



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 18, 2017 – 12:50 AM EST

PDB ID : 5TWV
EMDB ID: : EMD-8470
Title : Cryo-EM structure of the pancreatic ATP-sensitive K⁺ channel SUR1/Kir6.2
in the presence of ATP and glibenclamide
Authors : Martin, G.M.; Yoshioka, C.; Chen, J.Z.; Shyng, S.L.
Deposited on : 2016-11-14
Resolution : 6.30 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

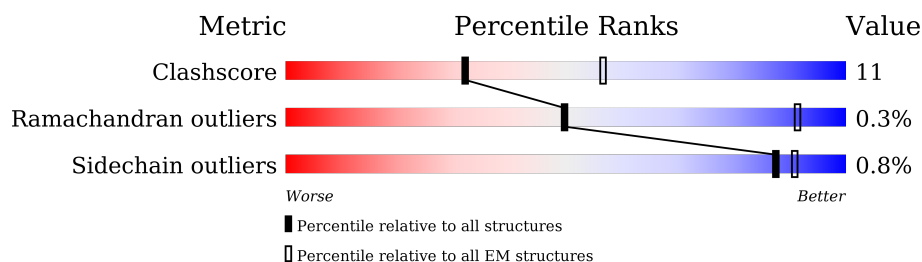
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	390	
1	C	390	
1	E	390	
1	G	390	
2	B	1590	
2	D	1590	
2	F	1590	
2	H	1590	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41080 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	325	Total	C	N	O	S	0	0
			2479	1598	422	444	15		
1	C	325	Total	C	N	O	S	0	0
			2479	1598	422	444	15		
1	E	325	Total	C	N	O	S	0	0
			2479	1598	422	444	15		
1	G	325	Total	C	N	O	S	0	0
			2479	1598	422	444	15		

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1375	Total	C	N	O	S	0	0
			7760	4866	1450	1439	5		
2	D	1375	Total	C	N	O	S	0	0
			7760	4866	1450	1439	5		
2	F	1375	Total	C	N	O	S	0	0
			7760	4866	1450	1439	5		
2	H	1375	Total	C	N	O	S	0	0
			7760	4866	1450	1439	5		

There are 32 discrepancies between the modelled and reference sequences:

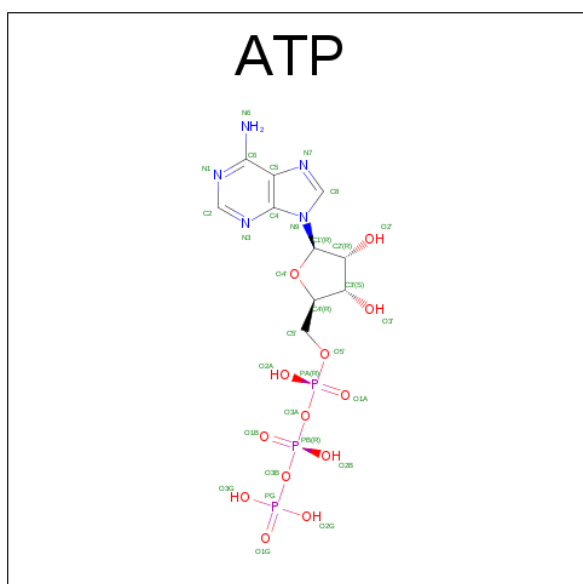
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	ASP	-	expression tag	UNP Q09427
B	-6	TYR	-	expression tag	UNP Q09427
B	-5	LYS	-	expression tag	UNP Q09427
B	-4	ASP	-	expression tag	UNP Q09427
B	-3	ASP	-	expression tag	UNP Q09427
B	-2	ASP	-	expression tag	UNP Q09427
B	-1	ASP	-	expression tag	UNP Q09427
B	0	LYS	-	expression tag	UNP Q09427
D	-7	ASP	-	expression tag	UNP Q09427

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	TYR	-	expression tag	UNP Q09427
D	-5	LYS	-	expression tag	UNP Q09427
D	-4	ASP	-	expression tag	UNP Q09427
D	-3	ASP	-	expression tag	UNP Q09427
D	-2	ASP	-	expression tag	UNP Q09427
D	-1	ASP	-	expression tag	UNP Q09427
D	0	LYS	-	expression tag	UNP Q09427
F	-7	ASP	-	expression tag	UNP Q09427
F	-6	TYR	-	expression tag	UNP Q09427
F	-5	LYS	-	expression tag	UNP Q09427
F	-4	ASP	-	expression tag	UNP Q09427
F	-3	ASP	-	expression tag	UNP Q09427
F	-2	ASP	-	expression tag	UNP Q09427
F	-1	ASP	-	expression tag	UNP Q09427
F	0	LYS	-	expression tag	UNP Q09427
H	-7	ASP	-	expression tag	UNP Q09427
H	-6	TYR	-	expression tag	UNP Q09427
H	-5	LYS	-	expression tag	UNP Q09427
H	-4	ASP	-	expression tag	UNP Q09427
H	-3	ASP	-	expression tag	UNP Q09427
H	-2	ASP	-	expression tag	UNP Q09427
H	-1	ASP	-	expression tag	UNP Q09427
H	0	LYS	-	expression tag	UNP Q09427

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

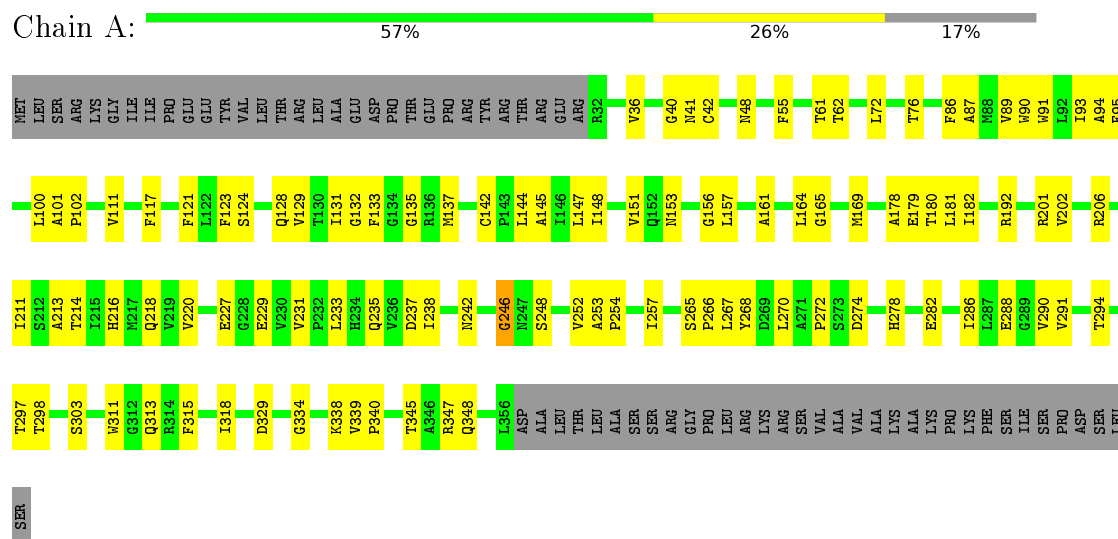


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0

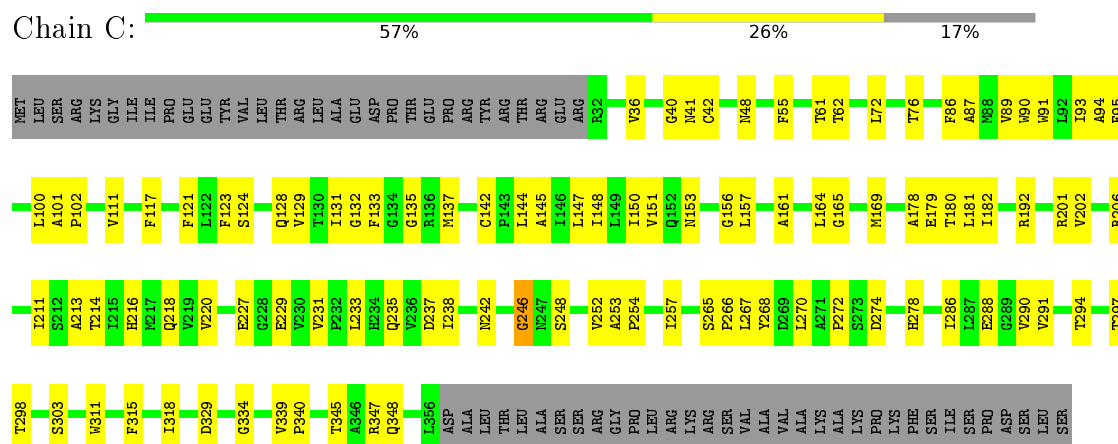
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

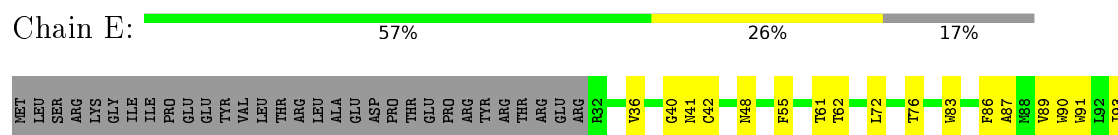
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

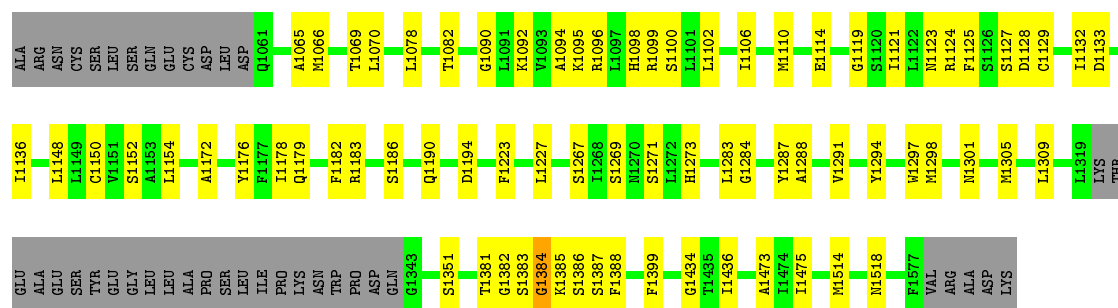


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



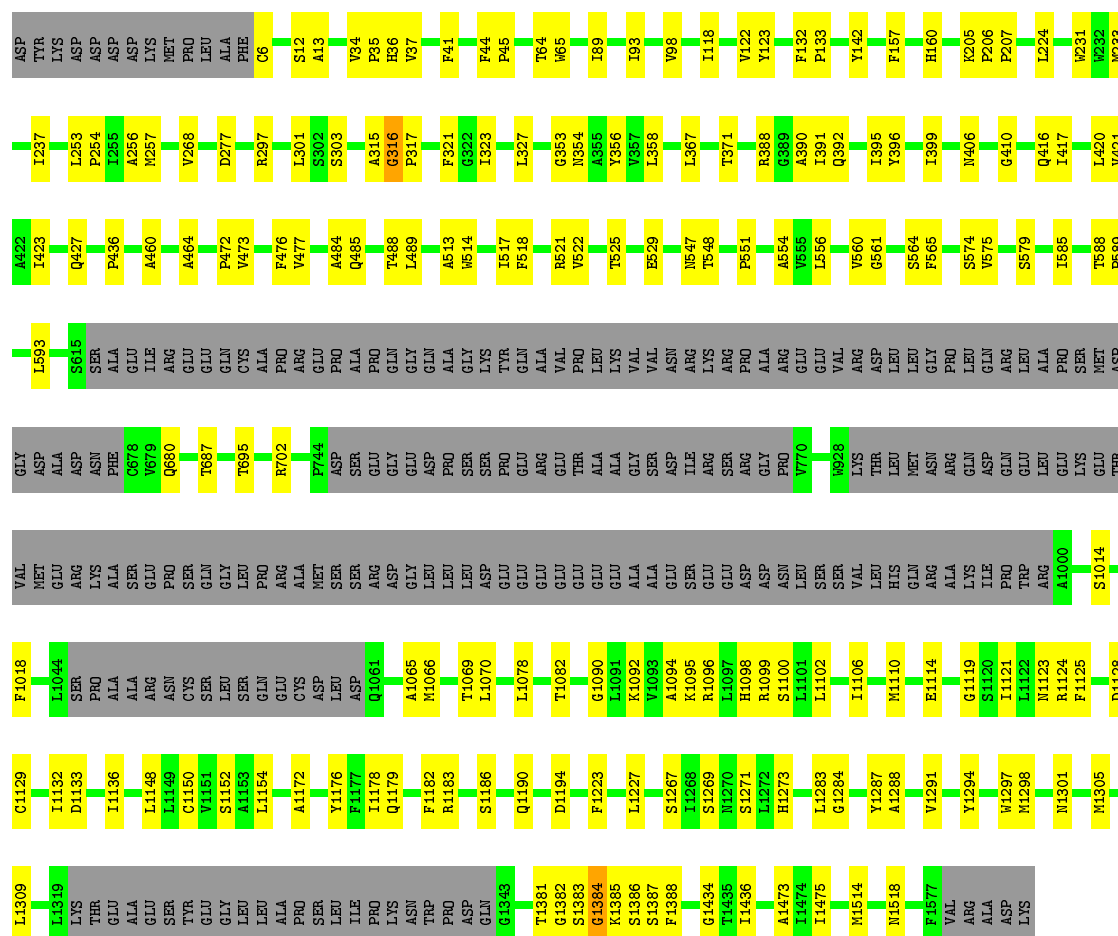
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11





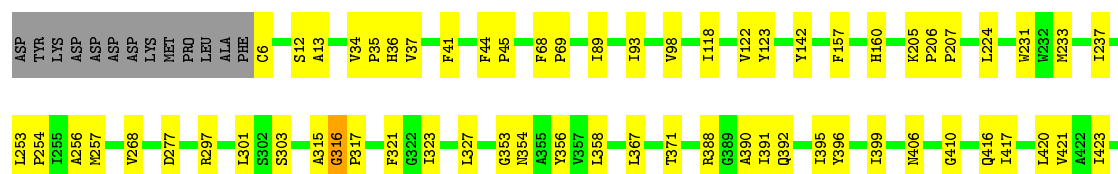
- Molecule 2: ATP-binding cassette sub-family C member 8

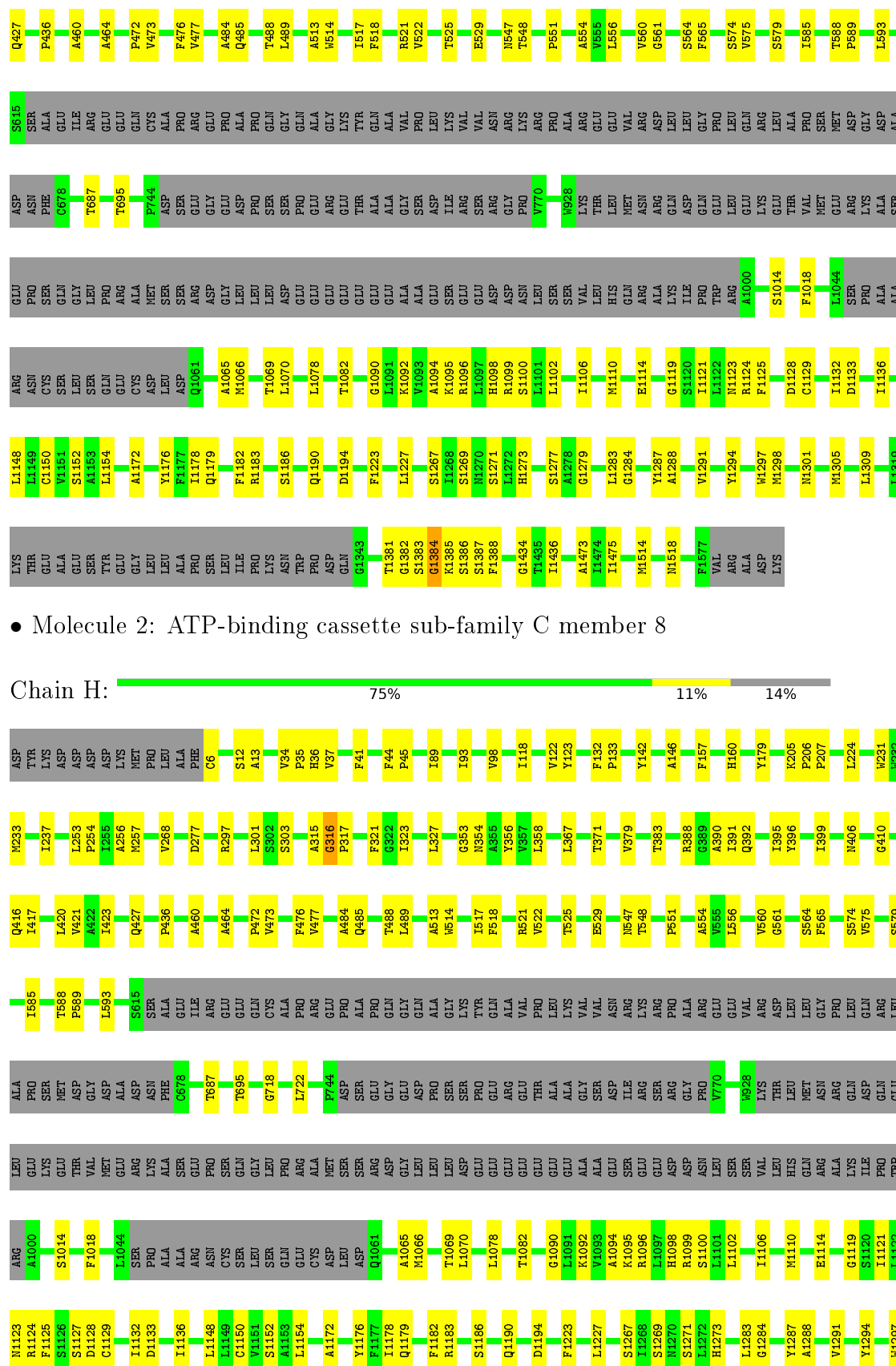
Chain D: 75% 11% 14%

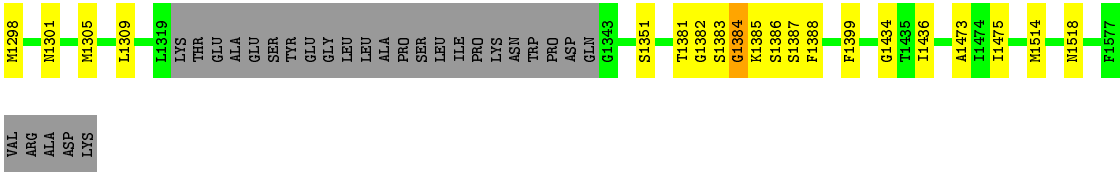


- Molecule 2: ATP-binding cassette sub-family C member 8

Chain F: 75% 11% 14%







4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	20000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	Not provided	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.32	0/2536	0.66	1/3459 (0.0%)
1	C	0.32	0/2536	0.66	1/3459 (0.0%)
1	E	0.32	0/2536	0.66	1/3459 (0.0%)
1	G	0.32	0/2536	0.66	1/3459 (0.0%)
2	B	0.29	0/7912	0.51	0/10995
2	D	0.29	0/7912	0.51	0/10995
2	F	0.29	0/7912	0.51	0/10995
2	H	0.29	0/7912	0.51	0/10995
All	All	0.30	0/41792	0.55	4/57816 (0.0%)

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
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	246	GLY	N-CA-C	5.18	126.05	113.10
1	C	246	GLY	N-CA-C	5.18	126.05	113.10
1	E	246	GLY	N-CA-C	5.18	126.05	113.10
1	G	246	GLY	N-CA-C	5.18	126.05	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1384	GLY	Peptide
2	D	1384	GLY	Peptide
2	F	1384	GLY	Peptide
2	H	1384	GLY	Peptide

5.2 Too-close contacts

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	2479	0	2442	89	0
1	C	2479	0	2442	91	0
1	E	2479	0	2442	92	0
1	G	2479	0	2442	94	0
2	B	7760	0	4559	115	0
2	D	7760	0	4559	115	0
2	F	7760	0	4559	114	0
2	H	7760	0	4559	119	0
3	A	31	0	12	7	0
3	C	31	0	12	7	0
3	E	31	0	12	7	0
3	G	31	0	12	7	0
All	All	41080	0	28052	784	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (784) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:206:PRO:HB2	2:F:207:PRO:HD3	1.64	0.80
2:H:206:PRO:HB2	2:H:207:PRO:HD3	1.64	0.80
2:B:206:PRO:HB2	2:B:207:PRO:HD3	1.64	0.78
2:D:206:PRO:HB2	2:D:207:PRO:HD3	1.64	0.78
2:F:233:MET:O	2:F:237:ILE:CB	2.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:233:MET:O	2:D:237:ILE:CB	2.37	0.72
1:E:213:ALA:HB1	1:E:288:GLU:O	1.89	0.72
2:H:233:MET:O	2:H:237:ILE:CB	2.37	0.72
2:B:233:MET:O	2:B:237:ILE:CB	2.37	0.71
1:C:213:ALA:HB1	1:C:288:GLU:O	1.89	0.71
1:G:213:ALA:HB1	1:G:288:GLU:O	1.89	0.71
1:A:213:ALA:HB1	1:A:288:GLU:O	1.89	0.71
1:E:48:ASN:O	3:E:401:ATP:N6	2.26	0.69
1:C:48:ASN:O	3:C:401:ATP:N6	2.26	0.69
1:A:48:ASN:O	3:A:401:ATP:N6	2.26	0.68
1:G:48:ASN:O	3:G:401:ATP:N6	2.26	0.68
2:H:44:PHE:HB2	2:H:45:PRO:HD3	1.77	0.67
1:G:257:ILE:HD12	1:G:257:ILE:N	2.10	0.66
1:E:257:ILE:N	1:E:257:ILE:HD12	2.10	0.66
2:B:44:PHE:HB2	2:B:45:PRO:HD3	1.77	0.66
2:F:44:PHE:HB2	2:F:45:PRO:HD3	1.77	0.66
1:G:220:VAL:O	1:G:220:VAL:HG13	1.96	0.66
2:D:44:PHE:HB2	2:D:45:PRO:HD3	1.77	0.66
2:B:1172:ALA:O	2:B:1176:TYR:HB2	1.96	0.65
1:G:339:VAL:HG13	1:G:340:PRO:HD2	1.78	0.65
1:A:257:ILE:HD12	1:A:257:ILE:N	2.10	0.65
1:A:220:VAL:O	1:A:220:VAL:HG13	1.96	0.65
1:C:257:ILE:N	1:C:257:ILE:HD12	2.10	0.65
2:D:1172:ALA:O	2:D:1176:TYR:HB2	1.96	0.65
1:A:339:VAL:HG13	1:A:340:PRO:HD2	1.78	0.65
2:F:1119:GLY:O	2:F:1123:ASN:HB2	1.97	0.65
1:E:220:VAL:HG13	1:E:220:VAL:O	1.96	0.65
2:H:1172:ALA:O	2:H:1176:TYR:HB2	1.96	0.65
1:C:339:VAL:HG13	1:C:340:PRO:HD2	1.78	0.65
2:B:1119:GLY:O	2:B:1123:ASN:HB2	1.97	0.65
1:C:220:VAL:HG13	1:C:220:VAL:O	1.96	0.64
1:E:36:VAL:HB	1:E:42:CYS:HB3	1.79	0.64
2:H:1119:GLY:O	2:H:1123:ASN:HB2	1.97	0.64
2:D:585:ILE:O	2:D:589:PRO:CD	2.45	0.64
2:F:1172:ALA:O	2:F:1176:TYR:HB2	1.96	0.64
2:H:585:ILE:O	2:H:589:PRO:CD	2.45	0.64
2:D:1119:GLY:O	2:D:1123:ASN:HB2	1.97	0.64
1:E:101:ALA:CB	2:F:12:SER:CB	2.76	0.64
2:F:585:ILE:O	2:F:589:PRO:CD	2.45	0.64
3:E:401:ATP:H3'	3:E:401:ATP:O3A	1.99	0.63
1:G:36:VAL:HB	1:G:42:CYS:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:HB	1:A:42:CYS:HB3	1.79	0.63
2:B:585:ILE:O	2:B:589:PRO:CD	2.45	0.63
2:B:1094:ALA:O	2:B:1098:HIS:HB3	1.99	0.63
1:C:90:TRP:CE2	1:C:123:PHE:CE2	2.86	0.63
1:E:339:VAL:HG13	1:E:340:PRO:HD2	1.78	0.63
1:A:101:ALA:CB	2:B:12:SER:CB	2.76	0.63
1:G:101:ALA:CB	2:H:12:SER:CB	2.76	0.63
1:E:90:TRP:CE2	1:E:123:PHE:CE2	2.86	0.63
1:C:101:ALA:CB	2:D:12:SER:CB	2.76	0.63
3:A:401:ATP:H3'	3:A:401:ATP:O3A	1.99	0.63
1:C:36:VAL:HB	1:C:42:CYS:HB3	1.79	0.63
3:C:401:ATP:H3'	3:C:401:ATP:O3A	1.99	0.63
1:A:90:TRP:CE2	1:A:123:PHE:CE2	2.86	0.62
1:G:90:TRP:CE2	1:G:123:PHE:CE2	2.86	0.62
2:H:1094:ALA:O	2:H:1098:HIS:HB3	1.99	0.62
1:C:101:ALA:HB3	2:D:12:SER:CB	2.30	0.62
3:G:401:ATP:O3A	3:G:401:ATP:H3'	1.99	0.62
1:A:101:ALA:HB3	2:B:12:SER:CB	2.30	0.62
1:A:135:GLY:HA3	1:G:137:MET:HE2	1.80	0.62
1:C:220:VAL:HG22	1:C:233:LEU:HD22	1.82	0.62
2:D:1094:ALA:O	2:D:1098:HIS:HB3	1.99	0.62
2:F:1094:ALA:O	2:F:1098:HIS:HB3	1.99	0.62
1:E:101:ALA:HB3	2:F:12:SER:CB	2.30	0.62
1:E:91:TRP:CE2	1:E:117:PHE:HD1	2.19	0.61
1:G:101:ALA:HB3	2:H:12:SER:CB	2.30	0.61
1:A:91:TRP:CE2	1:A:117:PHE:HD1	2.19	0.61
1:G:91:TRP:CE2	1:G:117:PHE:HD1	2.19	0.61
1:A:220:VAL:HG22	1:A:233:LEU:HD22	1.82	0.61
1:G:220:VAL:HG22	1:G:233:LEU:HD22	1.82	0.61
1:C:91:TRP:CE2	1:C:117:PHE:HD1	2.19	0.61
1:E:220:VAL:HG22	1:E:233:LEU:HD22	1.82	0.60
1:G:129:VAL:O	1:G:129:VAL:HG12	2.02	0.60
1:A:129:VAL:O	1:A:129:VAL:HG12	2.02	0.60
2:F:585:ILE:O	2:F:589:PRO:HD2	2.02	0.60
2:B:1223:PHE:O	2:B:1227:LEU:HB2	2.02	0.60
2:D:1223:PHE:O	2:D:1227:LEU:HB2	2.02	0.60
2:H:1223:PHE:O	2:H:1227:LEU:HB2	2.02	0.60
1:C:40:GLY:O	1:C:41:ASN:OD1	2.20	0.59
2:B:585:ILE:O	2:B:589:PRO:HD2	2.02	0.59
1:A:40:GLY:O	1:A:41:ASN:OD1	2.20	0.59
1:C:36:VAL:CG1	1:C:303:SER:HB2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:VAL:CG1	1:E:303:SER:HB2	2.33	0.59
1:A:36:VAL:CG1	1:A:303:SER:HB2	2.33	0.59
2:D:585:ILE:O	2:D:589:PRO:HD2	2.02	0.59
2:D:89:ILE:O	2:D:93:ILE:HG12	2.03	0.59
1:E:40:GLY:O	1:E:41:ASN:OD1	2.20	0.59
1:G:36:VAL:CG1	1:G:303:SER:HB2	2.33	0.59
1:E:129:VAL:HG12	1:E:129:VAL:O	2.02	0.59
2:B:89:ILE:O	2:B:93:ILE:HG12	2.03	0.59
1:G:40:GLY:O	1:G:41:ASN:OD1	2.20	0.59
1:C:169:MET:CE	1:E:294:THR:HG22	2.33	0.58
2:F:588:THR:CB	2:F:589:PRO:HD3	2.33	0.58
2:H:89:ILE:O	2:H:93:ILE:HG12	2.03	0.58
2:F:89:ILE:O	2:F:93:ILE:HG12	2.03	0.58
1:A:169:MET:CE	1:C:294:THR:HG22	2.33	0.58
2:D:588:THR:CB	2:D:589:PRO:HD3	2.33	0.58
1:E:169:MET:CE	1:G:294:THR:HG22	2.33	0.58
2:F:1223:PHE:O	2:F:1227:LEU:HB2	2.02	0.58
1:G:237:ASP:OD1	1:G:238:ILE:N	2.37	0.58
2:H:585:ILE:O	2:H:589:PRO:HD2	2.02	0.58
1:C:237:ASP:OD1	1:C:238:ILE:N	2.37	0.58
1:E:36:VAL:CB	1:E:42:CYS:HB3	2.34	0.58
1:E:237:ASP:OD1	1:E:238:ILE:N	2.37	0.58
1:C:36:VAL:CB	1:C:42:CYS:HB3	2.34	0.58
2:D:315:ALA:O	2:D:317:PRO:N	2.37	0.58
2:H:588:THR:CB	2:H:589:PRO:HD3	2.33	0.58
1:A:294:THR:HG22	1:G:169:MET:CE	2.33	0.57
2:F:315:ALA:O	2:F:317:PRO:N	2.37	0.57
1:G:128:GLN:OE1	1:G:156:GLY:HA3	2.04	0.57
2:H:315:ALA:O	2:H:317:PRO:N	2.37	0.57
1:A:128:GLN:OE1	1:A:156:GLY:HA3	2.04	0.57
1:C:137:MET:HE2	1:E:135:GLY:HA3	1.86	0.57
2:B:556:LEU:O	2:B:560:VAL:N	2.38	0.57
1:C:129:VAL:O	1:C:129:VAL:HG12	2.02	0.57
1:A:137:MET:HE2	1:C:135:GLY:HA3	1.86	0.57
2:B:588:THR:CB	2:B:589:PRO:HD3	2.33	0.57
1:E:102:PRO:HB3	2:F:13:ALA:CB	2.35	0.57
2:D:157:PHE:O	2:D:160:HIS:C	2.43	0.57
1:A:334:GLY:HA3	3:G:401:ATP:O1A	2.05	0.57
1:A:36:VAL:CB	1:A:42:CYS:HB3	2.34	0.57
1:G:36:VAL:CB	1:G:42:CYS:HB3	2.34	0.57
1:G:102:PRO:HB3	2:H:13:ALA:CB	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:157:PHE:O	2:H:160:HIS:C	2.43	0.57
1:A:102:PRO:HB3	2:B:13:ALA:HB1	1.87	0.57
1:A:237:ASP:OD1	1:A:238:ILE:N	2.37	0.57
1:C:102:PRO:HB3	2:D:13:ALA:HB1	1.87	0.56
1:E:102:PRO:HB3	2:F:13:ALA:HB1	1.87	0.56
2:H:556:LEU:O	2:H:560:VAL:N	2.38	0.56
3:E:401:ATP:O1A	1:E:334:GLY:HA3	2.04	0.56
1:A:290:VAL:HB	1:A:297:THR:HG22	1.88	0.56
2:D:556:LEU:O	2:D:560:VAL:N	2.38	0.56
2:F:157:PHE:O	2:F:160:HIS:C	2.43	0.56
2:H:1284:GLY:O	2:H:1288:ALA:HB2	2.06	0.56
1:C:128:GLN:OE1	1:C:156:GLY:HA3	2.04	0.56
1:C:290:VAL:HB	1:C:297:THR:HG22	1.88	0.56
2:F:1284:GLY:O	2:F:1288:ALA:HB2	2.06	0.56
2:B:315:ALA:O	2:B:317:PRO:N	2.37	0.56
1:G:102:PRO:HB3	2:H:13:ALA:HB1	1.87	0.56
1:A:102:PRO:HB3	2:B:13:ALA:CB	2.35	0.56
2:B:157:PHE:O	2:B:160:HIS:C	2.43	0.56
1:E:128:GLN:OE1	1:E:156:GLY:HA3	2.04	0.56
1:E:290:VAL:HB	1:E:297:THR:HG22	1.88	0.56
1:C:102:PRO:HB3	2:D:13:ALA:CB	2.35	0.56
1:G:290:VAL:HB	1:G:297:THR:HG22	1.88	0.56
2:F:1090:GLY:O	2:F:1094:ALA:HB2	2.06	0.56
2:B:1090:GLY:O	2:B:1094:ALA:HB2	2.06	0.55
2:B:1284:GLY:O	2:B:1288:ALA:HB2	2.06	0.55
2:D:1284:GLY:O	2:D:1288:ALA:HB2	2.06	0.55
2:F:556:LEU:O	2:F:560:VAL:N	2.38	0.55
2:B:472:PRO:O	2:B:476:PHE:HB3	2.07	0.55
3:E:401:ATP:O1A	1:G:334:GLY:HA3	2.06	0.55
1:E:137:MET:CE	1:G:135:GLY:HA3	2.36	0.55
2:H:206:PRO:CB	2:H:207:PRO:HD3	2.36	0.55
3:A:401:ATP:O1A	1:C:334:GLY:HA3	2.06	0.55
2:F:472:PRO:O	2:F:476:PHE:HB3	2.07	0.55
2:D:1090:GLY:O	2:D:1094:ALA:HB2	2.06	0.55
2:H:1090:GLY:O	2:H:1094:ALA:HB2	2.06	0.55
2:H:1294:TYR:O	2:H:1298:MET:CB	2.55	0.55
2:D:1294:TYR:O	2:D:1298:MET:CB	2.55	0.55
2:D:472:PRO:O	2:D:476:PHE:HB3	2.07	0.55
2:F:1294:TYR:O	2:F:1298:MET:CB	2.55	0.55
2:F:206:PRO:CB	2:F:207:PRO:HD3	2.36	0.55
2:D:206:PRO:CB	2:D:207:PRO:HD3	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:MET:CE	1:E:135:GLY:HA3	2.37	0.54
2:H:268:VAL:HG12	2:H:390:ALA:HB2	1.89	0.54
2:B:1223:PHE:O	2:B:1227:LEU:CB	2.56	0.54
2:D:1223:PHE:O	2:D:1227:LEU:CB	2.56	0.54
2:B:1294:TYR:O	2:B:1298:MET:CB	2.55	0.54
2:B:268:VAL:HG12	2:B:390:ALA:HB2	1.89	0.54
1:E:137:MET:HE2	1:G:135:GLY:HA3	1.88	0.54
1:E:272:PRO:HB3	1:E:311:TRP:CE2	2.43	0.54
2:H:472:PRO:O	2:H:476:PHE:HB3	2.07	0.54
1:G:290:VAL:HG22	1:G:291:VAL:N	2.23	0.54
2:H:1223:PHE:O	2:H:1227:LEU:CB	2.56	0.54
1:A:137:MET:CE	1:C:135:GLY:HA3	2.37	0.54
2:D:1383:SER:O	2:D:1387:SER:CB	2.56	0.54
2:F:1182:PHE:O	2:F:1186:SER:CB	2.56	0.54
2:F:1223:PHE:O	2:F:1227:LEU:CB	2.56	0.54
2:H:1182:PHE:O	2:H:1186:SER:CB	2.56	0.54
2:D:268:VAL:HG12	2:D:390:ALA:HB2	1.89	0.53
1:A:135:GLY:HA3	1:G:137:MET:CE	2.38	0.53
1:G:48:ASN:O	3:G:401:ATP:C6	2.61	0.53
1:A:290:VAL:HG22	1:A:291:VAL:N	2.23	0.53
2:B:1383:SER:O	2:B:1387:SER:CB	2.56	0.53
1:A:48:ASN:O	3:A:401:ATP:C6	2.61	0.53
1:C:272:PRO:HB3	1:C:311:TRP:CE2	2.43	0.53
2:B:575:VAL:O	2:B:579:SER:CB	2.57	0.53
1:C:290:VAL:HG22	1:C:291:VAL:N	2.23	0.53
2:D:575:VAL:O	2:D:579:SER:CB	2.57	0.53
1:G:272:PRO:HB3	1:G:311:TRP:CE2	2.43	0.53
2:H:1383:SER:O	2:H:1387:SER:CB	2.56	0.53
2:H:575:VAL:O	2:H:579:SER:CB	2.57	0.53
1:A:242:ASN:HB2	1:A:246:GLY:H	1.73	0.53
2:F:1383:SER:O	2:F:1387:SER:CB	2.56	0.53
3:G:401:ATP:H8	3:G:401:ATP:O1G	1.92	0.53
1:A:272:PRO:HB3	1:A:311:TRP:CE2	2.43	0.53
2:F:268:VAL:HG12	2:F:390:ALA:HB2	1.89	0.53
2:F:575:VAL:O	2:F:579:SER:CB	2.57	0.53
1:A:90:TRP:NE1	1:A:123:PHE:CE2	2.77	0.53
3:A:401:ATP:O1G	3:A:401:ATP:H8	1.92	0.53
2:B:1182:PHE:O	2:B:1186:SER:CB	2.56	0.53
3:C:401:ATP:O1G	3:C:401:ATP:H8	1.92	0.53
1:C:90:TRP:NE1	1:C:123:PHE:CE2	2.77	0.53
2:D:1182:PHE:O	2:D:1186:SER:CB	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:VAL:HG22	1:E:291:VAL:N	2.23	0.53
1:C:242:ASN:HB2	1:C:246:GLY:H	1.73	0.52
1:E:90:TRP:NE1	1:E:123:PHE:CE2	2.77	0.52
2:D:1287:TYR:O	2:D:1291:VAL:CB	2.58	0.52
2:D:253:LEU:O	2:D:257:MET:N	2.36	0.52
2:F:513:ALA:O	2:F:517:ILE:CB	2.58	0.52
1:G:242:ASN:HB2	1:G:246:GLY:H	1.73	0.52
1:G:90:TRP:NE1	1:G:123:PHE:CE2	2.77	0.52
2:B:1287:TYR:O	2:B:1291:VAL:CB	2.58	0.52
2:D:513:ALA:O	2:D:517:ILE:CB	2.58	0.52
2:H:1096:ARG:O	2:H:1100:SER:CB	2.58	0.52
2:H:1119:GLY:O	2:H:1123:ASN:CB	2.58	0.52
2:B:1119:GLY:O	2:B:1123:ASN:CB	2.58	0.52
1:C:48:ASN:O	3:C:401:ATP:C6	2.61	0.52
1:E:242:ASN:HB2	1:E:246:GLY:H	1.73	0.52
2:B:1096:ARG:O	2:B:1100:SER:CB	2.58	0.52
2:B:514:TRP:O	2:B:518:PHE:CB	2.58	0.52
2:D:514:TRP:O	2:D:518:PHE:CB	2.58	0.52
1:E:48:ASN:O	3:E:401:ATP:C6	2.61	0.52
1:G:86:PHE:HB2	1:G:124:SER:OG	2.10	0.52
2:H:513:ALA:O	2:H:517:ILE:CB	2.58	0.52
2:D:1382:GLY:O	2:D:1386:SER:CB	2.58	0.52
3:E:401:ATP:H8	3:E:401:ATP:O1G	1.92	0.52
1:A:201:ARG:CZ	1:A:315:PHE:HB3	2.40	0.52
2:B:1382:GLY:O	2:B:1386:SER:CB	2.58	0.52
2:D:1096:ARG:O	2:D:1100:SER:CB	2.58	0.52
2:F:1382:GLY:O	2:F:1386:SER:CB	2.58	0.52
2:H:1287:TYR:O	2:H:1291:VAL:CB	2.58	0.52
2:F:1096:ARG:O	2:F:1100:SER:CB	2.58	0.52
1:G:227:GLU:HB2	1:G:229:GLU:OE1	2.10	0.52
1:C:216:HIS:O	1:C:286:ILE:HB	2.10	0.52
1:A:86:PHE:HB2	1:A:124:SER:OG	2.10	0.51
2:B:513:ALA:O	2:B:517:ILE:CB	2.58	0.51
1:C:227:GLU:HB2	1:C:229:GLU:OE1	2.10	0.51
1:C:86:PHE:HB2	1:C:124:SER:OG	2.10	0.51
2:F:1119:GLY:O	2:F:1123:ASN:CB	2.58	0.51
1:G:201:ARG:CZ	1:G:315:PHE:HB3	2.40	0.51
2:F:1287:TYR:O	2:F:1291:VAL:CB	2.58	0.51
2:F:514:TRP:O	2:F:518:PHE:CB	2.58	0.51
2:H:514:TRP:O	2:H:518:PHE:CB	2.58	0.51
1:A:89:VAL:O	1:A:93:ILE:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1119:GLY:O	2:D:1123:ASN:CB	2.58	0.51
1:A:216:HIS:O	1:A:286:ILE:HB	2.10	0.51
1:C:89:VAL:O	1:C:93:ILE:HG23	2.11	0.51
2:D:1095:LYS:O	2:D:1099:ARG:CB	2.59	0.51
1:E:86:PHE:HB2	1:E:124:SER:OG	2.10	0.51
2:F:1095:LYS:O	2:F:1099:ARG:CB	2.59	0.51
1:G:111:VAL:HA	1:G:137:MET:O	2.11	0.51
2:H:1382:GLY:O	2:H:1386:SER:CB	2.58	0.51
2:B:1095:LYS:O	2:B:1099:ARG:CB	2.59	0.51
1:C:201:ARG:CZ	1:C:315:PHE:HB3	2.40	0.51
1:E:218:GLN:HG2	1:E:235:GLN:HB3	1.93	0.51
1:E:267:LEU:HA	1:E:270:LEU:HD13	1.93	0.51
1:E:48:ASN:O	3:E:401:ATP:N1	2.44	0.51
1:A:227:GLU:HB2	1:A:229:GLU:OE1	2.10	0.51
2:B:460:ALA:O	2:B:464:ALA:HB3	2.11	0.51
1:C:48:ASN:O	3:C:401:ATP:N1	2.44	0.51
2:D:1436:ILE:N	2:D:1473:ALA:O	2.41	0.51
1:E:227:GLU:HB2	1:E:229:GLU:OE1	2.10	0.51
1:E:89:VAL:O	1:E:93:ILE:HG23	2.11	0.51
2:F:253:LEU:O	2:F:257:MET:N	2.36	0.51
2:F:460:ALA:O	2:F:464:ALA:HB3	2.11	0.51
2:H:1095:LYS:O	2:H:1099:ARG:CB	2.59	0.51
1:A:267:LEU:HA	1:A:270:LEU:HD13	1.93	0.51
2:D:1381:THR:O	2:D:1385:LYS:CB	2.59	0.51
1:E:201:ARG:CZ	1:E:315:PHE:HB3	2.40	0.51
1:G:216:HIS:O	1:G:286:ILE:HB	2.10	0.51
1:G:218:GLN:HG2	1:G:235:GLN:HB3	1.93	0.51
1:E:111:VAL:HA	1:E:137:MET:O	2.11	0.50
2:H:1436:ILE:N	2:H:1473:ALA:O	2.41	0.50
1:A:111:VAL:HA	1:A:137:MET:O	2.11	0.50
1:A:218:GLN:HG2	1:A:235:GLN:HB3	1.93	0.50
1:C:218:GLN:HG2	1:C:235:GLN:HB3	1.93	0.50
1:C:55:PHE:CE1	1:E:206:ARG:HD3	2.47	0.50
1:E:216:HIS:O	1:E:286:ILE:HB	2.10	0.50
2:H:1381:THR:O	2:H:1385:LYS:CB	2.59	0.50
1:G:267:LEU:HA	1:G:270:LEU:HD13	1.93	0.50
2:B:1381:THR:O	2:B:1385:LYS:CB	2.59	0.50
1:C:111:VAL:HA	1:C:137:MET:O	2.11	0.50
1:G:48:ASN:O	3:G:401:ATP:N1	2.44	0.50
1:G:89:VAL:O	1:G:93:ILE:HG23	2.10	0.50
2:B:1190:GLN:O	2:B:1194:ASP:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:LEU:HA	1:C:270:LEU:HD13	1.93	0.50
2:D:460:ALA:O	2:D:464:ALA:HB3	2.11	0.50
2:H:1190:GLN:O	2:H:1194:ASP:CB	2.60	0.50
2:D:525:THR:O	2:D:529:GLU:CB	2.60	0.50
2:F:1381:THR:O	2:F:1385:LYS:CB	2.59	0.50
1:A:48:ASN:O	3:A:401:ATP:N1	2.44	0.50
2:B:1178:ILE:O	2:B:1182:PHE:HB3	2.12	0.50
2:D:321:PHE:HE1	2:D:574:SER:CB	2.25	0.50
2:F:525:THR:O	2:F:529:GLU:CB	2.60	0.50
2:H:460:ALA:O	2:H:464:ALA:HB3	2.11	0.50
1:A:165:GLY:O	1:A:169:MET:HG2	2.12	0.49
2:B:1436:ILE:N	2:B:1473:ALA:O	2.41	0.49
2:B:321:PHE:HE1	2:B:574:SER:CB	2.25	0.49
2:D:561:GLY:O	2:D:565:PHE:HB2	2.12	0.49
2:H:1178:ILE:O	2:H:1182:PHE:HB3	2.12	0.49
1:A:55:PHE:CE1	1:C:206:ARG:HD3	2.47	0.49
2:D:1305:MET:O	2:D:1309:LEU:CB	2.60	0.49
2:F:321:PHE:HE1	2:F:574:SER:CB	2.25	0.49
1:G:36:VAL:HG13	1:G:303:SER:HB2	1.94	0.49
2:H:1305:MET:O	2:H:1309:LEU:CB	2.61	0.49
1:E:101:ALA:N	1:E:102:PRO:HD2	2.28	0.49
1:G:211:ILE:O	1:G:290:VAL:HG12	2.12	0.49
2:H:353:GLY:HA2	2:H:356:TYR:HD2	1.77	0.49
2:F:1305:MET:O	2:F:1309:LEU:CB	2.61	0.49
2:H:321:PHE:HE1	2:H:574:SER:CB	2.25	0.49
1:E:211:ILE:O	1:E:290:VAL:HG12	2.12	0.49
2:B:353:GLY:HA2	2:B:356:TYR:HD2	1.77	0.49
1:C:211:ILE:O	1:C:290:VAL:HG12	2.12	0.49
2:D:1190:GLN:O	2:D:1194:ASP:CB	2.60	0.49
2:F:1190:GLN:O	2:F:1194:ASP:CB	2.60	0.49
1:G:165:GLY:O	1:G:169:MET:HG2	2.12	0.49
2:H:525:THR:O	2:H:529:GLU:CB	2.60	0.49
2:D:1178:ILE:O	2:D:1182:PHE:HB3	2.12	0.49
1:G:101:ALA:N	1:G:102:PRO:HD2	2.28	0.49
2:F:561:GLY:O	2:F:565:PHE:HB2	2.13	0.49
1:C:165:GLY:O	1:C:169:MET:HG2	2.12	0.49
2:F:1178:ILE:O	2:F:1182:PHE:HB3	2.12	0.49
2:F:354:ASN:O	2:F:358:LEU:CB	2.61	0.49
2:F:353:GLY:HA2	2:F:356:TYR:HD2	1.77	0.49
2:H:354:ASN:O	2:H:358:LEU:CB	2.61	0.49
1:A:36:VAL:HG13	1:A:303:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:525:THR:O	2:B:529:GLU:CB	2.60	0.49
2:D:548:THR:O	2:D:551:PRO:HD2	2.13	0.49
1:C:201:ARG:NH1	1:C:315:PHE:HB3	2.28	0.48
1:E:165:GLY:O	1:E:169:MET:HG2	2.13	0.48
2:B:1172:ALA:O	2:B:1176:TYR:CB	2.62	0.48
2:D:315:ALA:O	2:D:316:GLY:C	2.51	0.48
2:F:315:ALA:O	2:F:316:GLY:C	2.51	0.48
1:G:201:ARG:NH1	1:G:315:PHE:HB3	2.28	0.48
2:H:253:LEU:O	2:H:257:MET:N	2.36	0.48
1:A:201:ARG:NH1	1:A:315:PHE:HB3	2.28	0.48
1:A:211:ILE:O	1:A:290:VAL:HG12	2.12	0.48
2:B:37:VAL:CB	2:B:41:PHE:CE2	2.96	0.48
2:H:551:PRO:HA	2:H:554:ALA:HB3	1.95	0.48
1:A:101:ALA:N	1:A:102:PRO:HD2	2.27	0.48
1:A:206:ARG:HD3	1:G:55:PHE:CE1	2.47	0.48
2:B:548:THR:O	2:B:551:PRO:HD2	2.13	0.48
1:C:101:ALA:N	1:C:102:PRO:HD2	2.27	0.48
2:D:353:GLY:HA2	2:D:356:TYR:HD2	1.77	0.48
2:D:37:VAL:CB	2:D:41:PHE:CE2	2.96	0.48
3:C:401:ATP:O4'	1:E:182:ILE:HG21	2.13	0.48
2:F:548:THR:O	2:F:551:PRO:HD2	2.13	0.48
2:H:37:VAL:CB	2:H:41:PHE:CE2	2.96	0.48
2:H:548:THR:O	2:H:551:PRO:HD2	2.13	0.48
2:D:1172:ALA:O	2:D:1176:TYR:CB	2.62	0.48
2:D:551:PRO:HA	2:D:554:ALA:HB3	1.95	0.48
1:E:55:PHE:CE1	1:G:206:ARG:HD3	2.47	0.48
2:F:1436:ILE:N	2:F:1473:ALA:O	2.41	0.48
2:H:561:GLY:O	2:H:565:PHE:HB2	2.13	0.48
2:B:354:ASN:O	2:B:358:LEU:CB	2.61	0.48
2:D:1124:ARG:O	2:D:1128:ASP:CB	2.62	0.48
1:E:36:VAL:HG13	1:E:303:SER:HB2	1.94	0.48
2:B:1305:MET:O	2:B:1309:LEU:CB	2.61	0.48
2:B:253:LEU:O	2:B:257:MET:N	2.36	0.48
1:G:94:ALA:HB1	1:G:100:LEU:HD23	1.96	0.48
2:H:315:ALA:O	2:H:316:GLY:C	2.51	0.48
3:E:401:ATP:O4'	1:G:182:ILE:HG21	2.14	0.48
2:F:37:VAL:CB	2:F:41:PHE:CE2	2.96	0.48
2:F:551:PRO:HA	2:F:554:ALA:HB3	1.95	0.48
2:H:323:ILE:O	2:H:327:LEU:CB	2.62	0.48
2:B:1124:ARG:O	2:B:1128:ASP:CB	2.62	0.48
2:D:323:ILE:O	2:D:327:LEU:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:589:PRO:O	2:D:593:LEU:CB	2.62	0.48
1:A:94:ALA:HB1	1:A:100:LEU:HD23	1.96	0.48
1:A:182:ILE:HG21	3:G:401:ATP:O4'	2.14	0.48
2:B:561:GLY:O	2:B:565:PHE:HB2	2.13	0.48
2:B:589:PRO:O	2:B:593:LEU:CB	2.62	0.48
2:D:354:ASN:O	2:D:358:LEU:CB	2.61	0.48
2:F:367:LEU:O	2:F:371:THR:CB	2.62	0.48
2:H:1124:ARG:O	2:H:1128:ASP:CB	2.62	0.48
2:H:367:LEU:O	2:H:371:THR:CB	2.62	0.48
3:A:401:ATP:O4'	1:C:182:ILE:HG21	2.14	0.47
1:C:36:VAL:HG13	1:C:303:SER:HB2	1.94	0.47
1:E:201:ARG:NH1	1:E:315:PHE:HB3	2.28	0.47
2:B:315:ALA:O	2:B:316:GLY:C	2.51	0.47
2:B:323:ILE:O	2:B:327:LEU:CB	2.62	0.47
2:B:551:PRO:HA	2:B:554:ALA:HB3	1.95	0.47
2:F:1269:SER:O	2:F:1273:HIS:CB	2.62	0.47
2:F:323:ILE:O	2:F:327:LEU:CB	2.62	0.47
2:D:1269:SER:O	2:D:1273:HIS:CB	2.62	0.47
2:D:517:ILE:O	2:D:521:ARG:CB	2.63	0.47
1:E:257:ILE:N	1:E:257:ILE:CD1	2.77	0.47
2:F:1124:ARG:O	2:F:1128:ASP:CB	2.62	0.47
2:H:1269:SER:O	2:H:1273:HIS:CB	2.62	0.47
2:H:1297:TRP:O	2:H:1301:ASN:CB	2.63	0.47
2:H:423:ILE:O	2:H:427:GLN:CB	2.63	0.47
1:A:214:THR:HA	1:A:248:SER:HB3	1.97	0.47
1:A:318:ILE:HG23	1:A:329:ASP:O	2.15	0.47
2:F:1267:SER:O	2:F:1271:SER:CB	2.63	0.47
2:H:517:ILE:O	2:H:521:ARG:CB	2.63	0.47
2:B:423:ILE:O	2:B:427:GLN:CB	2.63	0.47
1:C:318:ILE:HG23	1:C:329:ASP:O	2.15	0.47
2:F:1172:ALA:O	2:F:1176:TYR:CB	2.62	0.47
2:F:517:ILE:O	2:F:521:ARG:CB	2.63	0.47
2:B:1129:CYS:O	2:B:1133:ASP:CB	2.63	0.47
2:B:1267:SER:O	2:B:1271:SER:CB	2.63	0.47
2:B:1269:SER:O	2:B:1273:HIS:CB	2.62	0.47
1:E:94:ALA:HB1	1:E:100:LEU:HD23	1.96	0.47
2:F:589:PRO:O	2:F:593:LEU:CB	2.62	0.47
1:G:318:ILE:HG23	1:G:329:ASP:O	2.15	0.47
2:H:417:ILE:O	2:H:421:VAL:CB	2.63	0.47
2:H:589:PRO:O	2:H:593:LEU:CB	2.62	0.47
2:B:367:LEU:O	2:B:371:THR:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:517:ILE:O	2:B:521:ARG:CB	2.63	0.47
1:C:214:THR:HA	1:C:248:SER:HB3	1.97	0.47
2:D:1129:CYS:O	2:D:1133:ASP:CB	2.63	0.47
2:F:423:ILE:O	2:F:427:GLN:CB	2.63	0.47
2:B:1297:TRP:O	2:B:1301:ASN:CB	2.63	0.47
2:D:1102:LEU:O	2:D:1106:ILE:CB	2.63	0.47
2:D:253:LEU:HA	2:D:256:ALA:HB3	1.97	0.47
2:D:367:LEU:O	2:D:371:THR:CB	2.62	0.47
2:F:1102:LEU:O	2:F:1106:ILE:CB	2.63	0.47
2:B:417:ILE:O	2:B:421:VAL:CB	2.63	0.46
2:D:1267:SER:O	2:D:1271:SER:CB	2.63	0.46
2:D:1297:TRP:O	2:D:1301:ASN:CB	2.63	0.46
1:E:214:THR:HA	1:E:248:SER:HB3	1.97	0.46
1:A:257:ILE:CD1	1:A:257:ILE:N	2.77	0.46
1:C:94:ALA:HB1	1:C:100:LEU:HD23	1.96	0.46
2:H:1129:CYS:O	2:H:1133:ASP:CB	2.63	0.46
2:B:206:PRO:CB	2:B:207:PRO:HD3	2.36	0.46
2:D:423:ILE:O	2:D:427:GLN:CB	2.63	0.46
2:F:1065:ALA:O	2:F:1069:THR:CB	2.63	0.46
2:F:253:LEU:HA	2:F:256:ALA:HB3	1.97	0.46
2:F:417:ILE:O	2:F:421:VAL:CB	2.63	0.46
2:H:1065:ALA:O	2:H:1069:THR:CB	2.63	0.46
2:H:1172:ALA:O	2:H:1176:TYR:CB	2.62	0.46
1:C:117:PHE:CD2	1:C:117:PHE:C	2.89	0.46
2:D:1150:CYS:O	2:D:1154:LEU:CB	2.64	0.46
2:F:1297:TRP:O	2:F:1301:ASN:CB	2.63	0.46
2:H:1267:SER:O	2:H:1271:SER:CB	2.63	0.46
2:B:1065:ALA:O	2:B:1069:THR:CB	2.63	0.46
2:B:1102:LEU:O	2:B:1106:ILE:CB	2.63	0.46
1:E:318:ILE:HG23	1:E:329:ASP:O	2.15	0.46
1:G:87:ALA:CB	1:G:121:PHE:HA	2.46	0.46
2:B:1150:CYS:O	2:B:1154:LEU:CB	2.64	0.46
2:B:253:LEU:HA	2:B:256:ALA:HB3	1.97	0.46
2:D:1121:ILE:O	2:D:1125:PHE:HB2	2.16	0.46
2:F:1129:CYS:O	2:F:1133:ASP:CB	2.63	0.46
2:H:1102:LEU:O	2:H:1106:ILE:CB	2.63	0.46
2:H:1150:CYS:O	2:H:1154:LEU:CB	2.64	0.46
1:C:257:ILE:N	1:C:257:ILE:CD1	2.77	0.46
1:E:117:PHE:C	1:E:117:PHE:CD2	2.89	0.46
1:E:87:ALA:CB	1:E:121:PHE:HA	2.46	0.46
1:G:214:THR:HA	1:G:248:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:560:VAL:O	2:H:564:SER:CB	2.64	0.46
2:B:1078:LEU:O	2:B:1082:THR:CB	2.64	0.46
2:D:1065:ALA:O	2:D:1069:THR:CB	2.63	0.46
2:D:1078:LEU:O	2:D:1082:THR:CB	2.64	0.46
2:D:560:VAL:O	2:D:564:SER:CB	2.64	0.46
1:A:117:PHE:CD2	1:A:117:PHE:C	2.89	0.45
2:D:37:VAL:O	2:D:41:PHE:CG	2.69	0.45
2:D:417:ILE:O	2:D:421:VAL:CB	2.63	0.45
1:E:142:CYS:SG	1:E:145:ALA:HB3	2.56	0.45
2:F:1150:CYS:O	2:F:1154:LEU:CB	2.64	0.45
2:D:1384:GLY:O	2:D:1388:PHE:CB	2.65	0.45
2:F:1121:ILE:O	2:F:1125:PHE:HB2	2.16	0.45
2:F:560:VAL:O	2:F:564:SER:CB	2.64	0.45
2:H:521:ARG:O	2:H:525:THR:CB	2.65	0.45
2:F:37:VAL:O	2:F:41:PHE:CG	2.69	0.45
1:G:117:PHE:CD2	1:G:117:PHE:C	2.89	0.45
2:H:253:LEU:HA	2:H:256:ALA:HB3	1.97	0.45
2:H:37:VAL:O	2:H:41:PHE:CG	2.70	0.45
2:B:1384:GLY:O	2:B:1388:PHE:CB	2.65	0.45
1:C:87:ALA:CB	1:C:121:PHE:HA	2.46	0.45
2:D:1092:LYS:O	2:D:1096:ARG:CB	2.65	0.45
2:F:396:TYR:HA	2:F:399:ILE:HG22	1.99	0.45
2:B:37:VAL:O	2:B:41:PHE:CG	2.69	0.45
2:D:321:PHE:CE1	2:D:574:SER:CB	3.00	0.45
2:F:1078:LEU:O	2:F:1082:THR:CB	2.64	0.45
2:F:1384:GLY:O	2:F:1388:PHE:CB	2.64	0.45
2:H:1092:LYS:O	2:H:1096:ARG:CB	2.65	0.45
2:H:1384:GLY:O	2:H:1388:PHE:CB	2.65	0.45
2:B:1110:MET:O	2:B:1114:GLU:CB	2.65	0.45
2:B:560:VAL:O	2:B:564:SER:CB	2.64	0.45
2:F:1092:LYS:O	2:F:1096:ARG:CB	2.65	0.45
2:F:1110:MET:O	2:F:1114:GLU:CB	2.65	0.45
2:H:396:TYR:HA	2:H:399:ILE:HG22	1.99	0.45
1:A:142:CYS:SG	1:A:145:ALA:HB3	2.56	0.45
2:B:521:ARG:O	2:B:525:THR:CB	2.65	0.45
1:C:178:ALA:HB2	1:C:298:THR:OG1	2.17	0.45
1:C:179:GLU:C	1:C:181:LEU:H	2.20	0.45
1:E:220:VAL:CG2	1:E:233:LEU:HD22	2.47	0.45
2:F:1121:ILE:O	2:F:1125:PHE:CB	2.65	0.45
1:G:142:CYS:SG	1:G:145:ALA:HB3	2.56	0.45
1:G:144:LEU:O	1:G:147:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLU:C	1:A:181:LEU:H	2.20	0.45
2:B:1121:ILE:O	2:B:1125:PHE:HB2	2.16	0.45
2:B:396:TYR:HA	2:B:399:ILE:HG22	1.99	0.45
2:B:556:LEU:O	2:B:560:VAL:CB	2.65	0.45
1:E:161:ALA:HB1	1:G:164:LEU:HD23	1.99	0.45
1:G:178:ALA:HB2	1:G:298:THR:OG1	2.17	0.45
1:G:43:ASN:N	1:G:43:ASN:OD1	2.44	0.45
2:H:1078:LEU:O	2:H:1082:THR:CB	2.64	0.45
2:B:1014:SER:O	2:B:1018:PHE:HB2	2.17	0.45
2:B:1092:LYS:O	2:B:1096:ARG:CB	2.65	0.45
2:D:396:TYR:HA	2:D:399:ILE:HG22	1.99	0.45
1:E:179:GLU:C	1:E:181:LEU:H	2.20	0.45
2:H:1110:MET:O	2:H:1114:GLU:CB	2.65	0.45
2:H:1121:ILE:O	2:H:1125:PHE:HB2	2.16	0.45
1:A:87:ALA:CB	1:A:121:PHE:HA	2.46	0.45
1:A:61:THR:HG23	1:A:62:THR:N	2.33	0.45
2:D:231:TRP:CE3	2:D:231:TRP:O	2.70	0.45
2:B:1121:ILE:O	2:B:1125:PHE:CB	2.65	0.44
2:D:1014:SER:O	2:D:1018:PHE:HB2	2.17	0.44
2:D:1110:MET:O	2:D:1114:GLU:CB	2.65	0.44
1:E:144:LEU:O	1:E:147:LEU:HG	2.17	0.44
1:E:274:ASP:O	1:E:278:HIS:HB2	2.17	0.44
2:F:1434:GLY:O	2:F:1475:ILE:N	2.44	0.44
2:F:231:TRP:O	2:F:231:TRP:CE3	2.70	0.44
1:G:220:VAL:CG2	1:G:233:LEU:HD22	2.47	0.44
1:G:345:THR:CG2	1:G:348:GLN:HB2	2.47	0.44
2:H:1121:ILE:O	2:H:1125:PHE:CB	2.65	0.44
2:H:556:LEU:O	2:H:560:VAL:CB	2.65	0.44
2:B:406:ASN:O	2:B:410:GLY:N	2.51	0.44
1:C:142:CYS:SG	1:C:145:ALA:HB3	2.56	0.44
2:D:521:ARG:O	2:D:525:THR:CB	2.65	0.44
1:E:144:LEU:O	1:E:148:ILE:HG12	2.17	0.44
2:F:321:PHE:CE1	2:F:574:SER:CB	3.00	0.44
2:H:321:PHE:CE1	2:H:574:SER:CB	3.00	0.44
1:C:144:LEU:O	1:C:147:LEU:HG	2.17	0.44
2:D:1121:ILE:O	2:D:1125:PHE:CB	2.65	0.44
2:D:556:LEU:O	2:D:560:VAL:CB	2.65	0.44
1:E:345:THR:CG2	1:E:348:GLN:HB2	2.47	0.44
2:F:521:ARG:O	2:F:525:THR:CB	2.65	0.44
2:F:556:LEU:O	2:F:560:VAL:CB	2.65	0.44
1:G:144:LEU:O	1:G:148:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:274:ASP:O	1:G:278:HIS:HB2	2.17	0.44
1:G:61:THR:HG23	1:G:62:THR:N	2.32	0.44
1:A:161:ALA:HB1	1:C:164:LEU:HD23	1.99	0.44
1:A:178:ALA:HB2	1:A:298:THR:OG1	2.17	0.44
1:C:144:LEU:O	1:C:148:ILE:HG12	2.17	0.44
1:C:61:THR:HG23	1:C:62:THR:N	2.33	0.44
1:G:252:VAL:HG23	1:G:253:ALA:N	2.33	0.44
2:B:388:ARG:O	2:B:392:GLN:CB	2.66	0.44
2:F:68:PHE:HA	2:F:69:PRO:HD3	1.86	0.44
2:H:1014:SER:O	2:H:1018:PHE:HB2	2.17	0.44
1:A:144:LEU:O	1:A:148:ILE:HG12	2.17	0.44
1:C:274:ASP:O	1:C:278:HIS:HB2	2.18	0.44
2:D:1283:LEU:O	2:D:1287:TYR:HB2	2.18	0.44
1:E:252:VAL:HG23	1:E:253:ALA:N	2.33	0.44
2:H:547:ASN:O	2:H:551:PRO:HD2	2.18	0.44
1:A:144:LEU:O	1:A:147:LEU:HG	2.17	0.44
2:B:1283:LEU:O	2:B:1287:TYR:HB2	2.18	0.44
2:B:231:TRP:O	2:B:231:TRP:CE3	2.70	0.44
2:B:321:PHE:CE1	2:B:574:SER:CB	3.00	0.44
1:E:137:MET:HE1	1:G:135:GLY:H	1.83	0.44
2:F:1179:GLN:O	2:F:1183:ARG:CB	2.66	0.44
2:F:547:ASN:O	2:F:551:PRO:HD2	2.18	0.44
1:A:164:LEU:HD23	1:G:161:ALA:HB1	2.00	0.44
1:C:202:VAL:O	1:C:254:PRO:HA	2.18	0.44
1:C:345:THR:CG2	1:C:348:GLN:HB2	2.47	0.44
1:E:178:ALA:HB2	1:E:298:THR:OG1	2.17	0.44
1:E:61:THR:HG23	1:E:62:THR:N	2.33	0.44
1:A:252:VAL:HG23	1:A:253:ALA:N	2.33	0.44
2:B:547:ASN:O	2:B:551:PRO:HD2	2.18	0.44
2:H:231:TRP:O	2:H:231:TRP:CE3	2.70	0.44
2:B:118:ILE:O	2:B:122:VAL:HG23	2.18	0.43
1:C:265:SER:HA	1:C:266:PRO:HD3	1.84	0.43
2:D:1179:GLN:O	2:D:1183:ARG:CB	2.66	0.43
2:F:1014:SER:O	2:F:1018:PHE:HB2	2.17	0.43
2:F:406:ASN:O	2:F:410:GLY:N	2.51	0.43
2:H:1179:GLN:O	2:H:1183:ARG:CB	2.66	0.43
2:H:388:ARG:O	2:H:392:GLN:CB	2.66	0.43
1:A:274:ASP:O	1:A:278:HIS:HB2	2.18	0.43
1:A:345:THR:CG2	1:A:348:GLN:HB2	2.47	0.43
2:B:36:HIS:HA	2:B:142:TYR:HE1	1.83	0.43
2:H:406:ASN:O	2:H:410:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:ILE:O	2:D:122:VAL:HG23	2.18	0.43
2:D:205:LYS:N	2:D:206:PRO:CD	2.82	0.43
2:D:388:ARG:O	2:D:392:GLN:CB	2.66	0.43
2:F:1283:LEU:O	2:F:1287:TYR:HB2	2.18	0.43
1:G:179:GLU:C	1:G:181:LEU:H	2.20	0.43
1:G:231:VAL:HG13	1:G:231:VAL:O	2.19	0.43
1:A:202:VAL:O	1:A:254:PRO:HA	2.18	0.43
2:B:1351:SER:O	2:B:1399:PHE:N	2.47	0.43
2:B:548:THR:C	2:B:551:PRO:HD2	2.39	0.43
2:D:547:ASN:O	2:D:551:PRO:HD2	2.18	0.43
1:C:55:PHE:HE1	1:E:206:ARG:CD	2.31	0.43
2:H:473:VAL:O	2:H:477:VAL:CB	2.67	0.43
1:A:153:ASN:O	1:A:157:LEU:HB2	2.19	0.43
1:A:178:ALA:HA	1:A:181:LEU:HD12	2.01	0.43
2:B:473:VAL:O	2:B:477:VAL:CB	2.67	0.43
2:D:547:ASN:O	2:D:551:PRO:CD	2.67	0.43
2:H:548:THR:C	2:H:551:PRO:HD2	2.39	0.43
1:C:178:ALA:HA	1:C:181:LEU:HD12	2.01	0.43
2:D:303:SER:HA	2:D:436:PRO:HB3	2.01	0.43
2:D:473:VAL:O	2:D:477:VAL:CB	2.67	0.43
2:D:548:THR:C	2:D:551:PRO:HD2	2.39	0.43
2:F:303:SER:HA	2:F:436:PRO:HB3	2.01	0.43
1:A:231:VAL:O	1:A:231:VAL:HG13	2.19	0.43
2:B:1179:GLN:O	2:B:1183:ARG:CB	2.66	0.43
2:B:37:VAL:O	2:B:41:PHE:CD2	2.72	0.43
1:C:161:ALA:HB1	1:E:164:LEU:HD23	1.99	0.43
2:F:388:ARG:O	2:F:392:GLN:CB	2.66	0.43
2:H:118:ILE:O	2:H:122:VAL:HG23	2.18	0.43
2:B:205:LYS:N	2:B:206:PRO:CD	2.82	0.43
2:F:118:ILE:O	2:F:122:VAL:HG23	2.18	0.43
2:H:1351:SER:O	2:H:1399:PHE:N	2.47	0.43
2:H:36:HIS:HA	2:H:142:TYR:HE1	1.83	0.43
1:C:220:VAL:O	1:C:220:VAL:CG1	2.66	0.43
1:E:178:ALA:HA	1:E:181:LEU:HD12	2.01	0.43
1:E:202:VAL:O	1:E:254:PRO:HA	2.18	0.43
2:F:473:VAL:O	2:F:477:VAL:CB	2.67	0.43
2:F:548:THR:C	2:F:551:PRO:HD2	2.39	0.43
1:G:202:VAL:O	1:G:254:PRO:HA	2.18	0.43
1:A:36:VAL:HG23	1:A:42:CYS:HB3	2.01	0.43
2:D:253:LEU:N	2:D:254:PRO:CD	2.82	0.43
1:E:231:VAL:O	1:E:231:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:PHE:HE1	1:G:206:ARG:CD	2.32	0.43
1:G:36:VAL:CG2	1:G:42:CYS:HB3	2.49	0.43
2:H:1132:ILE:O	2:H:1136:ILE:CB	2.67	0.43
2:H:1283:LEU:O	2:H:1287:TYR:HB2	2.18	0.43
2:D:37:VAL:O	2:D:41:PHE:CD2	2.72	0.42
2:H:379:VAL:O	2:H:383:THR:OG1	2.29	0.42
2:H:37:VAL:O	2:H:41:PHE:CD2	2.72	0.42
2:B:253:LEU:N	2:B:254:PRO:CD	2.82	0.42
1:A:132:GLY:HA3	1:C:131:ILE:O	2.19	0.42
1:C:36:VAL:CG2	1:C:42:CYS:HB3	2.49	0.42
2:D:36:HIS:HA	2:D:142:TYR:HE1	1.83	0.42
2:D:1434:GLY:O	2:D:1475:ILE:N	2.44	0.42
1:E:36:VAL:CG2	1:E:42:CYS:HB3	2.49	0.42
2:F:547:ASN:O	2:F:551:PRO:CD	2.67	0.42
1:G:153:ASN:O	1:G:157:LEU:HB2	2.19	0.42
1:G:178:ALA:HA	1:G:181:LEU:HD12	2.00	0.42
1:A:206:ARG:CD	1:G:55:PHE:HE1	2.32	0.42
2:B:303:SER:HA	2:B:436:PRO:HB3	2.01	0.42
2:B:588:THR:N	2:B:589:PRO:CD	2.82	0.42
2:F:36:HIS:HA	2:F:142:TYR:HE1	1.83	0.42
2:F:588:THR:N	2:F:589:PRO:CD	2.82	0.42
2:H:132:PHE:HA	2:H:133:PRO:HD3	1.81	0.42
2:H:687:THR:HA	2:H:695:THR:H	1.85	0.42
1:A:265:SER:HA	1:A:266:PRO:HD3	1.84	0.42
2:B:1132:ILE:O	2:B:1136:ILE:CB	2.67	0.42
1:C:153:ASN:O	1:C:157:LEU:HB2	2.19	0.42
2:D:1132:ILE:O	2:D:1136:ILE:CB	2.67	0.42
2:D:406:ASN:O	2:D:410:GLY:N	2.51	0.42
2:D:687:THR:HA	2:D:695:THR:H	1.85	0.42
2:F:205:LYS:N	2:F:206:PRO:CD	2.82	0.42
2:F:687:THR:HA	2:F:695:THR:H	1.84	0.42
2:H:547:ASN:O	2:H:551:PRO:CD	2.67	0.42
1:C:231:VAL:O	1:C:231:VAL:HG13	2.19	0.42
1:C:36:VAL:HG23	1:C:42:CYS:HB3	2.01	0.42
2:F:253:LEU:N	2:F:254:PRO:CD	2.82	0.42
1:A:142:CYS:O	1:A:142:CYS:SG	2.78	0.42
1:A:220:VAL:CG1	1:A:220:VAL:O	2.66	0.42
1:A:36:VAL:CG2	1:A:42:CYS:HB3	2.49	0.42
2:B:1514:MET:O	2:B:1518:ASN:CB	2.67	0.42
1:C:252:VAL:HG23	1:C:253:ALA:N	2.33	0.42
1:E:227:GLU:OE2	1:G:192:ARG:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1132:ILE:O	2:F:1136:ILE:CB	2.67	0.42
2:F:37:VAL:O	2:F:41:PHE:CD2	2.72	0.42
2:H:588:THR:N	2:H:589:PRO:CD	2.82	0.42
1:A:227:GLU:OE2	1:C:192:ARG:HA	2.18	0.42
1:C:268:TYR:CE2	1:C:347:ARG:HG2	2.55	0.42
2:D:1514:MET:O	2:D:1518:ASN:CB	2.67	0.42
1:E:153:ASN:O	1:E:157:LEU:HB2	2.19	0.42
2:F:1514:MET:O	2:F:1518:ASN:CB	2.67	0.42
2:H:1514:MET:O	2:H:1518:ASN:CB	2.68	0.42
2:H:518:PHE:O	2:H:522:VAL:CB	2.68	0.42
2:B:547:ASN:O	2:B:551:PRO:CD	2.67	0.42
1:A:55:PHE:HE1	1:C:206:ARG:CD	2.32	0.42
1:C:220:VAL:CG2	1:C:233:LEU:HD22	2.47	0.42
1:G:142:CYS:O	1:G:142:CYS:SG	2.78	0.42
1:G:257:ILE:CD1	1:G:257:ILE:N	2.77	0.42
1:G:341:THR:HA	1:G:342:PRO:HD3	1.88	0.42
2:H:1123:ASN:O	2:H:1127:SER:OG	2.26	0.42
2:H:253:LEU:N	2:H:254:PRO:CD	2.82	0.42
2:D:132:PHE:HA	2:D:133:PRO:HD3	1.81	0.42
1:C:132:GLY:HA3	1:E:131:ILE:O	2.20	0.42
1:E:132:GLY:HA3	1:G:131:ILE:O	2.20	0.42
1:A:192:ARG:HA	1:G:227:GLU:OE2	2.20	0.42
2:H:1434:GLY:O	2:H:1475:ILE:N	2.44	0.42
1:A:268:TYR:CE2	1:A:347:ARG:HG2	2.55	0.42
2:B:1066:MET:O	2:B:1070:LEU:CB	2.68	0.42
2:B:518:PHE:O	2:B:522:VAL:CB	2.68	0.42
2:B:687:THR:HA	2:B:695:THR:H	1.85	0.42
1:E:268:TYR:CE2	1:E:347:ARG:HG2	2.55	0.42
2:F:518:PHE:O	2:F:522:VAL:CB	2.68	0.42
1:G:36:VAL:HG23	1:G:42:CYS:HB3	2.01	0.42
2:H:205:LYS:N	2:H:206:PRO:CD	2.82	0.42
2:D:588:THR:N	2:D:589:PRO:CD	2.82	0.41
1:E:147:LEU:O	1:E:151:VAL:HG23	2.20	0.41
2:H:1066:MET:O	2:H:1070:LEU:CB	2.68	0.41
2:H:303:SER:HA	2:H:436:PRO:HB3	2.01	0.41
2:B:132:PHE:HA	2:B:133:PRO:HD3	1.81	0.41
1:C:339:VAL:HG13	1:C:340:PRO:CD	2.49	0.41
2:D:1066:MET:O	2:D:1070:LEU:CB	2.68	0.41
2:B:206:PRO:HB2	2:B:207:PRO:CD	2.44	0.41
1:C:72:LEU:O	1:C:76:THR:HG23	2.21	0.41
2:D:391:ILE:O	2:D:395:ILE:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:CYS:O	1:E:142:CYS:SG	2.78	0.41
2:B:485:GLN:O	2:B:489:LEU:CB	2.69	0.41
2:D:34:VAL:CB	2:D:35:PRO:CD	2.98	0.41
2:D:518:PHE:O	2:D:522:VAL:CB	2.68	0.41
1:E:36:VAL:HG23	1:E:42:CYS:HB3	2.01	0.41
1:G:345:THR:HG23	1:G:348:GLN:H	1.86	0.41
1:A:220:VAL:CG2	1:A:233:LEU:HD22	2.47	0.41
1:C:345:THR:HG23	1:C:348:GLN:H	1.86	0.41
2:D:416:GLN:O	2:D:420:LEU:HB2	2.21	0.41
2:B:391:ILE:O	2:B:395:ILE:CB	2.69	0.41
1:C:142:CYS:O	1:C:142:CYS:SG	2.78	0.41
2:F:391:ILE:O	2:F:395:ILE:CB	2.69	0.41
2:F:561:GLY:O	2:F:565:PHE:CB	2.69	0.41
1:A:131:ILE:O	1:G:132:GLY:HA3	2.20	0.41
1:G:147:LEU:O	1:G:151:VAL:HG23	2.20	0.41
1:G:72:LEU:O	1:G:76:THR:HG23	2.21	0.41
1:A:345:THR:HG23	1:A:348:GLN:H	1.86	0.41
1:C:147:LEU:O	1:C:151:VAL:HG23	2.20	0.41
1:G:268:TYR:CE2	1:G:347:ARG:HG2	2.55	0.41
2:H:44:PHE:N	2:H:45:PRO:CD	2.83	0.41
2:H:472:PRO:O	2:H:476:PHE:CB	2.69	0.41
1:A:72:LEU:O	1:A:76:THR:HG23	2.21	0.41
2:D:297:ARG:O	2:D:301:LEU:HB2	2.21	0.41
2:B:34:VAL:CB	2:B:35:PRO:CD	2.98	0.41
2:B:44:PHE:N	2:B:45:PRO:CD	2.83	0.41
2:B:561:GLY:O	2:B:565:PHE:CB	2.69	0.41
1:C:137:MET:HE1	1:E:135:GLY:H	1.86	0.41
1:C:238:ILE:HG13	1:C:238:ILE:O	2.21	0.41
2:D:64:THR:O	2:D:65:TRP:CG	2.74	0.41
2:F:1148:LEU:O	2:F:1152:SER:CB	2.69	0.41
2:F:297:ARG:O	2:F:301:LEU:HB2	2.21	0.41
2:F:34:VAL:CB	2:F:35:PRO:CD	2.98	0.41
2:H:561:GLY:O	2:H:565:PHE:CB	2.69	0.41
2:D:1148:LEU:O	2:D:1152:SER:CB	2.69	0.41
2:D:44:PHE:N	2:D:45:PRO:CD	2.83	0.41
1:C:227:GLU:OE2	1:E:192:ARG:HA	2.20	0.41
1:E:238:ILE:O	1:E:238:ILE:HG13	2.20	0.41
1:E:268:TYR:CD2	1:E:347:ARG:HG2	2.56	0.41
1:G:268:TYR:CD2	1:G:347:ARG:HG2	2.56	0.41
2:H:391:ILE:O	2:H:395:ILE:CB	2.69	0.41
2:B:1123:ASN:O	2:B:1127:SER:OG	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:680:GLN:HA	2:D:702:ARG:HG2	2.03	0.41
2:F:485:GLN:O	2:F:489:LEU:CB	2.69	0.41
1:G:200:LEU:HD23	1:G:200:LEU:HA	1.96	0.41
1:G:238:ILE:O	1:G:238:ILE:HG13	2.21	0.41
2:H:297:ARG:O	2:H:301:LEU:HB2	2.21	0.41
2:H:485:GLN:O	2:H:489:LEU:CB	2.69	0.41
2:B:1434:GLY:O	2:B:1475:ILE:N	2.44	0.40
2:B:484:ALA:O	2:B:488:THR:CB	2.69	0.40
1:E:345:THR:HG23	1:E:348:GLN:H	1.86	0.40
2:F:1066:MET:O	2:F:1070:LEU:CB	2.68	0.40
2:F:416:GLN:O	2:F:420:LEU:HB2	2.21	0.40
2:F:472:PRO:O	2:F:476:PHE:CB	2.69	0.40
1:G:265:SER:HA	1:G:266:PRO:HD3	1.84	0.40
1:G:313:GLN:HA	1:G:338:LYS:HA	2.03	0.40
2:H:416:GLN:O	2:H:420:LEU:HB2	2.21	0.40
1:A:220:VAL:HG12	1:A:282:GLU:O	2.22	0.40
1:A:313:GLN:HA	1:A:338:LYS:HA	2.03	0.40
2:B:64:THR:O	2:B:65:TRP:CG	2.74	0.40
1:C:150:ILE:HG23	1:E:83:TRP:HZ3	1.85	0.40
2:F:484:ALA:O	2:F:488:THR:CB	2.69	0.40
2:H:460:ALA:O	2:H:464:ALA:CB	2.70	0.40
2:H:484:ALA:O	2:H:488:THR:CB	2.69	0.40
1:A:268:TYR:CD2	1:A:347:ARG:HG2	2.56	0.40
1:C:268:TYR:CD2	1:C:347:ARG:HG2	2.56	0.40
2:D:472:PRO:O	2:D:476:PHE:CB	2.69	0.40
1:E:221:ARG:HG2	1:E:222:LYS:N	2.37	0.40
1:E:72:LEU:O	1:E:76:THR:HG23	2.21	0.40
2:F:44:PHE:N	2:F:45:PRO:CD	2.83	0.40
1:E:150:ILE:HG23	1:G:83:TRP:HZ3	1.85	0.40
2:H:718:GLY:O	2:H:722:LEU:N	2.48	0.40
1:A:147:LEU:O	1:A:151:VAL:HG23	2.20	0.40
2:B:1148:LEU:O	2:B:1152:SER:CB	2.69	0.40
2:B:297:ARG:O	2:B:301:LEU:HB2	2.21	0.40
2:D:485:GLN:O	2:D:489:LEU:CB	2.69	0.40
2:D:561:GLY:O	2:D:565:PHE:CB	2.69	0.40
2:H:34:VAL:CB	2:H:35:PRO:CD	2.98	0.40
2:D:484:ALA:O	2:D:488:THR:CB	2.69	0.40
2:F:1277:SER:OG	2:F:1279:GLY:O	2.32	0.40
1:E:55:PHE:HE1	1:G:206:ARG:HD3	1.87	0.40
2:H:1148:LEU:O	2:H:1152:SER:CB	2.69	0.40
2:H:146:ALA:HB1	2:H:179:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/390 (83%)	310 (96%)	12 (4%)	1 (0%)	46	83
1	C	323/390 (83%)	310 (96%)	12 (4%)	1 (0%)	46	83
1	E	323/390 (83%)	310 (96%)	12 (4%)	1 (0%)	46	83
1	G	323/390 (83%)	310 (96%)	12 (4%)	1 (0%)	46	83
2	B	1363/1590 (86%)	1303 (96%)	56 (4%)	4 (0%)	46	83
2	D	1363/1590 (86%)	1302 (96%)	57 (4%)	4 (0%)	46	83
2	F	1363/1590 (86%)	1303 (96%)	56 (4%)	4 (0%)	46	83
2	H	1363/1590 (86%)	1303 (96%)	56 (4%)	4 (0%)	46	83
All	All	6744/7920 (85%)	6451 (96%)	273 (4%)	20 (0%)	50	83

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	98	VAL
2	B	277	ASP
2	B	316	GLY
2	D	98	VAL
2	D	277	ASP
2	D	316	GLY
2	F	98	VAL
2	F	277	ASP
2	F	316	GLY
2	H	98	VAL
2	H	277	ASP
2	H	316	GLY
1	A	180	THR
1	C	180	THR

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Mol	Chain	Res	Type
1	E	180	THR
1	G	180	THR
2	B	224	LEU
2	D	224	LEU
2	F	224	LEU
2	H	224	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	264/341 (77%)	262 (99%)	2 (1%)	86	94
1	C	264/341 (77%)	262 (99%)	2 (1%)	86	94
1	E	264/341 (77%)	262 (99%)	2 (1%)	86	94
1	G	264/341 (77%)	262 (99%)	2 (1%)	86	94
2	B	224/1381 (16%)	222 (99%)	2 (1%)	84	93
2	D	224/1381 (16%)	222 (99%)	2 (1%)	84	93
2	F	224/1381 (16%)	222 (99%)	2 (1%)	84	93
2	H	224/1381 (16%)	222 (99%)	2 (1%)	84	93
All	All	1952/6888 (28%)	1936 (99%)	16 (1%)	87	94

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	PHE
1	A	133	PHE
2	B	6	CYS
2	B	123	TYR
1	C	95	PHE
1	C	133	PHE
2	D	6	CYS
2	D	123	TYR
1	E	95	PHE

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Mol	Chain	Res	Type
1	E	133	PHE
2	F	6	CYS
2	F	123	TYR
1	G	95	PHE
1	G	133	PHE
2	H	6	CYS
2	H	123	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	ATP	A	401	-	26,33,33	0.92	1 (3%)	26,52,52	1.76	3 (11%)
3	ATP	C	401	-	26,33,33	0.92	1 (3%)	26,52,52	1.76	3 (11%)
3	ATP	E	401	-	26,33,33	0.92	1 (3%)	26,52,52	1.76	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	G	401	-	26,33,33	0.92	1 (3%)	26,52,52	1.76	3 (11%)

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	ATP	A	401	-	-	0/18/38/38	0/3/3/3
3	ATP	C	401	-	-	0/18/38/38	0/3/3/3
3	ATP	E	401	-	-	0/18/38/38	0/3/3/3
3	ATP	G	401	-	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	ATP	C5-C4	2.44	1.46	1.40
3	G	401	ATP	C5-C4	2.44	1.46	1.40
3	A	401	ATP	C5-C4	2.44	1.46	1.40
3	C	401	ATP	C5-C4	2.45	1.46	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	ATP	N3-C2-N1	-6.00	124.16	128.87
3	E	401	ATP	N3-C2-N1	-6.00	124.16	128.87
3	G	401	ATP	N3-C2-N1	-6.00	124.16	128.87
3	A	401	ATP	N3-C2-N1	-6.00	124.16	128.87
3	E	401	ATP	C1'-N9-C4	-3.12	123.32	126.81
3	G	401	ATP	C1'-N9-C4	-3.09	123.36	126.81
3	A	401	ATP	C1'-N9-C4	-3.09	123.36	126.81
3	C	401	ATP	C1'-N9-C4	-3.09	123.36	126.81
3	E	401	ATP	N6-C6-N1	2.66	122.98	118.52
3	G	401	ATP	N6-C6-N1	2.67	123.00	118.52
3	A	401	ATP	N6-C6-N1	2.67	123.00	118.52
3	C	401	ATP	N6-C6-N1	2.67	123.00	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ATP	7	0
3	C	401	ATP	7	0
3	E	401	ATP	7	0
3	G	401	ATP	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.