Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 01:26 AM EDT

PDB ID	:	2IPI
Title	:	Crystal Structure of Aclacinomycin Oxidoreductase
Authors	:	Sultana, A.; Kursula, I.; Schneider, G.; Alexeev, I.; Niemi, J.; Mantsala, P.
Deposited on	:	2006-10-12
Resolution	:	1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

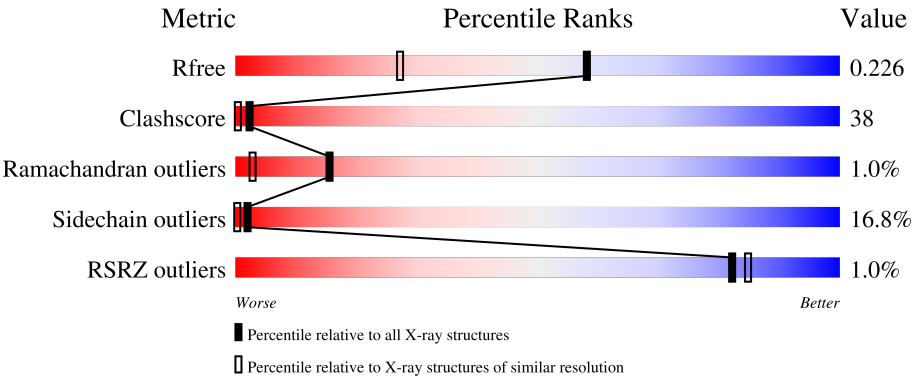
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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

Mol	Chain	Length	Quality of chain
1	A	521	44% 39% 11% 6%
1	B	521	37% 45% 11% 6%
1	C	521	44% 41% 9% 6%
1	D	521	41% 41% 11% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AKY	A	601[A]	X	-	-	-
3	FAD	B	801	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16589 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Aclacinomycin oxidoreductase (AknOx).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	67	2	0
			3836	2423	693	712	8			
1	B	492	Total	C	N	O	S	67	0	0
			3823	2415	690	710	8			
1	C	492	Total	C	N	O	S	55	1	0
			3828	2418	690	712	8			
1	D	492	Total	C	N	O	S	70	0	0
			3823	2415	690	710	8			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	INITIATING METHIONINE	UNP Q0PCD7
A	-17	ALA	-	CLONING ARTIFACT	UNP Q0PCD7
A	-16	HIS	-	EXPRESSION TAG	UNP Q0PCD7
A	-15	HIS	-	EXPRESSION TAG	UNP Q0PCD7
A	-14	HIS	-	EXPRESSION TAG	UNP Q0PCD7
A	-13	HIS	-	EXPRESSION TAG	UNP Q0PCD7
A	-12	HIS	-	EXPRESSION TAG	UNP Q0PCD7
A	-11	HIS	-	EXPRESSION TAG	UNP Q0PCD7
A	-10	HIS	-	EXPRESSION TAG	UNP Q0PCD7
A	-9	ARG	-	CLONING ARTIFACT	UNP Q0PCD7
A	-8	SER	-	CLONING ARTIFACT	UNP Q0PCD7
A	-7	ALA	-	CLONING ARTIFACT	UNP Q0PCD7
A	-6	ALA	-	CLONING ARTIFACT	UNP Q0PCD7
A	-5	GLY	-	CLONING ARTIFACT	UNP Q0PCD7
A	-4	THR	-	CLONING ARTIFACT	UNP Q0PCD7
A	-3	ILE	-	CLONING ARTIFACT	UNP Q0PCD7
A	-2	TRP	-	CLONING ARTIFACT	UNP Q0PCD7
A	-1	GLU	-	CLONING ARTIFACT	UNP Q0PCD7
A	0	PHE	-	CLONING ARTIFACT	UNP Q0PCD7
B	-18	MET	-	INITIATING METHIONINE	UNP Q0PCD7
B	-17	ALA	-	CLONING ARTIFACT	UNP Q0PCD7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	EXPRESSION TAG	UNP Q0PCD7
B	-15	HIS	-	EXPRESSION TAG	UNP Q0PCD7
B	-14	HIS	-	EXPRESSION TAG	UNP Q0PCD7
B	-13	HIS	-	EXPRESSION TAG	UNP Q0PCD7
B	-12	HIS	-	EXPRESSION TAG	UNP Q0PCD7
B	-11	HIS	-	EXPRESSION TAG	UNP Q0PCD7
B	-10	HIS	-	EXPRESSION TAG	UNP Q0PCD7
B	-9	ARG	-	CLONING ARTIFACT	UNP Q0PCD7
B	-8	SER	-	CLONING ARTIFACT	UNP Q0PCD7
B	-7	ALA	-	CLONING ARTIFACT	UNP Q0PCD7
B	-6	ALA	-	CLONING ARTIFACT	UNP Q0PCD7
B	-5	GLY	-	CLONING ARTIFACT	UNP Q0PCD7
B	-4	THR	-	CLONING ARTIFACT	UNP Q0PCD7
B	-3	ILE	-	CLONING ARTIFACT	UNP Q0PCD7
B	-2	TRP	-	CLONING ARTIFACT	UNP Q0PCD7
B	-1	GLU	-	CLONING ARTIFACT	UNP Q0PCD7
B	0	PHE	-	CLONING ARTIFACT	UNP Q0PCD7
C	-18	MET	-	INITIATING METHIONINE	UNP Q0PCD7
C	-17	ALA	-	CLONING ARTIFACT	UNP Q0PCD7
C	-16	HIS	-	EXPRESSION TAG	UNP Q0PCD7
C	-15	HIS	-	EXPRESSION TAG	UNP Q0PCD7
C	-14	HIS	-	EXPRESSION TAG	UNP Q0PCD7
C	-13	HIS	-	EXPRESSION TAG	UNP Q0PCD7
C	-12	HIS	-	EXPRESSION TAG	UNP Q0PCD7
C	-11	HIS	-	EXPRESSION TAG	UNP Q0PCD7
C	-10	HIS	-	EXPRESSION TAG	UNP Q0PCD7
C	-9	ARG	-	CLONING ARTIFACT	UNP Q0PCD7
C	-8	SER	-	CLONING ARTIFACT	UNP Q0PCD7
C	-7	ALA	-	CLONING ARTIFACT	UNP Q0PCD7
C	-6	ALA	-	CLONING ARTIFACT	UNP Q0PCD7
C	-5	GLY	-	CLONING ARTIFACT	UNP Q0PCD7
C	-4	THR	-	CLONING ARTIFACT	UNP Q0PCD7
C	-3	ILE	-	CLONING ARTIFACT	UNP Q0PCD7
C	-2	TRP	-	CLONING ARTIFACT	UNP Q0PCD7
C	-1	GLU	-	CLONING ARTIFACT	UNP Q0PCD7
C	0	PHE	-	CLONING ARTIFACT	UNP Q0PCD7
D	-18	MET	-	INITIATING METHIONINE	UNP Q0PCD7
D	-17	ALA	-	CLONING ARTIFACT	UNP Q0PCD7
D	-16	HIS	-	EXPRESSION TAG	UNP Q0PCD7
D	-15	HIS	-	EXPRESSION TAG	UNP Q0PCD7
D	-14	HIS	-	EXPRESSION TAG	UNP Q0PCD7
D	-13	HIS	-	EXPRESSION TAG	UNP Q0PCD7

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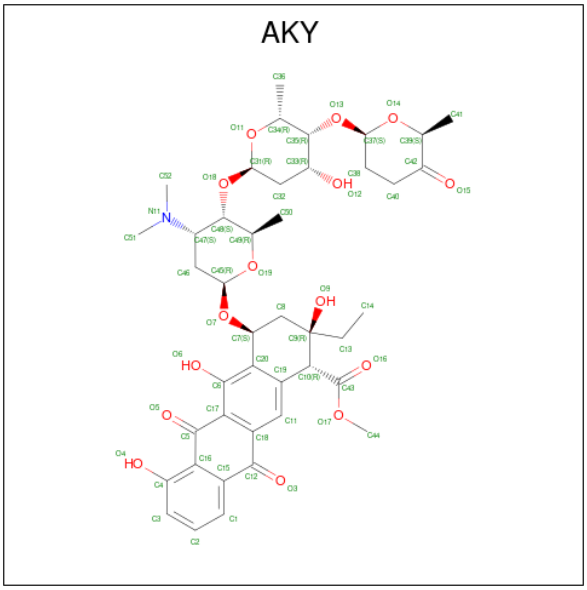
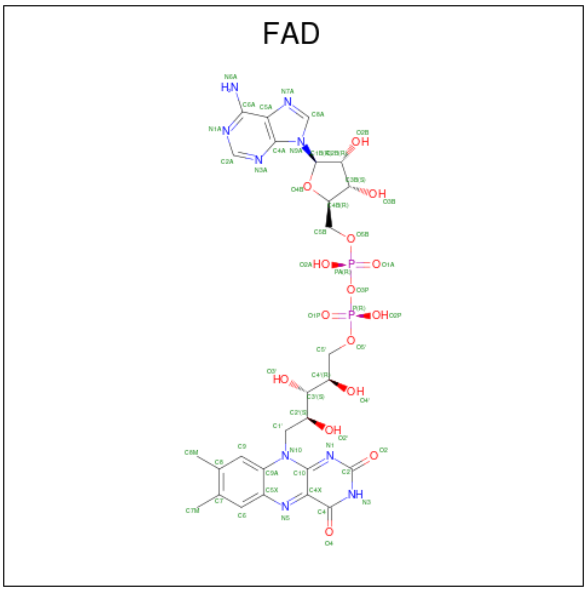
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	EXPRESSION TAG	UNP Q0PCD7
D	-11	HIS	-	EXPRESSION TAG	UNP Q0PCD7
D	-10	HIS	-	EXPRESSION TAG	UNP Q0PCD7
D	-9	ARG	-	CLONING ARTIFACT	UNP Q0PCD7
D	-8	SER	-	CLONING ARTIFACT	UNP Q0PCD7
D	-7	ALA	-	CLONING ARTIFACT	UNP Q0PCD7
D	-6	ALA	-	CLONING ARTIFACT	UNP Q0PCD7
D	-5	GLY	-	CLONING ARTIFACT	UNP Q0PCD7
D	-4	THR	-	CLONING ARTIFACT	UNP Q0PCD7
D	-3	ILE	-	CLONING ARTIFACT	UNP Q0PCD7
D	-2	TRP	-	CLONING ARTIFACT	UNP Q0PCD7
D	-1	GLU	-	CLONING ARTIFACT	UNP Q0PCD7
D	0	PHE	-	CLONING ARTIFACT	UNP Q0PCD7

- Molecule 2 is METHYL (2S,4R)-2-ETHYL-2,5,7-TRIHYDROXY-6,11-DIOXO-4-{[2,3,6-TRIDEOXY-4-O-{2,6-DIDEOXY-4-O-[(2S,6S)-6-METHYL-5-OXOTETRAHYDRO-2H-PYRAN-2-YL]-ALPHA-D-LYXO-HEXOPYRANOSYL}-3-(DIMETHYLAMINO)-D-RIBO-HEXOPYRANOSYL]OXY}-1,2,3,4,6,11-HEXAHYDROTETRACENE-1-CARBOXYLATE (three-letter code: AKY) (formula: $C_{42}H_{53}NO_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			58	42	1	15		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is water.

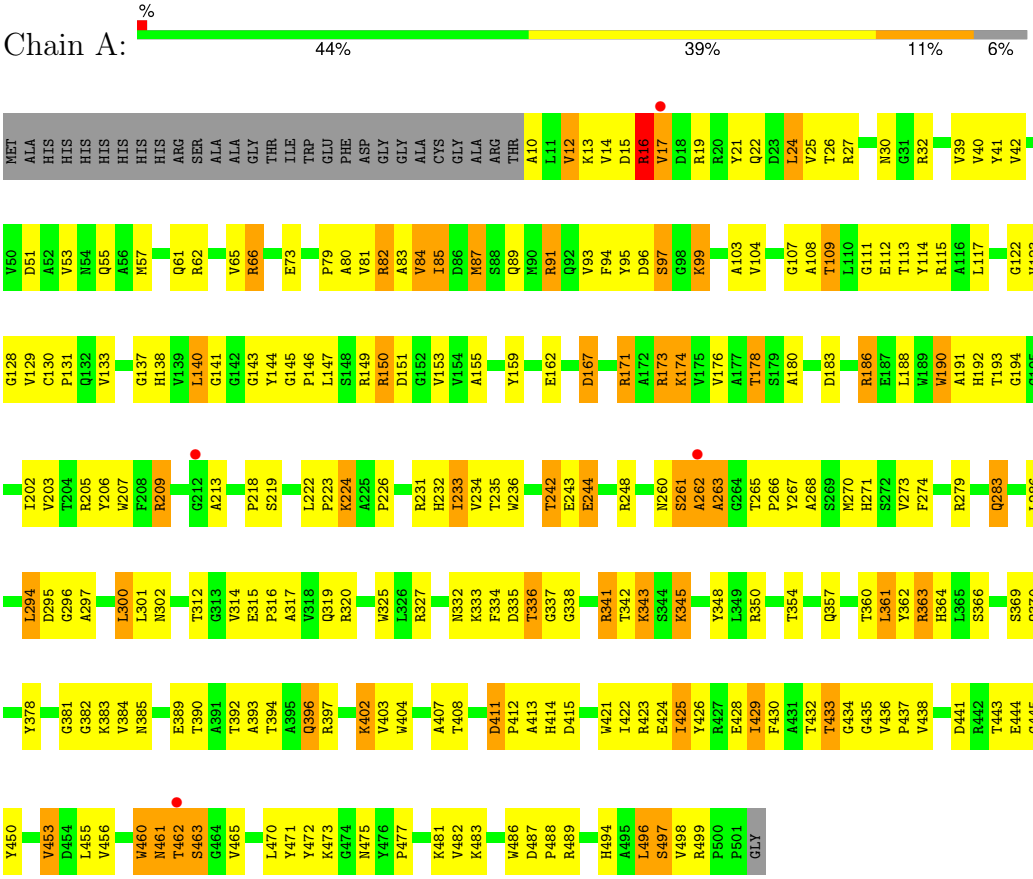
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	274	Total	O	0	0
			274	274		
4	B	212	Total	O	0	0
			212	212		
4	C	317	Total	O	0	0
			317	317		
4	D	206	Total	O	0	0
			206	206		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

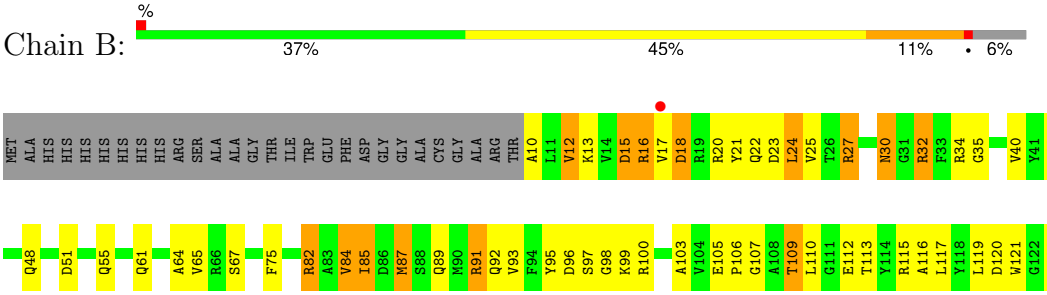
• Molecule 1: Aclacinomycin oxidoreductase (AknOx)

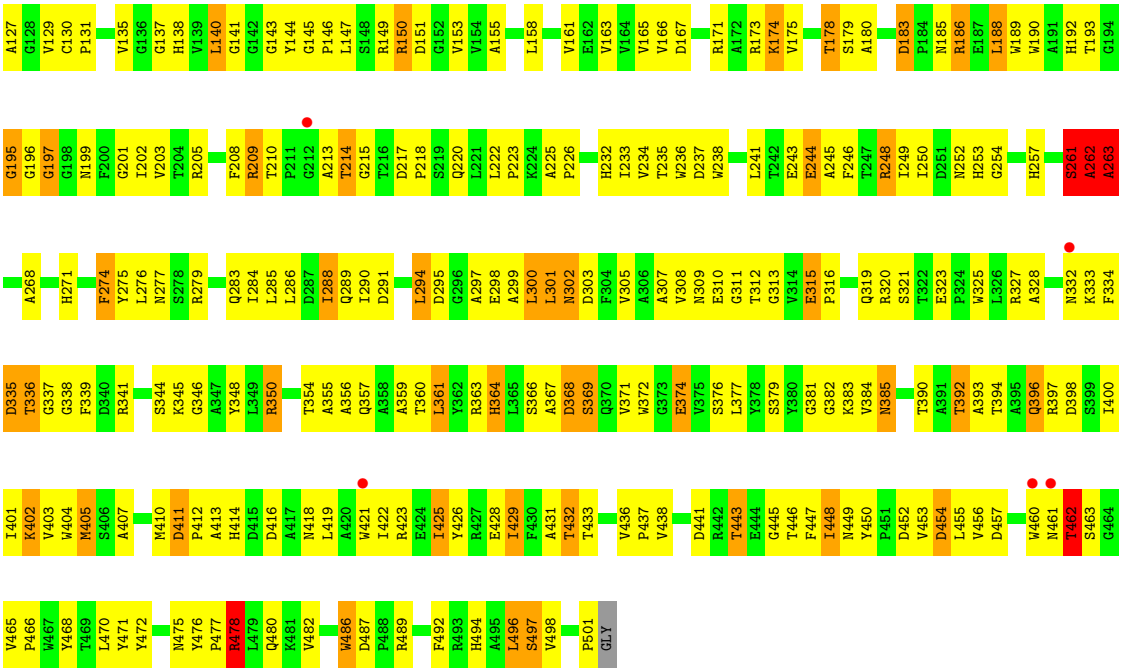
Chain A:



• Molecule 1: Aclacinomycin oxidoreductase (AknOx)

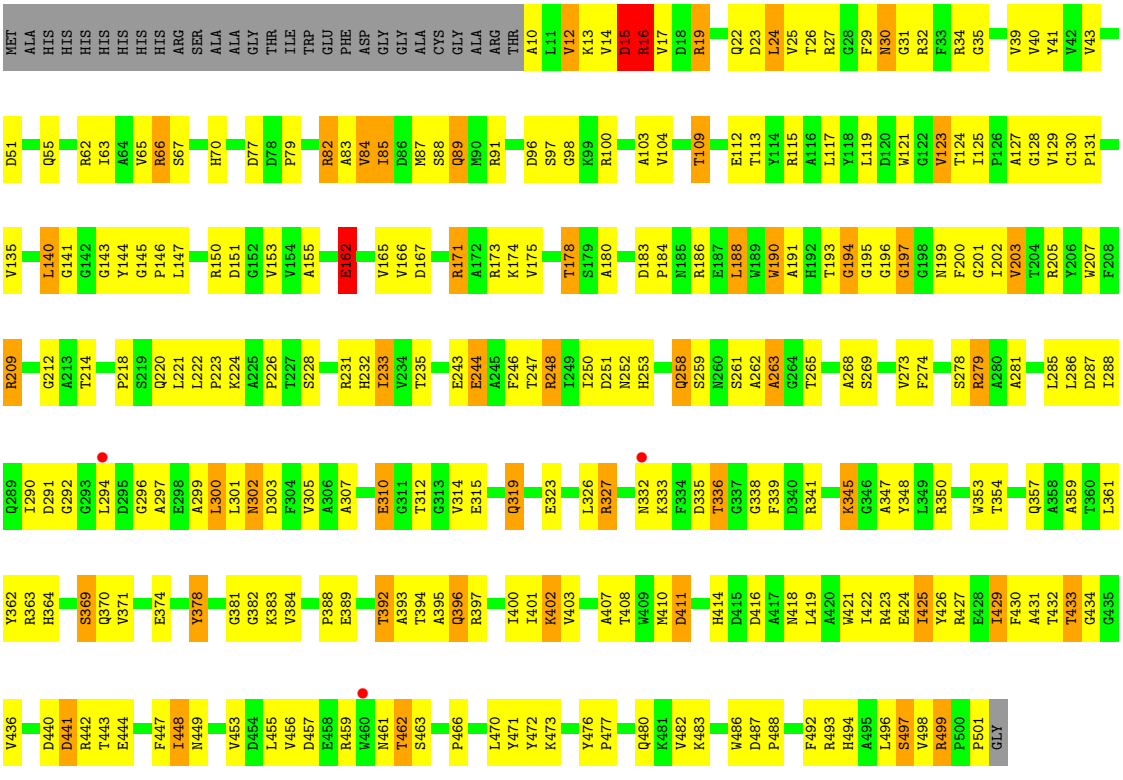
Chain B:





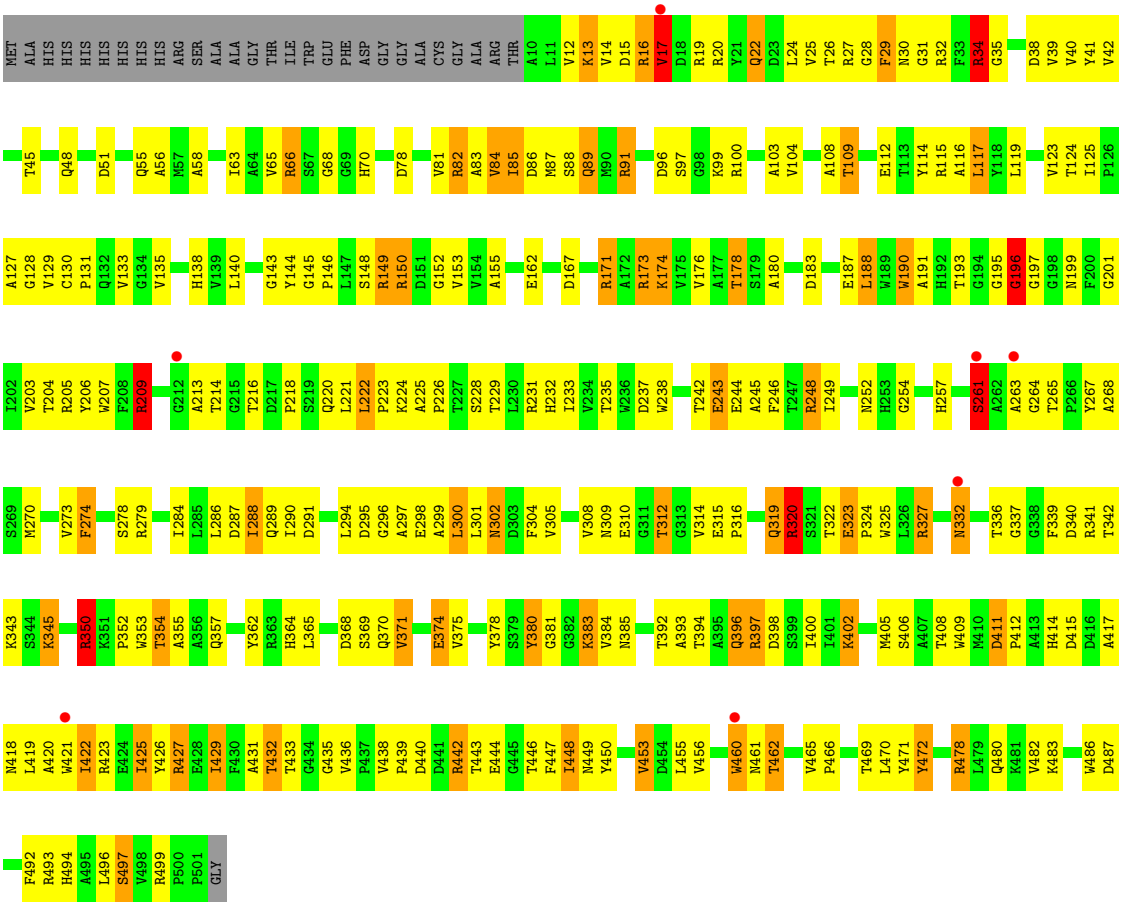
• Molecule 1: Aclacinomycin oxidoreductase (AknOx)

Chain C:



• Molecule 1: Aclacinomycin oxidoreductase (AknOx)

Chain D:


MET ALA HIS HIS HIS HIS HIS HIS ARG SER ALA ALA GLY THR ILE TRP GLU PHE ASP GLY GLY ALA CYS GLY ALA ARG THR A10 L11 V12 K13 V14 D15 R16 V17 D18 R19 R20 Y21 Q22 D23 L24 V25 T26 R27 G28 F29 N30 G31 R32 F33 R34 G35 D38 V39 V40 Y41 V42
T45 Q48 D51 Q55 A56 M57 A58 I63 A64 V65 R66 S67 G68 G69 H70 D78 V81 R82 A83 V84 I85 D86 M87 S88 Q89 M90 R91 D96 S97 G98 K99 R100 A103 V104 A108 T109 E112 T113 Y114 R115 A116 L117 Y118 L119 V123 T124 I125 P126
A127 G128 V129 C130 P131 Q132 V133 G134 V135 H138 V139 L140 G143 Y144 G145 P146 L147 S148 R149 R150 D151 G152 V153 V154 A155 E162 D167 R171 A172 R173 K174 V175 V176 A177 T178 S179 A180 D183 E187 L188 W189 W190 A191 H192 T193 G194 G195 G196 G197 G198 N199 P200 G201
I202 V203 T204 R205 Y206 W207 P208 R209 G212 A213 T214 G215 T216 D217 P218 S219 Q220 L221 L222 P223 K224 A225 P226 T227 S228 T229 L230 R231 H232 I233 V234 T235 W236 D237 W238 T242 E243 E244 A245 F246 T247 R248 I249 N252 H253 G254 H257 S261 A262 A263 G264 T265 P266 Y267 A268
S269 M270 V273 F274 S278 R279 I284 L285 L286 D287 I288 Q289 I290 D291 L294 D295 G296 A297 E298 A299 L300 L301 N302 D303 F304 V305 V308 N309 E310 G311 T312 G313 V314 E315 P316 Q319 R320 S321 T322 E323 P324 W325 L326 R327 N332 T336 G337 G338 F339 D340 R341 T342
K343 S344 K345 R350 K351 P352 W353 T354 A355 A356 Q357 Y362 R363 H364 L365 D368 S369 Q370 V371 E374 V375 Y378 S379 Y380 G381 G382 K383 V384 N385 T392 A393 T394 A395 Q396 R397 D398 S399 I400 I401 K402 M405 S406 A407 T408 W409 M410 D411 P412 A413 H414 D415 D416 A417
N418 L419 A420 W421 I422 R423 E424 I425 Y426 R427 E428 I429 F430 A431 T432 T433 G434 G435 V436 P437 V438 P439 D440 D441 R442 T443 E444 G445 T446 F447 I448 N449 Y450 W453 D454 L455 V456 W460 N461 T462 V465 P466 T469 L470 Y471 Y472 R478 L479 Q480 K481 V482 K483 W486 D487
F492 R493 H494 A495 L496 S497 V498 R499 P500 P501 GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.50Å 266.20Å 68.70Å 90.00° 119.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.65 19.76 – 1.67	Depositor EDS
% Data completeness (in resolution range)	95.9 (20.00-1.65) 98.5 (19.76-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 1.67Å)	Xtriage
Refinement program	REFMAC, SHELXL-97	Depositor
R, R_{free}	0.185 , 0.242 0.182 , 0.226	Depositor DCC
R_{free} test set	9545 reflections (3.87%)	wwPDB-VP
Wilson B-factor (Å^2)	13.2	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 57.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.31$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	0.128 for -h-l,k,h 0.128 for l,k,-h-l 0.130 for h,-k,-h-l 0.128 for -h-l,-k,l 0.430 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16589	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, AKY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.40	0/3946	1.14	19/5386 (0.4%)
1	B	0.41	0/3927	1.17	25/5361 (0.5%)
1	C	0.43	0/3935	1.19	22/5372 (0.4%)
1	D	0.39	0/3927	1.17	28/5361 (0.5%)
All	All	0.41	0/15735	1.16	94/21480 (0.4%)

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	B	0	3
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	82	ARG	NE-CZ-NH1	-12.09	114.25	120.30
1	D	196	GLY	C-N-CA	11.89	147.28	122.30
1	A	91	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	C	66	ARG	NE-CZ-NH1	9.87	125.24	120.30
1	C	66	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	B	263	ALA	C-N-CA	9.58	142.43	122.30
1	A	186	ARG	NE-CZ-NH1	-9.54	115.53	120.30
1	B	149	ARG	CD-NE-CZ	9.32	136.65	123.60
1	B	149	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	D	149	ARG	NE-CZ-NH2	8.87	124.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	196	GLY	C-N-CA	8.76	140.69	122.30
1	A	91	ARG	CD-NE-CZ	8.68	135.75	123.60
1	B	341	ARG	CD-NE-CZ	8.64	135.69	123.60
1	B	186	ARG	NE-CZ-NH2	8.60	124.60	120.30
1	C	263	ALA	C-N-CA	8.46	140.06	122.30
1	D	34	ARG	CD-NE-CZ	8.43	135.40	123.60
1	A	82	ARG	NE-CZ-NH1	-8.23	116.18	120.30
1	D	149	ARG	CD-NE-CZ	7.94	134.71	123.60
1	D	209	ARG	CD-NE-CZ	7.93	134.70	123.60
1	C	186	ARG	NE-CZ-NH2	7.79	124.19	120.30
1	B	261	SER	C-N-CA	7.67	140.87	121.70
1	C	194	GLY	C-N-CA	-7.62	106.29	122.30
1	A	16	ARG	CD-NE-CZ	7.56	134.18	123.60
1	B	186	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	D	397	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	D	66	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	C	82	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	A	16	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	66	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	B	275	TYR	CB-CG-CD1	6.90	125.14	121.00
1	C	186	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	C	378	TYR	CB-CG-CD2	6.77	125.06	121.00
1	B	32	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	B	91	ARG	CD-NE-CZ	6.56	132.78	123.60
1	B	91	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	B	82	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	D	493	ARG	C-N-CA	6.40	137.70	121.70
1	A	190	TRP	CH2-CZ2-CE2	6.36	123.76	117.40
1	D	350	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	B	478	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	C	341	ARG	NE-CZ-NH2	6.27	123.43	120.30
1	D	327	ARG	CD-NE-CZ	6.20	132.29	123.60
1	A	196	GLY	C-N-CA	6.18	135.29	122.30
1	D	320	ARG	CD-NE-CZ	6.10	132.14	123.60
1	C	209	ARG	CD-NE-CZ	6.07	132.10	123.60
1	B	478	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	91	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	66	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	209	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	363	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	B	275	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	D	222	LEU	CA-CB-CG	5.90	128.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	487	ASP	CB-CG-OD1	5.90	123.61	118.30
1	D	171	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	C	197	GLY	C-N-CA	-5.87	109.97	122.30
1	A	82	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	B	166	VAL	C-N-CA	5.79	136.19	121.70
1	C	197	GLY	O-C-N	-5.78	113.38	123.20
1	D	17	VAL	C-N-CA	5.77	136.12	121.70
1	D	205	ARG	CD-NE-CZ	5.75	131.65	123.60
1	B	457	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	C	499	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	C	194	GLY	O-C-N	-5.63	113.63	123.20
1	B	341	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	C	327	ARG	CD-NE-CZ	5.60	131.44	123.60
1	C	162	GLU	CA-CB-CG	5.56	125.62	113.40
1	C	197	GLY	N-CA-C	5.55	126.98	113.10
1	B	183	ASP	CB-CG-OD1	5.52	123.27	118.30
1	D	472	TYR	CD1-CE1-CZ	5.50	124.75	119.80
1	C	353	TRP	CA-CB-CG	5.45	124.06	113.70
1	A	341	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	D	380	TYR	CB-CG-CD1	5.43	124.26	121.00
1	D	406	SER	C-N-CA	5.36	135.11	121.70
1	D	150	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	197	GLY	N-CA-C	5.28	126.30	113.10
1	D	264	GLY	C-N-CA	5.27	134.88	121.70
1	D	320	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	66	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	295	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	27	ARG	CD-NE-CZ	5.14	130.80	123.60
1	A	205	ARG	CD-NE-CZ	5.14	130.79	123.60
1	C	16	ARG	N-CA-C	5.14	124.87	111.00
1	D	295	ASP	CB-CG-OD2	5.13	122.91	118.30
1	B	150	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	B	262	ALA	C-N-CA	5.11	134.47	121.70
1	A	341	ARG	CD-NE-CZ	5.11	130.75	123.60
1	D	442	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	310	GLU	CA-CB-CG	5.10	124.63	113.40
1	B	253	HIS	CA-CB-CG	5.09	122.25	113.60
1	A	17	VAL	C-N-CA	5.07	134.38	121.70
1	D	66	ARG	CD-NE-CZ	5.07	130.70	123.60
1	D	450	TYR	CB-CG-CD2	5.07	124.04	121.00
1	C	15	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	D	353	TRP	CA-CB-CG	5.02	123.24	113.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	261	SER	Peptide
1	B	262	ALA	Peptide
1	B	263	ALA	Peptide
1	D	261	SER	Peptide

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	3836	0	3697	280	2
1	B	3823	0	3678	302	0
1	C	3828	0	3688	309	0
1	D	3823	0	3683	277	0
2	A	58	0	48	13	0
3	A	53	0	29	3	0
3	B	53	0	28	9	0
3	C	53	0	30	9	0
3	D	53	0	30	12	0
4	A	274	0	0	52	0
4	B	212	0	0	50	1
4	C	317	0	0	61	1
4	D	206	0	0	40	0
All	All	16589	0	14911	1146	2

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 38.

All (1146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:CYS:SG	3:C:801:FAD:H6	1.28	1.65
1:D:130:CYS:SG	3:D:801:FAD:H6	1.13	1.61
1:D:70:HIS:ND1	3:D:801:FAD:HM83	0.97	1.30
1:C:130:CYS:SG	3:C:801:FAD:C6	2.25	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:HIS:CE1	3:D:801:FAD:HM83	1.91	1.05
1:C:392:THR:HG21	1:C:397:ARG:HH21	1.23	1.02
1:D:392:THR:HG21	1:D:397:ARG:HH21	1.22	1.02
1:A:392:THR:HG21	1:A:397:ARG:HH21	1.25	1.01
1:A:392:THR:HG23	1:A:394:THR:H	1.23	1.00
1:B:263:ALA:HB3	1:B:382:GLY:HA2	1.41	0.98
1:D:193:THR:HG23	1:D:393:ALA:H	1.30	0.95
1:B:392:THR:HG21	1:B:397:ARG:HH21	1.31	0.95
1:C:193:THR:HG23	1:C:393:ALA:H	1.27	0.94
1:C:392:THR:HG23	1:C:394:THR:H	1.30	0.94
1:C:434:GLY:HA3	1:C:463:SER:HB2	1.48	0.94
1:B:193:THR:HG23	1:B:393:ALA:H	1.34	0.93
1:C:291:ASP:HB3	1:C:294:LEU:HD23	1.48	0.92
1:D:231:ARG:HH12	1:D:289:GLN:HE21	1.16	0.91
1:C:178:THR:HG23	1:C:180:ALA:H	1.35	0.91
1:C:290:ILE:HG12	1:C:294:LEU:HD21	1.50	0.91
1:A:65:VAL:HG22	1:A:85:ILE:HD11	1.53	0.90
1:A:193:THR:HG23	1:A:393:ALA:H	1.34	0.90
1:B:392:THR:HG23	1:B:394:THR:H	1.36	0.90
1:C:436:VAL:HG13	1:C:461:ASN:HB3	1.54	0.89
1:B:65:VAL:HG22	1:B:85:ILE:HD11	1.55	0.89
1:A:354:THR:H	1:A:357:GLN:HE21	1.21	0.87
1:D:342:THR:HG22	1:D:408:THR:HG23	1.53	0.87
1:D:288:ILE:HD11	1:D:301:LEU:HG	1.56	0.86
1:C:354:THR:H	1:C:357:GLN:HE21	1.24	0.86
1:A:354:THR:HG23	1:A:357:GLN:H	1.38	0.85
1:C:251:ASP:HA	4:C:945:HOH:O	1.76	0.85
1:D:392:THR:HG23	1:D:394:THR:H	1.40	0.85
1:B:354:THR:H	1:B:357:GLN:HE21	1.24	0.85
1:B:24:LEU:HG	1:B:40:VAL:HG11	1.57	0.85
1:A:130:CYS:HB2	1:A:133:VAL:HG23	1.59	0.85
1:D:312:THR:HG22	1:D:314:VAL:HG13	1.58	0.85
1:B:195:GLY:HA3	1:B:472:TYR:HE1	1.40	0.84
1:B:300:LEU:HA	1:B:303:ASP:HB2	1.58	0.84
1:A:333:LYS:HB2	4:A:957:HOH:O	1.78	0.84
1:A:178:THR:HG23	1:A:180:ALA:H	1.40	0.84
1:B:109:THR:HG22	1:B:112:GLU:H	1.43	0.83
1:C:203:VAL:HG22	3:C:801:FAD:N6A	1.92	0.83
1:B:195:GLY:HA2	1:B:448:ILE:HG13	1.61	0.83
1:B:178:THR:HG23	1:B:180:ALA:H	1.42	0.82
1:B:354:THR:HG23	1:B:357:GLN:H	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ILE:HB	4:B:957:HOH:O	1.80	0.82
1:D:257:HIS:O	1:D:261:SER:HB2	1.78	0.82
1:C:19:ARG:HH22	1:D:224:LYS:HB3	1.43	0.81
1:C:162:GLU:HG3	1:C:205:ARG:HB3	1.63	0.81
1:C:203:VAL:HG13	3:C:801:FAD:N1A	1.96	0.80
1:A:190:TRP:O	1:A:193:THR:HG22	1.83	0.79
1:A:233:ILE:HG23	1:A:319:GLN:HB2	1.64	0.79
1:C:129:VAL:HG22	1:C:146:PRO:HD3	1.62	0.79
1:B:51:ASP:O	1:B:55:GLN:HG3	1.83	0.79
1:D:396:GLN:H	1:D:396:GLN:HE21	1.31	0.78
1:B:425:ILE:O	1:B:429:ILE:HG23	1.83	0.78
1:A:290:ILE:HD13	1:A:300:LEU:HD13	1.64	0.78
1:A:84:VAL:HG23	4:A:960:HOH:O	1.83	0.78
1:A:392:THR:HG22	4:A:822:HOH:O	1.83	0.78
1:B:17:VAL:HA	4:B:884:HOH:O	1.82	0.78
1:B:226:PRO:HB3	1:B:291:ASP:HB2	1.64	0.78
1:B:400:ILE:HG13	1:B:401:ILE:HG13	1.66	0.78
1:C:14:VAL:HG11	4:C:1046:HOH:O	1.83	0.78
1:A:244:GLU:HG2	4:A:1042:HOH:O	1.84	0.77
1:B:385:ASN:HB3	1:B:397:ARG:O	1.84	0.77
1:B:241:LEU:HD13	1:B:246:PHE:HD1	1.49	0.77
1:A:448:ILE:HG23	4:A:858:HOH:O	1.83	0.77
1:D:190:TRP:O	1:D:193:THR:HG22	1.83	0.77
1:D:365:LEU:HB2	4:D:945:HOH:O	1.83	0.77
1:B:448:ILE:HG23	4:B:878:HOH:O	1.85	0.77
1:B:93:VAL:HG11	4:B:937:HOH:O	1.84	0.76
1:D:296:GLY:O	1:D:300:LEU:HG	1.86	0.76
1:D:381:GLY:O	1:D:384:VAL:HG12	1.86	0.76
1:B:190:TRP:O	1:B:193:THR:HG22	1.86	0.76
1:C:381:GLY:O	1:C:384:VAL:HG12	1.86	0.76
1:B:12:VAL:HG21	4:B:816:HOH:O	1.86	0.76
1:B:116:ALA:HB3	4:B:937:HOH:O	1.85	0.75
1:C:109:THR:O	1:C:113:THR:HG23	1.86	0.75
1:D:17:VAL:HG12	4:D:963:HOH:O	1.86	0.75
1:A:381:GLY:O	1:A:384:VAL:HG12	1.86	0.75
1:C:16:ARG:HB2	4:C:895:HOH:O	1.85	0.75
1:D:162:GLU:HG2	4:D:899:HOH:O	1.86	0.75
1:C:65:VAL:HG22	1:C:85:ILE:HD11	1.69	0.75
1:B:232:HIS:O	1:B:288:ILE:HG23	1.86	0.74
1:B:248:ARG:HB3	4:B:948:HOH:O	1.86	0.74
1:A:24:LEU:HD11	1:B:119:LEU:HD22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:THR:HG22	1:A:357:GLN:HE21	1.53	0.74
1:A:312:THR:HG22	1:A:314:VAL:H	1.53	0.74
1:B:178:THR:HG22	1:B:183:ASP:OD2	1.87	0.74
1:A:477:PRO:HD2	4:A:1056:HOH:O	1.87	0.74
1:B:462:THR:HG22	1:B:465:VAL:O	1.88	0.74
1:C:263:ALA:HB3	1:C:268:ALA:HB2	1.70	0.74
1:C:212:GLY:HA3	4:C:881:HOH:O	1.88	0.73
1:B:141:GLY:O	1:B:448:ILE:HD11	1.88	0.73
1:D:242:THR:HG21	4:D:995:HOH:O	1.86	0.73
1:C:424:GLU:HB3	4:C:1003:HOH:O	1.86	0.73
1:B:350:ARG:HD3	1:B:441:ASP:O	1.89	0.73
1:C:224:LYS:HB2	4:C:812:HOH:O	1.88	0.73
1:A:103:ALA:HA	4:A:993:HOH:O	1.87	0.73
1:C:16:ARG:HD2	1:C:17:VAL:HG13	1.70	0.73
1:C:89:GLN:OE1	1:D:119:LEU:HB2	1.88	0.73
1:C:425:ILE:HB	4:C:1025:HOH:O	1.89	0.73
1:A:89:GLN:HE22	1:B:116:ALA:HA	1.54	0.73
1:C:190:TRP:O	1:C:193:THR:HG22	1.89	0.73
1:A:124:THR:HG23	4:A:820:HOH:O	1.87	0.73
1:B:65:VAL:HA	1:B:85:ILE:HG12	1.69	0.73
1:D:40:VAL:HG22	1:D:84:VAL:HG13	1.71	0.73
1:A:65:VAL:HG21	1:A:202:ILE:HG12	1.70	0.73
1:B:25:VAL:HG23	4:B:930:HOH:O	1.88	0.72
1:D:25:VAL:HG23	4:D:853:HOH:O	1.90	0.72
1:D:371:VAL:HB	1:D:418:ASN:ND2	2.03	0.72
1:B:381:GLY:O	1:B:384:VAL:HG12	1.90	0.72
1:C:396:GLN:HA	1:C:444:GLU:OE2	1.89	0.72
1:C:51:ASP:O	1:C:55:GLN:HG3	1.88	0.72
1:D:354:THR:H	1:D:357:GLN:HE21	1.37	0.72
1:A:360:THR:HG23	1:A:428:GLU:OE2	1.90	0.72
1:A:404:TRP:CD2	2:A:601[A]:AKY:H413	2.24	0.72
1:C:89:GLN:HA	1:D:115:ARG:HH22	1.53	0.72
1:C:247:THR:HG21	1:C:248:ARG:HH11	1.55	0.72
1:B:345:LYS:HG3	1:B:405:MET:HB2	1.71	0.72
1:D:341:ARG:NH1	1:D:412:PRO:HB3	2.05	0.72
1:C:233:ILE:HG13	1:C:285:LEU:HD21	1.71	0.71
1:C:394:THR:HG22	4:C:1006:HOH:O	1.90	0.71
1:A:149:ARG:NH2	1:A:270:MET:HB3	2.06	0.71
1:A:297:ALA:HA	1:A:300:LEU:HD11	1.71	0.71
1:D:242:THR:HB	4:D:941:HOH:O	1.90	0.71
1:C:312:THR:HG22	1:C:314:VAL:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.55	0.71
1:D:143:GLY:O	1:D:153:VAL:HG13	1.91	0.71
1:C:444:GLU:OE2	1:C:473:LYS:HE2	1.91	0.71
1:D:178:THR:HG23	1:D:180:ALA:H	1.55	0.71
1:C:167:ASP:HB2	1:C:171:ARG:H	1.55	0.71
1:A:297:ALA:O	1:A:300:LEU:HD12	1.90	0.70
1:B:297:ALA:O	1:B:300:LEU:HD12	1.91	0.70
1:C:140:LEU:HD23	1:C:203:VAL:HG11	1.71	0.70
1:A:494:HIS:O	1:A:497:SER:HB2	1.92	0.70
1:A:207:TRP:HA	4:A:993:HOH:O	1.90	0.70
1:C:392:THR:HG22	4:C:818:HOH:O	1.90	0.70
1:C:419:LEU:HB3	1:C:423:ARG:NH1	2.07	0.70
1:C:442:ARG:HG3	4:C:844:HOH:O	1.92	0.70
1:B:263:ALA:CB	1:B:382:GLY:HA2	2.18	0.70
1:A:193:THR:O	1:A:394:THR:HG23	1.91	0.69
1:C:31:GLY:HA2	1:C:34:ARG:NH2	2.07	0.69
1:A:432:THR:HG23	4:A:1027:HOH:O	1.92	0.69
1:D:244:GLU:O	1:D:248:ARG:HG2	1.92	0.69
1:C:203:VAL:HG22	3:C:801:FAD:H62A	1.58	0.69
1:B:137:GLY:HA3	3:B:801:FAD:H51A	1.75	0.69
1:D:384:VAL:HG13	1:D:385:ASN:OD1	1.92	0.69
1:D:427:ARG:HB2	4:D:942:HOH:O	1.93	0.69
1:A:93:VAL:HG13	1:A:104:VAL:HG12	1.76	0.68
1:A:460:TRP:HB3	1:A:461:ASN:OD1	1.93	0.68
1:C:14:VAL:HA	4:C:1033:HOH:O	1.91	0.68
1:C:178:THR:HG22	1:C:183:ASP:OD2	1.92	0.68
1:D:123:VAL:HG13	1:D:223:PRO:O	1.94	0.68
1:A:261:SER:HB2	4:A:826:HOH:O	1.92	0.68
1:A:354:THR:HG22	1:A:357:GLN:NE2	2.09	0.68
1:B:263:ALA:HB1	1:B:268:ALA:HB2	1.73	0.68
1:D:187:GLU:OE1	1:D:478:ARG:HD3	1.93	0.68
1:D:127:ALA:O	1:D:145:GLY:HA3	1.92	0.68
1:A:115:ARG:HH12	1:B:89:GLN:NE2	1.91	0.68
1:A:343:LYS:HE2	4:A:922:HOH:O	1.93	0.68
1:A:497:SER:HA	4:A:982:HOH:O	1.94	0.68
1:C:220:GLN:OE1	4:C:872:HOH:O	2.12	0.68
1:B:129:VAL:HG22	1:B:146:PRO:HD3	1.76	0.67
1:B:333:LYS:HA	4:B:978:HOH:O	1.93	0.67
1:D:114:TYR:OH	1:D:127:ALA:HB3	1.94	0.67
1:A:12:VAL:HG13	4:A:1040:HOH:O	1.93	0.67
1:A:366:SER:HA	4:A:916:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:THR:HG22	1:B:357:GLN:HE21	1.58	0.67
1:B:297:ALA:HA	1:B:300:LEU:HD11	1.75	0.67
1:D:108:ALA:O	1:D:135:VAL:HG23	1.95	0.67
1:A:66:ARG:HG3	4:A:985:HOH:O	1.93	0.67
1:C:119:LEU:HD22	1:D:24:LEU:HD11	1.77	0.67
1:C:212:GLY:HA2	4:C:969:HOH:O	1.95	0.67
1:C:231:ARG:HD3	1:C:287:ASP:OD2	1.94	0.67
1:C:232:HIS:HB2	1:C:288:ILE:HG12	1.77	0.67
1:D:352:PRO:HA	4:D:993:HOH:O	1.92	0.67
1:A:32:ARG:HG2	1:A:341:ARG:HH21	1.59	0.67
1:A:392:THR:HG23	1:A:394:THR:N	2.04	0.67
1:C:312:THR:HG22	1:C:314:VAL:HG13	1.76	0.67
1:C:493:ARG:HB3	4:C:1078:HOH:O	1.95	0.67
1:B:452:ASP:HA	4:B:952:HOH:O	1.94	0.66
1:C:121:TRP:HB2	1:C:123:VAL:HG23	1.77	0.66
1:B:138:HIS:HB2	3:B:801:FAD:H4'	1.78	0.66
1:C:233:ILE:HD11	1:C:285:LEU:HD11	1.78	0.66
3:A:801:FAD:O2A	4:A:985:HOH:O	2.12	0.66
1:A:147:LEU:HD22	1:A:150:ARG:HD3	1.78	0.66
1:C:297:ALA:HA	1:C:300:LEU:HD11	1.77	0.66
1:D:231:ARG:HH12	1:D:289:GLN:NE2	1.92	0.66
1:B:65:VAL:HG21	1:B:202:ILE:HG12	1.78	0.65
1:A:444:GLU:HG2	1:A:473:LYS:NZ	2.12	0.65
1:B:426:TYR:O	1:B:429:ILE:HD13	1.97	0.65
1:C:244:GLU:HG2	1:C:248:ARG:HH22	1.60	0.65
1:C:184:PRO:HB2	4:C:980:HOH:O	1.96	0.65
1:A:133:VAL:HG13	3:A:801:FAD:H5'2	1.77	0.65
1:B:443:THR:HG21	4:B:961:HOH:O	1.97	0.65
1:A:32:ARG:HA	1:A:341:ARG:NH2	2.11	0.65
1:C:422:ILE:HD12	1:C:423:ARG:N	2.12	0.65
1:A:350[B]:ARG:HH11	1:A:441:ASP:HA	1.61	0.65
1:A:441:ASP:HB3	4:A:1006:HOH:O	1.97	0.65
1:B:150:ARG:O	1:B:383:LYS:HE2	1.96	0.65
1:B:431:ALA:HA	4:B:934:HOH:O	1.97	0.65
1:D:392:THR:HG21	1:D:397:ARG:NH2	2.04	0.65
1:A:436:VAL:HG13	1:A:462:THR:H	1.61	0.64
1:B:437:PRO:O	1:B:445:GLY:HA2	1.97	0.64
1:D:16:ARG:NE	1:D:17:VAL:H	1.95	0.64
1:A:279:ARG:HB2	4:A:916:HOH:O	1.96	0.64
1:A:288:ILE:HD11	1:A:301:LEU:HG	1.80	0.64
1:B:96:ASP:HA	4:B:855:HOH:O	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:VAL:HG21	1:C:202:ILE:HG12	1.78	0.64
1:D:297:ALA:HA	1:D:300:LEU:HD11	1.78	0.64
1:D:68:GLY:HA3	3:D:801:FAD:O2P	1.97	0.64
1:B:124:THR:HG22	1:B:125:ILE:H	1.62	0.64
1:C:203:VAL:HB	4:C:1015:HOH:O	1.96	0.64
1:D:396:GLN:H	1:D:396:GLN:NE2	1.96	0.64
1:A:42:VAL:HG11	4:B:896:HOH:O	1.97	0.64
1:D:15:ASP:OD1	1:D:20:ARG:HB2	1.97	0.64
1:D:70:HIS:HB2	3:D:801:FAD:H5'1	1.79	0.64
1:B:121:TRP:O	1:B:123:VAL:HG23	1.97	0.64
1:D:32:ARG:HG2	1:D:341:ARG:HD3	1.78	0.64
1:B:354:THR:H	1:B:357:GLN:NE2	1.95	0.64
1:C:150:ARG:O	1:C:383:LYS:HE3	1.97	0.64
1:C:244:GLU:O	1:C:248:ARG:HG2	1.97	0.63
1:D:144:TYR:CE1	1:D:402:LYS:HE3	2.33	0.63
1:C:433:THR:HG22	1:C:436:VAL:O	1.98	0.63
1:B:400:ILE:HD11	4:B:953:HOH:O	1.97	0.63
1:C:220:GLN:HG2	4:C:905:HOH:O	1.98	0.63
1:C:350:ARG:NH1	1:C:444:GLU:HG2	2.13	0.63
1:B:188:LEU:HG	1:B:486:TRP:CD2	2.34	0.63
1:D:261:SER:HB3	1:D:400:ILE:HG22	1.79	0.63
1:A:178:THR:HG22	1:A:183:ASP:OD2	1.97	0.63
1:B:92:GLN:HB2	1:B:105:GLU:OE1	1.99	0.63
1:B:238:TRP:CD1	1:B:279:ARG:HA	2.34	0.63
1:B:288:ILE:HD11	1:B:301:LEU:HG	1.81	0.63
1:D:380:TYR:CE2	1:D:402:LYS:HE2	2.33	0.63
1:C:302:ASN:HA	1:C:305:VAL:HG22	1.80	0.62
1:A:186:ARG:HH12	1:A:190:TRP:HZ3	1.45	0.62
1:A:242:THR:HG22	4:A:1042:HOH:O	1.99	0.62
1:B:436:VAL:HG13	1:B:461:ASN:HB3	1.81	0.62
1:B:436:VAL:HG13	1:B:462:THR:H	1.63	0.62
1:C:130:CYS:CB	3:C:801:FAD:H6	2.28	0.62
1:D:216:THR:O	1:D:218:PRO:HD3	1.99	0.62
1:D:263:ALA:HB1	1:D:265:THR:OG1	1.99	0.62
1:D:436:VAL:HG22	4:D:950:HOH:O	1.99	0.62
1:B:233:ILE:HG23	1:B:319:GLN:HB2	1.79	0.62
1:D:150:ARG:NH2	1:D:226:PRO:HG3	2.14	0.62
1:C:359:ALA:O	1:C:363:ARG:HG3	1.99	0.62
1:B:245:ALA:HB1	1:B:312:THR:HG23	1.82	0.62
1:C:83:ALA:HB1	4:C:1011:HOH:O	1.99	0.62
1:C:155:ALA:HB1	1:C:193:THR:OG1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:LEU:O	1:C:462:THR:HG21	2.00	0.62
1:D:25:VAL:HG21	1:D:35:GLY:O	2.00	0.62
1:D:31:GLY:HA3	1:D:340:ASP:OD1	1.99	0.62
1:D:150:ARG:O	1:D:383:LYS:HD2	2.00	0.62
1:A:373:GLY:HA3	1:A:421:TRP:CZ2	2.35	0.61
1:D:109:THR:HG22	1:D:112:GLU:HG3	1.82	0.61
1:D:124:THR:HG22	1:D:125:ILE:H	1.65	0.61
1:A:149:ARG:HD3	4:A:892:HOH:O	1.99	0.61
1:C:19:ARG:NH2	1:D:224:LYS:HB3	2.13	0.61
1:C:363:ARG:HB2	4:C:853:HOH:O	1.99	0.61
1:D:483:LYS:HD2	1:D:487:ASP:HB3	1.81	0.61
1:C:25:VAL:HG21	1:C:35:GLY:O	2.00	0.61
1:C:123:VAL:HG11	1:C:222:LEU:HB2	1.83	0.61
1:B:448:ILE:HD12	4:B:938:HOH:O	2.00	0.61
1:C:425:ILE:HD12	4:C:1025:HOH:O	2.00	0.61
1:D:150:ARG:HB2	4:D:836:HOH:O	2.01	0.61
1:A:167:ASP:HB2	1:A:171:ARG:H	1.66	0.61
1:B:18:ASP:OD2	1:B:20:ARG:HB2	2.00	0.61
1:D:16:ARG:HD2	1:D:17:VAL:HG13	1.83	0.61
1:A:109:THR:HG22	1:A:112:GLU:H	1.65	0.61
1:B:276:LEU:HD11	1:B:377:LEU:HD11	1.83	0.61
1:D:195:GLY:H	1:D:448:ILE:HD11	1.64	0.61
1:D:362:TYR:HA	4:D:945:HOH:O	2.00	0.60
1:A:124:THR:HG22	1:A:125:ILE:H	1.65	0.60
1:A:198:GLY:H	1:A:494:HIS:HE1	1.48	0.60
1:D:201:GLY:HA2	1:D:492:PHE:CE1	2.36	0.60
1:B:316:PRO:HG2	4:B:919:HOH:O	1.99	0.60
1:C:291:ASP:O	1:C:294:LEU:HG	2.00	0.60
1:B:422:ILE:HD12	1:B:423:ARG:N	2.16	0.60
1:C:388:PRO:HG3	4:C:832:HOH:O	2.00	0.60
1:D:84:VAL:HG11	4:D:975:HOH:O	2.01	0.60
1:A:336:THR:HA	2:A:601[A]:AKY:H503	1.84	0.60
1:D:188:LEU:HG	1:D:486:TRP:CD2	2.36	0.60
1:D:246:PHE:O	1:D:249:ILE:HB	2.02	0.60
1:C:345:LYS:HB2	1:C:426:TYR:CE2	2.35	0.60
1:B:478:ARG:HB2	4:B:834:HOH:O	2.02	0.60
1:B:480:GLN:HB3	1:B:501:PRO:HG3	1.84	0.60
1:C:199:ASN:ND2	1:C:498:VAL:HG22	2.16	0.60
1:D:84:VAL:HG21	4:D:975:HOH:O	2.02	0.60
1:D:195:GLY:HA2	1:D:472:TYR:HE1	1.66	0.60
1:D:231:ARG:HD3	1:D:287:ASP:OD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:421:TRP:CD1	1:D:422:ILE:HG23	2.37	0.60
1:D:150:ARG:HH22	1:D:226:PRO:HG3	1.67	0.59
1:B:155:ALA:HB1	1:B:193:THR:OG1	2.02	0.59
1:D:99:LYS:HE3	1:D:207:TRP:CD1	2.37	0.59
1:B:348:TYR:CE1	1:B:402:LYS:HD3	2.37	0.59
1:D:103:ALA:HB2	1:D:207:TRP:CZ3	2.37	0.59
1:D:375:VAL:HG22	1:D:405:MET:HG2	1.84	0.59
1:A:290:ILE:HG21	1:A:301:LEU:HD11	1.83	0.59
1:A:384:VAL:O	1:A:397:ARG:HD2	2.02	0.59
1:C:150:ARG:HD2	1:C:151:ASP:OD1	2.02	0.59
1:C:233:ILE:HG23	1:C:319:GLN:HG3	1.83	0.59
1:A:433:THR:HG21	1:A:436:VAL:O	2.03	0.59
1:B:109:THR:CG2	1:B:112:GLU:H	2.16	0.59
1:C:396:GLN:H	1:C:396:GLN:HE21	1.47	0.59
1:B:354:THR:HG22	1:B:357:GLN:NE2	2.16	0.59
1:B:411:ASP:OD2	1:B:413:ALA:HB3	2.02	0.59
1:D:22:GLN:O	1:D:26:THR:HG23	2.03	0.59
1:D:133:VAL:HG13	3:D:801:FAD:H5'2	1.85	0.59
1:B:252:ASN:HB3	1:B:307:ALA:O	2.02	0.59
1:C:421:TRP:O	1:C:425:ILE:HG13	2.02	0.59
1:C:67:SER:HA	4:C:1000:HOH:O	2.02	0.59
1:C:297:ALA:O	1:C:300:LEU:HD12	2.03	0.59
1:A:45:THR:OG1	1:A:48:GLN:HG3	2.03	0.59
1:B:436:VAL:CG1	1:B:461:ASN:HB3	2.32	0.59
1:C:32:ARG:HD2	4:C:862:HOH:O	2.02	0.59
1:A:354:THR:H	1:A:357:GLN:NE2	1.97	0.58
1:D:85:ILE:HG12	1:D:85:ILE:O	2.03	0.58
1:A:411:ASP:OD2	1:A:413:ALA:HB3	2.04	0.58
1:A:446:THR:HG23	1:A:471:TYR:CE2	2.37	0.58
1:B:199:ASN:HB2	1:B:498:VAL:HG22	1.84	0.58
1:A:91:ARG:HB3	1:A:108:ALA:HA	1.85	0.58
1:A:123:VAL:HG13	1:A:223:PRO:O	2.03	0.58
1:A:297:ALA:O	1:A:301:LEU:HD13	2.04	0.58
1:B:226:PRO:HB3	1:B:291:ASP:CB	2.34	0.58
1:A:141:GLY:O	1:A:448:ILE:HD11	2.03	0.58
1:C:421:TRP:NE1	1:C:425:ILE:HD11	2.19	0.58
1:C:12:VAL:HB	4:C:1068:HOH:O	2.03	0.58
1:B:21:TYR:HB2	4:B:927:HOH:O	2.03	0.58
1:C:429:ILE:O	1:C:429:ILE:HG12	2.04	0.58
1:D:16:ARG:CZ	1:D:17:VAL:HG22	2.34	0.58
1:D:345:LYS:HD3	1:D:426:TYR:CG	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:478:ARG:O	1:D:482:VAL:HG23	2.04	0.58
1:D:455:LEU:O	1:D:462:THR:HG21	2.04	0.58
1:B:123:VAL:HG11	1:B:222:LEU:HB2	1.85	0.58
1:C:131:PRO:HG3	4:C:1057:HOH:O	2.04	0.58
1:C:312:THR:CG2	1:C:314:VAL:HG13	2.34	0.58
1:D:191:ALA:HB2	1:D:482:VAL:HG11	1.86	0.58
1:C:290:ILE:CG1	1:C:294:LEU:HD21	2.31	0.57
1:D:195:GLY:HA2	1:D:472:TYR:CE1	2.38	0.57
1:B:244:GLU:O	1:B:248:ARG:HG2	2.04	0.57
1:D:40:VAL:HG22	1:D:84:VAL:CG1	2.34	0.57
1:B:354:THR:N	1:B:357:GLN:HE21	2.00	0.57
1:A:65:VAL:HG13	1:A:85:ILE:HG12	1.87	0.57
1:B:201:GLY:HA2	1:B:492:PHE:CD1	2.40	0.57
1:C:24:LEU:HB3	1:C:40:VAL:HG21	1.87	0.57
1:C:288:ILE:CD1	1:C:301:LEU:HG	2.34	0.57
1:C:14:VAL:HG13	1:C:39:VAL:HG21	1.86	0.57
1:A:109:THR:CG2	1:A:112:GLU:H	2.18	0.57
1:B:419:LEU:O	1:B:423:ARG:HG3	2.05	0.57
1:D:423:ARG:HD3	1:D:460:TRP:CZ2	2.40	0.57
1:C:294:LEU:HD11	1:C:300:LEU:HD11	1.87	0.56
1:C:103:ALA:HB2	1:C:207:TRP:CZ3	2.40	0.56
1:A:350[B]:ARG:NH1	1:A:441:ASP:HA	2.21	0.56
1:A:433:THR:HG21	1:A:438:VAL:HG23	1.87	0.56
1:D:294:LEU:HD12	1:D:297:ALA:HB2	1.87	0.56
1:D:65:VAL:HG23	4:D:949:HOH:O	2.06	0.56
1:C:115:ARG:HB2	1:C:326:LEU:HD21	1.87	0.56
1:C:389:GLU:OE2	1:C:473:LYS:HE3	2.06	0.56
1:A:16:ARG:HG3	1:A:17:VAL:N	2.20	0.56
1:C:103:ALA:HB1	1:C:205:ARG:HD3	1.87	0.56
1:C:456:VAL:HG12	4:C:1056:HOH:O	2.05	0.56
1:A:248:ARG:HD3	4:A:967:HOH:O	2.06	0.56
1:C:244:GLU:HB2	4:C:804:HOH:O	2.06	0.56
1:D:178:THR:HG22	1:D:183:ASP:OD2	2.05	0.56
3:B:801:FAD:H2'	3:B:801:FAD:H9	1.88	0.56
1:D:130:CYS:CB	3:D:801:FAD:C6	2.84	0.56
1:A:140:LEU:HD21	1:A:197:GLY:HA2	1.88	0.56
1:A:389:GLU:OE2	1:A:473:LYS:HE2	2.05	0.56
1:B:233:ILE:HD11	1:B:285:LEU:HD11	1.88	0.56
1:C:109:THR:HG22	1:C:112:GLU:H	1.70	0.56
1:D:96:ASP:HB3	1:D:207:TRP:CZ3	2.40	0.56
1:D:494:HIS:O	1:D:497:SER:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ASP:HA	4:B:862:HOH:O	2.05	0.56
1:C:299:ALA:HA	1:C:302:ASN:OD1	2.05	0.56
1:D:81:VAL:HB	4:D:948:HOH:O	2.05	0.56
1:B:254:GLY:HA2	4:B:953:HOH:O	2.05	0.55
1:B:436:VAL:CG1	1:B:462:THR:H	2.18	0.55
1:B:360:THR:CG2	1:B:429:ILE:HG22	2.37	0.55
1:C:201:GLY:HA2	1:C:492:PHE:CE1	2.41	0.55
1:B:161:VAL:HG23	1:B:203:VAL:HG13	1.89	0.55
1:C:147:LEU:HA	4:C:939:HOH:O	2.05	0.55
1:C:22:GLN:O	1:C:26:THR:HG23	2.07	0.55
1:D:228:SER:HB2	1:D:323:GLU:O	2.06	0.55
1:D:238:TRP:HH2	4:D:945:HOH:O	1.88	0.55
1:A:122:GLY:O	1:A:224:LYS:HG3	2.05	0.55
1:B:18:ASP:HB2	4:B:815:HOH:O	2.05	0.55
1:B:301:LEU:O	1:B:305:VAL:HG13	2.06	0.55
1:B:432:THR:HG22	4:B:935:HOH:O	2.06	0.55
1:C:115:ARG:HE	1:D:91:ARG:NH2	2.04	0.55
1:C:201:GLY:HA2	1:C:492:PHE:CD1	2.42	0.55
1:C:364:HIS:CG	1:C:425:ILE:HG23	2.42	0.55
1:A:190:TRP:HZ2	1:A:390:THR:O	1.88	0.55
1:B:407:ALA:HB2	1:B:422:ILE:HG23	1.89	0.55
1:C:300:LEU:O	1:C:303:ASP:HB2	2.06	0.55
1:A:147:LEU:HD22	1:A:150:ARG:CD	2.36	0.55
2:A:601[A]:AKY:H141	4:A:1060:HOH:O	2.06	0.55
1:B:95:TYR:CE2	1:B:218:PRO:HG3	2.42	0.55
1:A:95:TYR:CE2	1:A:218:PRO:HG3	2.42	0.55
1:B:140:LEU:HD22	1:B:196:GLY:HA3	1.88	0.55
1:B:158:LEU:HD13	1:B:208:PHE:CE2	2.42	0.55
1:B:161:VAL:CG2	1:B:203:VAL:HG13	2.37	0.55
1:C:167:ASP:OD2	1:C:173:ARG:HD3	2.06	0.55
1:B:103:ALA:HB1	1:B:205:ARG:HD2	1.89	0.55
1:B:124:THR:HG23	4:B:936:HOH:O	2.07	0.55
1:A:243:GLU:HG3	1:A:362:TYR:CD2	2.42	0.55
1:B:323:GLU:HB2	1:B:328:ALA:HB2	1.89	0.55
1:D:267:TYR:CE1	1:D:300:LEU:HB2	2.42	0.54
1:B:27:ARG:HG2	1:B:27:ARG:HH21	1.71	0.54
1:B:140:LEU:H	1:B:140:LEU:HD12	1.72	0.54
1:B:392:THR:HG21	1:B:397:ARG:NH2	2.14	0.54
1:B:392:THR:CG2	1:B:394:THR:H	2.15	0.54
1:D:195:GLY:H	1:D:448:ILE:CD1	2.20	0.54
1:B:30:ASN:HD21	1:B:32:ARG:HG3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:TRP:CD2	1:B:279:ARG:HG3	2.42	0.54
1:D:448:ILE:HG21	1:D:472:TYR:CE1	2.42	0.54
1:B:100:ARG:HD2	1:B:215:GLY:O	2.07	0.54
1:B:201:GLY:HA2	1:B:492:PHE:CE1	2.42	0.54
1:C:400:ILE:HG13	1:C:401:ILE:HG13	1.89	0.54
1:D:431:ALA:O	1:D:432:THR:HG22	2.07	0.54
1:B:291:ASP:O	1:B:294:LEU:HG	2.07	0.54
1:D:193:THR:O	1:D:394:THR:HG23	2.07	0.54
1:B:354:THR:CG2	1:B:357:GLN:H	2.17	0.54
1:C:195:GLY:HA2	1:C:472:TYR:CE1	2.42	0.54
1:D:17:VAL:HA	4:D:936:HOH:O	2.07	0.54
1:B:363:ARG:O	1:B:367:ALA:HB2	2.06	0.54
1:C:41:TYR:HA	4:C:1033:HOH:O	2.08	0.54
1:D:297:ALA:O	1:D:300:LEU:HD12	2.07	0.54
1:B:300:LEU:CA	1:B:303:ASP:HB2	2.35	0.54
1:C:65:VAL:HG22	1:C:85:ILE:CD1	2.38	0.54
1:A:17:VAL:HG23	1:A:17:VAL:O	2.06	0.54
1:A:404:TRP:CD2	2:A:601[A]:AKY:C41	2.91	0.54
1:B:146:PRO:HA	1:B:271:HIS:CG	2.42	0.54
1:A:40:VAL:HG13	1:A:84:VAL:HG22	1.90	0.54
1:A:423:ARG:HD3	1:A:460:TRP:CZ2	2.43	0.54
1:B:233:ILE:CG2	1:B:319:GLN:HB2	2.38	0.54
1:B:447:PHE:CE2	1:B:449:ASN:HB2	2.43	0.54
1:B:113:THR:HA	4:B:937:HOH:O	2.08	0.53
1:B:249:ILE:HG12	4:B:963:HOH:O	2.06	0.53
1:C:263:ALA:HB1	1:C:265:THR:OG1	2.08	0.53
1:A:144:TYR:CE2	1:A:402:LYS:HE3	2.43	0.53
1:B:15:ASP:HB3	1:B:18:ASP:OD2	2.09	0.53
1:B:396:GLN:H	1:B:396:GLN:HE21	1.57	0.53
1:A:191:ALA:HB2	1:A:482:VAL:HG11	1.88	0.53
1:B:40:VAL:HG22	1:B:84:VAL:CG1	2.39	0.53
1:D:14:VAL:HG22	1:D:41:TYR:CD1	2.42	0.53
1:A:138:HIS:CE1	1:A:143:GLY:HA3	2.42	0.53
1:B:123:VAL:HG13	1:B:223:PRO:O	2.07	0.53
1:B:422:ILE:HD12	1:B:423:ARG:HG2	1.90	0.53
1:A:129:VAL:HG12	1:A:334:PHE:HZ	1.73	0.53
1:A:342:THR:HG22	1:A:408:THR:HG23	1.90	0.53
1:B:249:ILE:HA	4:B:963:HOH:O	2.07	0.53
1:C:143:GLY:O	1:C:153:VAL:HG13	2.08	0.53
1:B:112:GLU:O	1:B:115:ARG:HG2	2.07	0.53
1:B:245:ALA:HA	1:B:248:ARG:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:VAL:HG23	1:C:17:VAL:O	2.09	0.53
1:C:124:THR:HG22	1:C:125:ILE:H	1.74	0.53
1:D:123:VAL:HG11	1:D:222:LEU:HB2	1.91	0.53
1:D:419:LEU:HA	1:D:422:ILE:HD11	1.91	0.53
1:B:249:ILE:HG23	4:B:963:HOH:O	2.07	0.53
1:D:302:ASN:HA	1:D:305:VAL:HG22	1.90	0.53
1:A:123:VAL:CG1	1:A:222:LEU:HB2	2.38	0.53
1:A:174:LYS:NZ	1:A:174:LYS:HB3	2.17	0.53
1:A:233:ILE:CG2	1:A:319:GLN:HB2	2.36	0.53
1:C:16:ARG:CD	1:C:17:VAL:HG13	2.37	0.53
1:C:364:HIS:O	1:C:421:TRP:HZ2	1.90	0.53
1:D:254:GLY:HA2	4:D:993:HOH:O	2.08	0.53
1:A:273:VAL:HG22	1:A:378:TYR:CD2	2.43	0.53
1:C:432:THR:HG23	4:C:1010:HOH:O	2.08	0.53
1:C:109:THR:HG22	1:C:112:GLU:HB2	1.91	0.53
1:C:115:ARG:HH12	1:C:119:LEU:HD12	1.73	0.53
1:C:422:ILE:HD12	1:C:423:ARG:HG3	1.89	0.53
1:A:407:ALA:HB2	1:A:421:TRP:HD1	1.74	0.52
3:B:801:FAD:H5'1	4:B:837:HOH:O	2.09	0.52
1:C:123:VAL:HG12	1:C:223:PRO:O	2.09	0.52
1:D:174:LYS:HD3	4:D:899:HOH:O	2.09	0.52
1:A:354:THR:CG2	1:A:357:GLN:H	2.17	0.52
1:A:494:HIS:HD2	1:A:496:LEU:H	1.56	0.52
1:B:197:GLY:O	3:B:801:FAD:H1B	2.09	0.52
1:D:433:THR:HG22	1:D:433:THR:O	2.10	0.52
1:B:226:PRO:HD2	1:B:325:TRP:CD1	2.44	0.52
1:C:140:LEU:HD23	1:C:203:VAL:CG1	2.38	0.52
1:C:482:VAL:HG13	1:C:486:TRP:CE3	2.44	0.52
1:D:17:VAL:HG23	1:D:17:VAL:O	2.09	0.52
1:A:91:ARG:HD3	1:A:112:GLU:OE1	2.09	0.52
1:A:162:GLU:HG3	1:A:176:VAL:HG22	1.92	0.52
1:C:115:ARG:NH1	1:C:119:LEU:HD12	2.25	0.52
1:C:65:VAL:CG2	1:C:202:ILE:HG12	2.39	0.52
1:C:421:TRP:CD1	1:C:425:ILE:HD11	2.44	0.52
1:D:91:ARG:HB3	1:D:108:ALA:HA	1.90	0.52
1:D:261:SER:OG	1:D:380:TYR:O	2.27	0.52
1:D:278:SER:HA	1:D:365:LEU:HD22	1.91	0.52
1:D:371:VAL:HG21	1:D:421:TRP:CG	2.44	0.52
1:A:394:THR:HB	4:A:812:HOH:O	2.08	0.52
1:C:421:TRP:CE2	1:C:425:ILE:HD11	2.45	0.52
1:C:447:PHE:CE2	1:C:449:ASN:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:HG22	1:A:84:VAL:HG13	1.92	0.52
1:A:123:VAL:HG11	1:A:222:LEU:HB2	1.91	0.52
1:C:25:VAL:O	1:C:25:VAL:HG22	2.10	0.52
1:C:89:GLN:HE21	1:D:115:ARG:HH22	1.58	0.52
1:D:14:VAL:HG13	1:D:39:VAL:HG21	1.91	0.52
1:D:245:ALA:O	1:D:249:ILE:HG13	2.09	0.52
1:A:40:VAL:HG22	1:A:84:VAL:CG1	2.40	0.52
1:A:199:ASN:ND2	4:A:982:HOH:O	2.42	0.52
1:B:113:THR:HG21	1:B:135:VAL:HG21	1.92	0.51
1:B:354:THR:HG22	1:B:357:GLN:CG	2.40	0.51
1:B:396:GLN:H	1:B:396:GLN:NE2	2.07	0.51
1:C:30:ASN:ND2	1:C:32:ARG:HB2	2.26	0.51
1:D:45:THR:O	1:D:48:GLN:HB2	2.09	0.51
1:A:91:ARG:HH21	1:B:115:ARG:CZ	2.23	0.51
1:D:58:ALA:HB3	4:D:929:HOH:O	2.11	0.51
1:D:299:ALA:HA	1:D:302:ASN:OD1	2.10	0.51
1:A:327:ARG:HH12	1:B:34:ARG:HH22	1.57	0.51
1:C:247:THR:CG2	1:C:248:ARG:HH11	2.23	0.51
1:D:497:SER:HB3	4:D:909:HOH:O	2.10	0.51
1:B:150:ARG:NH1	1:B:226:PRO:HG3	2.25	0.51
1:B:262:ALA:H	1:B:263:ALA:CB	2.24	0.51
1:A:115:ARG:HH12	1:B:89:GLN:HE21	1.57	0.51
1:A:422:ILE:HD12	1:A:423:ARG:N	2.25	0.51
1:C:22:GLN:HA	1:C:22:GLN:OE1	2.08	0.51
1:A:25:VAL:HG13	1:A:26:THR:HG23	1.92	0.51
1:A:434:GLY:O	1:A:461:ASN:HB3	2.10	0.51
1:B:153:VAL:HG12	1:B:155:ALA:H	1.74	0.51
1:B:279:ARG:HG2	1:B:279:ARG:O	2.09	0.51
1:C:462:THR:HG23	1:C:470:LEU:HD11	1.92	0.51
1:D:16:ARG:NH1	1:D:17:VAL:HG22	2.26	0.51
1:D:149:ARG:NH2	1:D:261:SER:OG	2.44	0.51
1:A:131:PRO:HD3	1:A:334:PHE:CE1	2.45	0.51
1:A:364:HIS:HE1	1:A:428:GLU:OE1	1.94	0.51
1:A:447:PHE:CE2	1:A:449:ASN:HB2	2.46	0.51
1:C:113:THR:HG21	1:C:135:VAL:HG21	1.92	0.51
1:D:56:ALA:HB3	1:D:63:ILE:HD11	1.93	0.51
1:D:233:ILE:HG22	1:D:319:GLN:O	2.09	0.51
1:A:89:GLN:HA	1:B:115:ARG:HH22	1.76	0.51
1:A:128:GLY:HA2	1:A:144:TYR:O	2.11	0.51
1:B:13:LYS:HB2	1:B:42:VAL:HB	1.93	0.51
1:B:16:ARG:HD3	4:B:844:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:ALA:O	1:B:432:THR:HG22	2.10	0.51
1:C:115:ARG:NH2	1:D:91:ARG:HH21	2.09	0.51
1:A:21:TYR:HB2	4:A:1061:HOH:O	2.10	0.51
1:A:196:GLY:O	1:A:199:ASN:OD1	2.29	0.51
1:A:288:ILE:HD11	1:A:301:LEU:CG	2.40	0.51
1:B:226:PRO:HD2	1:B:325:TRP:NE1	2.26	0.51
1:A:455:LEU:HD13	1:A:470:LEU:HD12	1.92	0.51
1:A:434:GLY:HA3	1:A:463:SER:HB2	1.92	0.50
1:A:456:VAL:HG12	1:A:456:VAL:O	2.11	0.50
1:B:237:ASP:HA	1:B:283:GLN:HB3	1.93	0.50
1:B:311:GLY:HA3	4:B:866:HOH:O	2.11	0.50
1:D:299:ALA:O	1:D:302:ASN:OD1	2.29	0.50
1:D:494:HIS:HB2	1:D:497:SER:OG	2.12	0.50
1:A:408:THR:HG21	2:A:601[A]:AKY:H512	1.93	0.50
1:A:412:PRO:HA	1:A:415:ASP:OD1	2.12	0.50
1:B:433:THR:HB	4:B:935:HOH:O	2.12	0.50
1:C:338:GLY:O	1:C:410:MET:HB2	2.11	0.50
1:D:25:VAL:HG22	1:D:25:VAL:O	2.11	0.50
1:A:10:ALA:HB1	4:B:940:HOH:O	2.11	0.50
1:A:62:ARG:HD3	4:A:978:HOH:O	2.12	0.50
1:B:22:GLN:HA	1:B:25:VAL:HG12	1.92	0.50
3:B:801:FAD:HO3'	3:B:801:FAD:C10	2.24	0.50
1:D:350:ARG:HD2	1:D:444:GLU:HG3	1.94	0.50
1:A:149:ARG:HB3	1:A:268:ALA:O	2.12	0.50
1:B:123:VAL:HG12	1:B:124:THR:H	1.76	0.50
1:C:14:VAL:HG22	1:C:41:TYR:CD1	2.47	0.50
1:D:104:VAL:HG22	1:D:206:TYR:HB2	1.92	0.50
1:D:242:THR:HG22	1:D:243:GLU:H	1.77	0.50
1:A:209:ARG:HH11	1:A:209:ARG:HB3	1.77	0.50
1:A:296:GLY:O	1:A:300:LEU:HG	2.11	0.50
1:C:302:ASN:HB3	4:C:841:HOH:O	2.11	0.50
1:B:186:ARG:HG3	1:B:186:ARG:HH11	1.77	0.50
1:B:196:GLY:O	1:B:199:ASN:OD1	2.30	0.50
1:B:433:THR:HG21	4:B:961:HOH:O	2.11	0.50
1:B:462:THR:HG23	1:B:470:LEU:HD11	1.94	0.50
1:C:10:ALA:HB2	4:C:1031:HOH:O	2.12	0.50
1:C:41:TYR:HD2	4:C:1011:HOH:O	1.94	0.50
1:D:368:ASP:O	1:D:368:ASP:OD1	2.30	0.50
1:A:199:ASN:HB3	1:A:498:VAL:HG22	1.93	0.49
1:A:363:ARG:NH1	4:A:1073:HOH:O	2.45	0.49
1:C:299:ALA:O	1:C:302:ASN:OD1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ASN:O	1:B:422:ILE:HG13	2.11	0.49
1:C:115:ARG:NE	1:D:91:ARG:HH21	2.09	0.49
1:C:258:GLN:HG2	4:C:971:HOH:O	2.12	0.49
1:C:301:LEU:O	1:C:305:VAL:HG13	2.12	0.49
1:B:75:PHE:HZ	1:B:496:LEU:HD22	1.76	0.49
1:B:237:ASP:HA	1:B:283:GLN:CB	2.42	0.49
1:B:299:ALA:O	1:B:302:ASN:OD1	2.30	0.49
1:B:438:VAL:O	1:B:443:THR:OG1	2.30	0.49
1:C:124:THR:HG23	4:C:1009:HOH:O	2.11	0.49
1:A:85:ILE:HG13	1:A:202:ILE:HD13	1.95	0.49
1:A:404:TRP:CG	2:A:601[A]:AKY:H413	2.47	0.49
1:C:121:TRP:CD1	1:C:218:PRO:HB2	2.47	0.49
1:C:244:GLU:HG2	1:C:248:ARG:NH2	2.26	0.49
1:D:447:PHE:CE2	1:D:449:ASN:HB2	2.47	0.49
1:B:61:GLN:HB3	1:B:82:ARG:HB2	1.95	0.49
1:B:195:GLY:HA3	1:B:472:TYR:CE1	2.32	0.49
1:B:261:SER:N	1:B:262:ALA:HB2	2.27	0.49
1:C:180:ALA:HA	4:C:899:HOH:O	2.11	0.49
1:C:288:ILE:HD11	1:C:301:LEU:HG	1.95	0.49
1:C:384:VAL:O	1:C:397:ARG:HD2	2.12	0.49
1:A:232:HIS:O	1:A:288:ILE:HG23	2.12	0.49
1:A:394:THR:HG22	4:A:932:HOH:O	2.11	0.49
1:B:472:TYR:O	1:B:475:ASN:HB2	2.13	0.49
1:C:89:GLN:NE2	1:D:115:ARG:HH22	2.11	0.49
1:C:109:THR:HG22	1:C:112:GLU:CB	2.42	0.49
1:C:262:ALA:HA	1:C:382:GLY:H	1.76	0.49
1:D:341:ARG:HH11	1:D:412:PRO:HB3	1.75	0.49
1:A:40:VAL:HG13	1:A:84:VAL:HG13	1.92	0.49
1:B:447:PHE:HB3	1:B:450:TYR:CD1	2.47	0.49
1:C:441:ASP:HB3	4:C:844:HOH:O	2.12	0.49
1:A:407:ALA:HB2	1:A:422:ILE:HG23	1.94	0.49
2:A:601[A]:AKY:H513	2:A:601[A]:AKY:O18	2.12	0.49
1:C:30:ASN:ND2	1:C:32:ARG:H	2.11	0.49
1:C:153:VAL:HG12	1:C:155:ALA:H	1.78	0.49
1:D:274:PHE:CE2	1:D:284:ILE:HD12	2.47	0.49
1:A:137:GLY:HA2	1:A:140:LEU:HD11	1.94	0.49
1:A:226:PRO:HD2	1:A:325:TRP:CD1	2.48	0.49
1:A:193:THR:CG2	1:A:393:ALA:H	2.18	0.49
1:B:92:GLN:HB2	1:B:105:GLU:CD	2.33	0.49
1:C:203:VAL:HG13	3:C:801:FAD:C2A	2.43	0.49
1:C:220:GLN:NE2	4:C:1002:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:ILE:HD13	4:C:828:HOH:O	2.12	0.49
1:D:419:LEU:O	1:D:422:ILE:HD12	2.12	0.49
1:D:466:PRO:HG2	1:D:469:THR:OG1	2.12	0.49
1:A:396:GLN:H	1:A:396:GLN:NE2	2.11	0.48
1:C:476:TYR:HB3	1:C:477:PRO:HD3	1.95	0.48
1:D:85:ILE:HG13	1:D:87:MET:HE3	1.95	0.48
1:A:16:ARG:HG3	1:A:17:VAL:H	1.77	0.48
1:B:25:VAL:HG22	1:B:25:VAL:O	2.13	0.48
1:B:262:ALA:H	1:B:263:ALA:HB2	1.78	0.48
1:C:89:GLN:NE2	1:D:115:ARG:HH12	2.11	0.48
1:C:263:ALA:CB	1:C:268:ALA:HB2	2.39	0.48
1:D:174:LYS:HG3	4:D:899:HOH:O	2.13	0.48
1:D:291:ASP:O	1:D:294:LEU:HG	2.14	0.48
1:B:20:ARG:NH2	4:B:815:HOH:O	2.43	0.48
1:B:65:VAL:CG2	1:B:202:ILE:HG12	2.43	0.48
1:B:279:ARG:HB2	1:B:366:SER:HA	1.94	0.48
1:D:364:HIS:CG	1:D:425:ILE:HG23	2.49	0.48
1:A:14:VAL:HG22	1:A:41:TYR:CD1	2.48	0.48
1:A:345:LYS:HD3	1:A:426:TYR:CG	2.48	0.48
1:B:494:HIS:H	1:B:497:SER:HB2	1.78	0.48
1:C:109:THR:CG2	1:C:112:GLU:H	2.26	0.48
1:C:115:ARG:HE	1:D:91:ARG:HH21	1.60	0.48
1:C:195:GLY:HA2	1:C:472:TYR:HE1	1.78	0.48
1:A:65:VAL:HG22	1:A:85:ILE:CD1	2.35	0.48
1:B:40:VAL:HA	1:B:84:VAL:HG13	1.95	0.48
1:B:120:ASP:HB3	4:B:940:HOH:O	2.13	0.48
1:B:455:LEU:O	1:B:462:THR:HG21	2.14	0.48
1:C:115:ARG:HH21	1:D:91:ARG:HH21	1.61	0.48
1:A:143:GLY:HA2	3:A:801:FAD:O2	2.13	0.48
1:A:392:THR:HG21	1:A:394:THR:OG1	2.13	0.48
1:B:130:CYS:HB3	4:B:802:HOH:O	2.14	0.48
1:B:232:HIS:CE1	1:B:301:LEU:HB3	2.49	0.48
1:C:262:ALA:HA	1:C:382:GLY:N	2.29	0.48
1:D:343:LYS:HE2	4:D:956:HOH:O	2.13	0.48
1:A:370:GLN:NE2	4:A:1020:HOH:O	2.46	0.48
1:B:455:LEU:O	1:B:462:THR:OG1	2.30	0.48
1:B:456:VAL:HG12	1:B:456:VAL:O	2.13	0.48
1:D:124:THR:HG21	4:D:935:HOH:O	2.13	0.48
1:B:199:ASN:CB	1:B:498:VAL:HG22	2.43	0.48
1:B:245:ALA:HA	1:B:248:ARG:CG	2.44	0.48
1:B:263:ALA:HB1	1:B:268:ALA:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:GLU:OE2	1:C:395:ALA:O	2.30	0.48
1:D:193:THR:CG2	1:D:393:ALA:H	2.15	0.48
1:D:396:GLN:NE2	4:D:1004:HOH:O	2.47	0.48
1:B:195:GLY:HA2	1:B:448:ILE:CG1	2.39	0.48
1:B:338:GLY:O	1:B:410:MET:HG3	2.14	0.48
1:B:423:ARG:NH2	4:B:882:HOH:O	2.47	0.48
1:C:128:GLY:HA2	1:C:144:TYR:O	2.13	0.48
1:D:419:LEU:O	1:D:423:ARG:HD2	2.13	0.48
1:D:297:ALA:HA	1:D:300:LEU:CD1	2.42	0.48
1:A:146:PRO:HA	1:A:271:HIS:CG	2.49	0.47
1:A:422:ILE:HD12	1:A:423:ARG:HG3	1.96	0.47
1:A:444:GLU:HG2	1:A:473:LYS:HZ2	1.79	0.47
1:B:277:ASN:HA	1:B:374:GLU:HB3	1.94	0.47
1:C:214:THR:O	1:C:221:LEU:HD21	2.14	0.47
1:D:109:THR:HG22	1:D:112:GLU:CG	2.44	0.47
1:C:40:VAL:HA	1:C:84:VAL:HG13	1.96	0.47
1:D:14:VAL:HG22	1:D:41:TYR:CE1	2.50	0.47
1:D:128:GLY:HA2	1:D:144:TYR:O	2.14	0.47
1:D:429:ILE:O	1:D:429:ILE:HG12	2.08	0.47
1:A:159:TYR:OH	4:A:879:HOH:O	2.18	0.47
1:A:209:ARG:HB3	1:A:209:ARG:NH1	2.29	0.47
1:A:407:ALA:HB2	1:A:421:TRP:CD1	2.50	0.47
1:A:435:GLY:HA3	1:A:461:ASN:HB3	1.96	0.47
1:B:140:LEU:HA	1:B:192:HIS:O	2.14	0.47
1:B:288:ILE:HD11	1:B:301:LEU:CG	2.43	0.47
1:B:334:PHE:HE1	4:B:876:HOH:O	1.96	0.47
1:A:21:TYR:O	1:A:25:VAL:HG12	2.14	0.47
1:A:127:ALA:O	1:A:145:GLY:HA3	2.14	0.47
1:A:345:LYS:HE3	1:A:345:LYS:HB3	1.64	0.47
1:B:109:THR:HG21	4:B:926:HOH:O	2.14	0.47
1:B:290:ILE:HG22	1:B:301:LEU:HD21	1.97	0.47
1:B:433:THR:HG22	1:B:436:VAL:O	2.14	0.47
1:C:89:GLN:HA	1:D:115:ARG:NH2	2.26	0.47
1:B:305:VAL:HG21	4:B:913:HOH:O	2.13	0.47
1:B:344:SER:HB2	1:B:404:TRP:NE1	2.29	0.47
1:B:407:ALA:HB2	1:B:421:TRP:HD1	1.78	0.47
1:A:261:SER:OG	1:A:262:ALA:N	2.48	0.47
1:C:82:ARG:HH11	1:C:82:ARG:HD3	1.48	0.47
1:C:339:PHE:HB3	1:C:408:THR:HG22	1.95	0.47
1:A:81:VAL:HG23	4:A:978:HOH:O	2.13	0.47
1:B:10:ALA:HB3	1:B:44:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ASP:HA	1:B:412:PRO:HD2	1.76	0.47
1:B:494:HIS:HD2	1:B:496:LEU:H	1.62	0.47
1:C:23:ASP:OD1	1:D:324:PRO:HB2	2.15	0.47
1:C:30:ASN:HD22	1:C:32:ARG:H	1.62	0.47
1:C:433:THR:HB	4:C:848:HOH:O	2.14	0.47
1:D:173:ARG:HB2	4:D:862:HOH:O	2.15	0.47
1:A:290:ILE:CG2	1:A:301:LEU:HD11	2.45	0.47
1:B:45:THR:OG1	1:B:48:GLN:HG3	2.15	0.47
1:C:279:ARG:O	1:C:279:ARG:HG2	2.14	0.47
1:D:337:GLY:O	1:D:339:PHE:HD2	1.98	0.47
1:A:16:ARG:HG2	1:A:16:ARG:NH1	2.23	0.47
1:A:384:VAL:HG13	1:A:385:ASN:OD1	2.14	0.47
1:B:392:THR:CG2	1:B:397:ARG:HH21	2.14	0.47
1:C:296:GLY:O	1:C:299:ALA:HB3	2.15	0.47
1:D:103:ALA:HB2	1:D:207:TRP:CH2	2.49	0.47
1:D:124:THR:OG1	1:D:225:ALA:HB2	2.15	0.47
1:D:162:GLU:HB3	1:D:204:THR:CG2	2.46	0.47
1:D:309:ASN:ND2	1:D:316:PRO:HD3	2.29	0.47
1:A:444:GLU:HG2	1:A:473:LYS:HZ3	1.81	0.46
1:C:104:VAL:HG23	1:C:135:VAL:HG11	1.97	0.46
1:D:29:PHE:CE2	3:D:801:FAD:HM82	2.50	0.46
1:D:99:LYS:HE3	1:D:207:TRP:NE1	2.29	0.46
1:D:203:VAL:HG11	1:D:206:TYR:CZ	2.50	0.46
1:A:141:GLY:CA	1:A:448:ILE:HD11	2.45	0.46
1:C:246:PHE:O	1:C:250:ILE:HG12	2.15	0.46
1:C:494:HIS:O	1:C:497:SER:HB2	2.15	0.46
1:D:394:THR:OG1	1:D:397:ARG:NH2	2.49	0.46
1:A:140:LEU:HA	1:A:192:HIS:O	2.14	0.46
1:A:213:ALA:N	4:A:954:HOH:O	2.48	0.46
1:B:17:VAL:O	1:B:17:VAL:HG23	2.15	0.46
1:B:237:ASP:OD1	1:B:283:GLN:NE2	2.49	0.46
1:C:65:VAL:HG22	1:C:85:ILE:CG1	2.45	0.46
1:D:100:ARG:HH22	1:D:213:ALA:HB1	1.79	0.46
1:D:162:GLU:HG3	1:D:176:VAL:HG22	1.97	0.46
1:D:193:THR:OG1	1:D:392:THR:OG1	2.29	0.46
1:B:163:VAL:HG22	1:B:203:VAL:HG22	1.96	0.46
1:B:217:ASP:OD2	1:B:220:GLN:NE2	2.49	0.46
1:C:252:ASN:HB3	1:C:307:ALA:O	2.15	0.46
1:C:197:GLY:O	3:C:801:FAD:N3A	2.49	0.46
1:A:290:ILE:HG12	1:A:294:LEU:HD11	1.97	0.46
1:B:232:HIS:HB2	1:B:288:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ARG:NH1	4:A:824:HOH:O	2.49	0.46
1:A:290:ILE:HD13	1:A:300:LEU:CD1	2.40	0.46
3:B:801:FAD:O2'	4:B:971:HOH:O	2.21	0.46
1:C:434:GLY:CA	1:C:463:SER:HB2	2.34	0.46
1:D:27:ARG:HH11	1:D:66:ARG:HD2	1.81	0.46
1:A:421:TRP:HZ3	4:A:974:HOH:O	1.98	0.46
1:A:453:VAL:HG23	1:A:496:LEU:HD13	1.96	0.46
1:B:213:ALA:O	1:B:214:THR:OG1	2.29	0.46
1:C:231:ARG:HA	1:C:288:ILE:O	2.16	0.46
1:B:115:ARG:HG3	1:B:116:ALA:N	2.31	0.46
1:C:370:GLN:O	1:C:370:GLN:HG3	2.15	0.46
1:D:196:GLY:O	1:D:199:ASN:ND2	2.49	0.46
1:D:312:THR:CG2	1:D:314:VAL:HG13	2.37	0.46
1:B:67:SER:HB3	1:B:106:PRO:O	2.16	0.46
3:B:801:FAD:N1	3:B:801:FAD:O3'	2.49	0.46
1:C:88:SER:N	4:C:1000:HOH:O	2.49	0.46
1:C:103:ALA:HB2	1:C:207:TRP:CE3	2.51	0.46
1:C:199:ASN:ND2	1:C:497:SER:OG	2.49	0.46
1:C:462:THR:CG2	1:C:470:LEU:HD11	2.45	0.46
1:D:462:THR:N	4:D:950:HOH:O	2.47	0.46
1:A:162:GLU:CG	1:A:176:VAL:HG22	2.46	0.45
1:A:373:GLY:HA3	1:A:421:TRP:CE2	2.51	0.45
1:A:434:GLY:O	1:A:462:THR:N	2.50	0.45
1:A:437:PRO:O	1:A:445:GLY:HA2	2.15	0.45
1:C:62:ARG:NH2	1:C:494:HIS:HA	2.32	0.45
1:D:28:GLY:O	1:D:34:ARG:NH2	2.50	0.45
1:A:112:GLU:HA	1:A:115:ARG:HG2	1.98	0.45
1:A:149:ARG:NH1	1:A:267:TYR:O	2.49	0.45
1:A:261:SER:HB2	4:A:892:HOH:O	2.16	0.45
1:B:234:VAL:HG11	4:B:913:HOH:O	2.15	0.45
1:B:291:ASP:N	4:B:895:HOH:O	2.48	0.45
1:B:419:LEU:HD22	1:B:423:ARG:HH21	1.82	0.45
1:C:34:ARG:NH2	4:C:997:HOH:O	2.49	0.45
1:C:347:ALA:N	1:C:403:VAL:HG22	2.30	0.45
1:C:400:ILE:HD11	4:C:1007:HOH:O	2.17	0.45
1:C:422:ILE:HD12	1:C:423:ARG:H	1.81	0.45
1:D:232:HIS:CD2	1:D:320:ARG:HG2	2.51	0.45
1:A:14:VAL:HG22	1:A:41:TYR:CE1	2.51	0.45
1:A:85:ILE:CG1	1:A:87:MET:HE3	2.46	0.45
1:A:335:ASP:OD2	1:A:337:GLY:N	2.49	0.45
1:B:65:VAL:HG22	1:B:85:ILE:CD1	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ASN:HB2	1:B:308:VAL:O	2.17	0.45
1:B:298:GLU:OE2	1:B:320:ARG:NH1	2.50	0.45
1:D:78:ASP:N	4:D:948:HOH:O	2.49	0.45
1:D:427:ARG:O	1:D:431:ALA:N	2.49	0.45
1:A:265:THR:HB	1:A:266:PRO:HD2	1.98	0.45
1:A:450:TYR:CE2	2:A:601[A]:AKY:H412	2.51	0.45
1:B:150:ARG:NH2	1:B:151:ASP:OD2	2.50	0.45
1:C:115:ARG:NH2	1:D:88:SER:O	2.50	0.45
1:C:233:ILE:HG22	4:C:1001:HOH:O	2.17	0.45
1:C:243:GLU:OE1	1:C:362:TYR:HB3	2.17	0.45
1:C:354:THR:H	1:C:357:GLN:NE2	2.03	0.45
1:D:341:ARG:NE	4:D:959:HOH:O	2.49	0.45
1:A:140:LEU:HD12	1:A:140:LEU:H	1.81	0.45
1:A:279:ARG:N	4:A:916:HOH:O	2.49	0.45
1:B:335:ASP:OD2	1:B:337:GLY:N	2.50	0.45
1:C:109:THR:HG22	1:C:112:GLU:HG3	1.99	0.45
1:C:188:LEU:HG	1:C:486:TRP:CD2	2.52	0.45
1:A:17:VAL:HA	4:A:852:HOH:O	2.16	0.45
1:A:91:ARG:HG2	1:A:107:GLY:C	2.36	0.45
1:A:114:TYR:OH	1:A:127:ALA:HB3	2.17	0.45
1:B:109:THR:HG22	1:B:112:GLU:HG3	1.98	0.45
1:C:66:ARG:NH2	1:C:77:ASP:OD2	2.48	0.45
1:C:79:PRO:O	1:C:82:ARG:NH1	2.49	0.45
1:C:89:GLN:CD	1:D:115:ARG:HH12	2.20	0.45
1:C:109:THR:HG22	1:C:112:GLU:CG	2.47	0.45
1:C:171:ARG:NH2	4:C:877:HOH:O	2.50	0.45
1:D:354:THR:OG1	1:D:355:ALA:N	2.49	0.45
1:A:89:GLN:OE1	1:B:115:ARG:NH1	2.50	0.45
1:A:414:HIS:HA	4:A:853:HOH:O	2.17	0.45
2:A:601[A]:AKY:H143	2:A:601[A]:AKY:H81	1.70	0.45
1:B:96:ASP:OD2	1:B:98:GLY:N	2.49	0.45
1:B:299:ALA:HA	1:B:302:ASN:OD1	2.17	0.45
1:B:336:THR:OG1	1:B:339:PHE:O	2.29	0.45
1:C:127:ALA:O	1:C:145:GLY:HA3	2.16	0.45
1:C:429:ILE:HD11	1:C:430:PHE:CZ	2.52	0.45
1:D:350:ARG:HD2	4:D:915:HOH:O	2.16	0.45
1:A:155:ALA:HB1	1:A:193:THR:OG1	2.16	0.45
1:A:203:VAL:HG11	1:A:206:TYR:CZ	2.52	0.45
1:A:261:SER:OG	1:A:382:GLY:N	2.50	0.45
1:B:246:PHE:O	1:B:250:ILE:HG12	2.17	0.45
1:C:130:CYS:CB	3:C:801:FAD:C6	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ARG:NH1	1:C:151:ASP:OD2	2.49	0.45
1:D:148:SER:HA	1:D:152:GLY:O	2.16	0.45
1:D:254:GLY:HA3	1:D:352:PRO:HB3	1.99	0.45
1:D:352:PRO:O	1:D:442:ARG:NH2	2.50	0.45
1:D:369:SER:OG	1:D:370:GLN:N	2.50	0.45
1:D:432:THR:HG23	1:D:432:THR:O	2.16	0.45
1:A:62:ARG:NH2	4:A:1011:HOH:O	2.49	0.45
1:B:140:LEU:HD12	1:B:140:LEU:N	2.32	0.45
1:C:162:GLU:CG	1:C:205:ARG:HB3	2.42	0.45
1:C:396:GLN:H	1:C:396:GLN:NE2	2.14	0.45
1:C:456:VAL:HG12	1:C:456:VAL:O	2.17	0.45
1:D:191:ALA:CB	1:D:482:VAL:HG11	2.47	0.45
1:D:341:ARG:NH2	1:D:415:ASP:OD2	2.50	0.45
1:A:463:SER:N	4:A:895:HOH:O	2.49	0.45
1:B:64:ALA:O	1:B:84:VAL:HA	2.17	0.45
1:B:392:THR:HG23	1:B:393:ALA:N	2.30	0.45
1:C:173:ARG:NH2	4:C:990:HOH:O	2.50	0.45
1:C:448:ILE:HG22	1:C:471:TYR:HB3	1.98	0.45
1:D:427:ARG:HB3	1:D:461:ASN:CG	2.37	0.45
1:A:150:ARG:HG3	1:A:151:ASP:CG	2.38	0.44
1:A:234:VAL:HA	1:A:317:ALA:O	2.17	0.44
2:A:601[A]:AKY:O16	2:A:601[A]:AKY:H82	2.14	0.44
1:B:241:LEU:HD23	1:B:241:LEU:HA	1.85	0.44
1:B:354:THR:OG1	1:B:355:ALA:N	2.50	0.44
1:B:367:ALA:O	1:B:369:SER:N	2.50	0.44
1:B:446:THR:HG23	1:B:471:TYR:CE2	2.52	0.44
1:C:63:ILE:HG23	1:C:85:ILE:HD13	1.99	0.44
1:C:88:SER:O	1:D:115:ARG:NH2	2.50	0.44
1:D:425:ILE:H	1:D:425:ILE:HG13	1.58	0.44
1:D:427:ARG:HB3	1:D:461:ASN:ND2	2.32	0.44
1:A:61:GLN:HB3	1:A:83:ALA:HB2	2.00	0.44
1:A:96:ASP:CG	1:A:99:LYS:HD2	2.38	0.44
4:A:937:HOH:O	1:B:327:ARG:NE	2.50	0.44
1:B:356:ALA:O	1:B:359:ALA:HB3	2.17	0.44
1:B:426:TYR:N	4:B:957:HOH:O	2.50	0.44
1:C:14:VAL:HG22	1:C:41:TYR:CE1	2.52	0.44
1:A:112:GLU:O	1:A:115:ARG:HG2	2.16	0.44
1:A:263:ALA:N	4:A:896:HOH:O	2.51	0.44
1:C:97:SER:O	1:C:100:ARG:N	2.50	0.44
1:C:175:VAL:N	4:C:929:HOH:O	2.50	0.44
1:C:253:HIS:HE1	4:C:850:HOH:O	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:GLY:O	1:D:461:ASN:ND2	2.50	0.44
1:A:82:ARG:NE	4:A:1041:HOH:O	2.49	0.44
1:A:429:ILE:HD11	1:A:430:PHE:CE2	2.53	0.44
1:A:448:ILE:HD13	4:A:857:HOH:O	2.17	0.44
1:B:248:ARG:HG2	1:B:248:ARG:H	1.69	0.44
1:B:308:VAL:HG12	4:B:963:HOH:O	2.18	0.44
1:C:499:ARG:HH11	1:C:499:ARG:HD3	1.51	0.44
1:B:127:ALA:O	1:B:145:GLY:HA3	2.17	0.44
1:D:193:THR:HG23	1:D:393:ALA:N	2.14	0.44
1:D:270:MET:HB2	1:D:290:ILE:HD12	1.99	0.44
1:D:279:ARG:O	1:D:279:ARG:HG2	2.18	0.44
1:B:123:VAL:HG12	1:B:124:THR:N	2.33	0.44
1:B:233:ILE:HG12	1:B:319:GLN:OE1	2.17	0.44
1:D:138:HIS:NE2	1:D:143:GLY:HA3	2.32	0.44
1:D:232:HIS:NE2	1:D:298:GLU:OE2	2.50	0.44
1:D:288:ILE:HD12	1:D:304:PHE:CD1	2.53	0.44
1:D:453:VAL:HG12	4:D:875:HOH:O	2.17	0.44
1:D:480:GLN:HG2	1:D:499:ARG:O	2.18	0.44
1:B:454:ASP:OD2	1:B:454:ASP:N	2.49	0.44
1:C:27:ARG:HD2	4:C:1030:HOH:O	2.16	0.44
1:D:89:GLN:HE21	1:D:89:GLN:HA	1.82	0.44
1:D:244:GLU:HB2	4:D:941:HOH:O	2.17	0.44
1:D:436:VAL:HG13	1:D:461:ASN:HB3	1.98	0.44
1:A:85:ILE:HG12	1:A:85:ILE:O	2.18	0.44
1:C:115:ARG:NH2	1:D:89:GLN:HE21	2.15	0.44
1:C:425:ILE:HG13	1:C:425:ILE:H	1.53	0.44
1:D:82:ARG:HD3	1:D:82:ARG:HA	1.80	0.44
1:D:89:GLN:HB2	4:D:845:HOH:O	2.18	0.44
1:D:109:THR:HG22	1:D:112:GLU:H	1.81	0.44
1:A:79:PRO:O	1:A:82:ARG:NH1	2.49	0.44
1:A:424:GLU:OE2	4:A:990:HOH:O	2.21	0.44
1:A:483:LYS:NZ	1:A:487:ASP:OD2	2.50	0.44
1:B:185:ASN:N	1:B:185:ASN:OD1	2.50	0.44
1:B:238:TRP:CG	1:B:279:ARG:HG3	2.53	0.44
1:C:29:PHE:HB2	1:C:70:HIS:HA	2.00	0.44
1:C:115:ARG:CZ	1:D:91:ARG:HH21	2.31	0.44
1:C:129:VAL:HG22	1:C:146:PRO:CD	2.39	0.44
1:D:263:ALA:HB1	1:D:265:THR:HG23	1.98	0.44
1:D:374:GLU:HG3	4:D:835:HOH:O	2.17	0.44
1:A:89:GLN:OE1	1:B:115:ARG:NH2	2.50	0.43
1:A:209:ARG:HD3	1:A:213:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LEU:HG	1:B:40:VAL:CG1	2.38	0.43
1:B:205:ARG:NH1	4:B:887:HOH:O	2.48	0.43
1:B:257:HIS:NE2	1:B:379:SER:HB3	2.33	0.43
1:C:43:VAL:HG21	1:C:87:MET:HE1	1.99	0.43
1:D:209:ARG:HG3	1:D:221:LEU:HD13	1.99	0.43
1:A:94:PHE:O	1:A:103:ALA:N	2.49	0.43
1:A:383:LYS:N	4:A:972:HOH:O	2.50	0.43
1:A:483:LYS:HD3	1:A:498:VAL:HG23	1.99	0.43
1:B:123:VAL:CG1	1:B:222:LEU:HB2	2.47	0.43
1:C:480:GLN:HB3	1:C:501:PRO:HG3	1.98	0.43
1:D:51:ASP:O	1:D:55:GLN:HG3	2.17	0.43
1:B:193:THR:HG23	1:B:393:ALA:N	2.17	0.43
1:B:350:ARG:NE	4:B:811:HOH:O	2.42	0.43
1:B:385:ASN:OD1	1:B:385:ASN:N	2.50	0.43
1:B:466:PRO:HG2	1:B:468:TYR:CE2	2.53	0.43
1:C:457:ASP:HB2	4:C:882:HOH:O	2.17	0.43
1:D:70:HIS:HB3	3:D:801:FAD:HM81	2.00	0.43
1:A:62:ARG:NH1	1:A:80:ALA:HB3	2.33	0.43
1:B:236:TRP:NE1	1:B:309:ASN:OD1	2.50	0.43
1:C:113:THR:HG21	1:C:135:VAL:CG2	2.48	0.43
1:C:233:ILE:HD11	1:C:285:LEU:CD1	2.47	0.43
1:D:13:LYS:HB2	1:D:42:VAL:HB	2.00	0.43
1:B:144:TYR:CE2	1:B:402:LYS:HE2	2.54	0.43
1:C:305:VAL:HG21	4:C:987:HOH:O	2.18	0.43
1:A:95:TYR:CE2	1:A:97:SER:HA	2.53	0.43
1:A:236:TRP:CE2	1:A:316:PRO:HB3	2.54	0.43
1:C:312:THR:HG22	1:C:314:VAL:N	2.27	0.43
1:A:319:GLN:NE2	4:A:941:HOH:O	2.49	0.43
1:A:404:TRP:CE2	2:A:601[A]:AKY:C41	3.01	0.43
1:B:34:ARG:NE	4:B:970:HOH:O	2.49	0.43
1:B:241:LEU:HD11	1:B:284:ILE:HD13	2.00	0.43
1:B:315:GLU:HA	1:B:316:PRO:HD2	1.92	0.43
1:B:360:THR:HG21	1:B:429:ILE:HG22	2.01	0.43
1:D:129:VAL:HG22	1:D:146:PRO:HD3	2.00	0.43
1:D:341:ARG:HD2	1:D:415:ASP:OD1	2.18	0.43
1:A:262:ALA:HA	1:A:382:GLY:CA	2.49	0.43
1:A:371:VAL:HG21	1:A:421:TRP:CD1	2.54	0.43
1:A:425:ILE:O	1:A:429:ILE:HG23	2.19	0.43
1:C:348:TYR:CD2	1:C:396:GLN:HG2	2.53	0.43
1:C:350:ARG:HH11	1:C:350:ARG:HD2	1.67	0.43
1:C:411:ASP:O	1:C:411:ASP:OD2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:ILE:O	1:D:252:ASN:HB2	2.18	0.43
1:A:73:GLU:OE1	1:A:343:LYS:NZ	2.50	0.43
1:A:396:GLN:H	1:A:396:GLN:HE21	1.66	0.43
1:C:98:GLY:HA2	4:C:954:HOH:O	2.19	0.43
1:C:203:VAL:CB	4:C:1015:HOH:O	2.60	0.43
1:C:247:THR:HG22	1:C:248:ARG:HE	1.84	0.43
1:C:335:ASP:OD1	1:D:332:ASN:ND2	2.49	0.43
1:C:392:THR:CG2	1:C:394:THR:H	2.15	0.43
1:D:66:ARG:NH1	4:D:975:HOH:O	2.50	0.43
1:D:249:ILE:N	4:D:901:HOH:O	2.52	0.43
1:A:124:THR:HG22	1:A:125:ILE:N	2.32	0.43
1:A:361:LEU:HD12	1:A:361:LEU:HA	1.86	0.43
1:C:141:GLY:C	1:C:194:GLY:HA2	2.39	0.43
1:C:193:THR:HG23	1:C:393:ALA:N	2.12	0.43
1:C:233:ILE:CD1	1:C:285:LEU:HD11	2.48	0.43
1:C:422:ILE:CD1	1:C:423:ARG:HG3	2.49	0.43
1:A:14:VAL:HG13	1:A:39:VAL:HG21	2.00	0.42
1:A:140:LEU:HD12	1:A:140:LEU:N	2.34	0.42
1:A:147:LEU:O	1:A:150:ARG:HG2	2.18	0.42
1:A:279:ARG:HA	4:A:854:HOH:O	2.19	0.42
1:B:30:ASN:ND2	1:B:32:ARG:HB2	2.34	0.42
1:B:87:MET:O	1:B:107:GLY:HA3	2.19	0.42
1:C:336:THR:CG2	4:C:968:HOH:O	2.67	0.42
1:D:229:THR:O	1:D:322:THR:HA	2.19	0.42
3:D:801:FAD:H9	3:D:801:FAD:H1'2	1.65	0.42
1:A:25:VAL:O	1:A:25:VAL:HG22	2.19	0.42
1:A:290:ILE:CD1	1:A:300:LEU:HD13	2.43	0.42
1:A:354:THR:HG22	1:A:357:GLN:CG	2.49	0.42
1:B:130:CYS:HB3	3:B:801:FAD:HM73	2.00	0.42
1:B:364:HIS:HE1	1:B:428:GLU:OE2	2.03	0.42
1:B:411:ASP:HB3	1:B:414:HIS:CE1	2.54	0.42
1:C:65:VAL:HA	1:C:85:ILE:HG12	2.01	0.42
1:C:228:SER:OG	1:C:292:GLY:HA3	2.19	0.42
1:C:232:HIS:CE1	1:C:301:LEU:HB3	2.53	0.42
1:D:350:ARG:HG3	1:D:444:GLU:HG3	2.00	0.42
1:A:194:GLY:HA3	1:A:394:THR:HG22	2.00	0.42
1:A:336:THR:HG23	1:A:338:GLY:H	1.83	0.42
1:A:424:GLU:HG2	4:A:1053:HOH:O	2.19	0.42
1:C:231:ARG:NH1	1:C:287:ASP:OD2	2.50	0.42
1:C:281:ALA:HB2	4:C:817:HOH:O	2.20	0.42
1:C:297:ALA:HA	1:C:300:LEU:CD1	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ARG:CD	1:D:17:VAL:H	2.31	0.42
1:D:27:ARG:NE	1:D:86:ASP:OD1	2.50	0.42
1:D:265:THR:O	1:D:268:ALA:HB3	2.19	0.42
1:D:446:THR:HG23	1:D:471:TYR:CE2	2.54	0.42
1:B:131:PRO:HD3	1:B:334:PHE:CE1	2.55	0.42
1:B:147:LEU:HA	4:B:924:HOH:O	2.19	0.42
1:B:174:LYS:HB2	1:B:174:LYS:HE3	1.87	0.42
1:B:312:THR:HG22	1:B:313:GLY:N	2.33	0.42
1:C:165:VAL:HA	4:C:1050:HOH:O	2.19	0.42
1:C:466:PRO:O	1:C:470:LEU:HG	2.19	0.42
1:D:343:LYS:HD3	4:D:956:HOH:O	2.19	0.42
1:A:129:VAL:HG12	1:A:334:PHE:CZ	2.52	0.42
1:B:346:GLY:HA2	1:B:403:VAL:O	2.19	0.42
1:D:144:TYR:CD1	1:D:402:LYS:HE3	2.54	0.42
1:D:409:TRP:NE1	1:D:415:ASP:OD1	2.50	0.42
1:A:130:CYS:HB2	1:A:133:VAL:CG2	2.39	0.42
1:B:350:ARG:NE	1:B:398:ASP:OD1	2.52	0.42
1:B:482:VAL:HG13	1:B:486:TRP:CE3	2.55	0.42
1:C:96:ASP:HB3	1:C:207:TRP:HZ3	1.84	0.42
1:C:347:ALA:HB3	1:C:403:VAL:HG22	2.01	0.42
1:D:249:ILE:HG12	4:D:901:HOH:O	2.20	0.42
1:B:300:LEU:H	1:B:300:LEU:HG	1.63	0.42
1:B:312:THR:HG22	1:B:313:GLY:H	1.85	0.42
1:C:166:VAL:HG23	4:C:1050:HOH:O	2.19	0.42
1:C:294:LEU:O	1:C:297:ALA:HB2	2.20	0.42
1:C:191:ALA:HB1	1:C:200:PHE:CE2	2.55	0.42
1:D:29:PHE:CZ	3:D:801:FAD:HM82	2.55	0.42
1:D:263:ALA:HB1	1:D:265:THR:CG2	2.50	0.42
1:A:65:VAL:CG2	1:A:202:ILE:HG12	2.46	0.42
1:A:453:VAL:HG23	1:A:496:LEU:CD1	2.50	0.42
1:B:360:THR:HG22	1:B:429:ILE:HG22	2.01	0.42
1:C:27:ARG:NH2	4:C:854:HOH:O	2.51	0.42
1:C:290:ILE:HD13	1:C:300:LEU:CD1	2.50	0.42
1:C:348:TYR:OH	1:C:402:LYS:NZ	2.47	0.42
1:C:447:PHE:HA	4:C:900:HOH:O	2.20	0.42
1:D:130:CYS:SG	3:D:801:FAD:C5X	2.93	0.42
1:D:375:VAL:HG22	1:D:405:MET:CG	2.50	0.42
1:D:422:ILE:HD12	1:D:423:ARG:H	1.85	0.42
1:A:62:ARG:HH11	1:A:80:ALA:HB3	1.85	0.42
1:B:476:TYR:HB3	1:B:477:PRO:HD3	2.01	0.42
1:C:66:ARG:HH22	1:C:77:ASP:CG	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:LYS:HE2	4:D:980:HOH:O	2.20	0.42
1:D:231:ARG:HG3	1:D:231:ARG:HH11	1.85	0.42
1:D:462:THR:HG22	1:D:465:VAL:O	2.20	0.42
1:A:236:TRP:HD1	1:A:314:VAL:HG22	1.85	0.41
1:B:25:VAL:HG21	1:B:35:GLY:O	2.20	0.41
1:B:210:THR:O	1:B:213:ALA:HB2	2.20	0.41
1:B:354:THR:HG22	1:B:357:GLN:HG3	2.01	0.41
1:C:144:TYR:CE1	1:C:402:LYS:HE3	2.55	0.41
1:C:300:LEU:HA	1:C:303:ASP:HB2	2.02	0.41
1:A:27:ARG:NH2	1:A:66:ARG:HG2	2.35	0.41
1:A:51:ASP:OD1	1:A:55:GLN:NE2	2.50	0.41
1:A:53:VAL:O	1:A:57:MET:HG3	2.20	0.41
1:A:421:TRP:CE2	1:A:425:ILE:HD11	2.55	0.41
1:B:236:TRP:NE1	1:B:316:PRO:HD3	2.35	0.41
1:B:356:ALA:HA	1:B:359:ALA:HB3	2.02	0.41
1:D:153:VAL:HG12	1:D:155:ALA:H	1.85	0.41
1:A:109:THR:HG23	1:A:111:GLY:N	2.35	0.41
1:A:115:ARG:HH21	1:B:91:ARG:HD2	1.84	0.41
1:A:203:VAL:HG11	1:A:206:TYR:CE1	2.55	0.41
1:A:243:GLU:N	4:A:1042:HOH:O	2.53	0.41
1:B:390:THR:HG23	1:B:390:THR:O	2.19	0.41
1:C:262:ALA:HA	1:C:382:GLY:CA	2.50	0.41
1:C:347:ALA:HB3	1:C:403:VAL:CG2	2.50	0.41
1:C:392:THR:HG21	1:C:397:ARG:NH2	2.08	0.41
1:C:392:THR:HG23	1:C:393:ALA:N	2.34	0.41
1:C:455:LEU:HD22	1:C:470:LEU:CD1	2.50	0.41
1:D:115:ARG:HG3	1:D:116:ALA:N	2.33	0.41
1:D:417:ALA:O	1:D:420:ALA:HB3	2.19	0.41
1:D:456:VAL:HG12	1:D:456:VAL:O	2.20	0.41
1:A:262:ALA:HA	1:A:382:GLY:O	2.20	0.41
1:C:273:VAL:HG13	1:C:378:TYR:CD2	2.55	0.41
1:C:483:LYS:HD3	1:C:498:VAL:O	2.19	0.41
1:C:487:ASP:N	1:C:488:PRO:HD3	2.35	0.41
1:D:226:PRO:HD2	1:D:325:TRP:CD1	2.56	0.41
1:D:274:PHE:CZ	1:D:284:ILE:HD12	2.56	0.41
1:B:146:PRO:HA	1:B:271:HIS:CD2	2.55	0.41
1:B:426:TYR:OH	1:B:437:PRO:HD3	2.20	0.41
1:D:130:CYS:HB2	1:D:133:VAL:HG23	2.01	0.41
1:D:232:HIS:HB2	1:D:288:ILE:HG12	2.02	0.41
1:D:273:VAL:HG22	1:D:378:TYR:HD2	1.85	0.41
1:D:414:HIS:HB3	4:D:970:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:NH2	1:B:91:ARG:NE	2.69	0.41
1:C:16:ARG:HE	1:C:17:VAL:HG22	1.85	0.41
1:C:290:ILE:HD13	1:C:300:LEU:HD13	2.03	0.41
1:C:448:ILE:HA	1:C:471:TYR:CE2	2.56	0.41
1:D:418:ASN:O	1:D:421:TRP:HB3	2.20	0.41
1:A:404:TRP:CE2	2:A:601[A]:AKY:H411	2.55	0.41
1:A:462:THR:HG22	1:A:465:VAL:O	2.21	0.41
2:A:601[A]:AKY:O5	2:A:601[A]:AKY:O6	2.38	0.41
1:B:95:TYR:CZ	1:B:218:PRO:HG3	2.55	0.41
1:B:350:ARG:HG2	1:B:398:ASP:O	2.20	0.41
1:C:323:GLU:OE1	1:C:327:ARG:NH1	2.54	0.41
1:C:486:TRP:C	1:C:488:PRO:HD3	2.41	0.41
1:A:171:ARG:NH1	1:A:173:ARG:NH2	2.69	0.41
1:B:165:VAL:HG22	1:B:175:VAL:HG13	2.02	0.41
1:C:124:THR:HG22	1:C:125:ILE:N	2.34	0.41
1:D:288:ILE:HD12	1:D:304:PHE:HD1	1.85	0.41
1:A:231:ARG:O	1:A:320:ARG:HA	2.21	0.41
1:A:248:ARG:HB3	4:A:967:HOH:O	2.19	0.41
1:A:350[A]:ARG:HH12	1:A:473:LYS:HZ1	1.67	0.41
1:B:140:LEU:HD22	1:B:196:GLY:CA	2.51	0.41
1:B:179:SER:HB3	1:B:189:TRP:CE2	2.55	0.41
1:B:384:VAL:O	1:B:397:ARG:HD2	2.20	0.41
1:C:15:ASP:O	1:C:39:VAL:HA	2.20	0.41
1:C:296:GLY:O	1:C:300:LEU:HG	2.21	0.41
1:C:448:ILE:CG2	1:C:471:TYR:HB3	2.51	0.41
1:D:96:ASP:HB3	1:D:207:TRP:HZ3	1.83	0.41
1:D:109:THR:HG23	1:D:131:PRO:O	2.21	0.41
1:D:117:LEU:HD12	1:D:117:LEU:HA	1.90	0.41
1:D:252:ASN:HB3	1:D:308:VAL:HA	2.03	0.41
1:D:312:THR:HG22	1:D:314:VAL:H	1.85	0.41
1:D:411:ASP:HA	1:D:412:PRO:HD2	1.82	0.41
1:D:438:VAL:HG13	1:D:439:PRO:HD2	2.03	0.41
1:A:49:VAL:O	1:A:53:VAL:HG23	2.21	0.41
1:A:93:VAL:HG13	1:A:103:ALA:O	2.20	0.41
1:A:283:GLN:N	1:A:283:GLN:HE21	2.19	0.41
1:C:226:PRO:O	1:D:19:ARG:NH2	2.53	0.41
1:A:104:VAL:O	1:A:104:VAL:HG23	2.22	0.40
1:A:130:CYS:HA	1:A:131:PRO:HD3	1.87	0.40
1:A:348:TYR:CD2	1:A:396:GLN:HG2	2.56	0.40
1:B:91:ARG:HD3	1:B:112:GLU:OE1	2.22	0.40
1:B:110:LEU:HD23	1:B:110:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:THR:HG23	1:B:193:THR:O	2.21	0.40
1:B:371:VAL:HG23	1:B:372:TRP:N	2.36	0.40
1:D:27:ARG:NH1	1:D:66:ARG:HD2	2.36	0.40
1:D:38:ASP:OD1	1:D:82:ARG:HD2	2.21	0.40
1:A:297:ALA:HA	1:A:300:LEU:CD1	2.45	0.40
1:B:124:THR:OG1	1:B:225:ALA:HB2	2.22	0.40
1:B:143:GLY:O	1:B:153:VAL:HG13	2.21	0.40
1:B:361:LEU:HD12	1:B:361:LEU:HA	1.93	0.40
1:C:98:GLY:HA3	4:C:978:HOH:O	2.22	0.40
1:C:359:ALA:HB1	1:C:363:ARG:NH1	2.36	0.40
1:C:371:VAL:HB	1:C:418:ASN:OD1	2.21	0.40
1:C:407:ALA:HB2	1:C:422:ILE:HG23	2.04	0.40
1:C:457:ASP:OD2	1:C:459:ARG:N	2.54	0.40
1:D:63:ILE:HA	1:D:83:ALA:O	2.21	0.40
1:D:364:HIS:O	1:D:421:TRP:HH2	2.04	0.40
1:D:433:THR:HG22	1:D:438:VAL:HG23	2.03	0.40
1:A:345:LYS:HD3	1:A:426:TYR:HB2	2.04	0.40
1:B:274:PHE:O	1:B:376:SER:HA	2.22	0.40
1:B:354:THR:H	1:B:357:GLN:HB2	1.85	0.40
1:C:278:SER:O	1:C:281:ALA:HB3	2.22	0.40
1:C:431:ALA:O	1:C:432:THR:HG22	2.21	0.40
1:A:109:THR:O	1:A:113:THR:HG23	2.21	0.40
1:A:149:ARG:NH2	1:A:270:MET:HE2	2.36	0.40
1:A:199:ASN:OD1	1:A:199:ASN:N	2.53	0.40
1:B:188:LEU:HD22	1:B:192:HIS:CE1	2.57	0.40
1:C:89:GLN:NE2	1:D:115:ARG:NH1	2.70	0.40
1:C:199:ASN:HD21	1:C:498:VAL:H	1.68	0.40
1:D:427:ARG:HA	1:D:435:GLY:HA2	2.02	0.40
1:D:470:LEU:HD23	1:D:470:LEU:HA	1.93	0.40
1:A:350[A]:ARG:NH1	1:A:444:GLU:HG2	2.36	0.40
1:A:472:TYR:O	1:A:475:ASN:HB2	2.22	0.40
1:B:140:LEU:HD22	1:B:196:GLY:C	2.41	0.40
1:C:129:VAL:CG2	1:C:146:PRO:HD3	2.43	0.40
1:C:448:ILE:HG23	4:C:900:HOH:O	2.22	0.40
1:D:354:THR:HG23	1:D:357:GLN:H	1.86	0.40

All (2) 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:481:LYS:CD	4:C:1070:HOH:O[2_655]	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ARG:NH2	4:B:820:HOH:O[1_554]	2.18	0.02

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 X-ray entries followed by that with respect to entries of similar resolution.

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	492/521 (94%)	459 (93%)	29 (6%)	4 (1%)	19	5
1	B	490/521 (94%)	456 (93%)	27 (6%)	7 (1%)	11	1
1	C	491/521 (94%)	449 (91%)	39 (8%)	3 (1%)	25	8
1	D	490/521 (94%)	448 (91%)	37 (8%)	5 (1%)	15	3
All	All	1963/2084 (94%)	1812 (92%)	132 (7%)	19 (1%)	15	3

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	ALA
1	B	195	GLY
1	B	214	THR
1	B	368	ASP
1	B	460	TRP
1	D	196	GLY
1	D	197	GLY
1	D	398	ASP
1	B	197	GLY
1	B	432	THR
1	A	261	SER
1	A	460	TRP
1	C	369	SER
1	D	214	THR
1	D	460	TRP
1	A	263	ALA

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Mol	Chain	Res	Type
1	B	462	THR
1	C	279	ARG
1	C	333	LYS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	391/408 (96%)	323 (83%)	68 (17%)	2 0
1	B	389/408 (95%)	323 (83%)	66 (17%)	2 0
1	C	390/408 (96%)	327 (84%)	63 (16%)	2 0
1	D	389/408 (95%)	323 (83%)	66 (17%)	2 0
All	All	1559/1632 (96%)	1296 (83%)	263 (17%)	2 0

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	13	LYS
1	A	15	ASP
1	A	16	ARG
1	A	19	ARG
1	A	22	GLN
1	A	24	LEU
1	A	30	ASN
1	A	84	VAL
1	A	85	ILE
1	A	87	MET
1	A	97	SER
1	A	99	LYS
1	A	109	THR
1	A	117	LEU
1	A	140	LEU
1	A	150	ARG
1	A	153	VAL

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Mol	Chain	Res	Type
1	A	167	ASP
1	A	171	ARG
1	A	173	ARG
1	A	174	LYS
1	A	178	THR
1	A	188	LEU
1	A	199	ASN
1	A	209	ARG
1	A	219	SER
1	A	224	LYS
1	A	233	ILE
1	A	235	THR
1	A	242	THR
1	A	244	GLU
1	A	260	ASN
1	A	274	PHE
1	A	283	GLN
1	A	286	LEU
1	A	288	ILE
1	A	294	LEU
1	A	300	LEU
1	A	302	ASN
1	A	315	GLU
1	A	332	ASN
1	A	336	THR
1	A	343	LYS
1	A	345	LYS
1	A	361	LEU
1	A	369	SER
1	A	371	VAL
1	A	372	TRP
1	A	374	GLU
1	A	396	GLN
1	A	402	LYS
1	A	403	VAL
1	A	411	ASP
1	A	425	ILE
1	A	429	ILE
1	A	433	THR
1	A	443	THR
1	A	448	ILE
1	A	453	VAL

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Mol	Chain	Res	Type
1	A	461	ASN
1	A	462	THR
1	A	463	SER
1	A	486	TRP
1	A	488	PRO
1	A	489	ARG
1	A	496	LEU
1	A	497	SER
1	B	12	VAL
1	B	15	ASP
1	B	16	ARG
1	B	18	ASP
1	B	23	ASP
1	B	24	LEU
1	B	30	ASN
1	B	84	VAL
1	B	85	ILE
1	B	87	MET
1	B	97	SER
1	B	99	LYS
1	B	109	THR
1	B	117	LEU
1	B	140	LEU
1	B	167	ASP
1	B	171	ARG
1	B	173	ARG
1	B	174	LYS
1	B	178	THR
1	B	188	LEU
1	B	209	ARG
1	B	235	THR
1	B	243	GLU
1	B	244	GLU
1	B	248	ARG
1	B	274	PHE
1	B	286	LEU
1	B	288	ILE
1	B	289	GLN
1	B	294	LEU
1	B	295	ASP
1	B	300	LEU
1	B	301	LEU

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Mol	Chain	Res	Type
1	B	302	ASN
1	B	310	GLU
1	B	315	GLU
1	B	321	SER
1	B	332	ASN
1	B	335	ASP
1	B	336	THR
1	B	350	ARG
1	B	361	LEU
1	B	364	HIS
1	B	369	SER
1	B	374	GLU
1	B	385	ASN
1	B	392	THR
1	B	396	GLN
1	B	402	LYS
1	B	405	MET
1	B	411	ASP
1	B	416	ASP
1	B	425	ILE
1	B	429	ILE
1	B	443	THR
1	B	448	ILE
1	B	453	VAL
1	B	454	ASP
1	B	462	THR
1	B	463	SER
1	B	478	ARG
1	B	486	TRP
1	B	489	ARG
1	B	496	LEU
1	B	497	SER
1	C	12	VAL
1	C	13	LYS
1	C	15	ASP
1	C	16	ARG
1	C	19	ARG
1	C	24	LEU
1	C	30	ASN
1	C	84	VAL
1	C	85	ILE
1	C	89	GLN

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Mol	Chain	Res	Type
1	C	91	ARG
1	C	109	THR
1	C	117	LEU
1	C	123	VAL
1	C	140	LEU
1	C	162	GLU
1	C	171	ARG
1	C	174	LYS
1	C	178	THR
1	C	188	LEU
1	C	190	TRP
1	C	203	VAL
1	C	209	ARG
1	C	233	ILE
1	C	235	THR
1	C	244	GLU
1	C	248	ARG
1	C	258	GLN
1	C	259	SER
1	C	261	SER
1	C	269	SER
1	C	274	PHE
1	C	286	LEU
1	C	300	LEU
1	C	302	ASN
1	C	310	GLU
1	C	315	GLU
1	C	319	GLN
1	C	332	ASN
1	C	336	THR
1	C	345	LYS
1	C	361	LEU
1	C	369	SER
1	C	374	GLU
1	C	392	THR
1	C	396	GLN
1	C	402	LYS
1	C	411	ASP
1	C	414	HIS
1	C	416	ASP
1	C	425	ILE
1	C	427	ARG

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Mol	Chain	Res	Type
1	C	429	ILE
1	C	433	THR
1	C	440[A]	ASP
1	C	440[B]	ASP
1	C	441	ASP
1	C	443	THR
1	C	448	ILE
1	C	453	VAL
1	C	462	THR
1	C	496	LEU
1	C	497	SER
1	D	12	VAL
1	D	13	LYS
1	D	16	ARG
1	D	17	VAL
1	D	22	GLN
1	D	29	PHE
1	D	30	ASN
1	D	34	ARG
1	D	84	VAL
1	D	85	ILE
1	D	89	GLN
1	D	91	ARG
1	D	97	SER
1	D	109	THR
1	D	117	LEU
1	D	140	LEU
1	D	167	ASP
1	D	171	ARG
1	D	173	ARG
1	D	174	LYS
1	D	178	THR
1	D	188	LEU
1	D	190	TRP
1	D	209	ARG
1	D	220	GLN
1	D	235	THR
1	D	237	ASP
1	D	243	GLU
1	D	248	ARG
1	D	261	SER
1	D	274	PHE

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Mol	Chain	Res	Type
1	D	286	LEU
1	D	288	ILE
1	D	300	LEU
1	D	302	ASN
1	D	310	GLU
1	D	312	THR
1	D	315	GLU
1	D	319	GLN
1	D	320	ARG
1	D	323	GLU
1	D	327	ARG
1	D	332	ASN
1	D	336	THR
1	D	345	LYS
1	D	350	ARG
1	D	354	THR
1	D	371	VAL
1	D	374	GLU
1	D	383	LYS
1	D	396	GLN
1	D	402	LYS
1	D	411	ASP
1	D	422	ILE
1	D	425	ILE
1	D	427	ARG
1	D	429	ILE
1	D	432	THR
1	D	440	ASP
1	D	443	THR
1	D	448	ILE
1	D	453	VAL
1	D	462	THR
1	D	478	ARG
1	D	496	LEU
1	D	497	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	253	HIS
1	A	283	GLN

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Mol	Chain	Res	Type
1	A	319	GLN
1	A	332	ASN
1	A	357	GLN
1	A	364	HIS
1	A	370	GLN
1	A	396	GLN
1	A	494	HIS
1	B	30	ASN
1	B	89	GLN
1	B	220	GLN
1	B	253	HIS
1	B	260	ASN
1	B	283	GLN
1	B	332	ASN
1	B	357	GLN
1	B	364	HIS
1	B	396	GLN
1	B	494	HIS
1	C	30	ASN
1	C	89	GLN
1	C	199	ASN
1	C	220	GLN
1	C	253	HIS
1	C	309	ASN
1	C	357	GLN
1	C	364	HIS
1	C	396	GLN
1	C	494	HIS
1	D	30	ASN
1	D	89	GLN
1	D	271	HIS
1	D	283	GLN
1	D	289	GLN
1	D	319	GLN
1	D	357	GLN
1	D	396	GLN
1	D	418	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	FAD	C	801	1	54,58,58	1.79	14 (25%)	71,89,89	2.09	23 (32%)
2	AKY	A	601[A]	-	62,64,64	1.97	16 (25%)	87,98,98	1.96	22 (25%)
3	FAD	B	801	1	54,58,58	1.88	15 (27%)	71,89,89	1.88	19 (26%)
3	FAD	D	801	1	54,58,58	1.94	22 (40%)	71,89,89	1.84	16 (22%)
3	FAD	A	801	1	54,58,58	1.64	9 (16%)	71,89,89	1.81	17 (23%)

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	FAD	C	801	1	-	12/30/50/50	0/6/6/6
2	AKY	A	601[A]	-	7/7/18/18	6/25/105/105	0/7/7/7
3	FAD	B	801	1	1/1/9/9	10/30/50/50	0/6/6/6
3	FAD	D	801	1	-	11/30/50/50	0/6/6/6
3	FAD	A	801	1	-	9/30/50/50	0/6/6/6

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601[A]	AKY	C32-C33	-6.61	1.40	1.52
2	A	601[A]	AKY	C41-C39	-5.28	1.34	1.51
3	A	801	FAD	O2-C2	-4.35	1.15	1.24
2	A	601[A]	AKY	O12-C33	4.30	1.52	1.43
3	B	801	FAD	P-O1P	-4.13	1.36	1.50
3	A	801	FAD	C4A-N3A	-3.92	1.30	1.35
2	A	601[A]	AKY	O11-C31	3.91	1.52	1.42
2	A	601[A]	AKY	C32-C31	-3.80	1.41	1.50
3	D	801	FAD	O2-C2	-3.80	1.16	1.24
2	A	601[A]	AKY	O11-C34	3.73	1.53	1.44
3	B	801	FAD	P-O3P	-3.72	1.55	1.59
3	C	801	FAD	P-O1P	-3.64	1.38	1.50
3	B	801	FAD	O2-C2	-3.62	1.17	1.24
3	B	801	FAD	C4A-N3A	-3.49	1.30	1.35
3	C	801	FAD	P-O3P	3.47	1.63	1.59
3	D	801	FAD	P-O1P	-3.41	1.39	1.50
2	A	601[A]	AKY	C36-C34	-3.39	1.43	1.51
3	D	801	FAD	C4X-N5	3.32	1.37	1.30
3	B	801	FAD	PA-O3P	-3.31	1.55	1.59
2	A	601[A]	AKY	C18-C12	-3.29	1.41	1.48
2	A	601[A]	AKY	O9-C9	-3.26	1.39	1.44
3	A	801	FAD	P-O2P	-3.25	1.40	1.55
3	D	801	FAD	C5'-C4'	3.23	1.56	1.51
3	C	801	FAD	C6-C7	-3.21	1.35	1.39
3	D	801	FAD	O2'-C2'	-3.12	1.36	1.43
2	A	601[A]	AKY	C15-C12	-3.12	1.42	1.48
3	B	801	FAD	O4'-C4'	-3.09	1.36	1.43
3	B	801	FAD	O4B-C4B	-3.05	1.38	1.45
3	B	801	FAD	PA-O2A	-3.04	1.41	1.55
3	D	801	FAD	C9-C8	-3.03	1.35	1.39
3	C	801	FAD	C4A-N3A	-2.99	1.31	1.35
3	D	801	FAD	O4B-C4B	-2.97	1.38	1.45
3	C	801	FAD	PA-O2A	-2.91	1.41	1.55
3	B	801	FAD	C4X-N5	2.89	1.37	1.30
3	D	801	FAD	PA-O1A	-2.88	1.40	1.50
3	D	801	FAD	C8A-N7A	-2.88	1.29	1.34
3	D	801	FAD	P-O3P	-2.83	1.56	1.59
3	A	801	FAD	C4X-N5	2.82	1.36	1.30
3	A	801	FAD	O4'-C4'	-2.80	1.37	1.43
3	C	801	FAD	O2-C2	-2.78	1.18	1.24
3	B	801	FAD	PA-O1A	-2.76	1.41	1.50
2	A	601[A]	AKY	C40-C42	2.73	1.55	1.50
3	B	801	FAD	O2'-C2'	-2.72	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	FAD	PA-O1A	-2.69	1.41	1.50
3	C	801	FAD	PA-O1A	-2.68	1.41	1.50
3	D	801	FAD	C2'-C3'	-2.64	1.48	1.53
2	A	601[A]	AKY	C16-C5	-2.59	1.41	1.47
3	B	801	FAD	C2A-N3A	2.50	1.36	1.32
2	A	601[A]	AKY	C17-C5	-2.47	1.41	1.47
3	A	801	FAD	P-O1P	-2.46	1.42	1.50
3	A	801	FAD	C10-N1	2.42	1.38	1.33
3	C	801	FAD	C5X-N5	-2.42	1.35	1.39
3	D	801	FAD	C9A-C5X	-2.41	1.37	1.41
3	D	801	FAD	C1'-C2'	-2.39	1.49	1.52
2	A	601[A]	AKY	C38-C40	-2.36	1.47	1.53
3	D	801	FAD	C6-C5X	-2.36	1.36	1.40
3	C	801	FAD	C4X-N5	2.35	1.35	1.30
3	D	801	FAD	C9A-N10	-2.34	1.37	1.41
3	C	801	FAD	O3'-C3'	-2.33	1.37	1.43
3	D	801	FAD	C6-C7	-2.28	1.36	1.39
3	C	801	FAD	P-O2P	-2.27	1.44	1.55
3	D	801	FAD	O4'-C4'	-2.24	1.38	1.43
3	C	801	FAD	O2'-C2'	-2.20	1.38	1.43
3	C	801	FAD	C10-N1	2.19	1.37	1.33
3	B	801	FAD	C6-C7	-2.19	1.36	1.39
3	B	801	FAD	P-O2P	-2.18	1.45	1.55
3	D	801	FAD	C9-C9A	-2.17	1.36	1.39
3	D	801	FAD	PA-O2A	-2.14	1.45	1.55
3	C	801	FAD	C9A-C5X	-2.11	1.37	1.41
3	D	801	FAD	C5X-N5	-2.11	1.35	1.39
3	B	801	FAD	O5B-C5B	-2.08	1.36	1.44
3	D	801	FAD	O2B-C2B	-2.06	1.37	1.43
3	D	801	FAD	C4X-C10	-2.06	1.38	1.44
2	A	601[A]	AKY	C8-C7	-2.05	1.48	1.52
2	A	601[A]	AKY	C8-C9	-2.01	1.51	1.53
3	A	801	FAD	O4B-C4B	-2.00	1.40	1.45

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	801	FAD	O4B-C1B-N9A	6.68	117.61	108.75
3	B	801	FAD	N3A-C2A-N1A	-6.39	120.00	128.67
2	A	601[A]	AKY	O19-C49-C50	6.35	120.83	106.74
3	C	801	FAD	N3A-C2A-N1A	-6.20	120.26	128.67
3	D	801	FAD	N3A-C2A-N1A	-6.00	120.53	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	FAD	C4'-C3'-C2'	-5.73	104.03	113.57
2	A	601[A]	AKY	C14-C13-C9	-5.16	104.45	115.05
2	A	601[A]	AKY	O17-C43-C10	5.14	120.63	110.74
3	B	801	FAD	C5'-C4'-C3'	5.05	121.75	112.22
2	A	601[A]	AKY	C45-O19-C49	5.04	127.64	113.82
3	B	801	FAD	O4B-C1B-N9A	4.80	115.12	108.75
2	A	601[A]	AKY	C50-C49-C48	4.79	120.53	113.39
3	C	801	FAD	C9A-C5X-N5	-4.65	117.52	122.45
3	B	801	FAD	C4'-C3'-C2'	-4.52	106.05	113.57
3	D	801	FAD	O5'-C5'-C4'	4.49	121.35	109.36
3	D	801	FAD	O4-C4-C4X	-4.43	114.85	126.53
3	C	801	FAD	C5X-C9A-N10	4.40	121.94	117.97
3	C	801	FAD	C4A-C5A-N7A	-4.36	104.73	109.34
2	A	601[A]	AKY	O18-C31-C32	4.04	116.05	108.28
3	A	801	FAD	N3A-C2A-N1A	-4.03	123.21	128.67
3	A	801	FAD	C5'-C4'-C3'	3.90	119.58	112.22
3	D	801	FAD	C10-N1-C2	3.88	125.25	116.85
3	D	801	FAD	C4X-C4-N3	3.87	123.10	113.25
3	C	801	FAD	O3'-C3'-C2'	3.80	117.56	108.93
3	A	801	FAD	C9A-C5X-N5	-3.72	118.50	122.45
3	A	801	FAD	O3'-C3'-C4'	3.71	117.36	108.93
2	A	601[A]	AKY	C44-O17-C43	-3.65	107.63	115.92
3	D	801	FAD	C4-N3-C2	-3.62	119.21	125.64
3	B	801	FAD	C4X-C10-N10	3.56	121.58	116.48
3	A	801	FAD	O4B-C1B-N9A	3.54	113.44	108.75
2	A	601[A]	AKY	O5-C5-C17	-3.47	115.65	121.44
3	D	801	FAD	C4-C4X-N5	3.42	122.93	118.21
3	B	801	FAD	C4-C4X-N5	3.30	122.77	118.21
3	B	801	FAD	C10-C4X-N5	-3.21	118.26	124.81
2	A	601[A]	AKY	O14-C37-C38	3.18	118.01	111.23
2	A	601[A]	AKY	O17-C43-O16	-3.09	117.84	123.85
2	A	601[A]	AKY	O14-C39-C42	3.03	114.77	111.48
2	A	601[A]	AKY	O12-C33-C35	3.02	117.05	109.99
3	C	801	FAD	C4-N3-C2	-2.95	120.40	125.64
3	A	801	FAD	O2A-PA-O3P	2.93	115.20	107.27
2	A	601[A]	AKY	O11-C34-C35	2.92	114.60	109.19
3	B	801	FAD	N6A-C6A-N1A	2.91	124.55	118.33
2	A	601[A]	AKY	O9-C9-C13	2.90	114.62	107.86
2	A	601[A]	AKY	O15-C42-C40	-2.88	117.01	122.13
3	C	801	FAD	C4B-O4B-C1B	2.87	112.55	109.92
3	A	801	FAD	C5X-C9A-N10	2.87	120.56	117.97
3	D	801	FAD	O4B-C1B-N9A	2.84	112.51	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601[A]	AKY	C48-C47-N11	2.84	120.76	111.75
3	D	801	FAD	C1'-N10-C9A	-2.79	115.20	120.63
3	D	801	FAD	O3P-PA-O1A	-2.79	102.31	110.70
3	C	801	FAD	O4-C4-C4X	-2.79	119.18	126.53
3	C	801	FAD	C1'-C2'-C3'	2.75	117.10	109.66
3	D	801	FAD	C1'-C2'-C3'	2.74	117.09	109.66
3	A	801	FAD	C10-C4X-N5	-2.74	119.22	124.81
3	B	801	FAD	O5B-C5B-C4B	2.70	118.17	108.99
3	C	801	FAD	O2A-PA-O3P	2.69	114.53	107.27
3	A	801	FAD	O4'-C4'-C3'	2.69	115.53	109.25
3	A	801	FAD	C4-C4X-N5	2.68	121.91	118.21
3	D	801	FAD	O3'-C3'-C4'	2.66	114.98	108.93
3	C	801	FAD	O3'-C3'-C4'	2.58	114.79	108.93
3	A	801	FAD	O4'-C4'-C5'	-2.56	104.33	109.99
3	B	801	FAD	C4-N3-C2	-2.56	121.10	125.64
3	B	801	FAD	O4-C4-C4X	-2.52	119.89	126.53
3	B	801	FAD	C9A-C9-C8	2.51	124.26	119.22
3	C	801	FAD	C5A-C6A-N6A	2.47	124.08	120.31
2	A	601[A]	AKY	C46-C47-N11	2.44	122.45	115.59
3	D	801	FAD	C5X-C9A-N10	2.41	120.15	117.97
3	B	801	FAD	O3B-C3B-C4B	-2.41	104.16	111.08
3	D	801	FAD	C4X-C10-N1	-2.40	118.70	124.59
3	B	801	FAD	O3B-C3B-C2B	-2.40	104.12	111.82
3	A	801	FAD	C4X-C10-N10	2.39	119.91	116.48
3	B	801	FAD	C5A-C6A-N6A	-2.37	116.70	120.31
2	A	601[A]	AKY	O13-C35-C34	2.37	112.81	106.77
3	A	801	FAD	C10-N1-C2	2.36	121.96	116.85
3	B	801	FAD	C10-N1-C2	2.35	121.93	116.85
3	A	801	FAD	C4X-C4-N3	2.34	119.22	113.25
3	A	801	FAD	C5X-N5-C4X	2.32	121.84	118.09
3	D	801	FAD	C10-C4X-N5	-2.29	120.13	124.81
3	C	801	FAD	C4X-C4-N3	2.28	119.05	113.25
3	D	801	FAD	O2A-PA-O3P	2.25	113.36	107.27
2	A	601[A]	AKY	C52-N11-C47	2.23	119.57	113.15
2	A	601[A]	AKY	O12-C33-C32	2.22	115.39	109.86
3	B	801	FAD	C4X-C10-N1	-2.21	119.17	124.59
3	B	801	FAD	C9-C9A-N10	2.21	124.82	121.85
3	C	801	FAD	O3B-C3B-C4B	-2.20	104.77	111.08
3	C	801	FAD	C5X-N5-C4X	2.19	121.64	118.09
2	A	601[A]	AKY	O16-C43-C10	-2.19	121.53	125.22
3	C	801	FAD	C2'-C1'-N10	2.14	120.30	110.20
3	B	801	FAD	C4X-C4-N3	2.11	118.63	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	FAD	C9A-C9-C8	2.09	123.42	119.22
2	A	601[A]	AKY	C9-C8-C7	-2.08	110.40	114.58
3	C	801	FAD	C1B-N9A-C4A	-2.07	123.00	126.64
3	C	801	FAD	C6-C5X-N5	2.07	121.88	118.44
3	C	801	FAD	O2P-P-O3P	2.06	112.84	107.27
3	C	801	FAD	O5'-C5'-C4'	2.05	114.83	109.36
3	C	801	FAD	C4-C4X-C10	2.04	120.43	116.93
3	C	801	FAD	C4X-C10-N10	2.00	119.35	116.48

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601[A]	AKY	C34
2	A	601[A]	AKY	C37
2	A	601[A]	AKY	C35
2	A	601[A]	AKY	C33
2	A	601[A]	AKY	C39
2	A	601[A]	AKY	C31
2	A	601[A]	AKY	C49
3	B	801	FAD	C2'

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601[A]	AKY	C10-C43-O17-C44
2	A	601[A]	AKY	C46-C47-N11-C51
2	A	601[A]	AKY	C48-C47-N11-C52
3	A	801	FAD	N10-C1'-C2'-O2'
3	A	801	FAD	N10-C1'-C2'-C3'
3	A	801	FAD	C2'-C3'-C4'-C5'
3	A	801	FAD	O3'-C3'-C4'-C5'
3	A	801	FAD	C5'-O5'-P-O2P
3	B	801	FAD	C5B-O5B-PA-O1A
3	B	801	FAD	C5B-O5B-PA-O3P
3	C	801	FAD	N10-C1'-C2'-O2'
3	D	801	FAD	C1'-C2'-C3'-O3'
3	D	801	FAD	C1'-C2'-C3'-C4'
3	D	801	FAD	O2'-C2'-C3'-O3'
3	D	801	FAD	C3'-C4'-C5'-O5'
3	D	801	FAD	O4'-C4'-C5'-O5'
3	D	801	FAD	C5'-O5'-P-O2P
2	A	601[A]	AKY	O16-C43-O17-C44

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Mol	Chain	Res	Type	Atoms
3	A	801	FAD	O3'-C3'-C4'-O4'
3	C	801	FAD	O3'-C3'-C4'-O4'
3	A	801	FAD	C2'-C3'-C4'-O4'
3	D	801	FAD	O2'-C2'-C3'-C4'
3	C	801	FAD	O3'-C3'-C4'-C5'
2	A	601[A]	AKY	C48-C47-N11-C51
3	B	801	FAD	O2'-C2'-C3'-C4'
3	C	801	FAD	O2'-C2'-C3'-C4'
3	B	801	FAD	O2'-C2'-C3'-O3'
3	B	801	FAD	C3'-C4'-C5'-O5'
3	C	801	FAD	C3'-C4'-C5'-O5'
3	C	801	FAD	P-O3P-PA-O1A
3	D	801	FAD	P-O3P-PA-O5B
3	C	801	FAD	C2'-C3'-C4'-C5'
2	A	601[A]	AKY	C46-C47-N11-C52
3	C	801	FAD	N10-C1'-C2'-C3'
3	A	801	FAD	C5'-O5'-P-O1P
3	C	801	FAD	C5B-O5B-PA-O1A
3	C	801	FAD	C5B-O5B-PA-O2A
3	C	801	FAD	C5B-O5B-PA-O3P
3	D	801	FAD	C5'-O5'-P-O1P
3	D	801	FAD	C5'-O5'-P-O3P
3	D	801	FAD	C2'-C3'-C4'-O4'
3	B	801	FAD	C3B-C4B-C5B-O5B
3	B	801	FAD	C2'-C3'-C4'-C5'
3	C	801	FAD	P-O3P-PA-O2A
3	B	801	FAD	C1'-C2'-C3'-O3'
3	A	801	FAD	PA-O3P-P-O2P
3	B	801	FAD	O4B-C4B-C5B-O5B
3	B	801	FAD	O4'-C4'-C5'-O5'

There are no ring outliers.

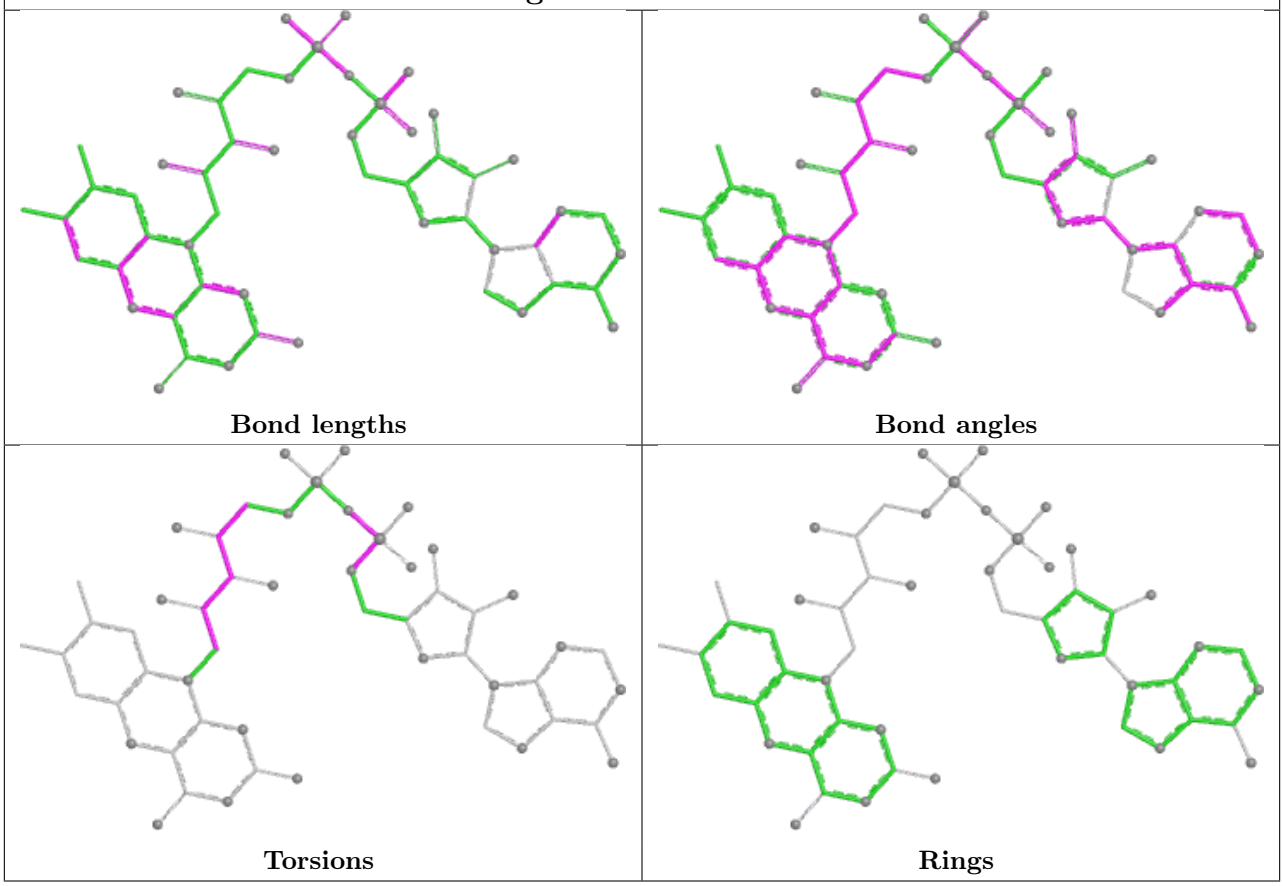
5 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	801	FAD	9	0
2	A	601[A]	AKY	13	0
3	B	801	FAD	9	0
3	D	801	FAD	12	0
3	A	801	FAD	3	0

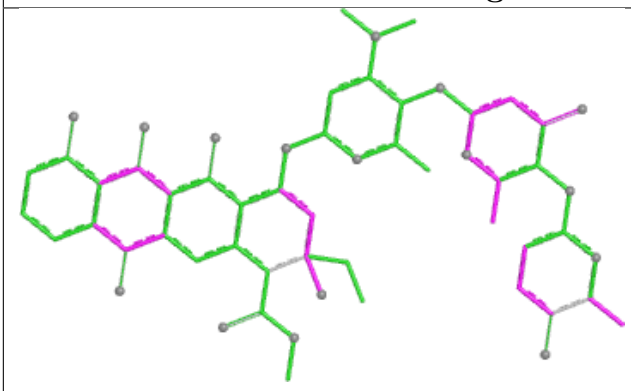
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

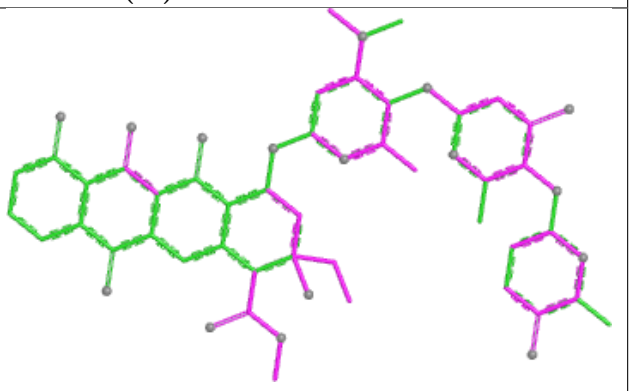
Ligand FAD C 801



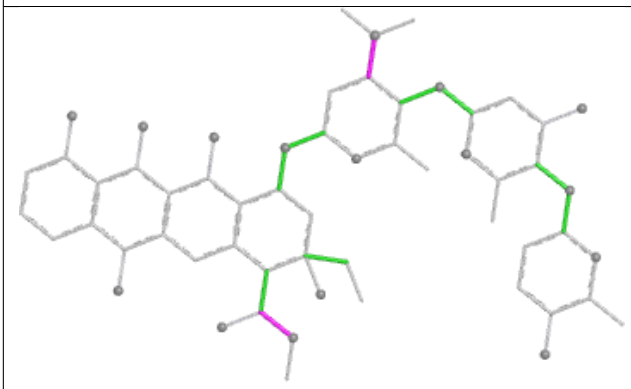
Ligand AKY A 601 (A)



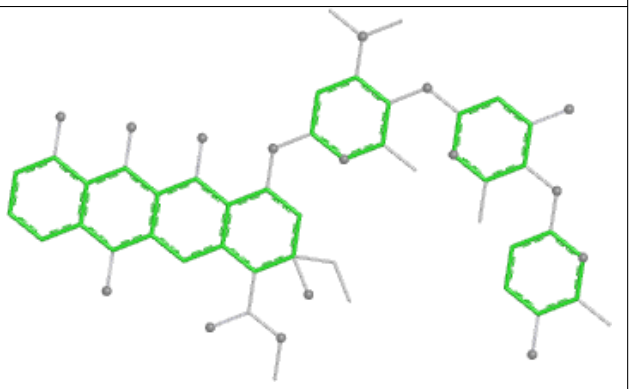
Bond lengths



Bond angles

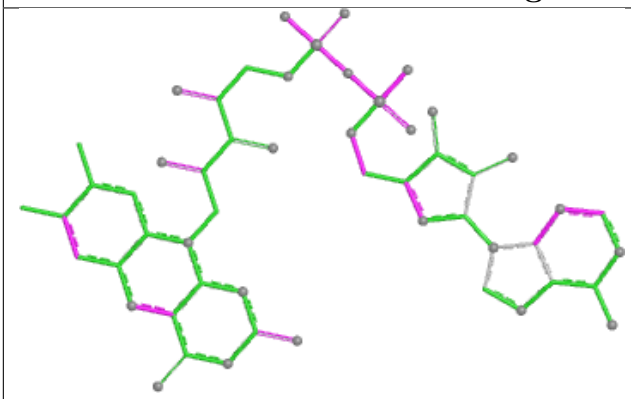


Torsions

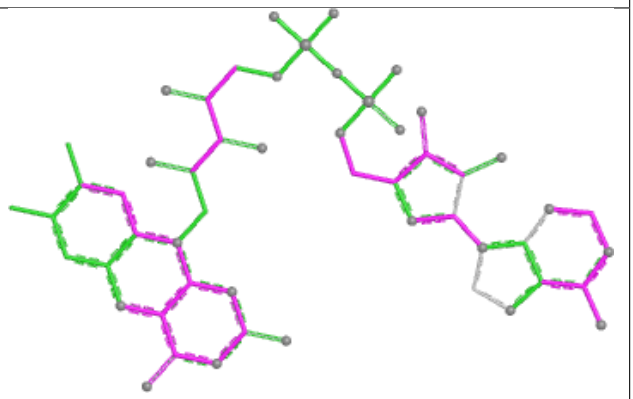


Rings

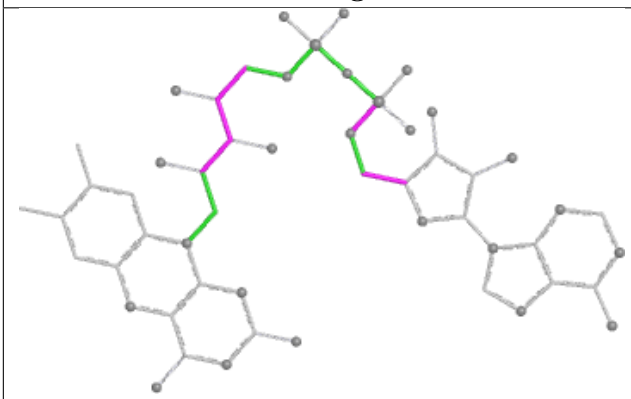
Ligand FAD B 801



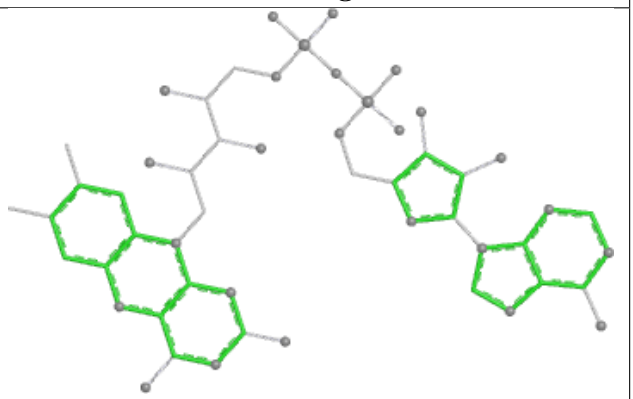
Bond lengths



Bond angles

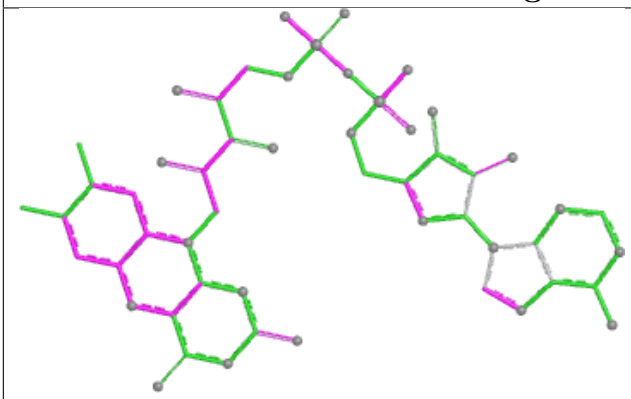


Torsions

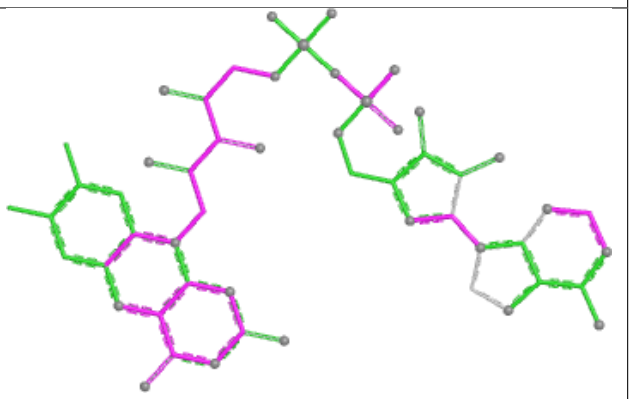


Rings

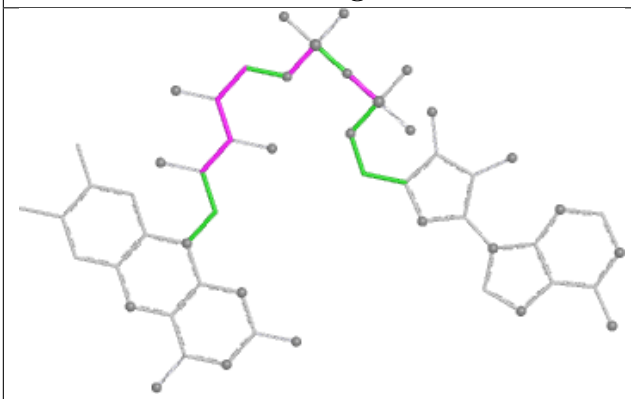
Ligand FAD D 801



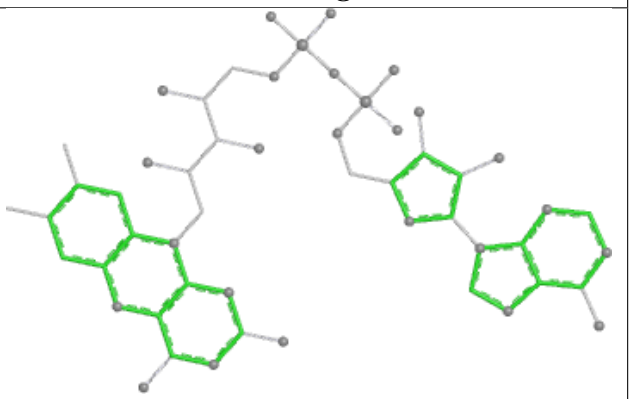
Bond lengths



Bond angles

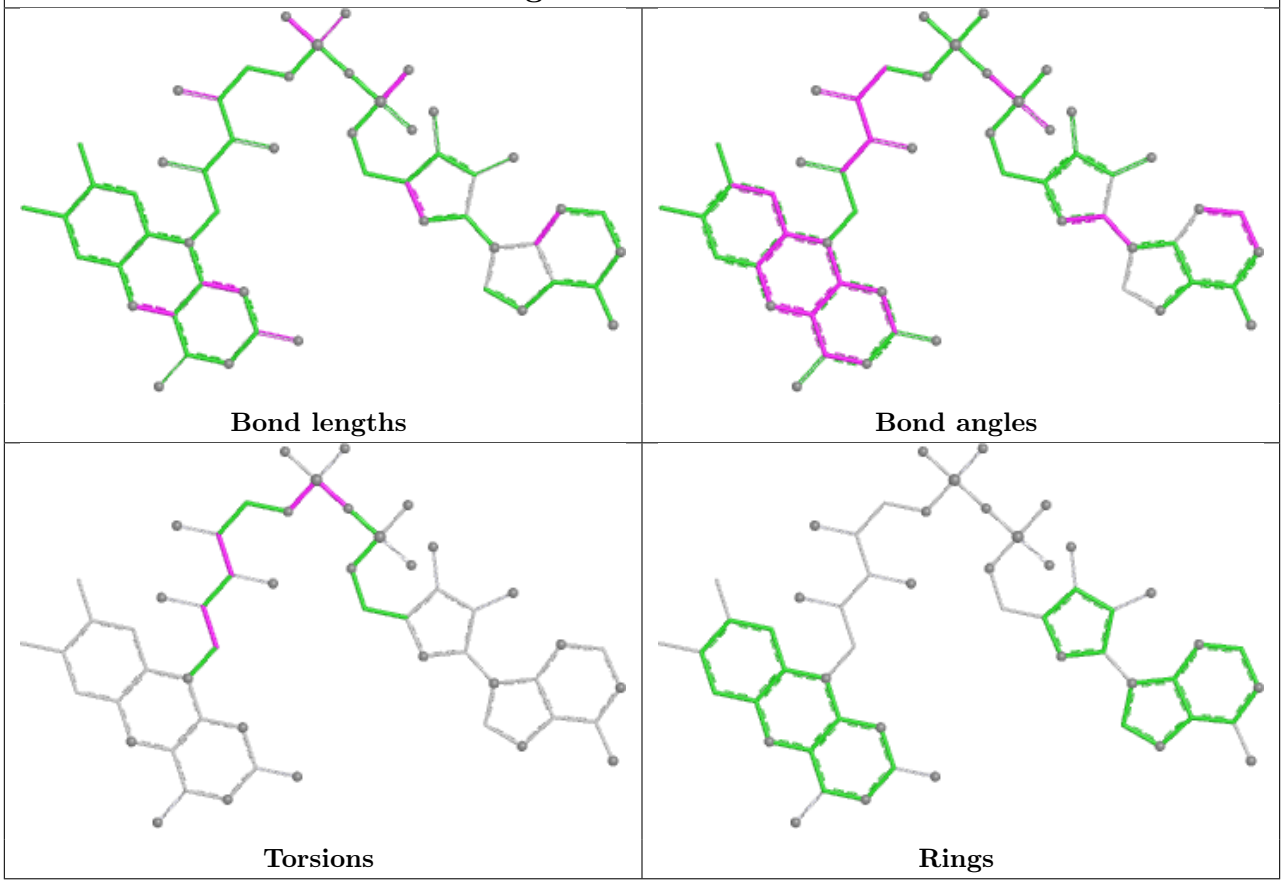


Torsions



Rings

Ligand FAD A 801



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	492/521 (94%)	-0.37	4 (0%)	86	88	3, 16, 31, 39	14 (2%)
1	B	492/521 (94%)	-0.36	6 (1%)	79	81	7, 17, 30, 39	14 (2%)
1	C	492/521 (94%)	-0.40	3 (0%)	89	90	7, 16, 30, 40	12 (2%)
1	D	492/521 (94%)	-0.33	7 (1%)	75	79	4, 17, 32, 43	15 (3%)
All	All	1968/2084 (94%)	-0.37	20 (1%)	82	85	3, 16, 31, 43	55 (2%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	17	VAL	4.2
1	D	263	ALA	3.8
1	D	212	GLY	3.3
1	B	17	VAL	3.3
1	B	460	TRP	3.1
1	B	212	GLY	3.1
1	A	17	VAL	3.0
1	A	212	GLY	2.9
1	D	261	SER	2.8
1	B	332	ASN	2.7
1	D	460	TRP	2.4
1	C	332	ASN	2.4
1	A	262	ALA	2.3
1	A	462	THR	2.3
1	B	461	ASN	2.2
1	C	460	TRP	2.2
1	D	332	ASN	2.1
1	C	294	LEU	2.1
1	D	421	TRP	2.0
1	B	421	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

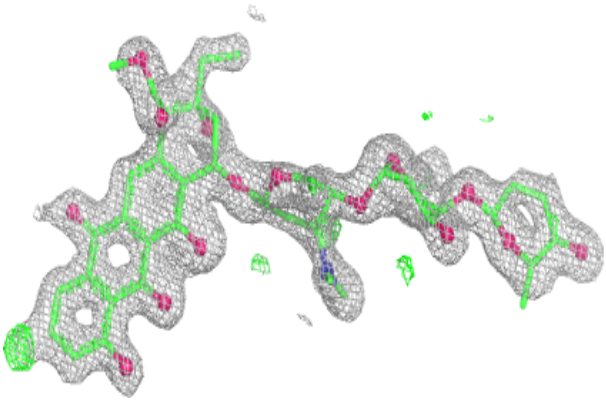
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

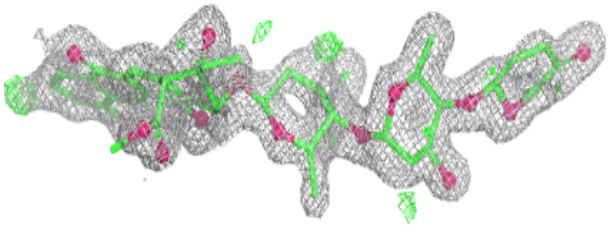
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AKY	A	601[A]	58/58	0.88	0.12	10,20,34,38	58
3	FAD	A	801	53/53	0.97	0.07	7,14,19,24	0
3	FAD	B	801	53/53	0.97	0.07	4,14,23,36	0
3	FAD	C	801	53/53	0.97	0.07	3,11,25,37	0
3	FAD	D	801	53/53	0.98	0.06	4,11,26,42	0

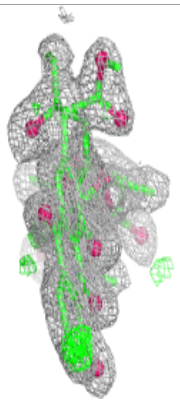
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AKY A 601 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

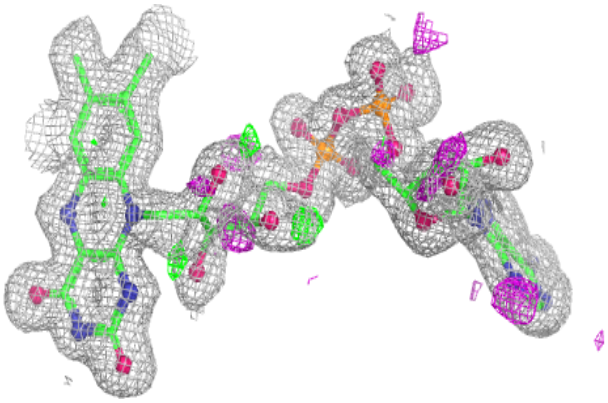


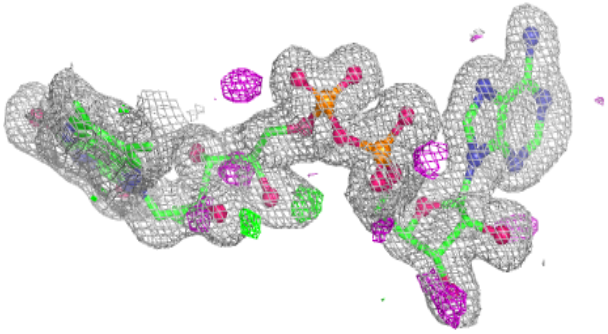


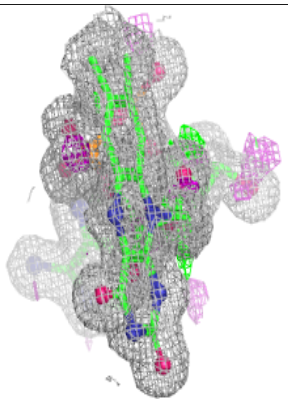


Electron density around FAD A 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

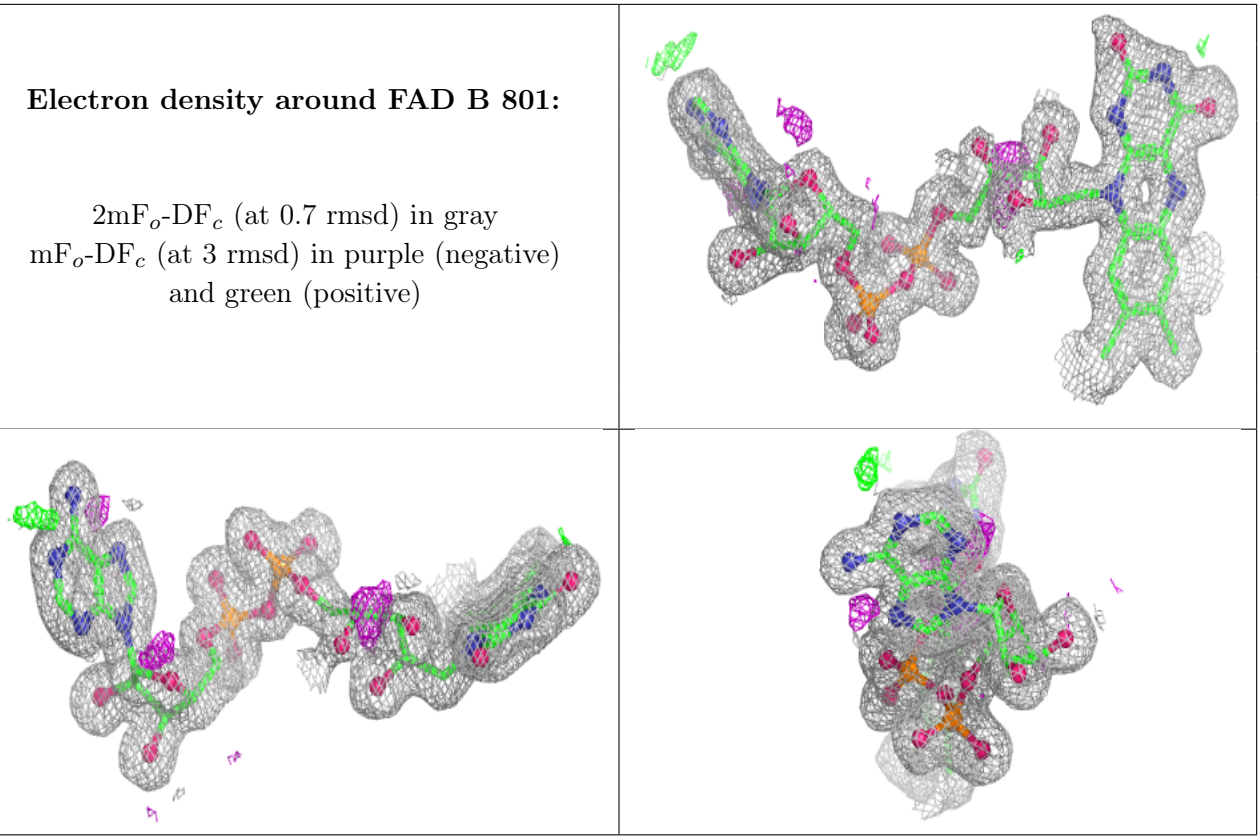






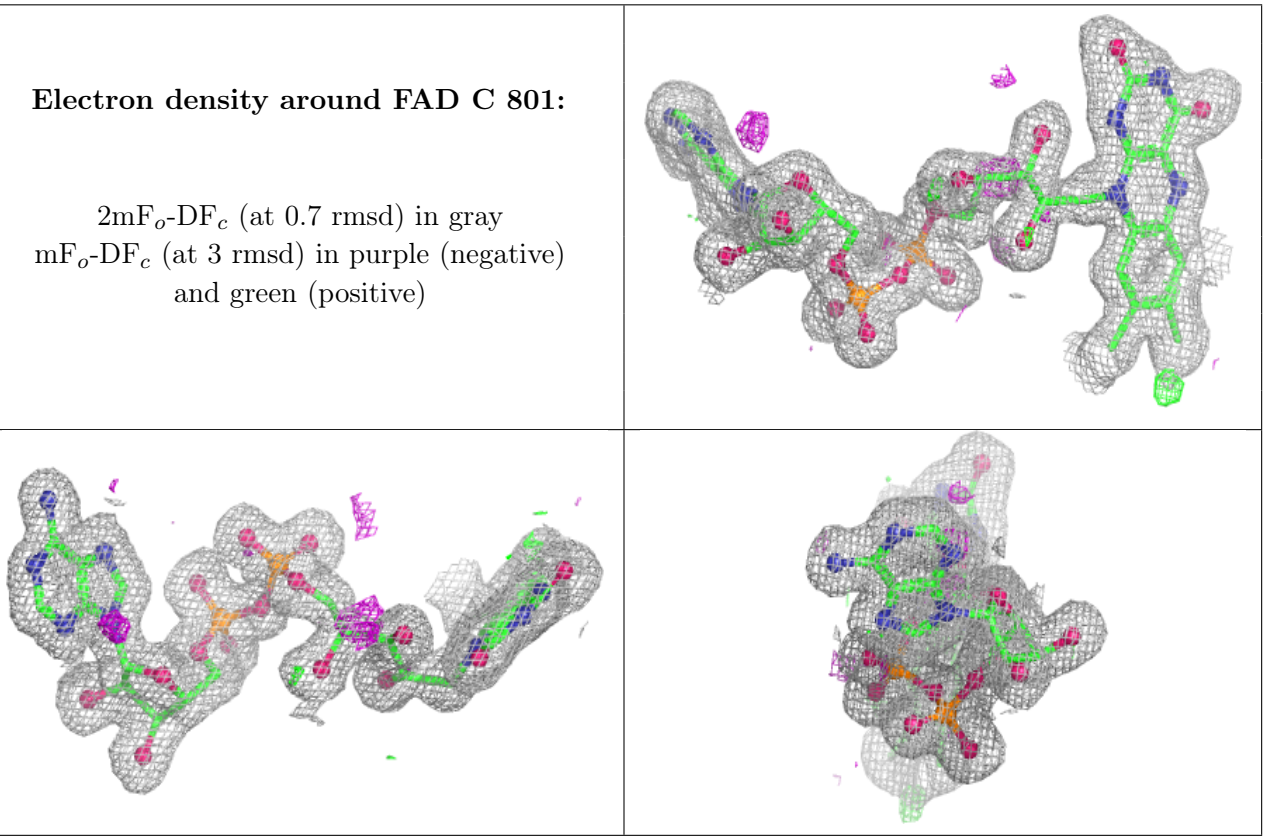
Electron density around FAD B 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



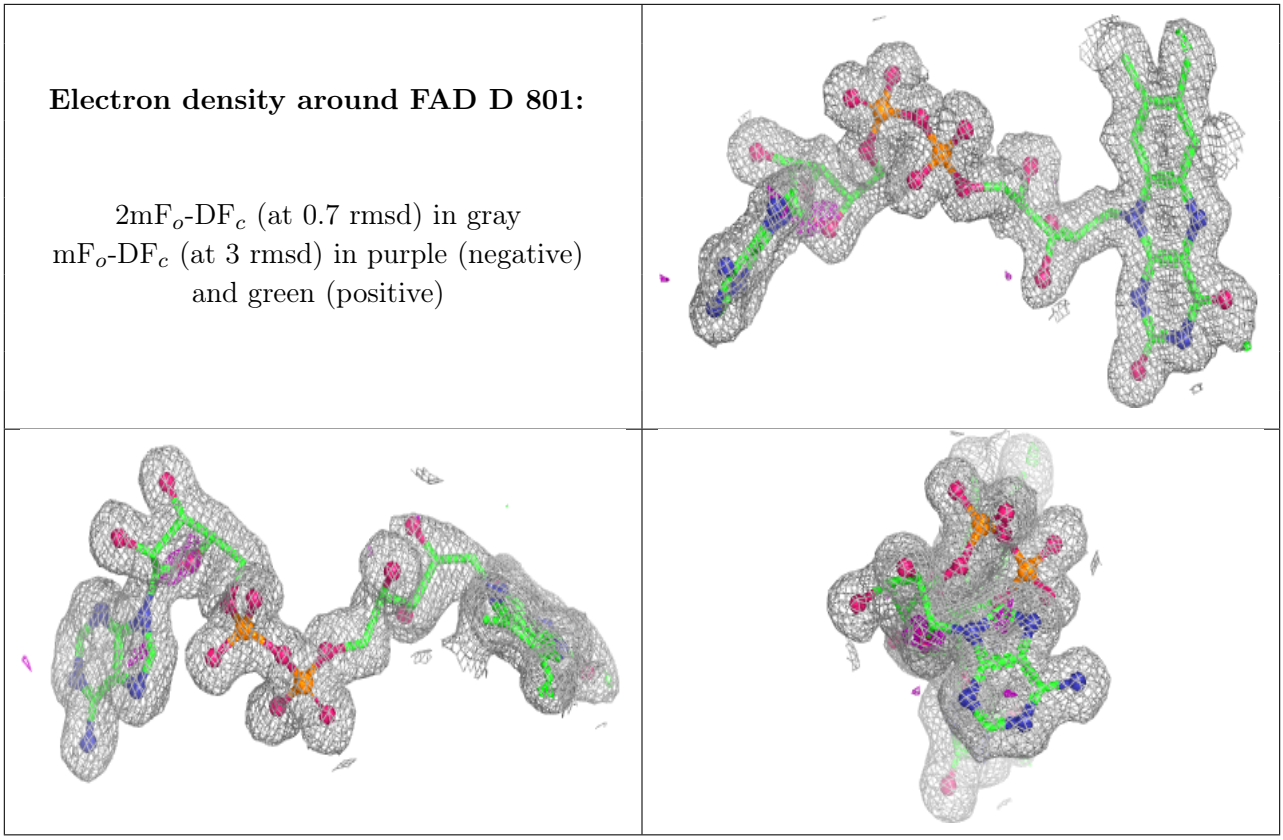
Electron density around FAD C 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FAD D 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.