARG:HH12	2:B:253:ARG:NH2	2.11	0.47
1:A:259:LEU:CB	1:A:380:ASN:HD21	2.27	0.47
1:A:262:TYR:CB	1:A:263:PRO:HD3	2.25	0.47
2:B:181:VAL:C	2:B:399:PHE:CE2	2.85	0.47
2:B:191:VAL:HG23	2:B:421:ALA:HA	1.87	0.47
1:A:23:LEU:CD2	1:A:233:GLN:HA	2.45	0.47
1:A:261:PRO:HB2	1:A:346:TRP:CH2	2.50	0.47
1:A:429:GLU:O	1:A:433:GLU:CG	2.51	0.47
2:B:64:ARG:NH2	2:B:125:GLU:C	2.67	0.47
2:B:158:ARG:HB2	2:B:197:ASN:ND2	2.01	0.47
2:B:275:LEU:CB	2:B:294:GLN:HE22	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:LEU:CD1	2:B:435:TYR:HD2	2.27	0.47
1:A:20:CYS:SG	1:A:138:PHE:CZ	3.06	0.47
1:A:103:TYR:HD2	1:A:189:LEU:HG	1.76	0.47
1:A:212:ILE:HB	1:A:216:ASN:HD22	1.79	0.47
2:B:112:ALA:HA	2:B:115:VAL:HB	1.96	0.47
2:B:248:LEU:HD23	2:B:353:THR:O	2.15	0.47
2:B:426:ASN:C	2:B:428:LEU:H	2.17	0.47
1:A:31:GLN:NE2	1:A:243:ARG:HB3	2.30	0.47
1:A:229:ARG:O	1:A:233:GLN:CG	2.52	0.47
1:A:271:THR:OG1	1:A:377:MET:N	2.48	0.47
2:B:170:SER:OG	2:B:203:CYS:CA	2.61	0.47
2:B:194:LEU:HD23	2:B:267:PHE:HZ	1.72	0.47
2:B:250:ALA:HB1	2:B:352:LYS:HZ3	1.80	0.47
2:B:261:PRO:HG3	2:B:314:THR:HG23	1.97	0.47
1:A:103:TYR:CD2	1:A:188:ILE:HG22	2.50	0.46
1:A:103:TYR:N	1:A:185:TYR:CE2	2.82	0.46
1:A:224:TYR:CB	2:B:325:MET:HB2	2.45	0.46
1:A:241:SER:HB2	1:A:356:ASN:CG	2.32	0.46
1:A:267:PHE:CE1	1:A:388:TRP:CH2	3.03	0.46
1:A:430:LYS:O	1:A:434:GLU:HG3	2.15	0.46
2:B:94:PHE:CZ	2:B:110:GLU:O	2.68	0.46
2:B:294:GLN:HG2	2:B:294:GLN:O	2.14	0.46
2:B:313:LEU:HA	2:B:344:VAL:CG2	2.30	0.46
1:A:20:CYS:SG	1:A:138:PHE:CE1	3.07	0.46
1:A:23:LEU:HD22	1:A:233:GLN:HA	1.96	0.46
1:A:48:SER:O	1:A:49:PHE:HB2	2.14	0.46
1:A:105:ARG:CZ	2:B:253:ARG:NH2	2.79	0.46
1:A:192:HIS:O	1:A:193:THR:C	2.53	0.46
1:A:197:HIS:O	1:A:198:SER:OG	2.34	0.46
1:A:334:THR:HA	1:A:337:THR:HG21	1.98	0.46
1:A:349:THR:O	1:A:351:PHE:N	2.48	0.46
2:B:27:GLU:CB	2:B:36:TYR:HB3	2.44	0.46
2:B:211:ASP:O	2:B:215:ARG:HB2	2.14	0.46
1:A:228:ASN:O	1:A:232:GLY:N	2.39	0.46
2:B:50:ASN:HB2	2:B:61:TYR:CB	2.45	0.46
2:B:74:THR:O	2:B:75:MET:O	2.33	0.46
2:B:222:PRO:C	2:B:223:THR:CG2	2.72	0.46
2:B:270:PRO:HA	2:B:377:PHE:O	2.14	0.46
2:B:273:ALA:HB1	2:B:294:GLN:HB3	1.97	0.46
2:B:433:GLN:C	2:B:435:TYR:N	2.67	0.46
1:A:3:GLU:CB	1:A:64:ARG:NH1	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASN:O	1:A:297:GLU:HG3	2.16	0.46
2:B:64:ARG:HH22	2:B:132:LEU:HD21	1.79	0.46
2:B:75:MET:CE	2:B:79:ARG:CB	2.90	0.46
2:B:151:THR:HG21	2:B:189:LEU:HA	1.96	0.46
1:A:87:PHE:HZ	1:A:92:LEU:HD21	1.80	0.46
1:A:109:THR:HG21	1:A:411:GLU:CB	2.44	0.46
1:A:153:LEU:O	1:A:153:LEU:HG	2.14	0.46
1:A:157:LEU:HB2	1:A:166:LYS:HE2	1.98	0.46
1:A:209:ILE:CD1	1:A:231:ILE:HG12	2.45	0.46
1:A:292:THR:CG2	1:A:319:TYR:CE2	2.98	0.46
1:A:344:VAL:HG12	1:A:345:ASP:H	1.81	0.46
1:A:3:GLU:HG3	1:A:131:GLY:O	2.16	0.46
1:A:170:SER:OG	1:A:202:PHE:O	2.34	0.46
1:A:217:LEU:O	1:A:218:ASP:OD1	2.33	0.46
1:A:223:THR:OG1	1:A:225:THR:OG1	2.10	0.46
1:A:340:THR:O	1:A:341:ILE:CD1	2.63	0.46
2:B:22:GLU:OE1	2:B:83:PHE:CG	2.67	0.46
2:B:94:PHE:CD1	2:B:94:PHE:C	2.68	0.46
2:B:102:ASN:CB	2:B:105:LYS:HE3	2.46	0.46
1:A:105:ARG:NH1	2:B:253:ARG:NE	2.62	0.46
1:A:187:SER:OG	1:A:188:ILE:N	2.49	0.46
1:A:312:TYR:HE1	1:A:341:ILE:HD12	1.81	0.46
2:B:33:THR:CG2	2:B:34:GLY:H	2.28	0.46
2:B:194:LEU:CA	2:B:265:LEU:HB2	2.38	0.46
2:B:212:ILE:HD12	2:B:302:MET:HB2	1.98	0.46
2:B:287:THR:C	2:B:290:GLU:HB3	2.36	0.46
1:A:14:VAL:CB	1:A:74:VAL:CG1	2.94	0.46
1:A:107:HIS:ND1	1:A:108:TYR:CD2	2.80	0.46
1:A:155:GLU:HG2	1:A:196:GLU:CB	2.46	0.46
1:A:289:ALA:CB	1:A:331:ALA:HB2	2.44	0.46
1:A:328:VAL:O	1:A:332:ILE:CG1	2.63	0.46
2:B:44:LEU:HG	2:B:85:GLN:CG	2.46	0.46
2:B:48:ARG:NH1	2:B:60:LYS:HG3	2.30	0.46
2:B:141:LEU:CD1	2:B:173:PRO:CD	2.91	0.46
1:A:3:GLU:HB2	1:A:64:ARG:NH2	2.30	0.46
1:A:172:TYR:CE2	1:A:388:TRP:HZ3	2.28	0.46
1:A:312:TYR:CD1	1:A:341:ILE:HG23	2.51	0.46
1:A:372:GLN:C	1:A:373:ARG:HG3	2.33	0.46
2:B:68:VAL:HA	2:B:92:PHE:HB2	1.98	0.46
2:B:143:GLY:H	2:B:147:SER:HG	1.56	0.46
2:B:273:ALA:CB	2:B:294:GLN:HB3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:SER:O	2:B:281:GLN:C	2.55	0.46
2:B:346:TRP:O	2:B:347:ILE:HG13	2.14	0.46
1:A:250:VAL:HG11	1:A:352:LYS:NZ	2.26	0.46
1:A:275:VAL:O	1:A:368:LEU:CD1	2.64	0.46
2:B:35:SER:CB	2:B:60:LYS:HE3	2.44	0.46
2:B:44:LEU:C	2:B:47:GLU:CG	2.56	0.46
2:B:56:ALA:HB1	2:B:62:VAL:N	2.31	0.46
2:B:57:ALA:C	2:B:64:ARG:N	2.69	0.46
2:B:179:ASP:O	2:B:180:THR:HG23	2.15	0.46
2:B:208:ALA:CB	2:B:303:ALA:C	2.81	0.46
2:B:249:ASN:O	2:B:249:ASN:OD1	2.34	0.46
2:B:435:TYR:O	2:B:436:GLN:CB	2.56	0.46
1:A:83:TYR:C	1:A:84:ARG:CG	2.73	0.45
1:A:267:PHE:CD1	1:A:388:TRP:HZ2	2.34	0.45
1:A:306:ASP:OD2	1:A:308:ARG:HB2	2.16	0.45
1:A:343:PHE:HE2	1:A:351:PHE:CZ	1.85	0.45
1:A:363:VAL:HG12	1:A:364:PRO:HG3	1.99	0.45
1:A:384:ILE:O	1:A:386:GLU:N	2.49	0.45
1:A:101:ASN:CA	3:A:500:GTP:O2G	2.61	0.45
1:A:141:PHE:CE1	1:A:170:SER:HB2	2.51	0.45
1:A:174:ALA:HB3	1:A:175:PRO:CD	2.10	0.45
1:A:175:PRO:HD2	1:A:207:GLU:HG2	1.98	0.45
1:A:341:ILE:O	1:A:342:GLN:C	2.52	0.45
2:B:14:ASN:HB3	2:B:74:THR:CB	2.43	0.45
2:B:241:CYS:O	2:B:242:LEU:CG	2.64	0.45
1:A:8:HIS:HB2	1:A:67:PHE:HA	1.98	0.45
2:B:22:GLU:CD	2:B:83:PHE:CD1	2.88	0.45
2:B:196:GLU:HA	2:B:196:GLU:OE1	2.15	0.45
2:B:318:VAL:HG22	2:B:354:ALA:HB3	1.98	0.45
2:B:384:ILE:HG22	2:B:388:PHE:HE2	1.77	0.45
1:A:123:ARG:O	1:A:127:ASP:OD1	2.34	0.45
1:A:238:ILE:CG2	1:A:255:PHE:CZ	2.99	0.45
1:A:277:SER:HB3	1:A:280:LYS:CE	2.36	0.45
2:B:102:ASN:HB2	2:B:105:LYS:HG3	1.98	0.45
2:B:140:SER:O	2:B:147:SER:OG	2.25	0.45
2:B:147:SER:HG	2:B:189:LEU:CD1	2.28	0.45
2:B:184:PRO:CA	2:B:395:PHE:CD1	2.98	0.45
1:A:103:TYR:CD2	1:A:148:GLY:N	2.85	0.45
1:A:272:TYR:CE1	1:A:274:PRO:C	2.70	0.45
1:A:278:ALA:N	1:A:368:LEU:HD22	2.32	0.45
2:B:103:TRP:CD1	2:B:147:SER:C	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:SER:CB	2:B:175:PRO:CD	2.89	0.45
2:B:295:MET:CE	2:B:375:ALA:HA	2.40	0.45
2:B:312:TYR:N	2:B:381:SER:CB	2.80	0.45
2:B:342:TYR:C	2:B:343:PHE:CG	2.90	0.45
2:B:427:ASP:O	2:B:431:GLU:HG3	2.16	0.45
1:A:31:GLN:OE1	1:A:243:ARG:HD3	2.01	0.45
1:A:116:ASP:C	1:A:118:VAL:N	2.68	0.45
1:A:309:HIS:CB	1:A:386:GLU:OE2	2.65	0.45
2:B:104:ALA:C	2:B:108:TYR:HD2	2.20	0.45
1:A:132:LEU:O	1:A:133:GLN:C	2.54	0.45
1:A:183:GLU:HB3	1:A:394:LYS:HB2	1.87	0.45
2:B:56:ALA:CB	2:B:62:VAL:N	2.80	0.45
2:B:312:TYR:C	2:B:381:SER:HA	2.36	0.45
2:B:411:GLU:OE1	2:B:411:GLU:HA	2.17	0.45
1:A:409:VAL:O	1:A:412:GLY:O	2.35	0.45
2:B:66:ILE:HG23	2:B:66:ILE:O	2.16	0.45
2:B:143:GLY:CA	2:B:185:TYR:CE1	2.87	0.45
2:B:217:LEU:CD2	2:B:275:LEU:O	2.65	0.45
2:B:273:ALA:CB	2:B:294:GLN:OE1	2.60	0.45
2:B:301:MET:CE	2:B:377:PHE:CD1	2.99	0.45
1:A:383:ALA:O	1:A:385:ALA:CA	2.60	0.45
2:B:35:SER:CB	2:B:60:LYS:CE	2.94	0.45
2:B:146:GLY:O	2:B:150:GLY:N	2.48	0.45
2:B:183:GLU:CD	2:B:394:GLN:HG3	2.34	0.45
2:B:194:LEU:HD21	2:B:267:PHE:HE2	1.65	0.45
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.51	0.45
2:B:274:PRO:C	2:B:276:THR:CG2	2.85	0.45
1:A:267:PHE:CE2	1:A:388:TRP:HZ2	2.35	0.45
2:B:94:PHE:CD2	2:B:114:LEU:CD2	3.00	0.45
2:B:250:ALA:HB1	2:B:352:LYS:NZ	2.32	0.45
2:B:313:LEU:HD22	2:B:346:TRP:CH2	2.51	0.45
2:B:319:PHE:O	2:B:355:VAL:HG13	2.16	0.45
1:A:35:GLN:N	1:A:60:LYS:HD3	2.31	0.44
1:A:169:PHE:CZ	1:A:235:VAL:CG2	2.78	0.44
1:A:217:LEU:C	1:A:218:ASP:OD1	2.55	0.44
1:A:267:PHE:HA	1:A:268:PRO:HD2	1.57	0.44
2:B:166:MET:HG2	2:B:197:ASN:O	2.16	0.44
2:B:313:LEU:H	2:B:381:SER:HA	1.81	0.44
1:A:9:VAL:HG13	1:A:150:THR:CG2	2.42	0.44
1:A:26:LEU:HD11	1:A:361:THR:HG23	1.83	0.44
1:A:291:ILE:HD11	1:A:373:ARG:HB2	1.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:TYR:C	1:A:313:MET:HG2	2.37	0.44
2:B:44:LEU:HD21	2:B:85:GLN:HB2	1.07	0.44
2:B:56:ALA:C	2:B:62:VAL:HB	2.38	0.44
2:B:71:GLU:HG2	2:B:99:ALA:H	1.65	0.44
2:B:75:MET:SD	2:B:93:VAL:HG21	2.57	0.44
2:B:230:LEU:HD21	2:B:302:MET:HG3	1.99	0.44
2:B:414:ASP:C	2:B:416:MET:N	2.68	0.44
1:A:16:ILE:O	1:A:19:ALA:HB3	2.16	0.44
1:A:182:VAL:O	1:A:183:GLU:O	2.34	0.44
1:A:184:PRO:HD2	1:A:398:MET:HB3	1.99	0.44
1:A:305:CYS:O	1:A:307:PRO:CD	2.56	0.44
1:A:345:ASP:OD2	1:A:439:SER:HA	2.17	0.44
2:B:192:HIS:O	2:B:196:GLU:HG3	1.87	0.44
2:B:344:VAL:HB	2:B:347:ILE:HD12	1.99	0.44
2:B:431:GLU:O	2:B:434:GLN:HB2	2.18	0.44
1:A:122:ILE:HD11	1:A:157:LEU:HD22	1.97	0.44
1:A:152:LEU:HD11	1:A:156:ARG:HH21	1.78	0.44
1:A:152:LEU:O	1:A:156:ARG:HG3	2.17	0.44
1:A:183:GLU:HG3	2:B:348:PRO:HB2	1.98	0.44
1:A:20:CYS:C	1:A:24:TYR:CD2	2.80	0.44
1:A:34:GLY:O	1:A:35:GLN:CB	2.64	0.44
1:A:97:GLU:OE2	1:A:114:ILE:HD11	2.16	0.44
2:B:151:THR:HG21	2:B:192:HIS:CG	2.36	0.44
2:B:157:ILE:O	2:B:161:TYR:HB2	2.18	0.44
2:B:265:LEU:HD23	2:B:267:PHE:HZ	1.67	0.44
1:A:137:VAL:CG2	1:A:168:GLU:HG2	2.48	0.44
1:A:190:THR:O	1:A:191:THR:C	2.52	0.44
1:A:197:HIS:C	1:A:198:SER:OG	2.56	0.44
1:A:335:ILE:C	1:A:337:THR:N	2.71	0.44
2:B:22:GLU:CD	2:B:83:PHE:CD2	2.69	0.44
2:B:66:ILE:HG21	2:B:66:ILE:HD13	1.78	0.44
2:B:295:MET:HE1	2:B:375:ALA:HB2	1.77	0.44
2:B:340:SER:OG	2:B:341:SER:N	2.38	0.44
2:B:346:TRP:C	2:B:347:ILE:HG13	2.37	0.44
1:A:40:LYS:C	1:A:42:ILE:N	2.65	0.44
1:A:206:ASN:OD1	3:A:500:GTP:N2	2.50	0.44
1:A:432:TYR:O	1:A:435:VAL:HB	2.17	0.44
2:B:166:MET:HG3	2:B:197:ASN:O	2.18	0.44
2:B:234:THR:HG23	2:B:270:PRO:HB2	2.00	0.44
2:B:289:PRO:CD	2:B:290:GLU:H	2.29	0.44
1:A:181:VAL:O	1:A:185:TYR:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASP:C	1:A:308:ARG:N	2.72	0.44
1:A:328:VAL:O	1:A:332:ILE:HB	2.17	0.44
1:A:437:VAL:O	1:A:437:VAL:CG1	2.64	0.44
2:B:12:CYS:C	2:B:16:ILE:HG12	2.20	0.44
2:B:29:GLY:O	2:B:58:GLY:HA3	2.18	0.44
2:B:70:LEU:C	2:B:71:GLU:HG3	2.38	0.44
2:B:243:ARG:CZ	2:B:252:LEU:HD21	2.45	0.44
2:B:333:LEU:HG	2:B:337:ASN:HD21	1.82	0.44
1:A:170:SER:OG	1:A:203:MET:CA	2.66	0.44
1:A:224:TYR:C	1:A:226:ASN:H	2.21	0.44
1:A:224:TYR:C	1:A:226:ASN:N	2.71	0.44
2:B:6:HIS:CE1	2:B:30:ILE:CG1	3.00	0.44
2:B:15:GLN:C	2:B:17:GLY:N	2.70	0.44
2:B:64:ARG:HH12	2:B:132:LEU:HD21	1.83	0.44
2:B:94:PHE:CE2	2:B:114:LEU:CB	3.01	0.44
2:B:103:TRP:CD1	2:B:148:GLY:N	2.83	0.44
2:B:133:GLN:NE2	2:B:253:ARG:HB2	2.33	0.44
2:B:259:MET:SD	2:B:378:ILE:CG2	3.05	0.44
1:A:184:PRO:HB3	1:A:187:SER:OG	2.18	0.43
1:A:229:ARG:HH11	1:A:229:ARG:HD2	1.40	0.43
1:A:362:VAL:HG13	1:A:367:ASP:CB	2.48	0.43
2:B:22:GLU:HB3	2:B:83:PHE:CE1	2.46	0.43
2:B:49:ILE:HA	2:B:61:TYR:HE2	1.82	0.43
2:B:194:LEU:HD21	2:B:267:PHE:CZ	2.48	0.43
2:B:236:SER:O	2:B:240:THR:HB	2.18	0.43
2:B:275:LEU:CD1	2:B:300:ASN:ND2	2.67	0.43
2:B:417:GLU:OE1	2:B:417:GLU:HA	2.17	0.43
1:A:71:GLU:HG2	1:A:99:ALA:HB2	1.01	0.43
1:A:76:ASP:O	1:A:76:ASP:OD1	2.37	0.43
1:A:241:SER:OG	1:A:242:LEU:N	2.51	0.43
1:A:361:THR:C	1:A:362:VAL:CG2	2.82	0.43
2:B:183:GLU:OE1	2:B:394:GLN:HB2	2.14	0.43
1:A:3:GLU:OE2	1:A:129:CYS:CB	2.59	0.43
1:A:12:ALA:HB1	1:A:171:ILE:HD12	2.00	0.43
1:A:222:PRO:CG	2:B:326:LYS:HD3	2.38	0.43
1:A:230:LEU:HG	1:A:302:MET:HE1	2.00	0.43
1:A:273:ALA:HB2	1:A:294:ALA:HB3	1.98	0.43
1:A:307:PRO:C	1:A:309:HIS:N	2.68	0.43
2:B:6:HIS:CD2	2:B:21:TRP:CZ2	3.03	0.43
2:B:115:VAL:HG11	2:B:152:LEU:HB3	2.00	0.43
2:B:265:LEU:HD21	2:B:267:PHE:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ARG:NH2	5:B:501:TXL:C27	2.78	0.43
2:B:385:GLN:OE1	2:B:433:GLN:HB2	2.17	0.43
1:A:31:GLN:NE2	1:A:243:ARG:NE	2.59	0.43
1:A:38:SER:HB3	1:A:45:GLY:HA3	2.00	0.43
1:A:115:ILE:HD11	1:A:156:ARG:CD	2.47	0.43
1:A:157:LEU:HB2	1:A:166:LYS:CE	2.49	0.43
1:A:259:LEU:CA	1:A:380:ASN:HD21	2.31	0.43
1:A:362:VAL:C	1:A:363:VAL:HG23	2.38	0.43
1:A:414:GLU:O	1:A:415:GLU:HB2	2.19	0.43
2:B:102:ASN:O	2:B:105:LYS:HB2	2.19	0.43
2:B:114:LEU:C	2:B:116:ASP:N	2.71	0.43
2:B:261:PRO:HB2	2:B:262:PHE:CE1	2.53	0.43
2:B:321:GLY:HA3	2:B:373:MET:CG	2.15	0.43
2:B:386:GLU:O	2:B:387:LEU:C	2.57	0.43
1:A:5:ILE:CB	1:A:135:PHE:CE1	3.01	0.43
1:A:7:ILE:HB	1:A:136:SER:O	2.18	0.43
1:A:26:LEU:O	1:A:27:GLU:CB	2.66	0.43
1:A:252:LEU:HD23	1:A:255:PHE:HE2	1.78	0.43
1:A:404:PHE:O	1:A:404:PHE:CG	2.72	0.43
1:A:411:GLU:OE1	1:A:411:GLU:HA	2.19	0.43
2:B:94:PHE:CE1	2:B:97:SER:HB3	2.52	0.43
2:B:296:PHE:CE2	2:B:335:VAL:CG1	2.98	0.43
2:B:318:VAL:O	2:B:376:THR:N	2.26	0.43
2:B:389:LYS:HG2	2:B:429:VAL:HG11	1.75	0.43
2:B:425:MET:O	2:B:428:LEU:CB	2.63	0.43
1:A:14:VAL:CG2	1:A:74:VAL:CG1	2.96	0.43
1:A:115:ILE:HD12	1:A:152:LEU:HD23	1.87	0.43
1:A:147:SER:OG	1:A:148:GLY:N	2.50	0.43
1:A:211:ASP:OD1	1:A:214:ARG:NH1	2.51	0.43
1:A:312:TYR:HD1	1:A:341:ILE:O	2.01	0.43
2:B:6:HIS:HE1	2:B:30:ILE:HD12	0.60	0.43
2:B:265:LEU:O	2:B:265:LEU:HG	2.19	0.43
2:B:280:SER:O	2:B:283:TYR:HD1	2.02	0.43
2:B:292:THR:HG22	2:B:332:MET:SD	2.58	0.43
1:A:97:GLU:HG3	1:A:110:ILE:HG23	1.92	0.43
1:A:108:TYR:OH	1:A:417:GLU:CD	2.56	0.43
1:A:119:LEU:HA	1:A:122:ILE:CG2	2.48	0.43
1:A:137:VAL:HB	1:A:168:GLU:CB	2.49	0.43
1:A:266:HIS:HD2	1:A:432:TYR:CZ	2.37	0.43
2:B:183:GLU:HB3	2:B:184:PRO:HD3	1.81	0.43
1:A:20:CYS:C	1:A:24:TYR:HD2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:O	1:A:79:ARG:HG3	2.18	0.43
2:B:4:ILE:HG21	2:B:30:ILE:HG22	1.99	0.43
2:B:21:TRP:CE3	2:B:24:ILE:HD12	2.53	0.43
2:B:24:ILE:CA	2:B:26:ASP:H	2.25	0.43
2:B:186:ASN:HA	2:B:189:LEU:HD12	2.01	0.43
2:B:344:VAL:H	2:B:350:ASN:HD21	1.67	0.43
1:A:64:ARG:CZ	1:A:132:LEU:CD2	2.86	0.43
1:A:192:HIS:O	1:A:196:GLU:CB	2.67	0.43
1:A:204:VAL:HG13	1:A:209:ILE:CD1	2.30	0.43
1:A:303:VAL:CG1	1:A:304:LYS:N	2.80	0.43
1:A:397:LEU:HA	1:A:401:LYS:HD2	2.00	0.43
1:A:409:VAL:O	1:A:412:GLY:N	2.40	0.43
1:A:437:VAL:HG12	1:A:438:ASP:OD1	2.19	0.43
2:B:20:PHE:HB2	2:B:235:MET:HE1	1.77	0.43
2:B:385:GLN:NE2	2:B:433:GLN:HB2	2.34	0.43
1:A:181:VAL:HG12	1:A:185:TYR:HB2	2.01	0.43
1:A:298:PRO:O	1:A:301:GLN:HB2	2.18	0.43
2:B:199:ASP:OD2	2:B:256:ALA:HB1	2.17	0.43
2:B:212:ILE:C	2:B:214:PHE:H	2.23	0.43
2:B:212:ILE:O	2:B:216:THR:OG1	2.35	0.43
2:B:258:ASN:O	2:B:314:THR:HG21	2.19	0.43
1:A:77:GLU:CA	1:A:80:THR:CB	2.84	0.42
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.86	0.42
1:A:277:SER:HA	1:A:368:LEU:CD2	2.38	0.42
1:A:341:ILE:H	1:A:342:GLN:HG3	1.84	0.42
2:B:27:GLU:HB2	2:B:36:TYR:CB	2.49	0.42
2:B:320:ARG:HH21	5:B:501:TXL:H27	1.76	0.42
2:B:324:SER:O	2:B:328:VAL:HG23	2.19	0.42
2:B:339:ASN:CA	2:B:342:TYR:HD1	2.32	0.42
2:B:384:ILE:HG21	2:B:388:PHE:HE2	1.79	0.42
2:B:398:MET:SD	2:B:399:PHE:CD2	3.12	0.42
1:A:31:GLN:NE2	1:A:243:ARG:CB	2.57	0.42
1:A:154:MET:HB2	1:A:192:HIS:HE1	1.75	0.42
2:B:3:GLU:CD	2:B:64:ARG:NH1	2.71	0.42
2:B:7:ILE:HG21	2:B:137:LEU:CD2	2.49	0.42
2:B:296:PHE:CD1	2:B:335:VAL:CG1	3.02	0.42
2:B:319:PHE:CE1	2:B:353:THR:HG21	2.44	0.42
2:B:405:LEU:O	2:B:409:THR:CB	2.67	0.42
1:A:101:ASN:O	1:A:102:ASN:CB	2.51	0.42
1:A:184:PRO:HG2	1:A:399:TYR:CD2	2.51	0.42
1:A:194:THR:CG2	1:A:195:LEU:N	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ARG:O	2:B:61:TYR:CE2	2.72	0.42
2:B:48:ARG:CZ	2:B:60:LYS:HA	2.46	0.42
2:B:152:LEU:O	2:B:155:SER:OG	2.34	0.42
2:B:243:ARG:HH21	2:B:252:LEU:CG	2.31	0.42
2:B:301:MET:HG3	2:B:307:PRO:HG3	2.00	0.42
2:B:313:LEU:HD22	2:B:346:TRP:CZ2	2.55	0.42
2:B:336:GLN:HE21	2:B:351:VAL:CB	2.29	0.42
1:A:252:LEU:HD23	1:A:255:PHE:CD2	2.54	0.42
2:B:27:GLU:OE2	2:B:40:SER:O	2.37	0.42
2:B:111:GLY:O	2:B:115:VAL:CA	2.66	0.42
2:B:114:LEU:O	2:B:118:VAL:HG23	2.20	0.42
2:B:191:VAL:HG23	2:B:421:ALA:HB1	2.00	0.42
2:B:216:THR:HG21	2:B:275:LEU:HD13	2.00	0.42
1:A:30:ILE:HB	1:A:64:ARG:HB3	1.90	0.42
1:A:273:ALA:HB1	1:A:294:ALA:HB1	1.98	0.42
1:A:312:TYR:HA	1:A:381:THR:CB	2.48	0.42
2:B:176:LYS:CD	2:B:207:GLU:OE2	2.67	0.42
2:B:250:ALA:HB2	2:B:352:LYS:HZ1	1.81	0.42
2:B:398:MET:CG	2:B:399:PHE:N	2.62	0.42
1:A:5:ILE:HB	1:A:135:PHE:CE1	2.55	0.42
1:A:98:ASP:CG	2:B:253:ARG:HH12	2.21	0.42
1:A:289:ALA:C	1:A:291:ILE:N	2.69	0.42
1:A:344:VAL:HG12	1:A:345:ASP:N	2.34	0.42
2:B:172:VAL:CG2	2:B:205:ASP:OD1	2.67	0.42
1:A:5:ILE:HG13	1:A:64:ARG:NH2	2.31	0.42
2:B:34:GLY:O	2:B:36:TYR:HD2	2.01	0.42
2:B:242:LEU:HD13	2:B:250:ALA:O	2.20	0.42
2:B:301:MET:CE	2:B:377:PHE:CE1	3.03	0.42
2:B:393:GLU:OE1	2:B:393:GLU:HA	2.20	0.42
1:A:276:ILE:HG22	1:A:277:SER:N	2.35	0.42
1:A:277:SER:C	1:A:368:LEU:HD22	2.40	0.42
1:A:362:VAL:O	1:A:363:VAL:HG23	2.19	0.42
1:A:397:LEU:CA	1:A:401:LYS:CB	2.84	0.42
2:B:96:GLN:OE1	2:B:96:GLN:HA	2.19	0.42
2:B:101:ASN:HD22	2:B:101:ASN:HA	1.47	0.42
2:B:196:GLU:O	2:B:197:ASN:HB3	2.19	0.42
2:B:292:THR:O	2:B:293:GLN:C	2.54	0.42
1:A:57:GLY:CA	1:A:61:HIS:NE2	2.78	0.42
1:A:209:ILE:O	1:A:213:CYS:SG	2.63	0.42
2:B:70:LEU:O	2:B:70:LEU:HG	2.20	0.42
2:B:236:SER:O	2:B:241:CYS:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:MET:HE2	2:B:379:GLY:H	1.79	0.42
2:B:431:GLU:CA	2:B:434:GLN:HG3	2.50	0.42
1:A:10:GLY:O	1:A:11:GLN:C	2.58	0.41
1:A:67:PHE:CB	1:A:92:LEU:CD2	2.97	0.41
1:A:147:SER:N	1:A:189:LEU:HD13	2.33	0.41
1:A:173:PRO:HG3	1:A:186:ASN:ND2	2.35	0.41
1:A:179:THR:HG21	1:A:181:VAL:CA	2.46	0.41
1:A:292:THR:HG22	1:A:319:TYR:HH	1.74	0.41
2:B:133:GLN:HE21	2:B:253:ARG:NH1	2.04	0.41
2:B:205:ASP:CG	2:B:304:ALA:N	2.72	0.41
2:B:213:CYS:CB	2:B:219:LEU:CD1	2.86	0.41
2:B:262:PHE:CB	2:B:263:PRO:CD	2.78	0.41
1:A:180:ALA:HB1	1:A:398:MET:HE3	2.02	0.41
1:A:282:TYR:CD2	1:A:284:GLU:O	2.74	0.41
2:B:35:SER:HB3	2:B:60:LYS:HE3	2.02	0.41
2:B:172:VAL:HG12	2:B:173:PRO:O	2.20	0.41
1:A:31:GLN:NE2	1:A:239:THR:HG23	2.35	0.41
1:A:73:THR:CG2	2:B:249:ASN:HD21	2.24	0.41
1:A:109:THR:HG1	1:A:110:ILE:H	1.68	0.41
1:A:170:SER:OG	1:A:203:MET:CB	2.42	0.41
2:B:103:TRP:HZ2	2:B:151:THR:HG1	1.66	0.41
2:B:151:THR:O	2:B:192:HIS:HD2	2.02	0.41
2:B:184:PRO:CB	2:B:395:PHE:CD1	3.00	0.41
2:B:263:PRO:O	2:B:264:ARG:C	2.57	0.41
1:A:102:ASN:HA	1:A:408:TYR:CE1	2.56	0.41
1:A:122:ILE:HD13	1:A:157:LEU:HD22	1.94	0.41
1:A:303:VAL:HG12	1:A:304:LYS:H	1.84	0.41
2:B:92:PHE:N	2:B:92:PHE:CD1	2.87	0.41
2:B:154:ILE:CD1	2:B:192:HIS:CE1	2.82	0.41
2:B:295:MET:HE2	2:B:376:THR:N	2.36	0.41
2:B:435:TYR:CB	2:B:436:GLN:HG3	2.51	0.41
1:A:101:ASN:HD22	3:A:500:GTP:PG	2.42	0.41
1:A:114:ILE:HD13	1:A:114:ILE:HG21	1.84	0.41
1:A:224:TYR:HH	3:A:500:GTP:C2'	2.04	0.41
2:B:260:VAL:HG12	2:B:262:PHE:H	1.85	0.41
2:B:346:TRP:CZ2	2:B:435:TYR:CD2	3.05	0.41
1:A:64:ARG:NH2	1:A:132:LEU:CB	2.83	0.41
1:A:407:TRP:CE2	2:B:256:ALA:O	2.74	0.41
2:B:4:ILE:CG2	2:B:30:ILE:HB	2.50	0.41
2:B:143:GLY:C	2:B:185:TYR:OH	2.59	0.41
2:B:253:ARG:HH11	2:B:253:ARG:CB	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:GLY:O	5:B:501:TXL:C18	2.37	0.41
5:B:501:TXL:C21	5:B:501:TXL:C18	2.91	0.41
1:A:9:VAL:HG12	1:A:146:GLY:HA2	2.02	0.41
1:A:70:LEU:CB	1:A:145:THR:HG22	2.36	0.41
1:A:75:ILE:HG23	1:A:76:ASP:N	2.36	0.41
1:A:382:THR:O	1:A:385:ALA:HB2	2.16	0.41
2:B:27:GLU:HG2	2:B:48:ARG:HH21	1.85	0.41
1:A:146:GLY:C	1:A:189:LEU:HD13	2.41	0.41
1:A:224:TYR:CB	2:B:325:MET:CB	2.98	0.41
1:A:416:GLY:O	1:A:417:GLU:HB2	2.19	0.41
2:B:14:ASN:ND2	2:B:69:ASP:HA	2.35	0.41
2:B:69:ASP:OD2	2:B:74:THR:HG22	2.15	0.41
2:B:243:ARG:CZ	2:B:252:LEU:HD11	2.48	0.41
1:A:34:GLY:C	1:A:60:LYS:HZ2	2.20	0.41
1:A:107:HIS:HD1	1:A:108:TYR:N	2.18	0.41
1:A:116:ASP:OD1	1:A:156:ARG:NH1	2.54	0.41
1:A:242:LEU:HD22	1:A:250:VAL:HB	2.03	0.41
1:A:287:SER:O	1:A:288:VAL:C	2.57	0.41
1:A:311:LYS:CG	1:A:342:GLN:O	2.69	0.41
2:B:150:GLY:O	2:B:154:ILE:CG1	2.45	0.41
2:B:174:SER:HB2	2:B:207:GLU:CG	2.51	0.41
2:B:48:ARG:HD2	2:B:60:LYS:CA	2.38	0.41
2:B:86:ILE:HB	2:B:87:PHE:H	1.29	0.41
2:B:157:ILE:HG21	2:B:166:MET:CE	2.49	0.41
2:B:236:SER:OG	5:B:501:TXL:H27	2.21	0.41
2:B:259:MET:HG3	2:B:378:ILE:CG2	2.50	0.41
1:A:130:THR:O	1:A:131:GLY:O	2.38	0.40
1:A:297:GLU:O	1:A:298:PRO:C	2.52	0.40
1:A:398:MET:SD	2:B:348:PRO:O	2.79	0.40
1:A:404:PHE:HE2	2:B:257:VAL:HG13	1.86	0.40
2:B:101:ASN:C	2:B:102:ASN:CG	2.78	0.40
2:B:183:GLU:HG3	2:B:398:MET:SD	2.59	0.40
2:B:194:LEU:HD11	2:B:428:LEU:HD22	2.03	0.40
2:B:224:TYR:O	2:B:225:GLY:C	2.54	0.40
2:B:405:LEU:CG	2:B:405:LEU:O	2.52	0.40
1:A:4:CYS:H	1:A:30:ILE:HG22	1.86	0.40
1:A:115:ILE:HD13	1:A:115:ILE:HG21	1.83	0.40
1:A:217:LEU:HD22	1:A:368:LEU:CG	2.51	0.40
1:A:230:LEU:HD23	1:A:302:MET:HE3	2.02	0.40
1:A:313:MET:HB2	1:A:380:ASN:HB2	2.03	0.40
2:B:50:ASN:N	2:B:61:TYR:CG	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:SER:CB	2:B:110:GLU:CD	2.60	0.40
2:B:165:ILE:HD12	2:B:256:ALA:CB	2.51	0.40
1:A:35:GLN:C	1:A:36:MET:CG	2.89	0.40
1:A:147:SER:N	1:A:189:LEU:CD1	2.80	0.40
1:A:191:THR:OG1	1:A:192:HIS:N	2.54	0.40
1:A:271:THR:CB	1:A:377:MET:HB3	2.50	0.40
1:A:311:LYS:O	1:A:382:THR:HG23	2.21	0.40
2:B:178:SER:O	2:B:179:ASP:CB	2.64	0.40
2:B:388:PHE:O	2:B:391:ILE:N	2.54	0.40
1:A:76:ASP:O	1:A:80:THR:HA	2.17	0.40
1:A:82:THR:C	1:A:84:ARG:N	2.73	0.40
1:A:150:THR:O	1:A:192:HIS:NE2	2.54	0.40
1:A:312:TYR:CG	1:A:381:THR:CG2	2.90	0.40
2:B:40:SER:O	2:B:41:ASP:HB2	2.21	0.40
2:B:201:THR:HG21	2:B:267:PHE:CE1	2.56	0.40
2:B:238:VAL:CG1	2:B:255:LEU:CD1	2.98	0.40
2:B:274:PRO:HB2	2:B:371:LEU:CD2	2.51	0.40
2:B:312:TYR:N	2:B:381:SER:HB2	2.36	0.40
1:A:14:VAL:CG1	1:A:74:VAL:HG13	2.52	0.40
1:A:103:TYR:CZ	1:A:148:GLY:HA2	2.56	0.40
1:A:116:ASP:O	1:A:119:LEU:HB2	2.22	0.40
1:A:154:MET:HB2	1:A:192:HIS:HE2	1.82	0.40
1:A:157:LEU:CB	1:A:166:LYS:HE2	2.50	0.40
1:A:342:GLN:O	1:A:343:PHE:C	2.58	0.40
2:B:62:VAL:HA	2:B:63:PRO:HD2	1.92	0.40
2:B:210:TYR:O	2:B:211:ASP:C	2.59	0.40
2:B:282:GLN:HA	2:B:282:GLN:OE1	2.21	0.40
2:B:315:VAL:HB	2:B:351:VAL:HG22	2.04	0.40

All (35) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:HIS:CG	1:A:420:GLU:CD[2_444]	0.73	1.47
1:A:1:MET:CE	2:B:72:PRO:CG[1_655]	1.00	1.20
1:A:283:HIS:CG	1:A:420:GLU:OE1[2_444]	1.01	1.19
1:A:283:HIS:ND1	1:A:420:GLU:CD[2_444]	1.11	1.09
1:A:283:HIS:CD2	1:A:420:GLU:CA[2_444]	1.18	1.02
1:A:283:HIS:CD2	1:A:420:GLU:CB[2_444]	1.19	1.01
1:A:283:HIS:NE2	1:A:420:GLU:CB[2_444]	1.42	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:HIS:CB	1:A:420:GLU:CD[2_444]	1.42	0.78
1:A:283:HIS:CG	1:A:420:GLU:CG[2_444]	1.42	0.78
1:A:440:VAL:C	2:B:402:LYS:CE[1_655]	1.45	0.75
1:A:283:HIS:ND1	1:A:420:GLU:OE1[2_444]	1.46	0.74
1:A:283:HIS:CB	1:A:420:GLU:OE2[2_444]	1.59	0.61
1:A:1:MET:CB	2:B:96:GLN:NE2[1_655]	1.61	0.59
1:A:326:LYS:NZ	2:B:214:PHE:CZ[1_655]	1.67	0.53
1:A:1:MET:CE	2:B:72:PRO:CB[1_655]	1.68	0.52
1:A:283:HIS:CD2	1:A:420:GLU:OE1[2_444]	1.75	0.45
1:A:283:HIS:ND1	1:A:420:GLU:CG[2_444]	1.75	0.45
1:A:349:THR:CB	2:B:177:VAL:CG1[1_655]	1.78	0.42
1:A:283:HIS:CD2	1:A:420:GLU:CG[2_444]	1.82	0.38
1:A:440:VAL:C	2:B:402:LYS:NZ[1_655]	1.82	0.38
1:A:1:MET:CA	2:B:96:GLN:NE2[1_655]	1.83	0.37
1:A:254:GLU:OE1	2:B:101:ASN:OD1[1_655]	1.87	0.33
1:A:283:HIS:CB	1:A:420:GLU:OE1[2_444]	1.90	0.30
1:A:283:HIS:CG	1:A:420:GLU:OE2[2_444]	1.90	0.30
1:A:283:HIS:ND1	1:A:420:GLU:OE2[2_444]	1.91	0.29
1:A:283:HIS:CG	1:A:420:GLU:CB[2_444]	1.98	0.22
1:A:283:HIS:CD2	1:A:420:GLU:CD[2_444]	2.01	0.19
1:A:440:VAL:O	2:B:402:LYS:CE[1_655]	2.02	0.18
2:B:284:ARG:NE	2:B:420:GLU:OE2[2_344]	2.05	0.15
1:A:2:ARG:NH2	2:B:71:GLU:OE1[1_655]	2.06	0.14
1:A:326:LYS:NZ	2:B:214:PHE:CE1[1_655]	2.06	0.14
1:A:133:GLN:NE2	2:B:96:GLN:O[1_655]	2.11	0.09
1:A:254:GLU:OE2	2:B:101:ASN:OD1[1_655]	2.13	0.07
1:A:283:HIS:NE2	1:A:420:GLU:CA[2_444]	2.17	0.03
1:A:283:HIS:CE1	1:A:420:GLU:CB[2_444]	2.17	0.03

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	438/440 (100%)	323 (74%)	62 (14%)	53 (12%)	0 4
2	B	425/427 (100%)	297 (70%)	49 (12%)	79 (19%)	0 1
All	All	863/867 (100%)	620 (72%)	111 (13%)	132 (15%)	0 3

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	33	ASP
1	A	35	GLN
1	A	39	ASP
1	A	42	ILE
1	A	46	ASP
1	A	50	ASN
1	A	51	THR
1	A	73	THR
1	A	83	TYR
1	A	129	CYS
1	A	133	GLN
1	A	174	ALA
1	A	177	VAL
1	A	183	GLU
1	A	185	TYR
1	A	193	THR
1	A	197	HIS
1	A	198	SER
1	A	219	ILE
1	A	248	LEU
1	A	265	GLY
1	A	268	PRO
1	A	275	VAL
1	A	281	ALA
1	A	283	HIS
1	A	284	GLU
1	A	312	TYR
1	A	341	ILE
1	A	344	VAL
1	A	348	PRO
1	A	359	PRO
1	A	364	PRO
1	A	368	LEU
1	A	369	ALA

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Mol	Chain	Res	Type
2	B	2	ARG
2	B	25	SER
2	B	33	THR
2	B	36	TYR
2	B	39	ASP
2	B	40	SER
2	B	41	ASP
2	B	42	LEU
2	B	43	GLN
2	B	47	GLU
2	B	54	ASN
2	B	60	LYS
2	B	61	TYR
2	B	80	SER
2	B	81	GLY
2	B	83	PHE
2	B	86	ILE
2	B	89	PRO
2	B	90	ASP
2	B	97	SER
2	B	99	ALA
2	B	102	ASN
2	B	177	VAL
2	B	179	ASP
2	B	195	VAL
2	B	204	ILE
2	B	219	LEU
2	B	245	PRO
2	B	261	PRO
2	B	270	PRO
2	B	274	PRO
2	B	280	SER
2	B	284	ARG
2	B	322	ARG
2	B	344	VAL
2	B	345	GLU
2	B	385	GLN
2	B	401	ARG
2	B	415	GLU
1	A	25	CYS
1	A	81	GLY
1	A	102	ASN

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Mol	Chain	Res	Type
1	A	131	GLY
1	A	350	GLY
1	A	384	ILE
1	A	417	GLU
1	A	427	ALA
2	B	30	ILE
2	B	32	PRO
2	B	50	ASN
2	B	72	PRO
2	B	75	MET
2	B	129	CYS
2	B	176	LYS
2	B	276	THR
2	B	285	ALA
2	B	341	SER
2	B	387	LEU
2	B	427	ASP
1	A	65	ALA
1	A	66	VAL
1	A	82	THR
1	A	194	THR
2	B	27	GLU
2	B	28	HIS
2	B	57	ALA
2	B	144	GLY
2	B	173	PRO
2	B	248	LEU
2	B	262	PHE
2	B	281	GLN
2	B	339	ASN
2	B	347	ILE
2	B	348	PRO
2	B	412	GLY
1	A	175	PRO
1	A	261	PRO
2	B	29	GLY
2	B	31	ASP
2	B	48	ARG
2	B	53	TYR
2	B	87	PHE
2	B	183	GLU
2	B	242	LEU

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Mol	Chain	Res	Type
2	B	340	SER
1	A	98	ASP
1	A	410	GLY
2	B	222	PRO
2	B	360	PRO
2	B	389	LYS
2	B	403	ALA
2	B	277	SER
2	B	314	THR
1	A	142	GLY
2	B	175	PRO
2	B	63	PRO
1	A	221	ARG

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	369/369 (100%)	351 (95%)	18 (5%)	25	56
2	B	368/368 (100%)	348 (95%)	20 (5%)	22	54
All	All	737/737 (100%)	699 (95%)	38 (5%)	27	55

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	101	ASN
1	A	172	TYR
1	A	184	PRO
1	A	192	HIS
1	A	206	ASN
1	A	212	ILE
1	A	214	ARG
1	A	219	ILE
1	A	229	ARG

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Mol	Chain	Res	Type
1	A	264	ARG
1	A	293	ASN
1	A	320	ARG
1	A	390	ARG
1	A	396	ASP
1	A	405	VAL
1	A	422	ARG
1	A	432	TYR
2	B	2	ARG
2	B	30	ILE
2	B	94	PHE
2	B	101	ASN
2	B	139	HIS
2	B	185	TYR
2	B	192	HIS
2	B	227	LEU
2	B	253	ARG
2	B	278	ARG
2	B	300	ASN
2	B	302	MET
2	B	308	ARG
2	B	319	PHE
2	B	390	ARG
2	B	416	MET
2	B	424	ASN
2	B	426	ASN
2	B	432	TYR
2	B	436	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	61	HIS
1	A	85	GLN
1	A	88	HIS
1	A	107	HIS
1	A	176	GLN
1	A	192	HIS
1	A	206	ASN
1	A	226	ASN
1	A	228	ASN

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Mol	Chain	Res	Type
1	A	300	ASN
1	A	356	ASN
1	A	380	ASN
1	A	406	HIS
2	B	6	HIS
2	B	28	HIS
2	B	50	ASN
2	B	59	ASN
2	B	101	ASN
2	B	102	ASN
2	B	107	HIS
2	B	133	GLN
2	B	136	GLN
2	B	193	GLN
2	B	197	ASN
2	B	247	GLN
2	B	249	ASN
2	B	294	GLN
2	B	336	GLN
2	B	337	ASN
2	B	349	ASN
2	B	350	ASN
2	B	406	HIS
2	B	426	ASN

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

3 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	GTP	A	500	1	26,34,34	1.92	8 (30%)	32,54,54	1.43	6 (18%)
5	TXL	B	501	2	63,63,63	4.25	46 (73%)	100,100,100	3.30	53 (53%)
4	GDP	B	500	2	24,30,30	1.73	5 (20%)	30,47,47	1.09	3 (10%)

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
3	GTP	A	500	1	-	0/18/38/38	0/3/3/3
5	TXL	B	501	2	-	0/38/124/124	0/6/6/6
4	GDP	B	500	2	-	4/12/32/32	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	TXL	O3-C4	-9.59	1.26	1.46
5	B	501	TXL	C41-C36	8.34	1.53	1.39
5	B	501	TXL	C8-C3	-7.74	1.38	1.57
5	B	501	TXL	C37-C36	-7.66	1.26	1.39
5	B	501	TXL	O6-C9	-7.61	1.08	1.21
5	B	501	TXL	C25-C24	-7.37	1.27	1.39
5	B	501	TXL	C14-C13	6.99	1.66	1.52
5	B	501	TXL	C13-C12	-6.89	1.37	1.51
5	B	501	TXL	O5-C7	-6.78	1.32	1.43
5	B	501	TXL	C16-C15	-6.59	1.40	1.53
5	B	501	TXL	C6-C7	5.79	1.63	1.53
5	B	501	TXL	C12-C11	-5.65	1.26	1.34
5	B	501	TXL	C43-C42	-5.63	1.30	1.49
5	B	501	TXL	C10-C11	-5.38	1.34	1.50
5	B	501	TXL	O8-C13	-5.17	1.36	1.45
5	B	501	TXL	C14-C1	-5.11	1.43	1.54
5	B	501	TXL	C20-C4	5.08	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	TXL	O4-C5	5.08	1.56	1.46
5	B	501	TXL	C17-C15	4.51	1.62	1.53
3	A	500	GTP	O4'-C1'	-4.31	1.35	1.41
5	B	501	TXL	C4-C3	4.30	1.64	1.54
5	B	501	TXL	C8-C9	4.10	1.67	1.55
5	B	501	TXL	C24-C23	-4.08	1.46	1.52
5	B	501	TXL	O11-C30	4.04	1.29	1.21
4	B	500	GDP	C2'-C1'	-3.98	1.47	1.53
5	B	501	TXL	O12-C30	-3.94	1.26	1.34
5	B	501	TXL	C30-N1	3.93	1.44	1.34
3	A	500	GTP	C5-C6	-3.88	1.39	1.47
5	B	501	TXL	O10-C22	3.79	1.49	1.42
5	B	501	TXL	C40-C39	-3.70	1.28	1.38
5	B	501	TXL	C28-C27	-3.62	1.28	1.38
5	B	501	TXL	C22-C21	-3.52	1.43	1.52
5	B	501	TXL	C40-C41	3.48	1.46	1.38
5	B	501	TXL	C23-N1	-3.47	1.39	1.46
5	B	501	TXL	O12-C31	3.38	1.54	1.48
3	A	500	GTP	O2'-C2'	-3.26	1.35	1.43
3	A	500	GTP	C2'-C1'	-3.20	1.48	1.53
5	B	501	TXL	C36-C35	-3.13	1.42	1.50
5	B	501	TXL	O2-C35	3.09	1.41	1.34
5	B	501	TXL	O4-C20	-2.79	1.38	1.45
5	B	501	TXL	O8-C21	2.77	1.40	1.34
5	B	501	TXL	C34-C31	-2.76	1.43	1.51
5	B	501	TXL	O13-C35	-2.73	1.15	1.22
4	B	500	GDP	C5-C6	-2.52	1.42	1.47
5	B	501	TXL	C10-C9	2.51	1.60	1.53
4	B	500	GDP	C8-N7	-2.47	1.30	1.35
4	B	500	GDP	PB-O2B	-2.45	1.45	1.54
5	B	501	TXL	C4-C5	-2.42	1.50	1.55
5	B	501	TXL	C6-C5	-2.42	1.47	1.52
4	B	500	GDP	PB-O1B	-2.41	1.42	1.50
5	B	501	TXL	O1-C1	-2.35	1.40	1.44
3	A	500	GTP	C3'-C4'	-2.33	1.47	1.53
5	B	501	TXL	O3-C42	2.29	1.40	1.35
5	B	501	TXL	C28-C29	-2.26	1.34	1.38
5	B	501	TXL	C39-C38	-2.21	1.32	1.38
5	B	501	TXL	C32-C31	-2.17	1.45	1.51
3	A	500	GTP	C4-N3	-2.15	1.32	1.37
3	A	500	GTP	C8-N7	-2.10	1.31	1.35
3	A	500	GTP	C5'-C4'	-2.09	1.45	1.51

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	501	TXL	C15-C1-C2	10.94	123.89	111.91
5	B	501	TXL	C39-C38-C37	8.99	133.89	120.19
5	B	501	TXL	C38-C37-C36	-8.08	110.78	120.34
5	B	501	TXL	O7-C10-C9	7.21	121.53	109.51
5	B	501	TXL	C8-C9-C10	6.23	131.96	122.69
5	B	501	TXL	C13-C12-C11	-6.02	108.07	117.72
5	B	501	TXL	O11-C30-N1	5.77	134.31	124.85
5	B	501	TXL	C11-C10-C9	-5.65	107.54	114.05
5	B	501	TXL	O2-C2-C1	5.29	115.97	104.76
5	B	501	TXL	C6-C5-C4	-5.10	112.44	119.61
5	B	501	TXL	C39-C40-C41	-5.04	112.51	120.19
5	B	501	TXL	C17-C15-C1	4.97	122.22	111.11
5	B	501	TXL	O4-C5-C6	4.67	122.11	113.21
5	B	501	TXL	C18-C12-C11	4.64	130.93	125.30
5	B	501	TXL	C10-C11-C12	-4.43	113.96	120.65
5	B	501	TXL	O12-C30-N1	-4.39	102.64	110.02
5	B	501	TXL	O10-C22-C23	4.37	122.24	109.80
5	B	501	TXL	C16-C15-C1	-4.36	101.36	111.11
5	B	501	TXL	C33-C31-C32	4.28	122.39	111.16
5	B	501	TXL	C14-C1-C15	-4.21	103.75	111.50
5	B	501	TXL	O12-C31-C32	-4.05	91.17	107.20
5	B	501	TXL	C2-O2-C35	4.01	125.37	117.79
5	B	501	TXL	O6-C9-C10	-3.96	112.85	117.37
5	B	501	TXL	C31-O12-C30	-3.83	115.10	120.99
5	B	501	TXL	O7-C10-C11	-3.73	105.45	111.48
5	B	501	TXL	C20-C4-C3	3.71	126.21	120.30
5	B	501	TXL	O3-C42-O14	3.69	130.39	123.61
5	B	501	TXL	O2-C35-C36	3.69	117.88	111.92
5	B	501	TXL	C19-C8-C9	3.67	116.53	106.55
5	B	501	TXL	C24-C23-N1	3.54	119.06	112.11
5	B	501	TXL	C15-C11-C12	3.42	124.33	119.61
3	A	500	GTP	O3G-PG-O3B	3.12	115.11	104.64
5	B	501	TXL	C13-O8-C21	-3.10	110.78	116.67
5	B	501	TXL	O5-C7-C6	3.01	115.25	109.12
5	B	501	TXL	C24-C23-C22	-2.91	103.87	111.36
3	A	500	GTP	PB-O3B-PG	-2.91	122.85	132.83
5	B	501	TXL	C1-C2-C3	-2.90	113.75	118.18
5	B	501	TXL	C20-C4-C5	-2.78	82.45	85.40
5	B	501	TXL	C34-C31-C33	-2.78	103.87	111.16
5	B	501	TXL	C23-N1-C30	-2.69	116.20	121.72
5	B	501	TXL	C37-C36-C35	-2.69	114.33	120.40
5	B	501	TXL	C18-C12-C13	2.69	120.92	116.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	GTP	PA-O3A-PB	-2.57	124.00	132.83
5	B	501	TXL	O12-C31-C34	2.50	117.08	107.20
5	B	501	TXL	O3-C42-C43	-2.49	106.15	110.68
5	B	501	TXL	O4-C5-C4	2.48	93.37	90.58
5	B	501	TXL	O8-C13-C12	-2.48	103.78	109.78
3	A	500	GTP	O6-C6-C5	2.44	129.13	124.37
5	B	501	TXL	O8-C21-O9	2.44	128.48	123.94
4	B	500	GDP	C3'-C2'-C1'	2.42	104.62	100.98
5	B	501	TXL	C41-C36-C35	2.42	125.86	120.40
5	B	501	TXL	C19-C8-C3	-2.41	105.67	113.15
3	A	500	GTP	C3'-C2'-C1'	2.37	104.54	100.98
5	B	501	TXL	C14-C1-C2	-2.36	107.45	111.70
5	B	501	TXL	O10-C22-C21	-2.33	103.74	110.17
4	B	500	GDP	O2B-PB-O1B	2.29	119.63	110.68
5	B	501	TXL	C3-C4-C5	2.23	123.68	119.52
5	B	501	TXL	O1-C1-C2	-2.23	100.61	105.49
5	B	501	TXL	O3-C4-C5	-2.18	107.09	112.28
3	A	500	GTP	O2G-PG-O3B	2.16	111.87	104.64
5	B	501	TXL	O2-C2-C3	-2.07	104.35	108.17
4	B	500	GDP	O6-C6-C5	2.03	128.33	124.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	500	GDP	PA-O3A-PB-O2B
4	B	500	GDP	PA-O3A-PB-O1B
4	B	500	GDP	PA-O3A-PB-O3B
4	B	500	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

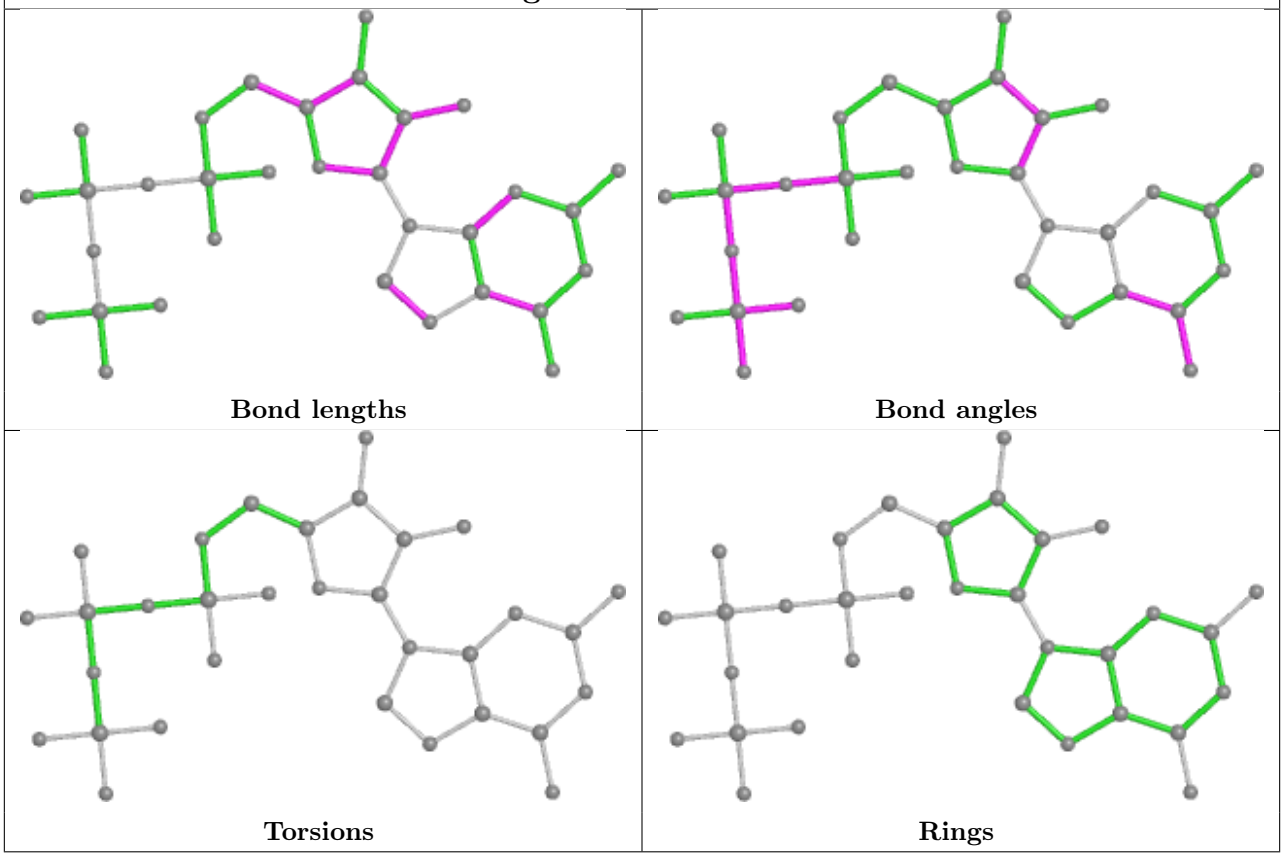
3 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	GTP	29	0
5	B	501	TXL	55	0
4	B	500	GDP	14	0

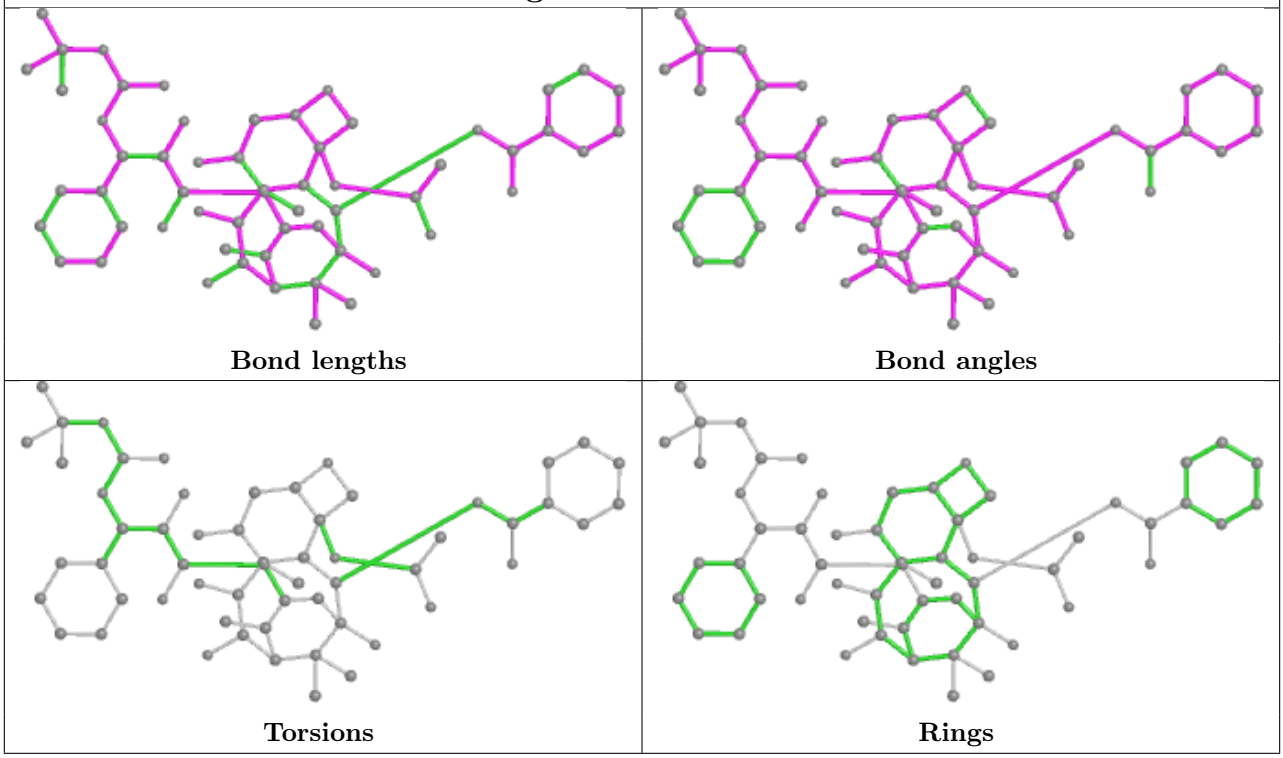
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

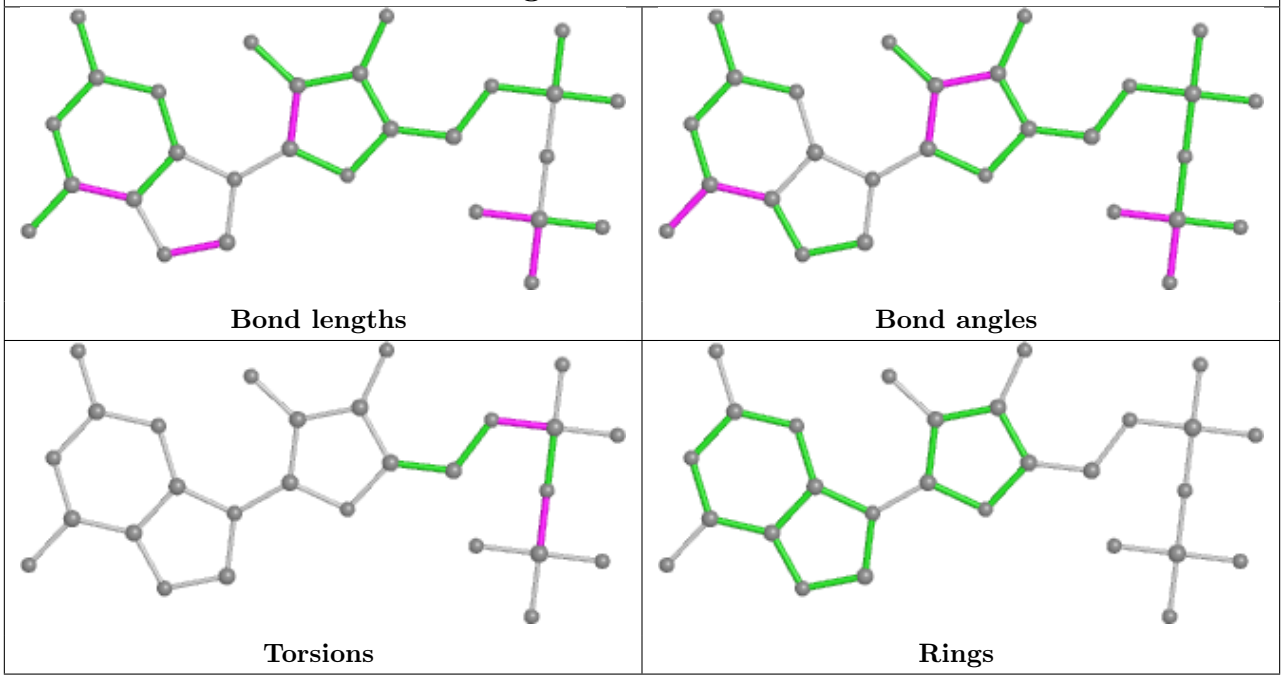
Ligand GTP A 500



Ligand TXL B 501



Ligand GDP B 500



5.7 Other polymers

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
2	B	52
1	A	41

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	387:LEU	C	388:PHE	N	1.63
1	A	283:HIS	C	284:GLU	N	1.20
1	A	380:ASN	C	381:THR	N	1.20
1	A	437:VAL	C	438:ASP	N	1.20
1	B	52:TYR	C	53:TYR	N	1.20
1	A	111:GLY	C	112:LYS	N	1.19
1	A	137:VAL	C	138:PHE	N	1.19
1	A	140:SER	C	141:PHE	N	1.19
1	A	146:GLY	C	147:SER	N	1.19
1	A	149:PHE	C	150:THR	N	1.19
1	A	377:MET	C	378:LEU	N	1.19
1	A	383:ALA	C	384:ILE	N	1.19
1	B	72:PRO	C	73:GLY	N	1.19
1	B	111:GLY	C	112:ALA	N	1.19
1	B	178:SER	C	179:ASP	N	1.19
1	B	193:GLN	C	194:LEU	N	1.19
1	B	194:LEU	C	195:VAL	N	1.19
1	B	234:THR	C	235:MET	N	1.19
1	B	259:MET	C	260:VAL	N	1.19
1	B	347:ILE	C	348:PRO	N	1.19
1	B	348:PRO	C	349:ASN	N	1.19
1	A	34:GLY	C	35:GLN	N	1.18
1	A	433:GLU	C	434:GLU	N	1.18
1	B	130:ASP	C	131:CYS	N	1.18
1	B	244:PHE	C	245:PRO	N	1.18
1	A	259:LEU	C	260:VAL	N	1.17
1	A	346:TRP	C	347:CYS	N	1.17
1	A	367:ASP	C	368:LEU	N	1.17
1	B	53:TYR	C	54:ASN	N	1.17
1	B	299:LYS	C	300:ASN	N	1.17
1	A	204:VAL	C	205:ASP	N	1.16
1	A	233:GLN	C	234:ILE	N	1.16
1	A	274:PRO	C	275:VAL	N	1.16
1	B	70:LEU	C	71:GLU	N	1.16

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	89:PRO	C	90:ASP	N	1.16
1	B	171:VAL	C	172:VAL	N	1.16
1	B	243:ARG	C	244:PHE	N	1.16
1	A	24:TYR	C	25:CYS	N	1.15
1	A	379:SER	C	380:ASN	N	1.15
1	B	154:ILE	C	155:SER	N	1.15
1	B	173:PRO	C	174:SER	N	1.15
1	B	337:ASN	C	338:LYS	N	1.15
1	B	151:THR	C	152:LEU	N	1.14
1	B	436:GLN	C	437:ASP	N	1.14
1	A	90:GLU	C	91:GLN	N	1.13
1	B	292:THR	C	293:GLN	N	1.13
1	A	33:ASP	C	34:GLY	N	1.12
1	A	280:LYS	C	281:ALA	N	1.12
1	B	273:ALA	C	274:PRO	N	1.12
1	A	87:PHE	C	88:HIS	N	1.11
1	B	64:ARG	C	65:ALA	N	1.11
1	B	334:ASN	C	335:VAL	N	1.11
1	B	414:ASP	C	415:GLU	N	1.11
1	B	60:LYS	C	61:TYR	N	1.10
1	B	179:ASP	C	180:THR	N	1.10
1	B	371:LEU	C	372:LYS	N	1.10
1	A	216:ASN	C	217:LEU	N	1.09
1	A	402:ARG	C	403:ALA	N	1.09
1	B	344:VAL	C	345:GLU	N	1.09
1	A	221:ARG	C	222:PRO	N	1.08
1	A	190:THR	C	191:THR	N	1.07
1	B	22:GLU	C	23:VAL	N	1.07
1	B	331:GLN	C	332:MET	N	1.07
1	A	31:GLN	C	32:PRO	N	1.06
1	B	71:GLU	C	72:PRO	N	1.06
1	B	127:GLU	C	128:SER	N	1.05
1	B	400:ARG	C	401:ARG	N	1.05
1	B	380:ASN	C	381:SER	N	1.04
1	A	69:ASP	C	70:LEU	N	1.03
1	A	405:VAL	C	406:HIS	N	1.03
1	A	415:GLU	C	416:GLY	N	1.03
1	A	371:VAL	C	372:GLN	N	1.02
1	B	203:CYS	C	204:ILE	N	1.02
1	B	275:LEU	C	276:THR	N	1.02
1	B	309:HIS	C	310:GLY	N	1.00
1	B	346:TRP	C	347:ILE	N	0.99

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	417:GLU	C	418:PHE	N	0.98
1	A	358:GLU	C	359:PRO	N	0.97
1	B	247:GLN	C	248:LEU	N	0.96
1	A	193:THR	C	194:THR	N	0.95
1	A	350:GLY	C	351:PHE	N	0.95
1	A	416:GLY	C	417:GLU	N	0.95
1	B	340:SER	C	341:SER	N	0.92
1	A	53:PHE	C	54:SER	N	0.90
1	B	182:VAL	C	183:GLU	N	0.90
1	B	197:ASN	C	198:THR	N	0.90
1	B	200:GLU	C	201:THR	N	0.90
1	A	347:CYS	C	348:PRO	N	0.89
1	B	321:GLY	C	322:ARG	N	0.88
1	A	218:ASP	C	219:ILE	N	0.84
1	B	105:LYS	C	106:GLY	N	0.80
1	A	38:SER	C	39:ASP	N	0.70
1	B	73:GLY	C	74:THR	N	0.69