



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:50 PM UTC

PDB ID : 5YWB / pdb_00005ywb
EMDB ID : EMD-6851
Title : Structure of pancreatic ATP-sensitive potassium channel bound with Mg-ADP
(CTD class2 at 5.2Å)
Authors : Chen, L.; Wu, J.X.
Deposited on : 2017-11-29
Resolution : 5.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

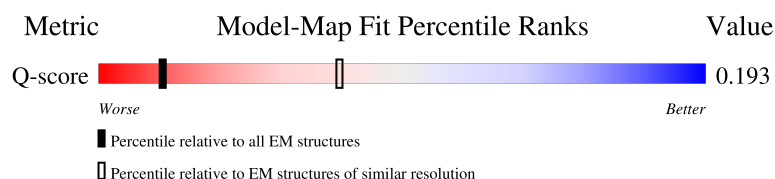
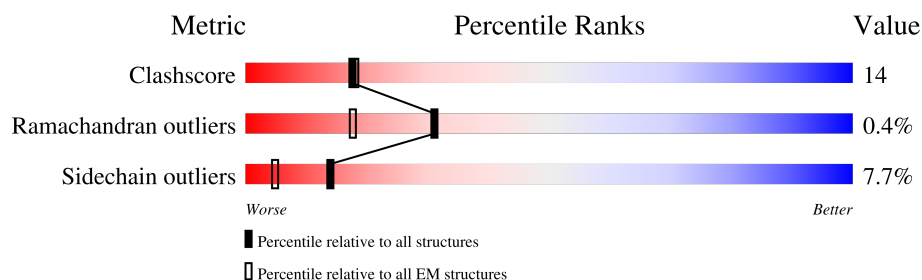
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 5.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	712 (4.70 - 5.70)

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

Mol	Chain	Length	Quality of chain
1	A	390	 7% 51% 28% • 17%
1	C	390	 7% 51% 29% • 17%
1	E	390	 7% 52% 28% • 17%
1	G	390	 7% 51% 29% • 17%

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Mol	Chain	Length	Quality of chain
2	B	1582	26% 60% 22% • 16%
2	D	1582	26% 60% 22% • 16%
2	F	1582	26% 60% 22% • 16%
2	H	1582	26% 60% 22% • 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50928 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.

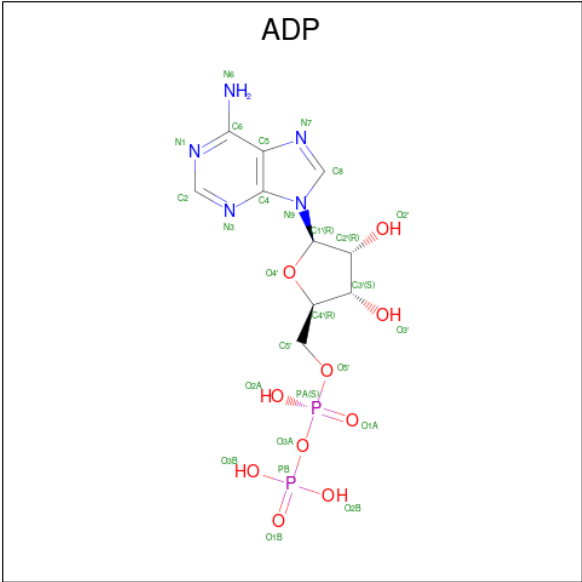
- Molecule 1 is a protein called ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	325	Total	C	N	O	S	0	0
			2424	1565	417	427	15		
1	C	325	Total	C	N	O	S	0	0
			2424	1565	417	427	15		
1	E	325	Total	C	N	O	S	0	0
			2424	1565	417	427	15		
1	G	325	Total	C	N	O	S	0	0
			2424	1565	417	427	15		

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8 isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1322	Total	C	N	O	S	0	0
			10225	6658	1727	1787	53		
2	D	1322	Total	C	N	O	S	0	0
			10225	6658	1727	1787	53		
2	F	1322	Total	C	N	O	S	0	0
			10225	6658	1727	1787	53		
2	H	1322	Total	C	N	O	S	0	0
			10225	6658	1727	1787	53		

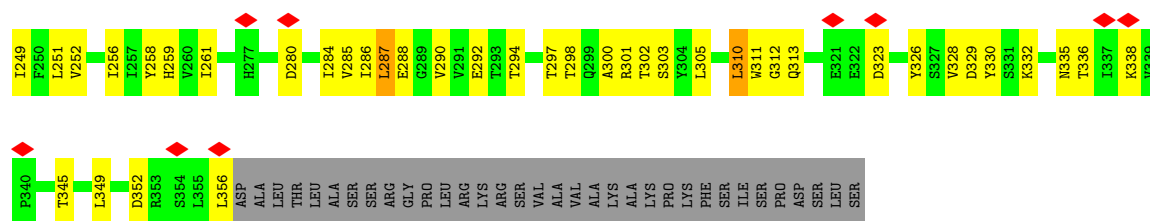
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



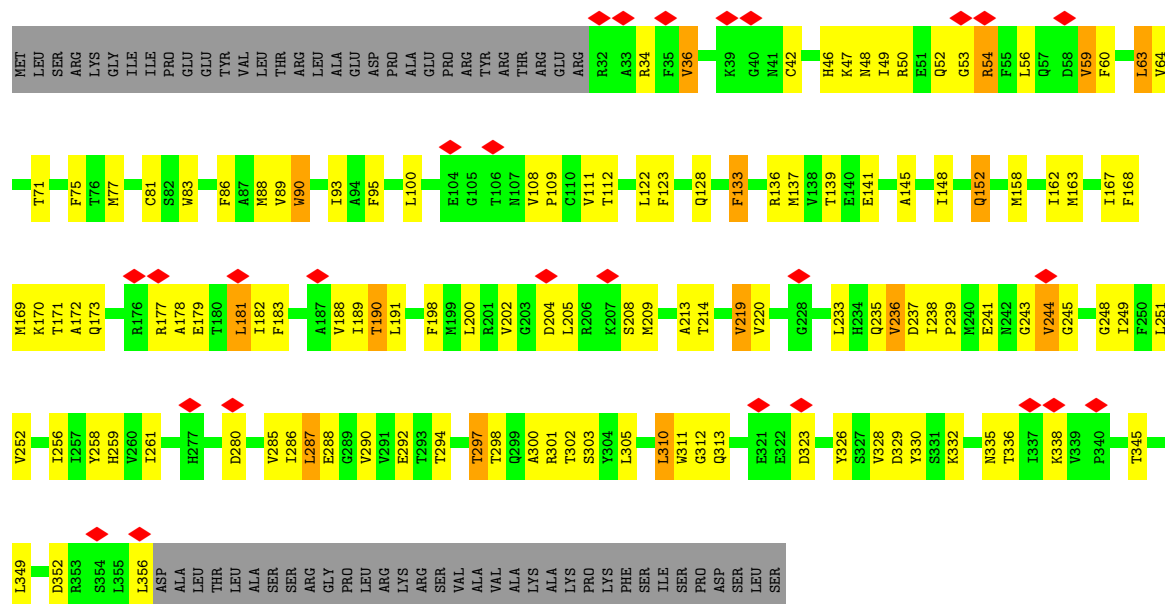
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	H	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

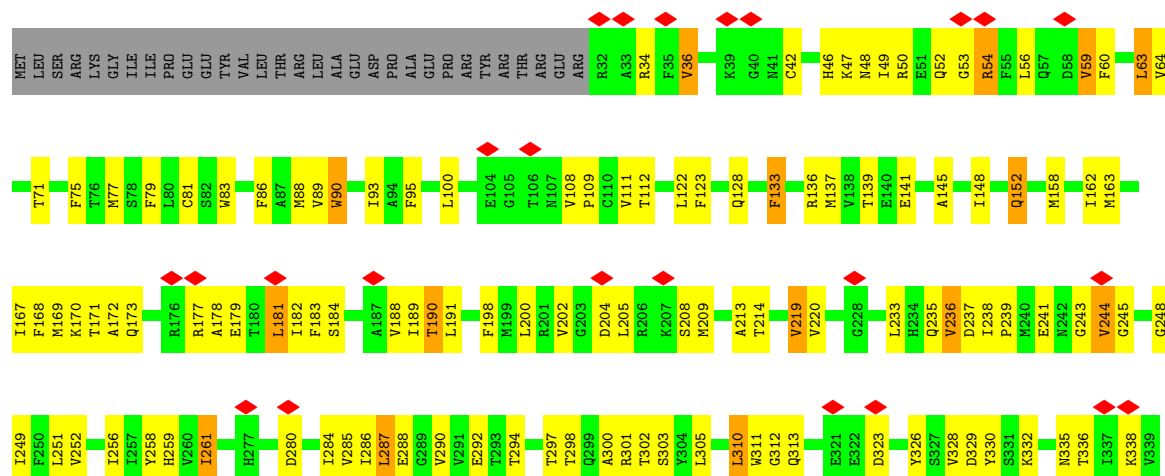
Mol	Chain	Residues	Atoms		AltConf
4	B	2	Total 2	Mg 2	0
4	D	2	Total 2	Mg 2	0
4	F	2	Total 2	Mg 2	0
4	H	2	Total 2	Mg 2	0

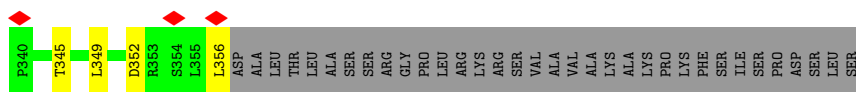


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

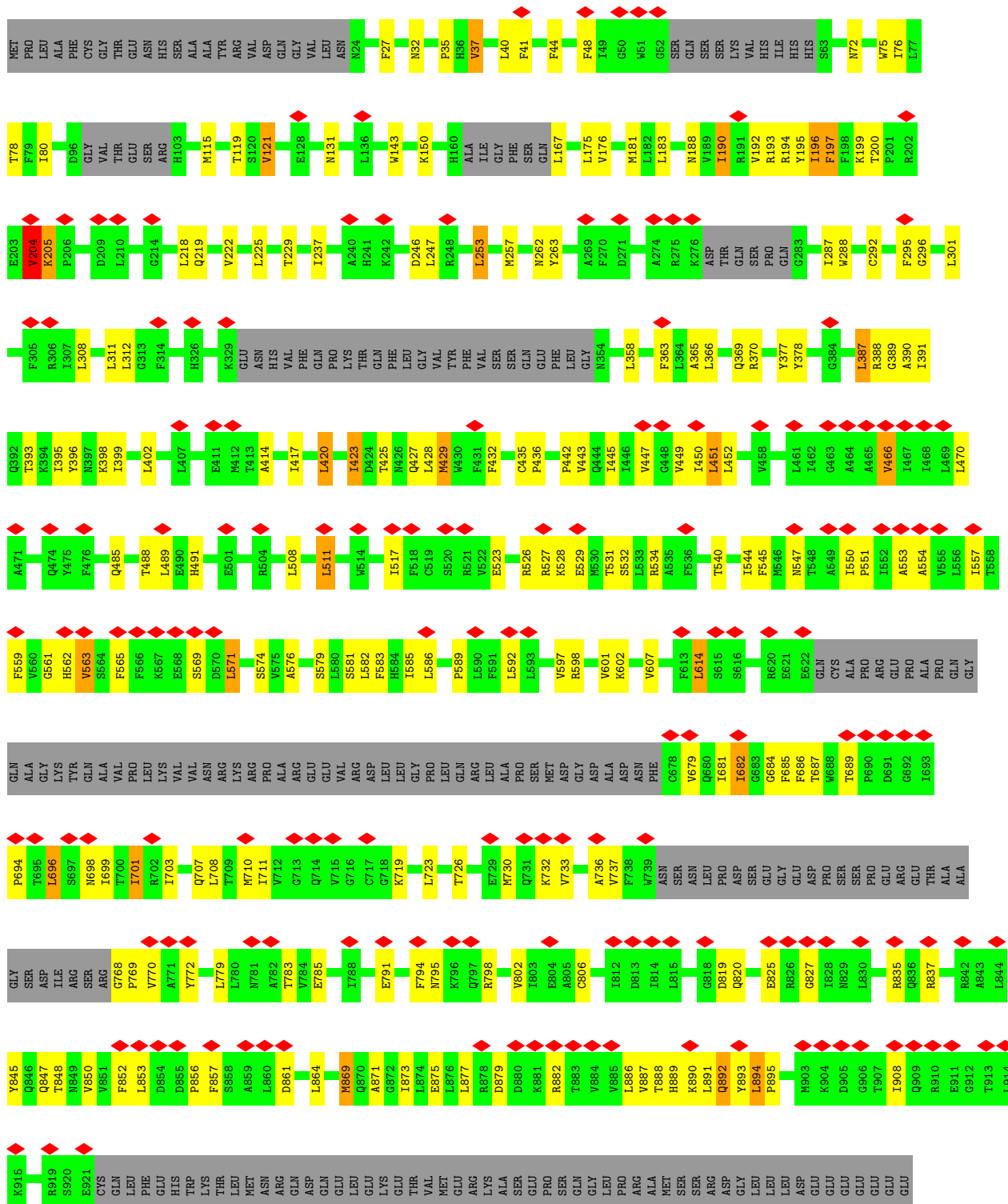


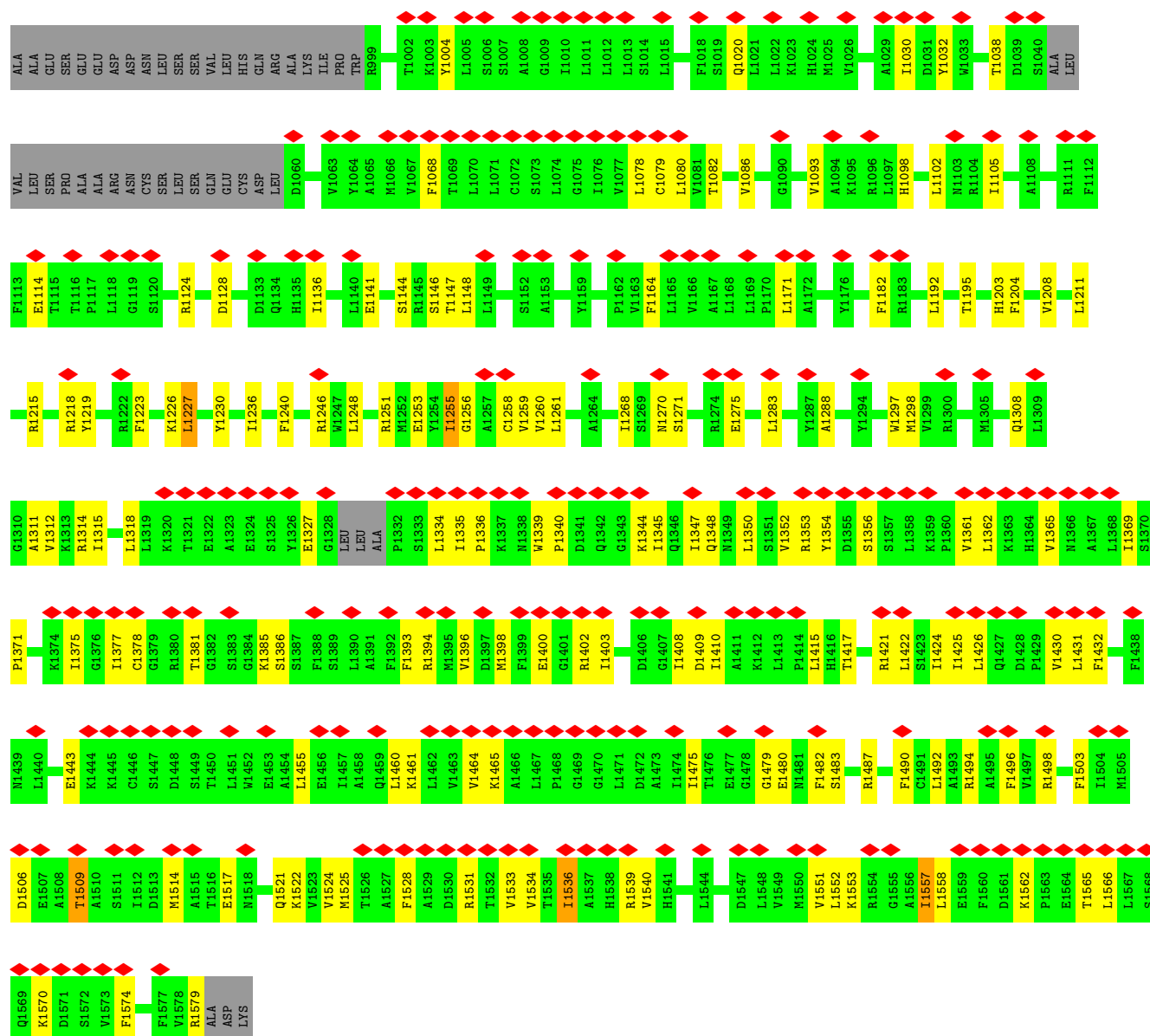
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



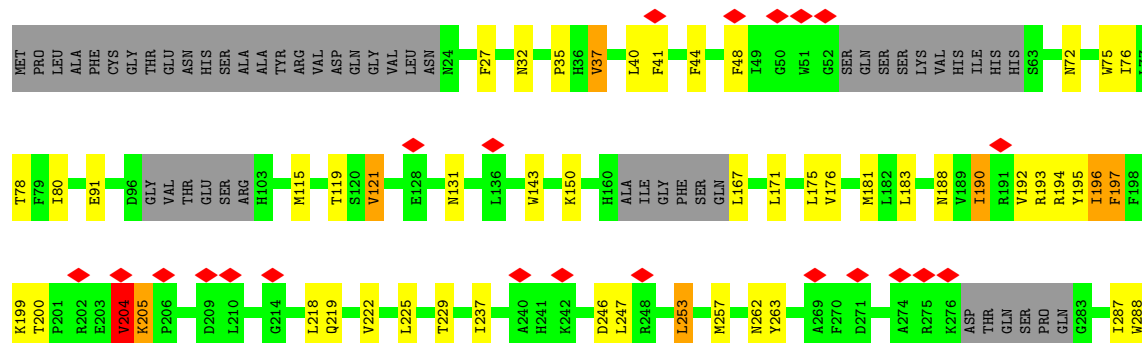


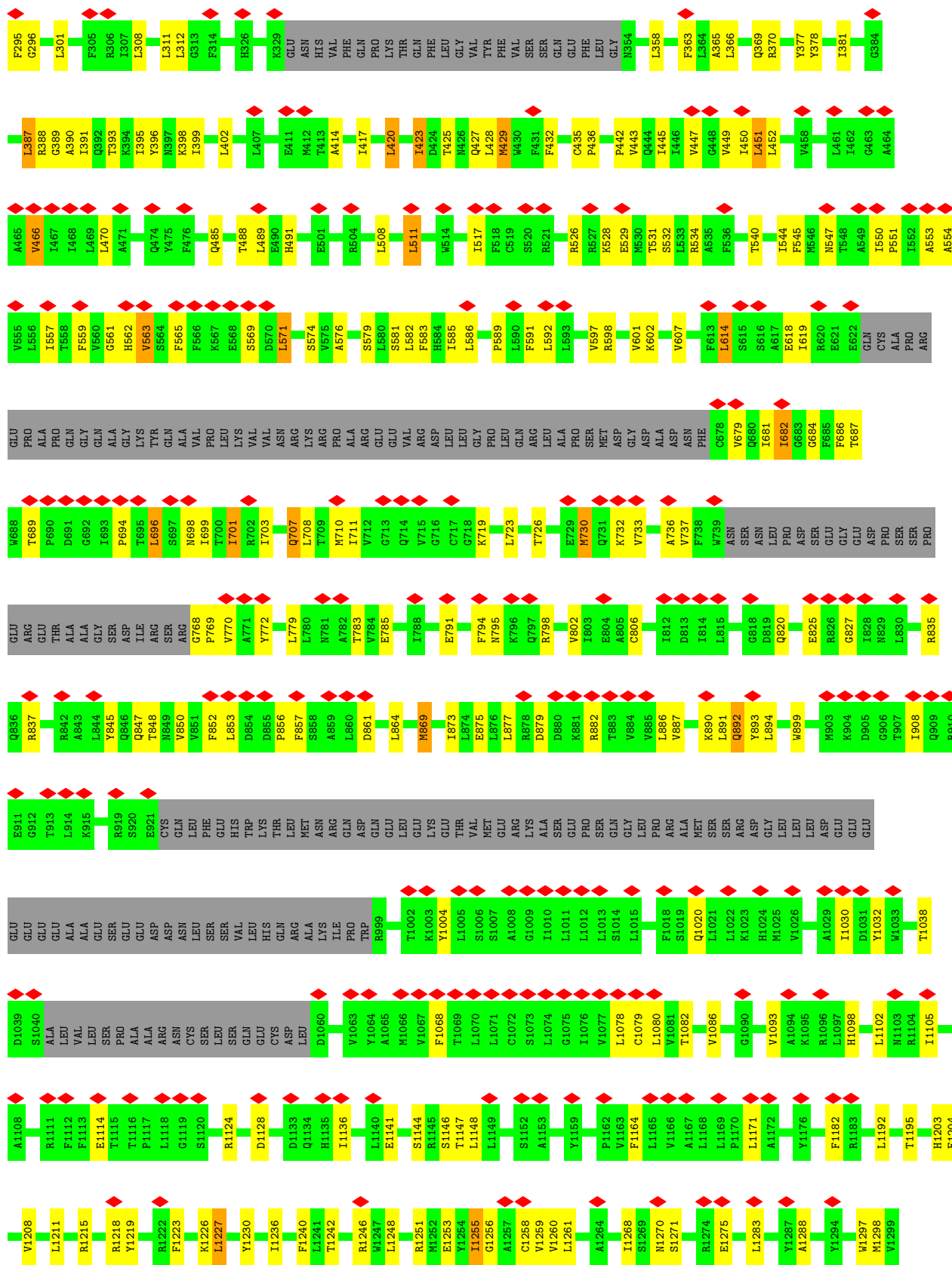
- Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

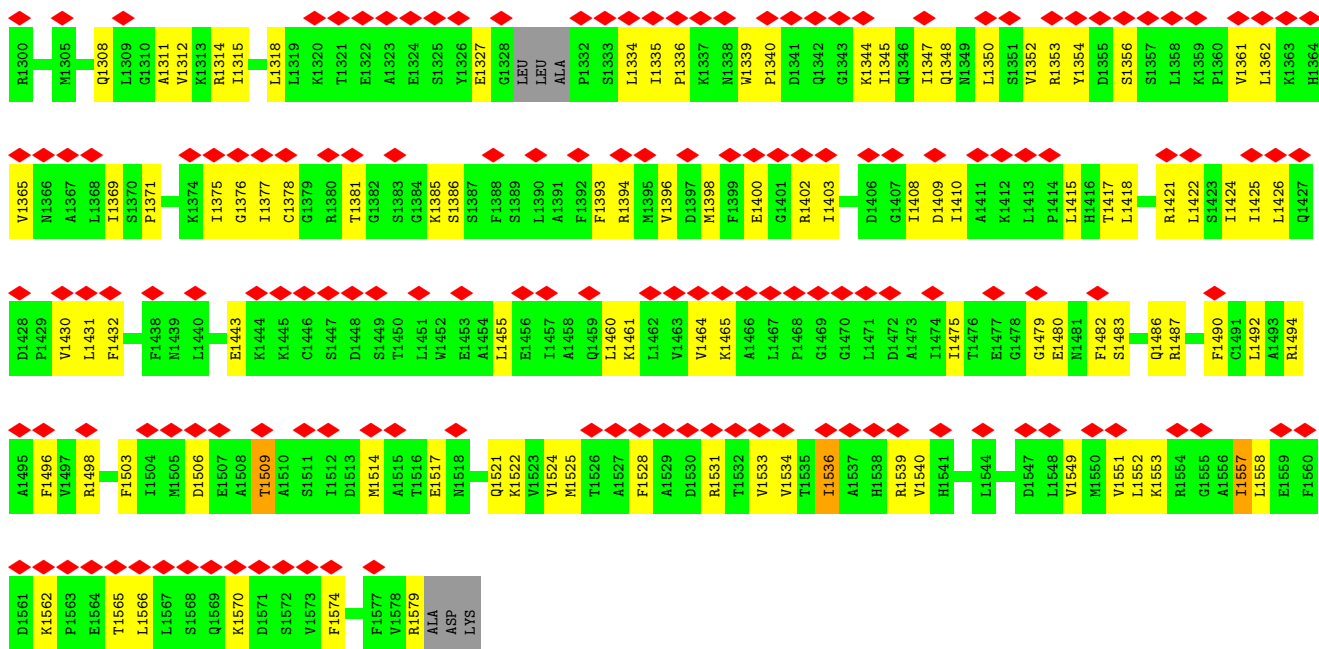




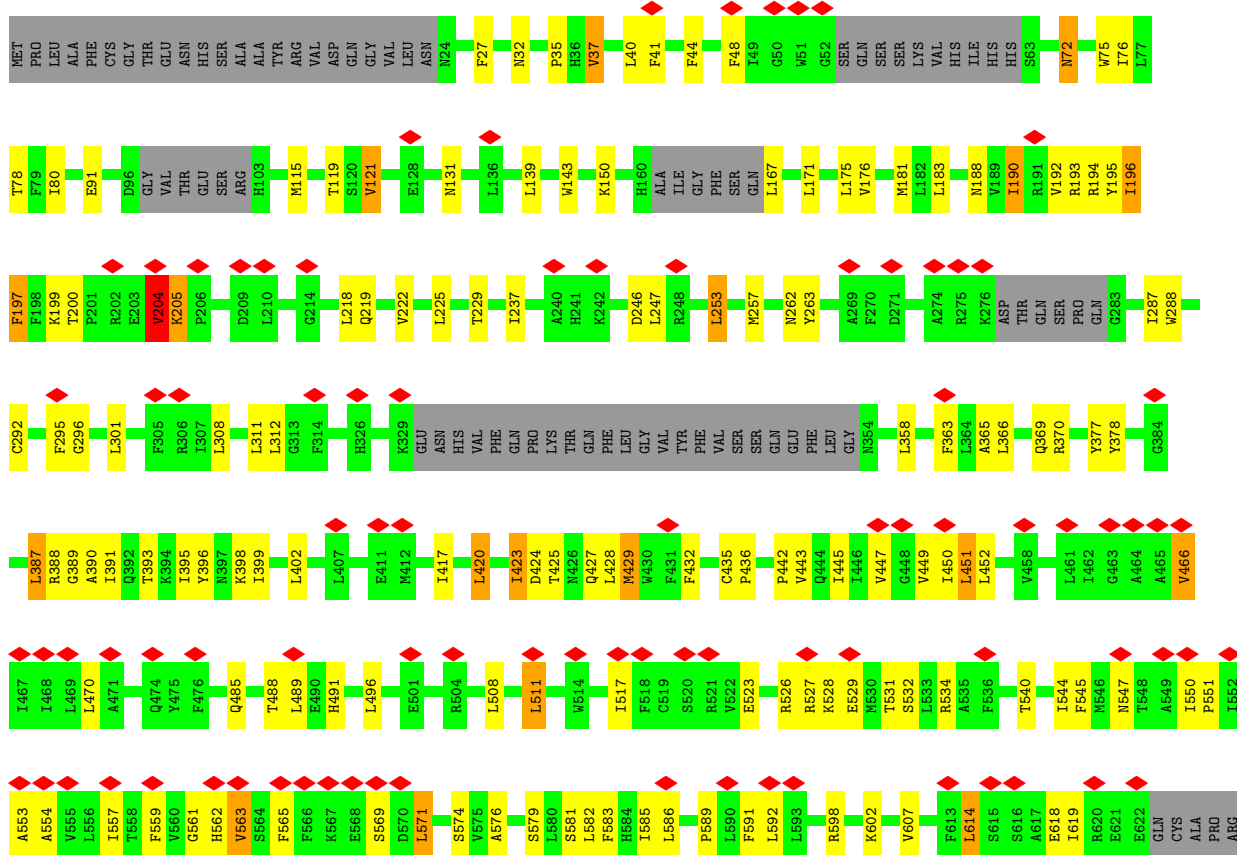
• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

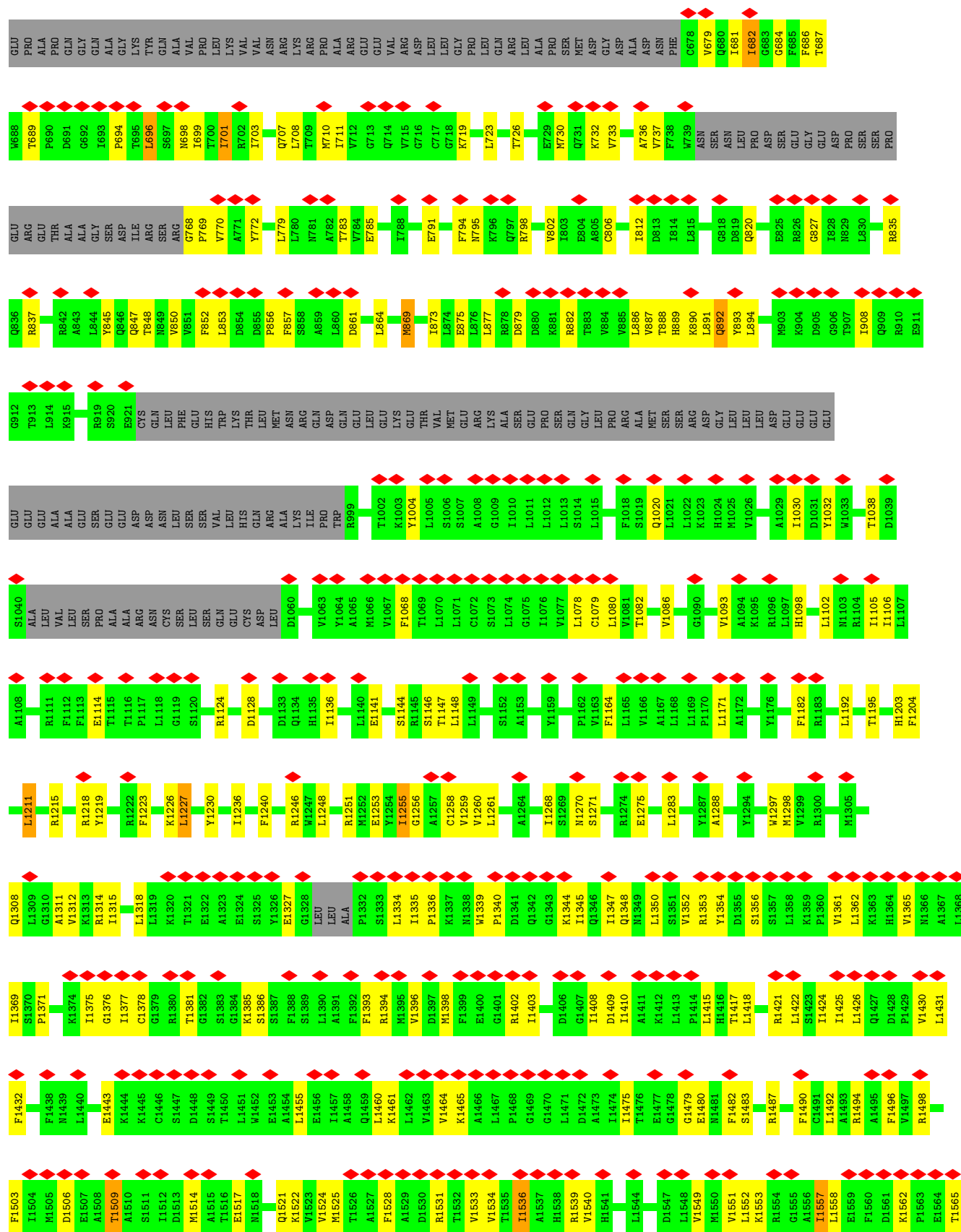


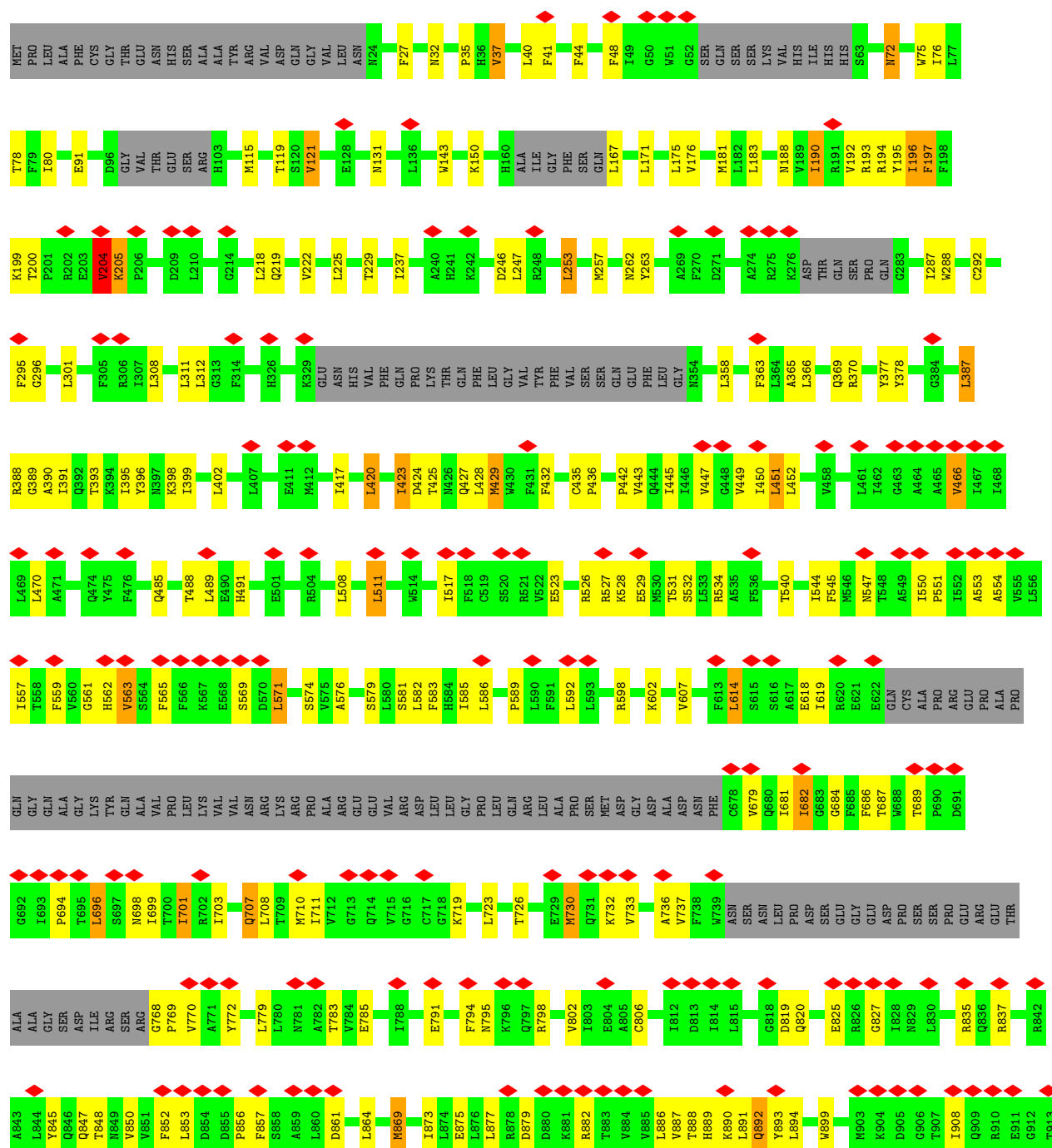




- Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56433	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	329.15997, 329.15997, 329.15997	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.18	0/2477	0.47	1/3380 (0.0%)
1	C	0.18	0/2477	0.47	1/3380 (0.0%)
1	E	0.18	0/2477	0.47	1/3380 (0.0%)
1	G	0.18	0/2477	0.47	1/3380 (0.0%)
2	B	0.20	1/10430 (0.0%)	0.42	5/14168 (0.0%)
2	D	0.20	1/10430 (0.0%)	0.42	5/14168 (0.0%)
2	F	0.20	1/10430 (0.0%)	0.42	5/14168 (0.0%)
2	H	0.20	1/10430 (0.0%)	0.42	5/14168 (0.0%)
All	All	0.20	4/51628 (0.0%)	0.43	24/70192 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	181	MET	C-N	-5.08	1.27	1.33
2	D	181	MET	C-N	-5.08	1.27	1.33
2	F	181	MET	C-N	-5.08	1.27	1.33
2	H	181	MET	C-N	-5.08	1.27	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	181	MET	O-C-N	-6.46	114.79	122.15
2	D	181	MET	O-C-N	-6.46	114.79	122.15
2	F	181	MET	O-C-N	-6.46	114.79	122.15
2	H	181	MET	O-C-N	-6.46	114.79	122.15
2	B	296	GLY	N-CA-C	6.28	122.88	110.77
2	D	296	GLY	N-CA-C	6.28	122.88	110.77
2	F	296	GLY	N-CA-C	6.28	122.88	110.77
2	H	296	GLY	N-CA-C	6.28	122.88	110.77
2	B	194	ARG	N-CA-C	6.14	120.85	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	194	ARG	N-CA-C	6.14	120.85	109.24
2	F	194	ARG	N-CA-C	6.14	120.85	109.24
2	H	194	ARG	N-CA-C	6.14	120.85	109.24
1	A	52	GLN	N-CA-C	5.86	119.64	111.74
1	C	52	GLN	N-CA-C	5.86	119.64	111.74
1	E	52	GLN	N-CA-C	5.86	119.64	111.74
1	G	52	GLN	N-CA-C	5.86	119.64	111.74
2	B	204	VAL	N-CA-C	5.23	115.96	110.62
2	D	204	VAL	N-CA-C	5.23	115.96	110.62
2	F	204	VAL	N-CA-C	5.23	115.96	110.62
2	H	204	VAL	N-CA-C	5.23	115.96	110.62
2	B	200	THR	N-CA-C	5.01	116.89	109.62
2	D	200	THR	N-CA-C	5.01	116.89	109.62
2	F	200	THR	N-CA-C	5.01	116.89	109.62
2	H	200	THR	N-CA-C	5.01	116.89	109.62

There are no chirality outliers.

There are no planarity outliers.

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	2424	0	2383	110	0
1	C	2424	0	2383	109	0
1	E	2424	0	2383	109	0
1	G	2424	0	2383	112	0
2	B	10225	0	10456	254	0
2	D	10225	0	10456	257	0
2	F	10225	0	10456	256	0
2	H	10225	0	10456	252	0
3	A	27	0	12	0	0
3	B	54	0	24	5	0
3	C	27	0	12	0	0
3	D	54	0	24	4	0
3	E	27	0	12	0	0
3	F	54	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	27	0	12	0	0
3	H	54	0	24	5	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
4	F	2	0	0	0	0
4	H	2	0	0	0	0
All	All	50928	0	51500	1385	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 14.

All (1385) 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:D:190:ILE:HG13	2:D:195:TYR:CB	1.79	1.13
2:F:190:ILE:HG13	2:F:195:TYR:CB	1.79	1.13
2:H:190:ILE:HG13	2:H:195:TYR:CB	1.79	1.12
2:B:190:ILE:HG13	2:B:195:TYR:CB	1.79	1.11
2:H:295:PHE:CZ	2:H:387:LEU:HB2	2.01	0.96
1:C:169:MET:HE1	1:E:172:ALA:HA	1.48	0.95
1:E:169:MET:HE1	1:G:172:ALA:HA	1.48	0.95
2:D:190:ILE:CG1	2:D:195:TYR:CB	2.44	0.95
2:D:295:PHE:CZ	2:D:387:LEU:HB2	2.01	0.94
2:F:190:ILE:CG1	2:F:195:TYR:CB	2.44	0.94
2:H:190:ILE:CG1	2:H:195:TYR:CB	2.44	0.94
2:B:295:PHE:CZ	2:B:387:LEU:HB2	2.01	0.94
2:F:295:PHE:CZ	2:F:387:LEU:HB2	2.01	0.94
2:B:190:ILE:CG1	2:B:195:TYR:CB	2.44	0.94
1:A:169:MET:HE1	1:C:172:ALA:HA	1.48	0.93
1:A:172:ALA:HA	1:G:169:MET:HE1	1.48	0.92
1:E:169:MET:CE	1:G:172:ALA:HA	2.02	0.90
1:A:169:MET:CE	1:C:172:ALA:HA	2.02	0.90
2:D:91:GLU:CD	2:D:171:LEU:HD12	1.96	0.90
1:A:172:ALA:HA	1:G:169:MET:CE	2.02	0.89
1:C:169:MET:CE	1:E:172:ALA:HA	2.02	0.89
1:E:168:PHE:O	1:E:171:THR:CG2	2.25	0.85
1:G:168:PHE:O	1:G:171:THR:CG2	2.25	0.85
1:A:168:PHE:O	1:A:171:THR:CG2	2.25	0.84
1:C:168:PHE:O	1:C:171:THR:CG2	2.25	0.84
1:A:243:GLY:HA3	1:G:237:ASP:HB3	1.62	0.81
1:A:182:ILE:HD12	1:A:182:ILE:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:ASP:HB3	1:G:243:GLY:HA3	1.62	0.81
1:C:237:ASP:HB3	1:E:243:GLY:HA3	1.62	0.81
1:C:182:ILE:HD12	1:C:182:ILE:O	1.81	0.81
1:G:182:ILE:HD12	1:G:182:ILE:O	1.81	0.81
1:A:237:ASP:HB3	1:C:243:GLY:HA3	1.62	0.80
1:E:182:ILE:HD12	1:E:182:ILE:O	1.81	0.80
1:G:168:PHE:HA	1:G:171:THR:CG2	2.12	0.80
1:G:168:PHE:O	1:G:171:THR:HG23	1.81	0.80
1:C:168:PHE:O	1:C:171:THR:HG23	1.81	0.80
1:C:168:PHE:HA	1:C:171:THR:CG2	2.12	0.80
1:A:168:PHE:HA	1:A:171:THR:CG2	2.12	0.80
1:E:168:PHE:HA	1:E:171:THR:CG2	2.12	0.79
1:E:168:PHE:O	1:E:171:THR:HG23	1.81	0.79
2:D:1124:ARG:HH11	2:D:1314:ARG:HD3	1.49	0.78
2:D:1271:SER:HA	2:D:1275:GLU:HB3	1.66	0.78
2:F:1271:SER:HA	2:F:1275:GLU:HB3	1.66	0.78
1:A:168:PHE:O	1:A:171:THR:HG23	1.81	0.78
2:F:1124:ARG:HH11	2:F:1314:ARG:HD3	1.49	0.78
1:G:214:THR:HA	1:G:248:GLY:HA2	1.65	0.78
1:E:214:THR:HA	1:E:248:GLY:HA2	1.65	0.78
2:B:204:VAL:O	2:B:205:LYS:HB3	1.83	0.77
2:D:204:VAL:O	2:D:205:LYS:HB3	1.83	0.77
2:H:1271:SER:HA	2:H:1275:GLU:HB3	1.66	0.77
1:C:214:THR:HA	1:C:248:GLY:HA2	1.65	0.77
2:B:1271:SER:HA	2:B:1275:GLU:HB3	1.66	0.77
2:B:1421:ARG:HG3	2:B:1422:LEU:HG	1.67	0.77
2:B:196:ILE:O	2:B:197:PHE:O	2.03	0.77
1:A:214:THR:HA	1:A:248:GLY:HA2	1.65	0.76
2:D:1421:ARG:HG3	2:D:1422:LEU:HG	1.67	0.76
2:F:204:VAL:O	2:F:205:LYS:HB3	1.83	0.76
2:B:150:LYS:HB3	2:B:176:VAL:HG22	1.67	0.76
2:H:204:VAL:O	2:H:205:LYS:HB3	1.83	0.76
2:B:150:LYS:HE3	2:B:175:LEU:HD13	1.67	0.76
2:F:1421:ARG:HG3	2:F:1422:LEU:HG	1.67	0.76
2:H:1124:ARG:HH11	2:H:1314:ARG:HD3	1.49	0.76
2:H:150:LYS:HB3	2:H:176:VAL:HG22	1.67	0.76
2:B:1124:ARG:HH11	2:B:1314:ARG:HD3	1.49	0.76
2:D:150:LYS:HE3	2:D:175:LEU:HD13	1.67	0.76
2:D:196:ILE:O	2:D:197:PHE:O	2.03	0.76
2:H:1421:ARG:HG3	2:H:1422:LEU:HG	1.67	0.75
1:A:177:ARG:HH22	1:A:208:SER:HB2	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:LYS:HB3	2:D:176:VAL:HG22	1.67	0.75
2:F:196:ILE:O	2:F:197:PHE:O	2.03	0.75
1:G:177:ARG:HH22	1:G:208:SER:HB2	1.51	0.75
2:H:150:LYS:HE3	2:H:175:LEU:HD13	1.67	0.75
2:H:196:ILE:O	2:H:197:PHE:O	2.03	0.75
2:F:150:LYS:HE3	2:F:175:LEU:HD13	1.67	0.75
1:C:177:ARG:HH22	1:C:208:SER:HB2	1.51	0.74
2:D:387:LEU:HD21	2:D:428:LEU:HB3	1.69	0.74
2:F:150:LYS:HB3	2:F:176:VAL:HG22	1.67	0.74
1:E:177:ARG:HH22	1:E:208:SER:HB2	1.51	0.73
2:B:387:LEU:HD21	2:B:428:LEU:HB3	1.69	0.73
2:H:387:LEU:HD21	2:H:428:LEU:HB3	1.69	0.73
2:F:387:LEU:HD21	2:F:428:LEU:HB3	1.69	0.72
2:H:1334:LEU:HD13	2:H:1408:ILE:HG23	1.72	0.72
1:E:177:ARG:NH2	1:E:208:SER:HB2	2.05	0.72
1:G:177:ARG:NH2	1:G:208:SER:HB2	2.05	0.72
1:C:219:VAL:HG13	1:C:236:VAL:HG23	1.72	0.71
1:A:169:MET:HE1	1:C:172:ALA:CA	2.21	0.71
2:B:150:LYS:CE	2:B:175:LEU:HD13	2.21	0.71
1:E:219:VAL:HG13	1:E:236:VAL:HG23	1.72	0.71
2:B:1334:LEU:HD13	2:B:1408:ILE:HG23	1.72	0.71
1:E:36:VAL:HG12	1:E:42:CYS:HA	1.72	0.71
1:G:36:VAL:HG12	1:G:42:CYS:HA	1.72	0.71
2:F:1334:LEU:HD13	2:F:1408:ILE:HG23	1.72	0.71
2:D:150:LYS:CE	2:D:175:LEU:HD13	2.21	0.71
1:E:169:MET:HE1	1:G:172:ALA:CA	2.21	0.71
1:A:36:VAL:HG12	1:A:42:CYS:HA	1.72	0.71
1:A:219:VAL:HG13	1:A:236:VAL:HG23	1.72	0.71
1:A:172:ALA:CA	1:G:169:MET:HE1	2.21	0.70
2:H:150:LYS:CE	2:H:175:LEU:HD13	2.21	0.70
2:H:301:LEU:C	2:H:301:LEU:HD23	2.17	0.70
1:C:169:MET:HE1	1:E:172:ALA:CA	2.21	0.70
2:F:682:ILE:HG23	2:F:736:ALA:HB3	1.73	0.70
1:C:177:ARG:NH2	1:C:208:SER:HB2	2.05	0.70
1:G:219:VAL:HG13	1:G:236:VAL:HG23	1.72	0.70
2:F:301:LEU:C	2:F:301:LEU:HD23	2.17	0.70
2:B:301:LEU:C	2:B:301:LEU:HD23	2.17	0.70
2:D:682:ILE:HG23	2:D:736:ALA:HB3	1.73	0.70
1:A:177:ARG:NH2	1:A:208:SER:HB2	2.05	0.70
2:D:204:VAL:O	2:D:205:LYS:CB	2.39	0.70
2:D:1334:LEU:HD13	2:D:1408:ILE:HG23	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:204:VAL:O	2:F:205:LYS:CB	2.39	0.70
1:G:168:PHE:C	1:G:171:THR:HG22	2.17	0.70
2:D:301:LEU:HD23	2:D:301:LEU:C	2.17	0.70
2:B:682:ILE:HG23	2:B:736:ALA:HB3	1.73	0.70
2:F:150:LYS:CE	2:F:175:LEU:HD13	2.21	0.69
1:A:168:PHE:C	1:A:171:THR:HG22	2.17	0.69
2:H:1394:ARG:HD2	2:H:1410:ILE:HG21	1.73	0.69
2:D:1394:ARG:HD2	2:D:1410:ILE:HG21	1.73	0.69
1:C:168:PHE:O	1:C:171:THR:HG22	1.92	0.69
1:C:168:PHE:C	1:C:171:THR:HG22	2.17	0.69
2:B:562:HIS:NE2	2:B:569:SER:O	2.26	0.69
1:C:36:VAL:HG12	1:C:42:CYS:HA	1.72	0.69
2:D:287:ILE:HD11	2:D:607:VAL:HG13	1.74	0.69
2:B:1394:ARG:HD2	2:B:1410:ILE:HG21	1.73	0.69
2:F:287:ILE:HD11	2:F:607:VAL:HG13	1.74	0.68
2:H:562:HIS:NE2	2:H:569:SER:O	2.26	0.68
2:H:682:ILE:HG23	2:H:736:ALA:HB3	1.73	0.68
2:B:287:ILE:HD11	2:B:607:VAL:HG13	1.74	0.68
1:C:183:PHE:CD2	1:C:202:VAL:HG12	2.29	0.68
1:E:168:PHE:C	1:E:171:THR:HG22	2.17	0.68
1:A:168:PHE:O	1:A:171:THR:HG22	1.92	0.68
1:A:168:PHE:HA	1:A:171:THR:HG22	1.76	0.68
2:D:562:HIS:NE2	2:D:569:SER:O	2.26	0.68
1:A:183:PHE:CD2	1:A:202:VAL:HG12	2.29	0.68
2:F:562:HIS:NE2	2:F:569:SER:O	2.26	0.68
1:E:168:PHE:O	1:E:171:THR:HG22	1.92	0.68
2:B:869:MET:HA	2:B:873:ILE:HD12	1.75	0.68
2:F:1394:ARG:HD2	2:F:1410:ILE:HG21	1.73	0.68
2:H:287:ILE:HD11	2:H:607:VAL:HG13	1.74	0.68
1:G:168:PHE:O	1:G:171:THR:HG22	1.92	0.67
1:E:167:ILE:O	1:E:171:THR:HG22	1.94	0.67
1:C:168:PHE:HA	1:C:171:THR:HG22	1.76	0.67
1:A:53:GLY:O	1:A:54:ARG:CB	2.43	0.67
1:E:168:PHE:HA	1:E:171:THR:HG22	1.76	0.67
1:G:168:PHE:HA	1:G:171:THR:HG22	1.76	0.67
2:B:204:VAL:O	2:B:205:LYS:CB	2.39	0.67
1:C:167:ILE:O	1:C:171:THR:HG22	1.94	0.67
2:B:873:ILE:HA	2:B:877:LEU:HD12	1.77	0.67
2:D:873:ILE:HA	2:D:877:LEU:HD12	1.77	0.67
1:E:183:PHE:CD2	1:E:202:VAL:HG12	2.29	0.67
2:F:551:PRO:HB3	2:F:583:PHE:CZ	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:869:MET:HA	2:F:873:ILE:HD12	1.75	0.67
2:F:873:ILE:HA	2:F:877:LEU:HD12	1.77	0.67
1:G:53:GLY:O	1:G:54:ARG:CB	2.43	0.67
1:G:183:PHE:CD2	1:G:202:VAL:HG12	2.29	0.67
2:H:869:MET:HA	2:H:873:ILE:HD12	1.75	0.67
2:H:873:ILE:HA	2:H:877:LEU:HD12	1.77	0.67
2:H:551:PRO:HB3	2:H:583:PHE:CZ	2.30	0.67
2:D:869:MET:HA	2:D:873:ILE:HD12	1.75	0.66
2:D:466:VAL:HG11	2:D:554:ALA:HB2	1.76	0.66
1:G:167:ILE:O	1:G:171:THR:HG22	1.94	0.66
2:H:466:VAL:HG11	2:H:554:ALA:HB2	1.76	0.66
1:A:167:ILE:O	1:A:171:THR:HG22	1.94	0.66
1:G:168:PHE:CA	1:G:171:THR:HG22	2.26	0.66
2:H:204:VAL:O	2:H:205:LYS:CB	2.39	0.66
2:B:466:VAL:HG11	2:B:554:ALA:HB2	1.76	0.66
2:B:551:PRO:HB3	2:B:583:PHE:CZ	2.30	0.66
1:C:53:GLY:O	1:C:54:ARG:CB	2.43	0.66
2:D:551:PRO:HB3	2:D:583:PHE:CZ	2.30	0.66
1:A:168:PHE:CA	1:A:171:THR:HG22	2.26	0.66
2:F:466:VAL:HG11	2:F:554:ALA:HB2	1.76	0.66
1:G:123:PHE:HD2	1:G:136:ARG:HG3	1.61	0.66
1:E:53:GLY:O	1:E:54:ARG:CB	2.43	0.65
1:E:123:PHE:HD2	1:E:136:ARG:HG3	1.61	0.65
1:C:181:LEU:N	1:C:181:LEU:HD22	2.12	0.65
1:A:181:LEU:N	1:A:181:LEU:HD22	2.12	0.65
2:B:1509:THR:HG23	2:B:1517:GLU:HG2	1.79	0.65
1:E:168:PHE:CA	1:E:171:THR:HG22	2.26	0.65
1:A:123:PHE:HD2	1:A:136:ARG:HG3	1.61	0.65
2:D:511:LEU:HD23	2:D:1426:LEU:HD21	1.79	0.65
2:F:511:LEU:HD23	2:F:1426:LEU:HD21	1.79	0.65
2:D:1509:THR:HG23	2:D:1517:GLU:HG2	1.79	0.65
2:B:710:MET:HE3	2:B:893:TYR:HB3	1.79	0.65
2:H:710:MET:HE3	2:H:893:TYR:HB3	1.79	0.65
2:H:1509:THR:HG23	2:H:1517:GLU:HG2	1.79	0.65
1:C:123:PHE:HD2	1:C:136:ARG:HG3	1.61	0.64
1:C:168:PHE:CA	1:C:171:THR:HG22	2.26	0.64
1:G:183:PHE:HZ	1:G:287:LEU:HD23	1.62	0.64
2:D:1480:GLU:OE1	3:D:2501:ADP:N6	2.30	0.64
2:H:1480:GLU:OE1	3:H:2501:ADP:N6	2.30	0.64
2:F:1480:GLU:OE1	3:F:2501:ADP:N6	2.30	0.64
1:E:181:LEU:HD22	1:E:181:LEU:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:710:MET:HE3	2:F:893:TYR:HB3	1.79	0.64
2:B:1032:TYR:HA	2:B:1283:LEU:HD11	1.80	0.64
2:F:150:LYS:NZ	2:F:175:LEU:HD13	2.13	0.64
2:H:365:ALA:O	2:H:369:GLN:HG3	1.98	0.64
2:H:681:ILE:HB	2:H:701:ILE:HG23	1.79	0.64
2:B:1480:GLU:OE1	3:B:2501:ADP:N6	2.30	0.64
2:D:365:ALA:O	2:D:369:GLN:HG3	1.98	0.64
2:D:1032:TYR:HA	2:D:1283:LEU:HD11	1.80	0.64
2:D:1506:ASP:HA	2:D:1536:ILE:HG13	1.80	0.64
2:B:365:ALA:O	2:B:369:GLN:HG3	1.98	0.63
2:D:681:ILE:HB	2:D:701:ILE:HG23	1.79	0.63
2:D:710:MET:HE3	2:D:893:TYR:HB3	1.79	0.63
2:B:190:ILE:CB	2:B:195:TYR:CB	2.77	0.63
2:B:783:THR:HB	2:B:820:GLN:HA	1.80	0.63
1:G:181:LEU:N	1:G:181:LEU:HD22	2.12	0.63
2:D:190:ILE:CB	2:D:195:TYR:CB	2.77	0.63
2:D:592:LEU:HD11	2:D:1297:TRP:HH2	1.63	0.63
2:F:1347:ILE:HG23	2:F:1403:ILE:HG12	1.80	0.63
2:H:190:ILE:CB	2:H:195:TYR:CB	2.77	0.63
1:A:183:PHE:HZ	1:A:287:LEU:HD23	1.62	0.63
1:E:109:PRO:HG2	1:E:112:THR:HA	1.81	0.63
1:E:183:PHE:HZ	1:E:287:LEU:HD23	1.62	0.63
2:F:1509:THR:HG23	2:F:1517:GLU:HG2	1.79	0.63
2:B:1506:ASP:HA	2:B:1536:ILE:HG13	1.80	0.63
2:H:1506:ASP:HA	2:H:1536:ILE:HG13	1.80	0.63
2:B:511:LEU:HD23	2:B:1426:LEU:HD21	1.79	0.63
1:C:109:PRO:HG2	1:C:112:THR:HA	1.81	0.63
2:D:1347:ILE:HG23	2:D:1403:ILE:HG12	1.80	0.63
2:H:150:LYS:NZ	2:H:175:LEU:HD13	2.13	0.63
2:F:681:ILE:HB	2:F:701:ILE:HG23	1.79	0.63
2:H:511:LEU:HD23	2:H:1426:LEU:HD21	1.79	0.63
2:H:551:PRO:HB3	2:H:583:PHE:HZ	1.64	0.63
2:B:592:LEU:HD11	2:B:1297:TRP:HH2	1.63	0.63
2:F:295:PHE:HZ	2:F:387:LEU:HB2	1.63	0.63
2:B:150:LYS:NZ	2:B:175:LEU:HD13	2.13	0.62
2:D:295:PHE:HZ	2:D:387:LEU:HB2	1.63	0.62
2:F:365:ALA:O	2:F:369:GLN:HG3	1.98	0.62
2:F:1506:ASP:HA	2:F:1536:ILE:HG13	1.80	0.62
2:H:783:THR:HB	2:H:820:GLN:HA	1.80	0.62
2:D:150:LYS:NZ	2:D:175:LEU:HD13	2.13	0.62
2:F:783:THR:HB	2:F:820:GLN:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:PHE:HZ	1:C:287:LEU:HD23	1.62	0.62
2:D:551:PRO:HB3	2:D:583:PHE:HZ	1.64	0.62
2:F:1032:TYR:HA	2:F:1283:LEU:HD11	1.80	0.62
2:H:592:LEU:HD11	2:H:1297:TRP:HH2	1.63	0.62
2:H:369:GLN:HB2	2:H:370:ARG:NH2	2.15	0.62
2:D:783:THR:HB	2:D:820:GLN:HA	1.80	0.62
2:H:1032:TYR:HA	2:H:1283:LEU:HD11	1.80	0.62
2:B:681:ILE:HB	2:B:701:ILE:HG23	1.79	0.61
2:D:561:GLY:HA2	2:D:565:PHE:HB3	1.82	0.61
2:H:1347:ILE:HG23	2:H:1403:ILE:HG12	1.80	0.61
2:B:551:PRO:HB3	2:B:583:PHE:HZ	1.64	0.61
2:F:190:ILE:CB	2:F:195:TYR:CB	2.77	0.61
2:F:592:LEU:HD11	2:F:1297:TRP:HH2	1.63	0.61
2:B:369:GLN:HB2	2:B:370:ARG:NH2	2.15	0.61
2:F:369:GLN:HB2	2:F:370:ARG:NH2	2.15	0.61
1:G:109:PRO:HG2	1:G:112:THR:HA	1.81	0.61
1:A:213:ALA:HA	1:A:288:GLU:O	2.01	0.61
2:B:561:GLY:HA2	2:B:565:PHE:HB3	1.82	0.61
2:B:1347:ILE:HG23	2:B:1403:ILE:HG12	1.80	0.61
1:A:109:PRO:HG2	1:A:112:THR:HA	1.81	0.61
1:C:237:ASP:HB3	1:E:243:GLY:CA	2.31	0.61
2:D:369:GLN:HB2	2:D:370:ARG:NH2	2.15	0.61
2:F:551:PRO:HB3	2:F:583:PHE:HZ	1.64	0.61
2:H:699:ILE:HG23	2:H:908:ILE:HD11	1.82	0.61
2:D:301:LEU:HD23	2:D:301:LEU:O	2.01	0.61
2:D:1350:LEU:HB3	2:D:1365:VAL:HB	1.83	0.61
2:D:699:ILE:HG23	2:D:908:ILE:HD11	1.82	0.61
1:E:183:PHE:CE2	1:E:202:VAL:HG12	2.36	0.61
2:F:301:LEU:HD23	2:F:301:LEU:O	2.01	0.61
2:B:1350:LEU:HB3	2:B:1365:VAL:HB	1.83	0.60
1:C:181:LEU:HD22	1:C:181:LEU:H	1.66	0.60
2:D:1362:LEU:HD13	2:D:1365:VAL:HG21	1.84	0.60
2:F:561:GLY:HA2	2:F:565:PHE:HB3	1.82	0.60
2:B:1171:LEU:HD11	2:B:1255:ILE:HG23	1.84	0.60
1:C:183:PHE:CE2	1:C:202:VAL:HG12	2.36	0.60
1:C:213:ALA:HA	1:C:288:GLU:O	2.01	0.60
2:F:699:ILE:HG23	2:F:908:ILE:HD11	1.82	0.60
2:H:1171:LEU:HD11	2:H:1255:ILE:HG23	1.84	0.60
1:E:213:ALA:HA	1:E:288:GLU:O	2.01	0.60
1:G:312:GLY:O	1:G:313:GLN:NE2	2.35	0.60
2:H:389:GLY:O	2:H:393:THR:HG22	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:561:GLY:HA2	2:H:565:PHE:HB3	1.82	0.60
1:A:183:PHE:CE2	1:A:202:VAL:HG12	2.36	0.60
1:C:170:LYS:O	1:C:173:GLN:NE2	2.35	0.60
2:H:295:PHE:HZ	2:H:387:LEU:HB2	1.63	0.60
1:A:168:PHE:HA	1:A:171:THR:HG21	1.84	0.60
2:D:1171:LEU:HD11	2:D:1255:ILE:HG23	1.84	0.60
2:F:1171:LEU:HD11	2:F:1255:ILE:HG23	1.84	0.60
1:G:183:PHE:CE2	1:G:202:VAL:HG12	2.36	0.60
2:H:301:LEU:HD23	2:H:301:LEU:O	2.01	0.60
1:A:172:ALA:CA	1:G:169:MET:CE	2.79	0.60
1:E:169:MET:CE	1:G:172:ALA:CA	2.79	0.60
2:F:1362:LEU:HD13	2:F:1365:VAL:HG21	1.84	0.60
1:A:312:GLY:O	1:A:313:GLN:NE2	2.35	0.60
2:B:190:ILE:HB	2:B:195:TYR:CB	2.32	0.60
2:B:295:PHE:HZ	2:B:387:LEU:HB2	1.63	0.60
2:B:301:LEU:HD23	2:B:301:LEU:O	2.01	0.60
1:C:168:PHE:HA	1:C:171:THR:HG21	1.84	0.60
2:D:190:ILE:HB	2:D:195:TYR:CB	2.32	0.60
2:D:312:LEU:HB2	2:D:369:GLN:HG2	1.84	0.60
2:D:389:GLY:O	2:D:393:THR:HG22	2.02	0.60
1:E:95:PHE:HD1	1:E:100:LEU:HD23	1.67	0.60
1:E:181:LEU:HD22	1:E:181:LEU:H	1.66	0.60
1:G:213:ALA:HA	1:G:288:GLU:O	2.01	0.60
1:A:95:PHE:HD1	1:A:100:LEU:HD23	1.67	0.59
2:F:389:GLY:O	2:F:393:THR:HG22	2.02	0.59
2:F:1350:LEU:HB3	2:F:1365:VAL:HB	1.83	0.59
1:G:183:PHE:CZ	1:G:287:LEU:HD23	2.37	0.59
2:H:190:ILE:HB	2:H:195:TYR:CB	2.32	0.59
2:H:785:GLU:HB3	2:H:794:PHE:HZ	1.67	0.59
1:E:312:GLY:O	1:E:313:GLN:NE2	2.35	0.59
2:F:190:ILE:HB	2:F:195:TYR:CB	2.32	0.59
2:H:1362:LEU:HD13	2:H:1365:VAL:HG21	1.84	0.59
2:B:785:GLU:HB3	2:B:794:PHE:HZ	1.67	0.59
2:B:1553:LYS:HE3	2:B:1558:LEU:HB2	1.83	0.59
2:F:785:GLU:HB3	2:F:794:PHE:HZ	1.67	0.59
1:G:95:PHE:HD1	1:G:100:LEU:HD23	1.67	0.59
1:G:168:PHE:HA	1:G:171:THR:HG21	1.84	0.59
1:G:181:LEU:HD22	1:G:181:LEU:H	1.66	0.59
2:H:1350:LEU:HB3	2:H:1365:VAL:HB	1.83	0.59
1:E:168:PHE:HA	1:E:171:THR:HG21	1.84	0.59
2:F:312:LEU:HB2	2:F:369:GLN:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1553:LYS:HE3	2:H:1558:LEU:HB2	1.83	0.59
1:C:95:PHE:HD1	1:C:100:LEU:HD23	1.67	0.59
2:D:785:GLU:HB3	2:D:794:PHE:HZ	1.67	0.59
1:E:170:LYS:O	1:E:173:GLN:NE2	2.35	0.59
1:A:170:LYS:O	1:A:173:GLN:NE2	2.35	0.59
2:B:699:ILE:HG23	2:B:908:ILE:HD11	1.82	0.59
2:D:1377:ILE:HB	2:D:1536:ILE:HG23	1.85	0.59
2:D:1553:LYS:HE3	2:D:1558:LEU:HB2	1.83	0.59
1:G:170:LYS:O	1:G:173:GLN:NE2	2.35	0.59
2:B:389:GLY:O	2:B:393:THR:HG22	2.02	0.59
1:A:243:GLY:CA	1:G:237:ASP:HB3	2.31	0.59
1:A:183:PHE:CZ	1:A:287:LEU:HD23	2.37	0.58
1:C:312:GLY:O	1:C:313:GLN:NE2	2.35	0.58
2:H:312:LEU:HB2	2:H:369:GLN:HG2	1.84	0.58
2:F:1553:LYS:HE3	2:F:1558:LEU:HB2	1.83	0.58
2:B:1362:LEU:HD13	2:B:1365:VAL:HG21	1.84	0.58
1:C:183:PHE:CZ	1:C:287:LEU:HD23	2.37	0.58
1:A:169:MET:CE	1:C:172:ALA:CA	2.79	0.58
1:A:181:LEU:HD22	1:A:181:LEU:H	1.66	0.58
2:B:312:LEU:HB2	2:B:369:GLN:HG2	1.84	0.58
2:D:75:TRP:CZ3	2:D:225:LEU:CB	2.87	0.58
1:E:183:PHE:CZ	1:E:287:LEU:HD23	2.37	0.58
2:H:545:PHE:HB2	2:H:1080:LEU:HD13	1.86	0.58
2:B:686:PHE:H	2:B:696:LEU:HB3	1.69	0.58
2:H:1377:ILE:HB	2:H:1536:ILE:HG23	1.85	0.58
2:D:366:LEU:O	2:D:370:ARG:HG2	2.04	0.58
2:F:1344:LYS:HB2	2:F:1371:PRO:HG3	1.85	0.58
2:F:1377:ILE:HB	2:F:1536:ILE:HG23	1.85	0.58
2:B:75:TRP:CZ3	2:B:225:LEU:CB	2.87	0.58
2:H:75:TRP:CZ3	2:H:225:LEU:CB	2.87	0.58
2:B:1377:ILE:HB	2:B:1536:ILE:HG23	1.85	0.58
1:C:169:MET:CE	1:E:172:ALA:CA	2.79	0.58
2:H:686:PHE:H	2:H:696:LEU:HB3	1.69	0.58
1:A:237:ASP:HB3	1:C:243:GLY:CA	2.31	0.57
2:F:686:PHE:H	2:F:696:LEU:HB3	1.69	0.57
2:H:366:LEU:O	2:H:370:ARG:HG2	2.04	0.57
2:D:686:PHE:H	2:D:696:LEU:HB3	1.69	0.57
1:E:237:ASP:HB3	1:G:243:GLY:CA	2.31	0.57
2:F:1385:LYS:HB2	2:F:1536:ILE:HG21	1.86	0.57
2:B:681:ILE:HD11	2:B:726:THR:HG22	1.87	0.57
2:B:1344:LYS:HB2	2:B:1371:PRO:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:681:ILE:HD11	2:H:726:THR:HG22	1.87	0.57
2:B:366:LEU:O	2:B:370:ARG:HG2	2.04	0.57
2:B:377:TYR:HB3	2:B:1246:ARG:HE	1.70	0.57
2:B:545:PHE:HB2	2:B:1080:LEU:HD13	1.86	0.57
2:F:75:TRP:CZ3	2:F:225:LEU:CB	2.87	0.57
2:F:366:LEU:O	2:F:370:ARG:HG2	2.04	0.57
2:H:1344:LYS:HB2	2:H:1371:PRO:HG3	1.85	0.57
2:D:545:PHE:HB2	2:D:1080:LEU:HD13	1.86	0.57
2:D:681:ILE:HD11	2:D:726:THR:HG22	1.87	0.57
2:F:545:PHE:HB2	2:F:1080:LEU:HD13	1.86	0.57
2:D:1344:LYS:HB2	2:D:1371:PRO:HG3	1.85	0.57
2:B:466:VAL:HG13	2:B:550:ILE:HG22	1.87	0.56
2:D:91:GLU:OE2	2:D:171:LEU:HD12	2.04	0.56
2:F:377:TYR:HB3	2:F:1246:ARG:HE	1.70	0.56
2:D:91:GLU:CD	2:D:171:LEU:CD1	2.76	0.56
1:E:352:ASP:O	1:E:356:LEU:N	2.39	0.56
2:F:681:ILE:HD11	2:F:726:THR:HG22	1.87	0.56
1:A:352:ASP:O	1:A:356:LEU:N	2.39	0.56
2:B:1385:LYS:HB2	2:B:1536:ILE:HG21	1.86	0.56
2:D:466:VAL:HG13	2:D:550:ILE:HG22	1.87	0.56
2:D:1475:ILE:HD12	2:D:1482:PHE:HE2	1.71	0.56
2:B:1475:ILE:HD12	2:B:1482:PHE:HE2	1.71	0.56
2:H:1475:ILE:HD12	2:H:1482:PHE:HE2	1.71	0.56
1:C:168:PHE:CA	1:C:171:THR:CG2	2.83	0.56
1:C:352:ASP:O	1:C:356:LEU:N	2.39	0.56
2:D:377:TYR:HB3	2:D:1246:ARG:HE	1.70	0.56
2:F:466:VAL:HG13	2:F:550:ILE:HG22	1.87	0.56
1:G:181:LEU:H	1:G:181:LEU:CD2	2.19	0.56
2:H:377:TYR:HB3	2:H:1246:ARG:HE	1.70	0.56
2:H:466:VAL:HG13	2:H:550:ILE:HG22	1.87	0.56
1:A:34:ARG:HG2	1:A:305:LEU:HD21	1.88	0.56
2:D:1385:LYS:HB2	2:D:1536:ILE:HG21	1.86	0.56
1:E:34:ARG:HG2	1:E:305:LEU:HD21	1.88	0.56
2:H:1385:LYS:HB2	2:H:1536:ILE:HG21	1.86	0.56
2:H:1528:PHE:HD1	2:H:1531:ARG:HD2	1.71	0.56
1:A:168:PHE:CA	1:A:171:THR:CG2	2.83	0.55
2:B:1528:PHE:HD1	2:B:1531:ARG:HD2	1.71	0.55
2:B:1540:VAL:HG11	2:B:1579:ARG:HA	1.88	0.55
2:D:1540:VAL:HG11	2:D:1579:ARG:HA	1.88	0.55
2:H:1455:LEU:HD13	2:H:1464:VAL:HG21	1.88	0.55
2:B:686:PHE:HD1	2:B:733:VAL:HG23	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:352:ASP:O	1:G:356:LEU:N	2.39	0.55
2:B:1086:VAL:HG11	2:B:1141:GLU:HB2	1.89	0.55
1:E:181:LEU:H	1:E:181:LEU:CD2	2.19	0.55
1:C:34:ARG:HG2	1:C:305:LEU:HD21	1.88	0.55
2:F:1475:ILE:HD12	2:F:1482:PHE:HE2	1.71	0.55
2:D:1086:VAL:HG11	2:D:1141:GLU:HB2	1.89	0.55
2:D:1455:LEU:HD13	2:D:1464:VAL:HG21	1.88	0.55
1:G:168:PHE:CA	1:G:171:THR:CG2	2.83	0.55
1:A:181:LEU:H	1:A:181:LEU:CD2	2.19	0.55
2:D:686:PHE:HD1	2:D:733:VAL:HG23	1.71	0.55
2:F:1455:LEU:HD13	2:F:1464:VAL:HG21	1.88	0.55
2:F:1353:ARG:HE	2:F:1398:MET:HE3	1.71	0.55
2:B:363:PHE:HB2	2:B:1261:LEU:HD13	1.90	0.55
2:H:686:PHE:HD1	2:H:733:VAL:HG23	1.71	0.55
2:H:1226:LYS:HG2	2:H:1230:TYR:HE1	1.72	0.55
2:B:1226:LYS:HG2	2:B:1230:TYR:HE1	1.72	0.54
2:B:1353:ARG:HE	2:B:1398:MET:HE3	1.71	0.54
2:D:1353:ARG:HE	2:D:1398:MET:HE3	1.71	0.54
1:E:83:TRP:CD1	1:E:128:GLN:HG2	2.43	0.54
2:F:686:PHE:HD1	2:F:733:VAL:HG23	1.71	0.54
2:F:1086:VAL:HG11	2:F:1141:GLU:HB2	1.89	0.54
1:C:83:TRP:CD1	1:C:128:GLN:HG2	2.43	0.54
2:D:526:ARG:HE	2:D:1098:HIS:CG	2.25	0.54
2:H:363:PHE:HB2	2:H:1261:LEU:HD13	1.90	0.54
2:B:1455:LEU:HD13	2:B:1464:VAL:HG21	1.88	0.54
2:F:1562:LYS:HB3	2:F:1565:THR:HB	1.89	0.54
1:G:83:TRP:CD1	1:G:128:GLN:HG2	2.43	0.54
2:H:1086:VAL:HG11	2:H:1141:GLU:HB2	1.89	0.54
1:A:83:TRP:CD1	1:A:128:GLN:HG2	2.43	0.54
1:C:181:LEU:H	1:C:181:LEU:CD2	2.19	0.54
2:D:1562:LYS:HB3	2:D:1565:THR:HB	1.89	0.54
2:F:1528:PHE:HD1	2:F:1531:ARG:HD2	1.71	0.54
1:G:34:ARG:HG2	1:G:305:LEU:HD21	1.88	0.54
2:D:1528:PHE:HD1	2:D:1531:ARG:HD2	1.71	0.54
2:F:526:ARG:HE	2:F:1098:HIS:CG	2.25	0.54
2:B:1311:ALA:O	2:B:1314:ARG:HG2	2.08	0.54
2:F:366:LEU:HD23	2:F:1260:VAL:HG11	1.89	0.54
2:F:719:LYS:HB3	2:F:887:VAL:HG11	1.90	0.54
2:F:791:GLU:HB3	2:F:1219:TYR:HE2	1.73	0.54
2:H:1353:ARG:HE	2:H:1398:MET:HE3	1.71	0.54
2:H:1562:LYS:HB3	2:H:1565:THR:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:363:PHE:HB2	2:D:1261:LEU:HD13	1.90	0.54
2:D:366:LEU:HD23	2:D:1260:VAL:HG11	1.89	0.54
2:F:1311:ALA:O	2:F:1314:ARG:HG2	2.08	0.54
2:F:1540:VAL:HG11	2:F:1579:ARG:HA	1.88	0.54
2:H:1540:VAL:HG11	2:H:1579:ARG:HA	1.88	0.54
2:B:719:LYS:HB3	2:B:887:VAL:HG11	1.90	0.54
2:B:366:LEU:HD23	2:B:1260:VAL:HG11	1.89	0.53
2:B:526:ARG:HE	2:B:1098:HIS:CG	2.25	0.53
2:B:442:PRO:O	2:B:445:ILE:HG13	2.08	0.53
2:D:1226:LYS:HG2	2:D:1230:TYR:HE1	1.72	0.53
2:F:1226:LYS:HG2	2:F:1230:TYR:HE1	1.72	0.53
2:D:791:GLU:HB3	2:D:1219:TYR:HE2	1.73	0.53
2:H:366:LEU:HD23	2:H:1260:VAL:HG11	1.89	0.53
2:H:562:HIS:CD2	2:H:571:LEU:HD23	2.44	0.53
2:H:1311:ALA:O	2:H:1314:ARG:HG2	2.08	0.53
2:H:1386:SER:OG	3:H:2502:ADP:O2B	2.26	0.53
2:B:1562:LYS:HB3	2:B:1565:THR:HB	1.89	0.53
2:F:363:PHE:HB2	2:F:1261:LEU:HD13	1.90	0.53
2:H:526:ARG:HE	2:H:1098:HIS:CG	2.25	0.53
2:B:517:ILE:HD11	2:B:1443:GLU:HG2	1.91	0.53
2:F:827:GLY:O	2:F:835:ARG:NH2	2.42	0.53
2:H:791:GLU:HB3	2:H:1219:TYR:HE2	1.73	0.53
2:H:827:GLY:O	2:H:835:ARG:NH2	2.42	0.53
2:B:562:HIS:CD2	2:B:571:LEU:HD23	2.44	0.53
2:D:719:LYS:HB3	2:D:887:VAL:HG11	1.90	0.53
2:D:1311:ALA:O	2:D:1314:ARG:HG2	2.08	0.53
2:D:517:ILE:HD11	2:D:1443:GLU:HG2	1.91	0.53
2:D:1124:ARG:NH1	2:D:1314:ARG:HD3	2.22	0.53
1:E:168:PHE:CA	1:E:171:THR:CG2	2.83	0.53
2:F:442:PRO:O	2:F:445:ILE:HG13	2.08	0.53
2:B:1393:PHE:CZ	2:B:1422:LEU:HB2	2.44	0.53
2:D:442:PRO:O	2:D:445:ILE:HG13	2.08	0.53
2:H:442:PRO:O	2:H:445:ILE:HG13	2.08	0.53
2:H:719:LYS:HB3	2:H:887:VAL:HG11	1.90	0.53
2:B:1386:SER:OG	3:B:2502:ADP:O2B	2.26	0.52
2:B:559:PHE:O	2:B:563:VAL:HG22	2.10	0.52
2:B:827:GLY:O	2:B:835:ARG:NH2	2.42	0.52
2:D:562:HIS:CD2	2:D:571:LEU:HD23	2.44	0.52
1:G:168:PHE:C	1:G:171:THR:CG2	2.81	0.52
2:H:1393:PHE:CZ	2:H:1422:LEU:HB2	2.44	0.52
2:B:791:GLU:HB3	2:B:1219:TYR:HE2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:517:ILE:HD11	2:F:1443:GLU:HG2	1.91	0.52
2:F:1393:PHE:CZ	2:F:1422:LEU:HB2	2.44	0.52
2:H:559:PHE:O	2:H:563:VAL:HG22	2.10	0.52
2:D:1386:SER:OG	3:D:2502:ADP:O2B	2.26	0.52
2:F:562:HIS:CD2	2:F:571:LEU:HD23	2.44	0.52
2:H:1528:PHE:CD1	2:H:1531:ARG:HD2	2.45	0.52
2:H:517:ILE:HD11	2:H:1443:GLU:HG2	1.91	0.52
2:F:1124:ARG:NH1	2:F:1314:ARG:HD3	2.22	0.52
2:B:150:LYS:NZ	2:B:175:LEU:CD1	2.73	0.52
2:B:1528:PHE:CD1	2:B:1531:ARG:HD2	2.45	0.52
2:D:1393:PHE:CZ	2:D:1422:LEU:HB2	2.44	0.52
2:F:150:LYS:NZ	2:F:175:LEU:CD1	2.73	0.52
2:H:779:LEU:HD11	2:H:835:ARG:HG2	1.92	0.52
2:D:779:LEU:HD11	2:D:835:ARG:HG2	1.92	0.52
2:B:143:TRP:HB3	2:B:183:LEU:HG	1.92	0.52
2:F:559:PHE:O	2:F:563:VAL:HG22	2.10	0.52
2:D:827:GLY:O	2:D:835:ARG:NH2	2.42	0.52
2:H:687:THR:HB	2:H:694:PRO:HA	1.92	0.52
2:H:1455:LEU:HD22	2:H:1460:LEU:HD23	1.92	0.52
2:B:679:VAL:HB	2:B:703:ILE:HD12	1.92	0.51
2:D:308:LEU:O	2:D:311:LEU:HG	2.11	0.51
2:F:1528:PHE:CD1	2:F:1531:ARG:HD2	2.45	0.51
2:B:1124:ARG:NH1	2:B:1314:ARG:HD3	2.22	0.51
2:F:679:VAL:HB	2:F:703:ILE:HD12	1.92	0.51
2:F:779:LEU:HD11	2:F:835:ARG:HG2	1.92	0.51
2:F:1455:LEU:HD22	2:F:1460:LEU:HD23	1.92	0.51
2:H:150:LYS:NZ	2:H:175:LEU:CD1	2.73	0.51
2:H:423:ILE:O	2:H:427:GLN:HG2	2.11	0.51
2:H:1124:ARG:NH1	2:H:1314:ARG:HD3	2.22	0.51
2:H:308:LEU:O	2:H:311:LEU:HG	2.11	0.51
2:H:679:VAL:HB	2:H:703:ILE:HD12	1.92	0.51
2:B:779:LEU:HD11	2:B:835:ARG:HG2	1.92	0.51
2:F:91:GLU:CD	2:F:171:LEU:HD12	2.36	0.51
2:F:687:THR:HB	2:F:694:PRO:HA	1.92	0.51
2:H:686:PHE:HB2	2:H:732:LYS:HA	1.93	0.51
2:D:423:ILE:O	2:D:427:GLN:HG2	2.11	0.51
2:D:679:VAL:HB	2:D:703:ILE:HD12	1.92	0.51
2:F:768:GLY:O	2:F:1218:ARG:NH2	2.44	0.51
2:H:143:TRP:HB3	2:H:183:LEU:HG	1.92	0.51
2:H:295:PHE:CE1	2:H:387:LEU:HB2	2.46	0.51
2:D:150:LYS:NZ	2:D:175:LEU:CD1	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:559:PHE:O	2:D:563:VAL:HG22	2.10	0.51
2:F:143:TRP:HB3	2:F:183:LEU:HG	1.92	0.51
2:H:686:PHE:CD1	2:H:733:VAL:HG23	2.46	0.51
2:D:687:THR:HB	2:D:694:PRO:HA	1.92	0.51
2:F:308:LEU:O	2:F:311:LEU:HG	2.11	0.51
2:F:847:GLN:HA	2:F:882:ARG:HH12	1.76	0.51
1:A:239:PRO:HG3	1:C:244:VAL:CB	2.41	0.51
1:A:285:VAL:HG22	1:A:302:THR:HG22	1.93	0.51
2:B:768:GLY:O	2:B:1218:ARG:NH2	2.44	0.51
1:C:239:PRO:HG3	1:E:244:VAL:CB	2.41	0.51
2:D:1528:PHE:CD1	2:D:1531:ARG:HD2	2.45	0.51
2:F:686:PHE:HB2	2:F:732:LYS:HA	1.93	0.51
1:C:285:VAL:HG22	1:C:302:THR:HG22	1.93	0.50
2:D:768:GLY:O	2:D:1218:ARG:NH2	2.44	0.50
2:B:686:PHE:CD1	2:B:733:VAL:HG23	2.46	0.50
1:C:202:VAL:HG23	1:C:251:LEU:HD21	1.94	0.50
2:D:1455:LEU:HD22	2:D:1460:LEU:HD23	1.92	0.50
1:E:168:PHE:C	1:E:171:THR:CG2	2.81	0.50
1:E:285:VAL:HG22	1:E:302:THR:HG22	1.93	0.50
2:F:76:ILE:O	2:F:80:ILE:HG13	2.12	0.50
2:H:76:ILE:O	2:H:80:ILE:HG13	2.12	0.50
2:B:686:PHE:HB2	2:B:732:LYS:HA	1.93	0.50
2:D:686:PHE:CD1	2:D:733:VAL:HG23	2.46	0.50
2:H:768:GLY:O	2:H:1218:ARG:NH2	2.44	0.50
2:H:798:ARG:NH2	2:H:847:GLN:OE1	2.45	0.50
2:B:769:PRO:O	2:B:848:THR:OG1	2.26	0.50
2:D:76:ILE:O	2:D:80:ILE:HG13	2.12	0.50
2:D:143:TRP:HB3	2:D:183:LEU:HG	1.92	0.50
2:D:847:GLN:HA	2:D:882:ARG:HH12	1.76	0.50
1:E:239:PRO:HG3	1:G:244:VAL:CB	2.41	0.50
1:A:202:VAL:HG23	1:A:251:LEU:HD21	1.94	0.50
2:B:196:ILE:C	2:B:197:PHE:O	2.55	0.50
2:B:423:ILE:O	2:B:427:GLN:HG2	2.11	0.50
2:B:798:ARG:NH2	2:B:847:GLN:OE1	2.45	0.50
2:D:402:LEU:O	2:D:1215:ARG:NH1	2.45	0.50
2:D:864:LEU:HD11	2:D:1381:THR:HG21	1.94	0.50
2:F:295:PHE:CE1	2:F:387:LEU:HB2	2.46	0.50
2:F:769:PRO:O	2:F:848:THR:OG1	2.26	0.50
1:G:202:VAL:HG23	1:G:251:LEU:HD21	1.94	0.50
1:A:244:VAL:CB	1:G:239:PRO:HG3	2.41	0.50
2:B:308:LEU:O	2:B:311:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:LEU:O	2:B:1215:ARG:NH1	2.45	0.50
2:B:847:GLN:HA	2:B:882:ARG:HH12	1.76	0.50
1:G:47:LYS:HG3	1:G:48:ASN:ND2	2.27	0.50
2:H:196:ILE:C	2:H:197:PHE:O	2.55	0.50
2:H:769:PRO:O	2:H:848:THR:OG1	2.26	0.50
1:A:46:HIS:HA	1:C:328:VAL:CG2	2.42	0.50
2:B:508:LEU:HD13	2:B:1430:VAL:HG12	1.94	0.50
2:B:1455:LEU:HD22	2:B:1460:LEU:HD23	1.92	0.50
1:E:202:VAL:HG23	1:E:251:LEU:HD21	1.94	0.50
2:F:423:ILE:O	2:F:427:GLN:HG2	2.11	0.50
1:G:285:VAL:HG22	1:G:302:THR:HG22	1.93	0.50
2:H:847:GLN:HA	2:H:882:ARG:HH12	1.76	0.50
1:A:47:LYS:HG3	1:A:48:ASN:ND2	2.27	0.50
2:D:1004:TYR:HE1	2:D:1093:VAL:HG11	1.77	0.50
1:E:46:HIS:HA	1:G:328:VAL:CG2	2.42	0.50
2:F:798:ARG:NH2	2:F:847:GLN:OE1	2.45	0.50
2:F:1004:TYR:HE1	2:F:1093:VAL:HG11	1.77	0.50
2:H:508:LEU:HD13	2:H:1430:VAL:HG12	1.94	0.50
1:A:328:VAL:CG2	1:G:46:HIS:HA	2.42	0.50
2:B:301:LEU:C	2:B:301:LEU:CD2	2.85	0.50
2:B:1496:PHE:HA	2:B:1528:PHE:HZ	1.77	0.50
2:D:196:ILE:C	2:D:197:PHE:O	2.55	0.50
1:E:47:LYS:HG3	1:E:48:ASN:ND2	2.27	0.50
1:E:198:PHE:HE1	1:E:200:LEU:HB2	1.77	0.50
2:B:687:THR:HB	2:B:694:PRO:HA	1.92	0.49
2:D:686:PHE:HB2	2:D:732:LYS:HA	1.93	0.49
2:F:196:ILE:C	2:F:197:PHE:O	2.55	0.49
2:F:508:LEU:HD13	2:F:1430:VAL:HG12	1.94	0.49
1:C:36:VAL:HG23	1:C:303:SER:OG	2.13	0.49
2:D:1347:ILE:HG21	2:D:1350:LEU:HD22	1.93	0.49
2:F:864:LEU:HD11	2:F:1381:THR:HG21	1.94	0.49
1:A:198:PHE:HE1	1:A:200:LEU:HB2	1.77	0.49
1:A:220:VAL:HG12	1:A:235:GLN:HG2	1.95	0.49
2:B:1004:TYR:HE1	2:B:1093:VAL:HG11	1.77	0.49
2:D:301:LEU:C	2:D:301:LEU:CD2	2.85	0.49
2:F:686:PHE:CD1	2:F:733:VAL:HG23	2.46	0.49
2:F:1347:ILE:HG21	2:F:1350:LEU:HD22	1.93	0.49
2:B:76:ILE:O	2:B:80:ILE:HG13	2.12	0.49
2:H:1353:ARG:HE	2:H:1398:MET:HB3	1.77	0.49
1:C:220:VAL:HG12	1:C:235:GLN:HG2	1.95	0.49
2:D:1553:LYS:HZ1	2:D:1558:LEU:HD13	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1570:LYS:HD3	2:D:1574:PHE:HB2	1.95	0.49
2:F:1496:PHE:HA	2:F:1528:PHE:HZ	1.77	0.49
1:A:328:VAL:HG23	1:G:46:HIS:HA	1.94	0.49
2:D:798:ARG:NH2	2:D:847:GLN:OE1	2.45	0.49
1:E:36:VAL:HG23	1:E:303:SER:OG	2.13	0.49
1:G:198:PHE:HE1	1:G:200:LEU:HB2	1.77	0.49
2:H:131:ASN:OD1	2:H:131:ASN:N	2.43	0.49
2:B:1353:ARG:HE	2:B:1398:MET:HB3	1.77	0.49
1:C:46:HIS:HA	1:E:328:VAL:CG2	2.42	0.49
1:C:243:GLY:O	1:C:245:GLY:N	2.46	0.49
2:D:508:LEU:HD13	2:D:1430:VAL:HG12	1.94	0.49
2:D:1353:ARG:NE	2:D:1398:MET:HE3	2.28	0.49
2:H:301:LEU:C	2:H:301:LEU:CD2	2.85	0.49
2:H:864:LEU:HD11	2:H:1381:THR:HG21	1.94	0.49
1:A:46:HIS:HA	1:C:328:VAL:HG23	1.94	0.49
2:B:1182:PHE:CD2	2:B:1248:LEU:HD22	2.48	0.49
2:B:1347:ILE:HG21	2:B:1350:LEU:HD22	1.93	0.49
2:D:295:PHE:CE1	2:D:387:LEU:HB2	2.46	0.49
1:E:220:VAL:HG12	1:E:235:GLN:HG2	1.95	0.49
2:F:402:LEU:O	2:F:1215:ARG:NH1	2.45	0.49
2:F:785:GLU:OE1	2:F:820:GLN:NE2	2.41	0.49
2:F:1339:TRP:CD2	2:F:1340:PRO:HD2	2.48	0.49
1:A:36:VAL:HG23	1:A:303:SER:OG	2.13	0.49
2:B:864:LEU:HD11	2:B:1381:THR:HG21	1.94	0.49
2:B:1353:ARG:NE	2:B:1398:MET:HE3	2.28	0.49
2:B:1570:LYS:HD3	2:B:1574:PHE:HB2	1.95	0.49
1:C:47:LYS:HG3	1:C:48:ASN:ND2	2.27	0.49
1:G:243:GLY:O	1:G:245:GLY:N	2.46	0.49
2:H:1182:PHE:CD2	2:H:1248:LEU:HD22	2.48	0.49
2:B:363:PHE:CD1	2:B:1261:LEU:HB2	2.48	0.49
2:B:526:ARG:NH1	2:B:529:GLU:OE1	2.46	0.49
1:C:139:THR:HG23	1:C:141:GLU:H	1.77	0.49
2:D:1353:ARG:HE	2:D:1398:MET:HB3	1.77	0.49
2:F:363:PHE:CD1	2:F:1261:LEU:HB2	2.48	0.49
1:G:139:THR:HG23	1:G:141:GLU:H	1.77	0.49
2:H:526:ARG:NH1	2:H:529:GLU:OE1	2.46	0.49
2:H:1004:TYR:HE1	2:H:1093:VAL:HG11	1.77	0.49
2:B:1339:TRP:CD2	2:B:1340:PRO:HD2	2.48	0.48
2:D:253:LEU:HD13	2:D:1236:ILE:HB	1.95	0.48
1:G:220:VAL:HG12	1:G:235:GLN:HG2	1.95	0.48
2:H:402:LEU:O	2:H:1215:ARG:NH1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1347:ILE:HG21	2:H:1350:LEU:HD22	1.93	0.48
2:H:1496:PHE:HA	2:H:1528:PHE:HZ	1.77	0.48
1:A:139:THR:HG23	1:A:141:GLU:H	1.77	0.48
2:B:795:ASN:HB2	2:B:798:ARG:HB3	1.95	0.48
2:D:795:ASN:HB2	2:D:798:ARG:HB3	1.95	0.48
2:D:1182:PHE:CD2	2:D:1248:LEU:HD22	2.48	0.48
2:F:253:LEU:HD13	2:F:1236:ILE:HB	1.95	0.48
2:F:1353:ARG:NE	2:F:1398:MET:HE3	2.28	0.48
2:F:1553:LYS:HZ1	2:F:1558:LEU:HD13	1.78	0.48
2:B:1461:LYS:HE2	2:B:1465:LYS:HE2	1.95	0.48
2:B:1553:LYS:HZ1	2:B:1558:LEU:HD13	1.77	0.48
2:D:526:ARG:NH1	2:D:529:GLU:OE1	2.46	0.48
2:F:449:VAL:HA	2:F:452:LEU:HG	1.96	0.48
2:F:526:ARG:NH1	2:F:529:GLU:OE1	2.46	0.48
2:F:1353:ARG:HE	2:F:1398:MET:HB3	1.77	0.48
2:F:1570:LYS:HD3	2:F:1574:PHE:HB2	1.95	0.48
1:A:181:LEU:N	1:A:181:LEU:CD2	2.76	0.48
2:D:581:SER:O	2:D:585:ILE:HG12	2.14	0.48
1:E:46:HIS:HA	1:G:328:VAL:HG23	1.94	0.48
2:F:1182:PHE:CD2	2:F:1248:LEU:HD22	2.48	0.48
2:H:449:VAL:HA	2:H:452:LEU:HG	1.96	0.48
2:H:1226:LYS:HG2	2:H:1230:TYR:CE1	2.48	0.48
2:H:1339:TRP:CD2	2:H:1340:PRO:HD2	2.48	0.48
2:H:1353:ARG:NE	2:H:1398:MET:HE3	2.28	0.48
2:B:449:VAL:HA	2:B:452:LEU:HG	1.96	0.48
1:C:198:PHE:HE1	1:C:200:LEU:HB2	1.77	0.48
2:D:363:PHE:CD1	2:D:1261:LEU:HB2	2.48	0.48
2:D:449:VAL:HA	2:D:452:LEU:HG	1.96	0.48
2:D:1496:PHE:HA	2:D:1528:PHE:HZ	1.77	0.48
1:E:181:LEU:N	1:E:181:LEU:CD2	2.76	0.48
2:F:301:LEU:C	2:F:301:LEU:CD2	2.85	0.48
2:H:32:ASN:O	2:H:35:PRO:HD2	2.14	0.48
1:A:243:GLY:O	1:A:245:GLY:N	2.46	0.48
2:B:32:ASN:O	2:B:35:PRO:HD2	2.14	0.48
2:D:711:ILE:HB	2:D:887:VAL:HG13	1.96	0.48
1:E:77:MET:HG2	2:F:48:PHE:CE2	2.48	0.48
2:F:581:SER:O	2:F:585:ILE:HG12	2.14	0.48
2:F:1461:LYS:HE2	2:F:1465:LYS:HE2	1.95	0.48
1:G:36:VAL:HG23	1:G:303:SER:OG	2.13	0.48
2:H:526:ARG:HE	2:H:1098:HIS:CD2	2.32	0.48
2:H:1570:LYS:HD3	2:H:1574:PHE:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1226:LYS:HG2	2:B:1230:TYR:CE1	2.48	0.48
2:D:526:ARG:HE	2:D:1098:HIS:CD2	2.32	0.48
2:D:1339:TRP:CD2	2:D:1340:PRO:HD2	2.48	0.48
1:E:243:GLY:O	1:E:245:GLY:N	2.46	0.48
2:H:363:PHE:CD1	2:H:1261:LEU:HB2	2.48	0.48
2:H:1128:ASP:OD1	2:H:1311:ALA:HB1	2.14	0.48
2:H:1553:LYS:HZ1	2:H:1558:LEU:HD13	1.78	0.48
1:C:46:HIS:HA	1:E:328:VAL:HG23	1.94	0.48
2:H:488:THR:OG1	2:H:532:SER:HB3	2.14	0.48
2:B:253:LEU:HD13	2:B:1236:ILE:HB	1.95	0.48
2:B:550:ILE:HB	2:B:551:PRO:HD3	1.96	0.48
2:D:1079:CYS:O	2:D:1082:THR:OG1	2.27	0.48
2:H:581:SER:O	2:H:585:ILE:HG12	2.14	0.48
1:A:64:VAL:HG13	1:A:170:LYS:CB	2.44	0.47
1:C:77:MET:HG2	2:D:48:PHE:CE2	2.48	0.47
1:C:128:GLN:NE2	1:C:152:GLN:OE1	2.47	0.47
1:C:168:PHE:C	1:C:171:THR:CG2	2.81	0.47
2:D:32:ASN:O	2:D:35:PRO:HD2	2.14	0.47
1:E:128:GLN:NE2	1:E:152:GLN:OE1	2.47	0.47
1:G:77:MET:HG2	2:H:48:PHE:CE2	2.48	0.47
2:H:553:ALA:O	2:H:557:ILE:HG12	2.15	0.47
2:D:550:ILE:HB	2:D:551:PRO:HD3	1.96	0.47
2:D:1246:ARG:HA	2:D:1246:ARG:HD3	1.65	0.47
1:E:139:THR:HG23	1:E:141:GLU:H	1.77	0.47
2:B:396:TYR:CD1	2:B:1227:LEU:HD13	2.50	0.47
2:B:1128:ASP:OD1	2:B:1311:ALA:HB1	2.14	0.47
2:D:1078:LEU:O	2:D:1082:THR:HG23	2.15	0.47
1:E:46:HIS:HD2	1:G:330:TYR:OH	1.98	0.47
2:F:526:ARG:HE	2:F:1098:HIS:CD2	2.32	0.47
1:G:181:LEU:N	1:G:181:LEU:CD2	2.76	0.47
2:B:1078:LEU:O	2:B:1082:THR:HG23	2.15	0.47
2:D:396:TYR:CD1	2:D:1227:LEU:HD13	2.50	0.47
1:E:95:PHE:HE2	2:F:27:PHE:HB2	1.80	0.47
2:F:711:ILE:HB	2:F:887:VAL:HG13	1.96	0.47
2:F:1375:ILE:HB	2:F:1534:VAL:HG22	1.97	0.47
2:H:550:ILE:HB	2:H:551:PRO:HD3	1.96	0.47
2:H:802:VAL:HG11	2:H:845:TYR:HB2	1.97	0.47
2:H:1078:LEU:O	2:H:1082:THR:HG23	2.15	0.47
2:H:1461:LYS:HE2	2:H:1465:LYS:HE2	1.95	0.47
1:A:128:GLN:NE2	1:A:152:GLN:OE1	2.47	0.47
2:B:131:ASN:OD1	2:B:131:ASN:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:553:ALA:O	2:D:557:ILE:HG12	2.15	0.47
2:D:785:GLU:OE1	2:D:820:GLN:NE2	2.41	0.47
2:F:550:ILE:HB	2:F:551:PRO:HD3	1.96	0.47
2:F:1425:ILE:HD13	2:F:1492:LEU:HD12	1.97	0.47
1:G:64:VAL:HG13	1:G:170:LYS:CB	2.44	0.47
1:G:95:PHE:HE2	2:H:27:PHE:HB2	1.80	0.47
1:A:46:HIS:HD2	1:C:330:TYR:OH	1.98	0.47
1:A:77:MET:HG2	2:B:48:PHE:CE2	2.48	0.47
1:A:330:TYR:OH	1:G:46:HIS:HD2	1.98	0.47
2:B:526:ARG:HE	2:B:1098:HIS:CD2	2.32	0.47
2:D:1425:ILE:HD13	2:D:1492:LEU:HD12	1.97	0.47
2:F:795:ASN:HB2	2:F:798:ARG:HB3	1.95	0.47
2:H:253:LEU:HD13	2:H:1236:ILE:HB	1.95	0.47
2:B:370:ARG:HD2	2:B:1253:GLU:CD	2.40	0.47
2:B:581:SER:O	2:B:585:ILE:HG12	2.14	0.47
2:B:869:MET:HE3	2:B:869:MET:HB3	1.77	0.47
1:C:46:HIS:HD2	1:E:330:TYR:OH	1.98	0.47
2:D:370:ARG:HD2	2:D:1253:GLU:CD	2.40	0.47
2:D:488:THR:OG1	2:D:532:SER:HB3	2.14	0.47
2:F:32:ASN:O	2:F:35:PRO:HD2	2.14	0.47
2:F:485:GLN:HE22	2:F:598:ARG:HG3	1.80	0.47
2:F:592:LEU:HD11	2:F:1297:TRP:CH2	2.48	0.47
2:F:1128:ASP:OD1	2:F:1311:ALA:HB1	2.14	0.47
2:F:1226:LYS:HG2	2:F:1230:TYR:CE1	2.48	0.47
2:F:1345:ILE:HD11	2:F:1369:ILE:HD12	1.97	0.47
2:H:370:ARG:HD2	2:H:1253:GLU:CD	2.40	0.47
2:H:396:TYR:CD1	2:H:1227:LEU:HD13	2.50	0.47
2:H:711:ILE:HB	2:H:887:VAL:HG13	1.96	0.47
2:H:795:ASN:HB2	2:H:798:ARG:HB3	1.95	0.47
2:H:1345:ILE:HD11	2:H:1369:ILE:HD12	1.97	0.47
2:B:553:ALA:O	2:B:557:ILE:HG12	2.15	0.47
1:E:181:LEU:HG	1:E:300:ALA:HB2	1.97	0.47
2:F:488:THR:OG1	2:F:532:SER:HB3	2.14	0.47
1:A:95:PHE:HE2	2:B:27:PHE:HB2	1.80	0.47
2:B:488:THR:OG1	2:B:532:SER:HB3	2.14	0.47
2:B:853:LEU:HB2	2:B:886:LEU:HG	1.97	0.47
2:B:1425:ILE:HD13	2:B:1492:LEU:HD12	1.97	0.47
2:D:853:LEU:HB2	2:D:886:LEU:HG	1.97	0.47
2:D:1128:ASP:OD1	2:D:1311:ALA:HB1	2.14	0.47
2:F:396:TYR:OH	2:F:1223:PHE:HB3	2.15	0.47
2:F:489:LEU:HD11	2:F:602:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1375:ILE:HB	2:B:1534:VAL:HG22	1.97	0.47
2:F:370:ARG:HD2	2:F:1253:GLU:CD	2.40	0.47
1:G:128:GLN:NE2	1:G:152:GLN:OE1	2.47	0.47
1:A:280:ASP:OD1	1:A:280:ASP:N	2.48	0.46
2:B:1503:PHE:HB2	2:B:1533:VAL:HG22	1.97	0.46
1:C:64:VAL:HG13	1:C:170:LYS:CB	2.44	0.46
2:D:769:PRO:O	2:D:848:THR:OG1	2.26	0.46
1:E:209:MET:HE3	1:E:209:MET:HB3	1.86	0.46
2:F:388:ARG:HD3	2:F:429:MET:SD	2.55	0.46
2:D:1345:ILE:HD11	2:D:1369:ILE:HD12	1.97	0.46
2:F:853:LEU:HB2	2:F:886:LEU:HG	1.97	0.46
2:H:190:ILE:CD1	2:H:195:TYR:CB	2.94	0.46
2:H:398:LYS:HE3	2:H:398:LYS:HB3	1.81	0.46
2:H:447:VAL:HA	2:H:450:ILE:HG22	1.98	0.46
2:H:1375:ILE:HB	2:H:1534:VAL:HG22	1.97	0.46
2:H:1503:PHE:HB2	2:H:1533:VAL:HG22	1.97	0.46
1:A:172:ALA:HA	1:G:169:MET:HE2	1.95	0.46
2:B:396:TYR:OH	2:B:1223:PHE:HB3	2.15	0.46
2:B:785:GLU:OE1	2:B:820:GLN:NE2	2.41	0.46
1:C:95:PHE:HE2	2:D:27:PHE:HB2	1.80	0.46
2:D:1375:ILE:HB	2:D:1534:VAL:HG22	1.97	0.46
2:D:1503:PHE:HB2	2:D:1533:VAL:HG22	1.97	0.46
2:F:553:ALA:O	2:F:557:ILE:HG12	2.15	0.46
2:H:1352:VAL:HG13	2:H:1361:VAL:HB	1.97	0.46
2:B:150:LYS:HB3	2:B:176:VAL:CG2	2.41	0.46
2:B:711:ILE:HB	2:B:887:VAL:HG13	1.96	0.46
1:C:169:MET:HE2	1:E:172:ALA:HA	1.95	0.46
2:D:150:LYS:HB3	2:D:176:VAL:CG2	2.41	0.46
2:D:388:ARG:HD3	2:D:429:MET:SD	2.55	0.46
2:D:396:TYR:OH	2:D:1223:PHE:HB3	2.15	0.46
2:D:701:ILE:HD11	2:D:703:ILE:HD11	1.98	0.46
2:D:1226:LYS:HG2	2:D:1230:TYR:CE1	2.48	0.46
2:D:1260:VAL:HG23	2:D:1288:ALA:HB1	1.98	0.46
1:E:177:ARG:HH22	1:E:208:SER:CB	2.25	0.46
2:H:701:ILE:HD11	2:H:703:ILE:HD11	1.98	0.46
2:B:1345:ILE:HD11	2:B:1369:ILE:HD12	1.97	0.46
2:B:1356:SER:HA	2:B:1398:MET:HE2	1.98	0.46
2:D:489:LEU:HD11	2:D:602:LYS:HE3	1.97	0.46
2:D:802:VAL:HG11	2:D:845:TYR:HB2	1.97	0.46
2:F:398:LYS:CD	2:F:614:LEU:HA	2.45	0.46
2:F:1490:PHE:O	2:F:1494:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:396:TYR:OH	2:H:1223:PHE:HB3	2.15	0.46
2:H:1356:SER:HA	2:H:1398:MET:HE2	1.98	0.46
1:A:181:LEU:HG	1:A:300:ALA:HB2	1.97	0.46
2:B:190:ILE:CD1	2:B:195:TYR:CB	2.94	0.46
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.98	0.46
2:B:1514:MET:HG2	2:B:1539:ARG:NH2	2.31	0.46
2:D:1461:LYS:HE2	2:D:1465:LYS:HE2	1.95	0.46
2:F:396:TYR:CD1	2:F:1227:LEU:HD13	2.50	0.46
2:F:802:VAL:HG11	2:F:845:TYR:HB2	1.97	0.46
2:F:1514:MET:HG2	2:F:1539:ARG:NH2	2.31	0.46
2:H:489:LEU:HD11	2:H:602:LYS:HE3	1.97	0.46
2:H:853:LEU:HB2	2:H:886:LEU:HG	1.97	0.46
2:B:388:ARG:HD3	2:B:429:MET:SD	2.55	0.46
2:B:398:LYS:CD	2:B:614:LEU:HA	2.45	0.46
2:B:485:GLN:HE22	2:B:598:ARG:HG3	1.80	0.46
2:B:802:VAL:HG11	2:B:845:TYR:HB2	1.97	0.46
2:D:263:TYR:HB2	2:D:393:THR:HG21	1.98	0.46
2:D:398:LYS:CD	2:D:614:LEU:HA	2.45	0.46
2:D:1352:VAL:HG13	2:D:1361:VAL:HB	1.97	0.46
2:F:1260:VAL:HG23	2:F:1288:ALA:HB1	1.98	0.46
1:G:190:THR:HG22	1:G:191:LEU:H	1.81	0.46
1:A:190:THR:HG22	1:A:191:LEU:H	1.81	0.46
2:B:1260:VAL:HG23	2:B:1288:ALA:HB1	1.98	0.46
2:B:1490:PHE:O	2:B:1494:ARG:HG3	2.16	0.46
1:C:181:LEU:HG	1:C:300:ALA:HB2	1.97	0.46
1:E:190:THR:HG22	1:E:191:LEU:H	1.81	0.46
1:E:280:ASP:OD1	1:E:280:ASP:N	2.48	0.46
2:F:1078:LEU:O	2:F:1082:THR:HG23	2.15	0.46
1:G:181:LEU:HG	1:G:300:ALA:HB2	1.97	0.46
1:G:280:ASP:OD1	1:G:280:ASP:N	2.48	0.46
2:H:253:LEU:HG	2:H:257:MET:HB3	1.98	0.46
2:H:388:ARG:HD3	2:H:429:MET:SD	2.55	0.46
2:H:398:LYS:CD	2:H:614:LEU:HA	2.45	0.46
2:B:253:LEU:HG	2:B:257:MET:HB3	1.98	0.46
1:C:90:TRP:HA	1:C:93:ILE:HG22	1.98	0.46
1:C:178:ALA:O	1:C:181:LEU:CD2	2.64	0.46
2:F:701:ILE:HD11	2:F:703:ILE:HD11	1.98	0.46
2:F:1352:VAL:HG13	2:F:1361:VAL:HB	1.97	0.46
2:F:1356:SER:HA	2:F:1398:MET:HE2	1.98	0.46
2:F:1503:PHE:HB2	2:F:1533:VAL:HG22	1.97	0.46
1:G:313:GLN:HB3	1:G:336:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:485:GLN:HE22	2:H:598:ARG:HG3	1.80	0.46
2:H:1425:ILE:HD13	2:H:1492:LEU:HD12	1.97	0.46
1:A:178:ALA:O	1:A:181:LEU:CD2	2.64	0.46
1:A:261:ILE:H	1:A:261:ILE:HG13	1.61	0.46
2:B:447:VAL:HA	2:B:450:ILE:HG22	1.98	0.46
2:B:1352:VAL:HG13	2:B:1361:VAL:HB	1.97	0.46
1:C:177:ARG:HH22	1:C:208:SER:CB	2.25	0.46
2:D:253:LEU:HG	2:D:257:MET:HB3	1.98	0.46
1:E:64:VAL:HG13	1:E:170:LYS:CB	2.44	0.46
1:E:178:ALA:O	1:E:181:LEU:CD2	2.64	0.46
2:D:447:VAL:HA	2:D:450:ILE:HG22	1.98	0.45
2:D:1102:LEU:HD23	2:D:1102:LEU:HA	1.76	0.45
1:E:90:TRP:HA	1:E:93:ILE:HG22	1.98	0.45
2:F:190:ILE:CD1	2:F:195:TYR:CB	2.94	0.45
2:H:1327:GLU:HB3	2:H:1415:LEU:H	1.82	0.45
1:A:168:PHE:C	1:A:171:THR:CG2	2.81	0.45
1:C:280:ASP:N	1:C:280:ASP:OD1	2.48	0.45
2:D:1356:SER:HA	2:D:1398:MET:HE2	1.98	0.45
2:F:263:TYR:HB2	2:F:393:THR:HG21	1.98	0.45
2:F:447:VAL:HA	2:F:450:ILE:HG22	1.98	0.45
1:G:313:GLN:HE22	1:G:338:LYS:HD2	1.82	0.45
1:A:313:GLN:HE22	1:A:338:LYS:HD2	1.82	0.45
2:B:576:ALA:O	2:B:579:SER:OG	2.34	0.45
1:C:190:THR:HG22	1:C:191:LEU:H	1.81	0.45
1:C:209:MET:HB3	1:C:209:MET:HE3	1.86	0.45
2:D:485:GLN:HE22	2:D:598:ARG:HG3	1.80	0.45
2:D:511:LEU:HD12	2:D:511:LEU:HA	1.73	0.45
2:D:1514:MET:HG2	2:D:1539:ARG:NH2	2.31	0.45
1:G:90:TRP:HA	1:G:93:ILE:HG22	1.98	0.45
1:A:313:GLN:HB3	1:A:336:THR:CG2	2.46	0.45
2:B:489:LEU:HD11	2:B:602:LYS:HE3	1.97	0.45
1:C:313:GLN:HE22	1:C:338:LYS:HD2	1.82	0.45
2:D:190:ILE:CD1	2:D:195:TYR:CB	2.94	0.45
2:D:398:LYS:HE3	2:D:398:LYS:HB3	1.81	0.45
2:F:150:LYS:CB	2:F:176:VAL:HG22	2.44	0.45
2:F:892:GLN:H	2:F:892:GLN:HG3	1.41	0.45
2:F:1079:CYS:O	2:F:1082:THR:OG1	2.27	0.45
1:G:177:ARG:HH22	1:G:208:SER:CB	2.25	0.45
1:G:178:ALA:O	1:G:181:LEU:CD2	2.64	0.45
2:H:785:GLU:OE1	2:H:820:GLN:NE2	2.41	0.45
2:H:1260:VAL:HG23	2:H:1288:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:ASP:OD1	2:B:247:LEU:N	2.49	0.45
2:B:288:TRP:CE3	2:B:607:VAL:HG11	2.52	0.45
2:B:312:LEU:CB	2:B:369:GLN:HG2	2.47	0.45
2:B:1327:GLU:HB3	2:B:1415:LEU:H	1.82	0.45
1:C:313:GLN:HB3	1:C:336:THR:CG2	2.46	0.45
2:D:1327:GLU:HB3	2:D:1415:LEU:H	1.82	0.45
2:D:1490:PHE:O	2:D:1494:ARG:HG3	2.16	0.45
1:E:56:LEU:O	1:E:59:VAL:HG22	2.17	0.45
2:F:37:VAL:HG13	2:F:41:PHE:CE2	2.52	0.45
2:F:1353:ARG:O	2:F:1398:MET:HB2	2.17	0.45
2:H:1030:ILE:HD11	2:H:1068:PHE:CE1	2.52	0.45
2:H:1102:LEU:HD23	2:H:1102:LEU:HA	1.76	0.45
2:H:1490:PHE:O	2:H:1494:ARG:HG3	2.16	0.45
2:H:1514:MET:HG2	2:H:1539:ARG:NH2	2.31	0.45
2:D:196:ILE:O	2:D:197:PHE:C	2.60	0.45
1:E:313:GLN:HB3	1:E:336:THR:CG2	2.46	0.45
2:F:253:LEU:HG	2:F:257:MET:HB3	1.98	0.45
2:H:37:VAL:HG13	2:H:41:PHE:CE2	2.52	0.45
1:A:90:TRP:HA	1:A:93:ILE:HG22	1.98	0.45
2:D:37:VAL:HG13	2:D:41:PHE:CE2	2.52	0.45
2:D:540:THR:O	2:D:544:ILE:HG12	2.17	0.45
1:E:169:MET:HE2	1:G:172:ALA:HA	1.95	0.45
1:E:313:GLN:HE22	1:E:338:LYS:HD2	1.82	0.45
2:F:511:LEU:HD12	2:F:511:LEU:HA	1.73	0.45
1:G:56:LEU:O	1:G:59:VAL:HG22	2.17	0.45
2:D:288:TRP:CE3	2:D:607:VAL:HG11	2.52	0.45
2:F:540:THR:O	2:F:544:ILE:HG12	2.17	0.45
2:H:1353:ARG:O	2:H:1398:MET:HB2	2.17	0.45
1:A:56:LEU:O	1:A:59:VAL:HG22	2.17	0.45
1:A:177:ARG:HH22	1:A:208:SER:CB	2.25	0.45
2:B:1246:ARG:HA	2:B:1246:ARG:HD3	1.65	0.45
1:C:56:LEU:O	1:C:59:VAL:HG22	2.17	0.45
2:D:592:LEU:HD21	2:D:1297:TRP:CH2	2.52	0.45
2:D:853:LEU:HD23	2:D:856:PRO:HG3	1.99	0.45
2:F:288:TRP:CE3	2:F:607:VAL:HG11	2.52	0.45
2:F:312:LEU:CB	2:F:369:GLN:HG2	2.47	0.45
2:H:592:LEU:HD11	2:H:1297:TRP:CH2	2.48	0.45
2:H:1460:LEU:HD21	2:H:1490:PHE:CE1	2.52	0.45
2:B:592:LEU:HD21	2:B:1297:TRP:CH2	2.52	0.45
2:B:1030:ILE:HD11	2:B:1068:PHE:CE1	2.52	0.45
2:D:312:LEU:CB	2:D:369:GLN:HG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:395:ILE:O	2:D:399:ILE:HG13	2.17	0.45
2:F:196:ILE:O	2:F:197:PHE:C	2.60	0.45
2:F:219:GLN:HG2	2:F:378:TYR:CZ	2.52	0.45
2:H:263:TYR:HB2	2:H:393:THR:HG21	1.98	0.45
2:H:540:THR:O	2:H:544:ILE:HG12	2.17	0.45
2:B:37:VAL:HG13	2:B:41:PHE:CE2	2.52	0.44
2:B:1020:GLN:HB3	2:B:1148:LEU:HD11	1.99	0.44
2:D:246:ASP:OD1	2:D:247:LEU:N	2.49	0.44
2:F:592:LEU:HD21	2:F:1297:TRP:CH2	2.52	0.44
2:H:196:ILE:O	2:H:197:PHE:C	2.60	0.44
2:H:288:TRP:CE3	2:H:607:VAL:HG11	2.52	0.44
2:H:551:PRO:CB	2:H:583:PHE:HZ	2.30	0.44
2:H:853:LEU:HD23	2:H:856:PRO:HG3	1.99	0.44
1:A:34:ARG:O	1:C:326:TYR:HE1	2.00	0.44
1:A:60:PHE:HA	1:A:63:LEU:HD23	1.99	0.44
1:A:241:GLU:HG3	1:A:259:HIS:HD2	1.82	0.44
2:D:1353:ARG:O	2:D:1398:MET:HB2	2.17	0.44
2:H:91:GLU:CD	2:H:171:LEU:HD12	2.41	0.44
2:H:312:LEU:CB	2:H:369:GLN:HG2	2.47	0.44
2:H:395:ILE:O	2:H:399:ILE:HG13	2.17	0.44
2:B:853:LEU:HD23	2:B:856:PRO:HG3	1.99	0.44
2:D:1004:TYR:CE1	2:D:1093:VAL:HG11	2.53	0.44
2:B:219:GLN:HG2	2:B:378:TYR:CZ	2.52	0.44
2:B:1256:GLY:O	2:B:1260:VAL:HG12	2.18	0.44
2:B:1353:ARG:O	2:B:1398:MET:HB2	2.17	0.44
2:D:1020:GLN:HB3	2:D:1148:LEU:HD11	1.99	0.44
2:D:1256:GLY:O	2:D:1260:VAL:HG12	2.18	0.44
2:D:1460:LEU:HD21	2:D:1490:PHE:CE1	2.52	0.44
2:F:395:ILE:O	2:F:399:ILE:HG13	2.17	0.44
2:F:576:ALA:O	2:F:579:SER:OG	2.34	0.44
2:F:853:LEU:HD23	2:F:856:PRO:HG3	1.99	0.44
2:F:1256:GLY:O	2:F:1260:VAL:HG12	2.18	0.44
2:F:1460:LEU:HD21	2:F:1490:PHE:CE1	2.52	0.44
2:B:1483:SER:O	2:B:1487:ARG:HG3	2.18	0.44
2:D:219:GLN:HG2	2:D:378:TYR:CZ	2.52	0.44
2:F:1369:ILE:HD13	2:F:1375:ILE:HG13	2.00	0.44
2:F:1509:THR:HG21	2:F:1539:ARG:HB2	2.00	0.44
1:G:60:PHE:HA	1:G:63:LEU:HD23	1.99	0.44
2:H:219:GLN:HG2	2:H:378:TYR:CZ	2.52	0.44
2:H:491:HIS:CE1	2:H:528:LYS:HB3	2.53	0.44
2:H:869:MET:HE3	2:H:869:MET:HB3	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1004:TYR:CE1	2:H:1093:VAL:HG11	2.53	0.44
2:B:263:TYR:HB2	2:B:393:THR:HG21	1.98	0.44
2:B:295:PHE:CE1	2:B:387:LEU:HB2	2.46	0.44
2:B:391:ILE:O	2:B:395:ILE:HG23	2.18	0.44
2:D:1030:ILE:HD11	2:D:1068:PHE:CE1	2.52	0.44
2:D:1369:ILE:HD13	2:D:1375:ILE:HG13	2.00	0.44
2:F:40:LEU:O	2:F:44:PHE:HD2	2.01	0.44
2:H:246:ASP:OD1	2:H:247:LEU:N	2.49	0.44
2:H:819:ASP:OD1	2:H:820:GLN:N	2.41	0.44
2:D:391:ILE:O	2:D:395:ILE:HG23	2.18	0.44
2:D:1479:GLY:O	2:D:1487:ARG:NH1	2.51	0.44
2:D:1509:THR:HG21	2:D:1539:ARG:HB2	2.00	0.44
2:F:1030:ILE:HD11	2:F:1068:PHE:CE1	2.52	0.44
2:F:1483:SER:O	2:F:1487:ARG:HG3	2.18	0.44
2:H:40:LEU:O	2:H:44:PHE:HD2	2.01	0.44
2:H:684:GLY:O	2:H:698:ASN:N	2.51	0.44
2:H:1431:LEU:HD12	2:H:1487:ARG:HG2	2.00	0.44
2:B:491:HIS:CE1	2:B:528:LYS:HB3	2.53	0.44
2:B:540:THR:O	2:B:544:ILE:HG12	2.17	0.44
2:B:1460:LEU:HD21	2:B:1490:PHE:CE1	2.52	0.44
2:D:253:LEU:HD12	2:D:253:LEU:HA	1.77	0.44
1:E:241:GLU:HG3	1:E:259:HIS:HD2	1.82	0.44
2:F:684:GLY:O	2:F:698:ASN:N	2.51	0.44
2:F:1192:LEU:HA	2:F:1195:THR:HG22	2.00	0.44
2:F:1327:GLU:HB3	2:F:1415:LEU:H	1.82	0.44
2:B:1004:TYR:CE1	2:B:1093:VAL:HG11	2.53	0.44
2:D:40:LEU:O	2:D:44:PHE:HD2	2.01	0.44
2:F:288:TRP:HE3	2:F:607:VAL:HG11	1.83	0.44
2:F:1105:ILE:HD11	2:F:1318:LEU:HD21	2.00	0.44
2:H:730:MET:HE3	2:H:730:MET:HB3	1.89	0.44
2:H:806:CYS:O	2:H:837:ARG:HD2	2.18	0.44
2:H:1256:GLY:O	2:H:1260:VAL:HG12	2.18	0.44
2:H:1345:ILE:HG12	2:H:1369:ILE:HB	2.00	0.44
2:B:40:LEU:O	2:B:44:PHE:HD2	2.01	0.43
2:B:150:LYS:CB	2:B:176:VAL:HG22	2.44	0.43
2:B:395:ILE:O	2:B:399:ILE:HG13	2.17	0.43
1:C:241:GLU:HG3	1:C:259:HIS:HD2	1.82	0.43
2:D:825:GLU:OE1	2:D:825:GLU:N	2.48	0.43
2:D:1255:ILE:HD13	2:D:1255:ILE:HA	1.93	0.43
2:F:1386:SER:OG	3:F:2502:ADP:O1A	2.36	0.43
2:F:1479:GLY:O	2:F:1487:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1479:GLY:O	2:H:1487:ARG:NH1	2.51	0.43
2:B:295:PHE:HZ	2:B:387:LEU:CD1	2.30	0.43
2:B:398:LYS:HE3	2:B:398:LYS:HB3	1.81	0.43
2:D:772:TYR:HD1	2:D:852:PHE:HB2	1.83	0.43
2:D:892:GLN:H	2:D:892:GLN:HG3	1.41	0.43
1:E:332:LYS:HD3	1:E:335:ASN:OD1	2.18	0.43
1:A:46:HIS:CD2	1:C:330:TYR:OH	2.72	0.43
1:A:169:MET:HE2	1:C:172:ALA:CB	2.48	0.43
2:B:806:CYS:O	2:B:837:ARG:HD2	2.18	0.43
2:B:1105:ILE:HD11	2:B:1318:LEU:HD21	2.00	0.43
2:B:1479:GLY:O	2:B:1487:ARG:NH1	2.51	0.43
2:D:592:LEU:HD11	2:D:1297:TRP:CH2	2.48	0.43
2:D:592:LEU:HD21	2:D:1297:TRP:CZ2	2.54	0.43
2:D:806:CYS:O	2:D:837:ARG:HD2	2.18	0.43
2:D:1105:ILE:HD11	2:D:1318:LEU:HD21	2.00	0.43
2:D:1483:SER:O	2:D:1487:ARG:HG3	2.18	0.43
1:E:60:PHE:HA	1:E:63:LEU:HD23	1.99	0.43
2:F:1020:GLN:HB3	2:F:1148:LEU:HD11	1.99	0.43
2:H:1105:ILE:HD11	2:H:1318:LEU:HD21	2.00	0.43
2:B:1354:TYR:HA	2:B:1396:VAL:HG13	2.00	0.43
1:C:34:ARG:O	1:E:326:TYR:HE1	2.00	0.43
1:C:60:PHE:HA	1:C:63:LEU:HD23	1.99	0.43
2:D:295:PHE:HZ	2:D:387:LEU:CD1	2.30	0.43
1:E:34:ARG:O	1:G:326:TYR:HE1	2.00	0.43
2:F:491:HIS:CE1	2:F:528:LYS:HB3	2.53	0.43
2:F:592:LEU:HD21	2:F:1297:TRP:CZ2	2.54	0.43
2:H:150:LYS:HB3	2:H:176:VAL:CG2	2.41	0.43
2:H:892:GLN:H	2:H:892:GLN:HG3	1.41	0.43
2:H:1114:GLU:OE1	3:H:2502:ADP:N6	2.52	0.43
1:C:332:LYS:HD3	1:C:335:ASN:OD1	2.18	0.43
2:D:684:GLY:O	2:D:698:ASN:N	2.51	0.43
2:F:262:ASN:HB3	2:F:390:ALA:HB2	2.00	0.43
2:H:150:LYS:CB	2:H:176:VAL:HG22	2.44	0.43
2:H:592:LEU:HD21	2:H:1297:TRP:CH2	2.52	0.43
2:H:592:LEU:HD21	2:H:1297:TRP:CZ2	2.54	0.43
2:H:1192:LEU:HA	2:H:1195:THR:HG22	2.00	0.43
1:A:326:TYR:HE1	1:G:34:ARG:O	2.00	0.43
2:B:262:ASN:HB3	2:B:390:ALA:HB2	2.00	0.43
2:B:819:ASP:OD1	2:B:820:GLN:N	2.41	0.43
2:B:1431:LEU:HD12	2:B:1487:ARG:HG2	2.00	0.43
1:C:169:MET:HE2	1:E:172:ALA:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1353:ARG:NH1	2:D:1400:GLU:OE2	2.45	0.43
2:D:1354:TYR:HA	2:D:1396:VAL:HG13	2.00	0.43
1:E:46:HIS:CD2	1:G:330:TYR:OH	2.72	0.43
2:F:551:PRO:CB	2:F:583:PHE:HZ	2.30	0.43
2:H:288:TRP:HE3	2:H:607:VAL:HG11	1.83	0.43
2:H:391:ILE:O	2:H:395:ILE:HG23	2.18	0.43
2:H:586:LEU:O	2:H:589:PRO:HD2	2.19	0.43
2:H:825:GLU:OE1	2:H:825:GLU:N	2.48	0.43
2:H:1020:GLN:HB3	2:H:1148:LEU:HD11	1.99	0.43
2:H:1369:ILE:HD13	2:H:1375:ILE:HG13	2.00	0.43
1:A:172:ALA:CB	1:G:169:MET:HE2	2.48	0.43
1:C:46:HIS:CD2	1:E:330:TYR:OH	2.72	0.43
2:D:219:GLN:HG2	2:D:378:TYR:OH	2.19	0.43
2:D:491:HIS:CE1	2:D:528:LYS:HB3	2.53	0.43
2:D:1431:LEU:HD12	2:D:1487:ARG:HG2	2.00	0.43
1:E:169:MET:HE2	1:G:172:ALA:CB	2.48	0.43
2:F:131:ASN:OD1	2:F:131:ASN:N	2.43	0.43
2:F:295:PHE:HZ	2:F:387:LEU:CD1	2.30	0.43
2:H:219:GLN:HG2	2:H:378:TYR:OH	2.19	0.43
2:H:263:TYR:HB2	2:H:393:THR:CG2	2.49	0.43
2:H:295:PHE:HZ	2:H:387:LEU:CD1	2.30	0.43
2:H:1079:CYS:O	2:H:1082:THR:OG1	2.27	0.43
2:H:1353:ARG:NH1	2:H:1400:GLU:OE2	2.45	0.43
2:B:253:LEU:HA	2:B:253:LEU:HD12	1.77	0.43
2:B:263:TYR:HB2	2:B:393:THR:CG2	2.49	0.43
2:B:592:LEU:HD21	2:B:1297:TRP:CZ2	2.54	0.43
2:B:1369:ILE:HD13	2:B:1375:ILE:HG13	2.00	0.43
2:D:1192:LEU:HA	2:D:1195:THR:HG22	2.00	0.43
2:F:391:ILE:O	2:F:395:ILE:HG23	2.18	0.43
2:F:586:LEU:O	2:F:589:PRO:HD2	2.19	0.43
2:F:772:TYR:HD1	2:F:852:PHE:HB2	1.83	0.43
1:G:241:GLU:HG3	1:G:259:HIS:HD2	1.82	0.43
2:H:1483:SER:O	2:H:1487:ARG:HG3	2.18	0.43
2:B:684:GLY:O	2:B:698:ASN:N	2.51	0.43
2:D:262:ASN:HB3	2:D:390:ALA:HB2	2.00	0.43
2:F:150:LYS:HB3	2:F:176:VAL:CG2	2.41	0.43
2:F:1102:LEU:HD23	2:F:1102:LEU:HA	1.76	0.43
2:F:1106:ILE:HD13	2:F:1106:ILE:HA	1.89	0.43
2:F:1431:LEU:HD12	2:F:1487:ARG:HG2	2.00	0.43
2:H:262:ASN:HB3	2:H:390:ALA:HB2	2.00	0.43
2:H:1494:ARG:O	2:H:1498:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1114:GLU:OE1	3:B:2502:ADP:N6	2.52	0.43
2:B:1203:HIS:CD2	2:B:1227:LEU:HD12	2.54	0.43
2:F:806:CYS:O	2:F:837:ARG:HD2	2.18	0.43
1:G:183:PHE:O	1:G:184:SER:C	2.62	0.43
1:G:332:LYS:HD3	1:G:335:ASN:OD1	2.18	0.43
2:H:772:TYR:HD1	2:H:852:PHE:HB2	1.83	0.43
2:B:288:TRP:HE3	2:B:607:VAL:HG11	1.83	0.42
1:C:183:PHE:O	1:C:184:SER:C	2.62	0.42
2:D:1114:GLU:OE1	3:D:2502:ADP:N6	2.52	0.42
2:F:1004:TYR:CE1	2:F:1093:VAL:HG11	2.53	0.42
1:A:178:ALA:O	1:A:181:LEU:HD23	2.20	0.42
1:A:330:TYR:OH	1:G:46:HIS:CD2	2.72	0.42
2:B:586:LEU:O	2:B:589:PRO:HD2	2.19	0.42
2:D:263:TYR:HB2	2:D:393:THR:CG2	2.49	0.42
2:D:576:ALA:O	2:D:579:SER:OG	2.34	0.42
2:D:1494:ARG:O	2:D:1498:ARG:HG3	2.19	0.42
2:F:44:PHE:HD1	2:F:48:PHE:CE2	2.37	0.42
2:F:1345:ILE:HG12	2:F:1369:ILE:HB	2.00	0.42
1:G:209:MET:HE3	1:G:209:MET:HB3	1.86	0.42
2:H:1509:THR:HG21	2:H:1539:ARG:HB2	2.00	0.42
1:A:332:LYS:HD3	1:A:335:ASN:OD1	2.18	0.42
2:B:772:TYR:HD1	2:B:852:PHE:HB2	1.83	0.42
2:B:1509:THR:HG21	2:B:1539:ARG:HB2	2.00	0.42
2:F:263:TYR:HB2	2:F:393:THR:CG2	2.49	0.42
2:F:875:GLU:O	2:F:879:ASP:HB2	2.20	0.42
2:H:78:THR:HG21	2:H:121:VAL:HG23	2.01	0.42
2:H:1521:GLN:HA	2:H:1524:VAL:HG12	2.01	0.42
2:B:1345:ILE:HG12	2:B:1369:ILE:HB	2.00	0.42
2:D:586:LEU:O	2:D:589:PRO:HD2	2.19	0.42
2:F:78:THR:HG21	2:F:121:VAL:HG23	2.01	0.42
2:F:1494:ARG:O	2:F:1498:ARG:HG3	2.19	0.42
2:D:78:THR:HG21	2:D:121:VAL:HG23	2.01	0.42
2:D:288:TRP:HE3	2:D:607:VAL:HG11	1.83	0.42
2:D:875:GLU:O	2:D:879:ASP:HB2	2.20	0.42
2:D:1345:ILE:HG12	2:D:1369:ILE:HB	2.00	0.42
2:F:869:MET:HB3	2:F:869:MET:HE3	1.77	0.42
2:F:1256:GLY:HA2	2:F:1259:VAL:HG12	2.02	0.42
2:F:1354:TYR:HA	2:F:1396:VAL:HG13	2.00	0.42
1:A:86:PHE:HA	1:A:89:VAL:HG12	2.02	0.42
1:A:183:PHE:O	1:A:184:SER:C	2.62	0.42
2:B:592:LEU:HD11	2:B:1297:TRP:CH2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1192:LEU:HA	2:B:1195:THR:HG22	2.00	0.42
2:D:1020:GLN:HB3	2:D:1148:LEU:CD1	2.50	0.42
2:D:1256:GLY:HA2	2:D:1259:VAL:HG12	2.02	0.42
2:D:1521:GLN:O	2:D:1525:MET:HG2	2.20	0.42
2:F:1146:SER:HB3	2:F:1298:MET:HB2	2.02	0.42
1:G:86:PHE:HA	1:G:89:VAL:HG12	2.02	0.42
1:A:286:ILE:HD12	1:A:301:ARG:HG2	2.02	0.42
2:B:219:GLN:HG2	2:B:378:TYR:OH	2.19	0.42
2:B:1020:GLN:HB3	2:B:1148:LEU:CD1	2.50	0.42
2:B:1079:CYS:O	2:B:1082:THR:OG1	2.27	0.42
2:B:1308:GLN:O	2:B:1312:VAL:HG23	2.20	0.42
1:C:188:VAL:HG12	1:C:310:LEU:HD11	2.02	0.42
2:D:869:MET:HE3	2:D:869:MET:HB3	1.77	0.42
2:D:1335:ILE:N	2:D:1336:PRO:HD2	2.35	0.42
2:D:1521:GLN:HA	2:D:1524:VAL:HG12	2.01	0.42
2:F:571:LEU:O	2:F:571:LEU:HD12	2.20	0.42
2:F:1521:GLN:HA	2:F:1524:VAL:HG12	2.01	0.42
1:G:243:GLY:O	1:G:244:VAL:C	2.63	0.42
1:G:286:ILE:HD12	1:G:301:ARG:HG2	2.02	0.42
2:H:44:PHE:HD1	2:H:48:PHE:CE2	2.37	0.42
2:H:1335:ILE:N	2:H:1336:PRO:HD2	2.35	0.42
1:A:209:MET:HB2	1:A:292:GLU:OE2	2.20	0.42
2:B:196:ILE:O	2:B:197:PHE:C	2.60	0.42
2:D:1164:PHE:HZ	2:D:1259:VAL:HG23	1.85	0.42
1:E:145:ALA:HA	1:E:148:ILE:HG22	2.02	0.42
1:E:178:ALA:O	1:E:181:LEU:HD23	2.20	0.42
2:F:219:GLN:HG2	2:F:378:TYR:OH	2.19	0.42
1:G:79:PHE:HD1	1:G:79:PHE:HA	1.74	0.42
1:G:178:ALA:O	1:G:181:LEU:HD23	2.20	0.42
2:H:531:THR:O	2:H:534:ARG:HG2	2.20	0.42
2:H:571:LEU:HD12	2:H:571:LEU:O	2.20	0.42
2:H:576:ALA:O	2:H:579:SER:OG	2.34	0.42
2:H:1020:GLN:HB3	2:H:1148:LEU:CD1	2.50	0.42
1:A:137:MET:SD	1:C:133:PHE:HB3	2.60	0.42
2:B:511:LEU:HA	2:B:511:LEU:HD12	1.73	0.42
2:B:857:PHE:HE2	2:B:886:LEU:HD21	1.85	0.42
2:B:875:GLU:O	2:B:879:ASP:HB2	2.20	0.42
2:B:1353:ARG:NH1	2:B:1400:GLU:OE2	2.45	0.42
2:D:44:PHE:HD1	2:D:48:PHE:CE2	2.37	0.42
2:D:1308:GLN:O	2:D:1312:VAL:HG23	2.20	0.42
2:F:1203:HIS:CD2	2:F:1227:LEU:HD12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1226:LYS:O	2:H:1230:TYR:HD1	2.03	0.42
2:B:44:PHE:HD1	2:B:48:PHE:CE2	2.37	0.42
2:B:1335:ILE:N	2:B:1336:PRO:HD2	2.35	0.42
2:B:1494:ARG:O	2:B:1498:ARG:HG3	2.19	0.42
1:C:145:ALA:HA	1:C:148:ILE:HG22	2.02	0.42
2:D:857:PHE:HE2	2:D:886:LEU:HD21	1.85	0.42
2:D:1203:HIS:CD2	2:D:1227:LEU:HD12	2.54	0.42
2:D:1226:LYS:O	2:D:1230:TYR:HD1	2.03	0.42
1:E:220:VAL:HB	1:E:233:LEU:HG	2.02	0.42
1:E:338:LYS:HB3	1:E:338:LYS:HE3	1.87	0.42
2:F:188:ASN:O	2:F:192:VAL:HG23	2.20	0.42
2:F:417:ILE:O	2:F:420:LEU:HB3	2.20	0.42
2:H:451:LEU:HD13	2:H:582:LEU:HD21	2.01	0.42
2:H:1146:SER:HB3	2:H:1298:MET:HB2	2.02	0.42
2:H:1246:ARG:HA	2:H:1246:ARG:HD3	1.65	0.42
2:H:1354:TYR:HA	2:H:1396:VAL:HG13	2.00	0.42
2:B:435:CYS:HB3	2:B:436:PRO:HD3	2.02	0.41
2:B:531:THR:O	2:B:534:ARG:HG2	2.20	0.41
2:B:825:GLU:OE1	2:B:825:GLU:N	2.48	0.41
1:C:49:ILE:H	1:C:49:ILE:HG13	1.58	0.41
1:C:338:LYS:HE3	1:C:338:LYS:HB3	1.87	0.41
2:D:435:CYS:HB3	2:D:436:PRO:HD3	2.02	0.41
1:E:148:ILE:HD12	1:E:148:ILE:HA	1.91	0.41
2:F:531:THR:O	2:F:534:ARG:HG2	2.20	0.41
2:F:857:PHE:HE2	2:F:886:LEU:HD21	1.85	0.41
2:F:1020:GLN:HB3	2:F:1148:LEU:CD1	2.50	0.41
2:F:1255:ILE:HD13	2:F:1255:ILE:HA	1.93	0.41
2:H:888:THR:OG1	2:H:889:HIS:N	2.53	0.41
1:A:329:ASP:OD1	1:G:48:ASN:ND2	2.53	0.41
2:B:892:GLN:H	2:B:892:GLN:HG3	1.41	0.41
2:B:1386:SER:OG	3:B:2502:ADP:O1A	2.36	0.41
2:B:1521:GLN:O	2:B:1525:MET:HG2	2.20	0.41
1:C:137:MET:SD	1:E:133:PHE:HB3	2.60	0.41
1:C:286:ILE:HG23	1:C:301:ARG:HG2	2.02	0.41
2:D:451:LEU:HD13	2:D:582:LEU:HD21	2.01	0.41
1:G:145:ALA:HA	1:G:148:ILE:HG22	2.02	0.41
2:H:435:CYS:HB3	2:H:436:PRO:HD3	2.02	0.41
2:H:1203:HIS:CD2	2:H:1227:LEU:HD12	2.54	0.41
1:A:48:ASN:ND2	1:C:329:ASP:OD1	2.53	0.41
1:A:243:GLY:O	1:A:244:VAL:C	2.63	0.41
1:A:286:ILE:HG23	1:A:301:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:VAL:HB	1:C:233:LEU:HG	2.02	0.41
2:D:571:LEU:HD12	2:D:571:LEU:O	2.20	0.41
2:D:1348:GLN:CG	2:D:1402:ARG:HB2	2.51	0.41
1:E:209:MET:HB2	1:E:292:GLU:OE2	2.20	0.41
2:F:812:ILE:HD13	2:F:812:ILE:HA	1.91	0.41
2:F:1164:PHE:HZ	2:F:1259:VAL:HG23	1.85	0.41
2:H:188:ASN:O	2:H:192:VAL:HG23	2.20	0.41
2:H:417:ILE:O	2:H:420:LEU:HB3	2.20	0.41
2:H:1124:ARG:O	2:H:1128:ASP:HB2	2.21	0.41
1:A:133:PHE:HB3	1:G:137:MET:SD	2.60	0.41
1:A:145:ALA:HA	1:A:148:ILE:HG22	2.02	0.41
1:A:188:VAL:HG12	1:A:310:LEU:HD11	2.02	0.41
2:B:547:ASN:O	2:B:551:PRO:HG2	2.21	0.41
2:B:888:THR:OG1	2:B:889:HIS:N	2.53	0.41
2:B:1553:LYS:CE	2:B:1558:LEU:HB2	2.50	0.41
1:C:243:GLY:O	1:C:244:VAL:C	2.63	0.41
2:D:40:LEU:HD11	2:D:115:MET:HB2	2.03	0.41
2:D:417:ILE:O	2:D:420:LEU:HB3	2.20	0.41
1:E:137:MET:SD	1:G:133:PHE:HB3	2.60	0.41
2:F:1144:SER:O	2:F:1147:THR:HG22	2.21	0.41
2:F:1521:GLN:O	2:F:1525:MET:HG2	2.20	0.41
1:G:158:MET:O	1:G:162:ILE:HG22	2.20	0.41
2:H:890:LYS:HB2	2:H:893:TYR:CE2	2.55	0.41
2:B:571:LEU:HD12	2:B:571:LEU:O	2.20	0.41
2:B:1124:ARG:O	2:B:1128:ASP:HB2	2.21	0.41
2:B:1144:SER:O	2:B:1147:THR:HG22	2.21	0.41
2:B:1521:GLN:HA	2:B:1524:VAL:HG12	2.01	0.41
2:D:427:GLN:OE1	2:D:602:LYS:HD3	2.21	0.41
2:D:1146:SER:HB3	2:D:1298:MET:HB2	2.02	0.41
2:F:1246:ARG:HA	2:F:1246:ARG:HD3	1.65	0.41
2:F:1394:ARG:HE	2:F:1415:LEU:HD11	1.86	0.41
1:G:209:MET:HB2	1:G:292:GLU:OE2	2.20	0.41
2:H:1308:GLN:O	2:H:1312:VAL:HG23	2.20	0.41
2:B:78:THR:HG21	2:B:121:VAL:HG23	2.01	0.41
2:B:188:ASN:O	2:B:192:VAL:HG23	2.20	0.41
2:B:427:GLN:OE1	2:B:602:LYS:HD3	2.21	0.41
1:C:158:MET:O	1:C:162:ILE:HG22	2.20	0.41
2:D:890:LYS:HB2	2:D:893:TYR:CE2	2.55	0.41
2:F:435:CYS:HB3	2:F:436:PRO:HD3	2.02	0.41
2:F:1335:ILE:N	2:F:1336:PRO:HD2	2.35	0.41
2:F:1552:LEU:HD23	2:F:1557:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:875:GLU:O	2:H:879:ASP:HB2	2.20	0.41
2:H:1256:GLY:HA2	2:H:1259:VAL:HG12	2.02	0.41
2:B:40:LEU:HD11	2:B:115:MET:HB2	2.03	0.41
2:B:1552:LEU:HD23	2:B:1557:ILE:HG12	2.03	0.41
1:C:48:ASN:ND2	1:E:329:ASP:OD1	2.53	0.41
1:C:178:ALA:O	1:C:181:LEU:HD23	2.20	0.41
1:C:241:GLU:HB2	1:C:258:TYR:O	2.21	0.41
2:D:188:ASN:O	2:D:192:VAL:HG23	2.20	0.41
2:D:547:ASN:O	2:D:551:PRO:HG2	2.21	0.41
2:D:1394:ARG:HE	2:D:1415:LEU:HD11	1.86	0.41
1:E:86:PHE:HA	1:E:89:VAL:HG12	2.02	0.41
1:E:241:GLU:HB2	1:E:258:TYR:O	2.21	0.41
1:E:243:GLY:O	1:E:244:VAL:C	2.63	0.41
2:F:1308:GLN:O	2:F:1312:VAL:HG23	2.20	0.41
1:G:286:ILE:HG23	1:G:301:ARG:HG2	2.02	0.41
2:H:1144:SER:O	2:H:1147:THR:HG22	2.21	0.41
1:A:158:MET:O	1:A:162:ILE:HG22	2.20	0.41
2:B:451:LEU:HD13	2:B:582:LEU:HD21	2.01	0.41
2:B:1226:LYS:O	2:B:1230:TYR:HD1	2.03	0.41
2:B:1256:GLY:HA2	2:B:1259:VAL:HG12	2.02	0.41
2:D:531:THR:O	2:D:534:ARG:HG2	2.20	0.41
1:E:158:MET:O	1:E:162:ILE:HG22	2.20	0.41
1:E:297:THR:O	1:E:297:THR:OG1	2.37	0.41
2:F:253:LEU:HD12	2:F:253:LEU:HA	1.77	0.41
2:F:496:LEU:HD23	2:F:496:LEU:HA	1.88	0.41
2:F:1114:GLU:OE1	3:F:2502:ADP:N6	2.52	0.41
1:G:220:VAL:HB	1:G:233:LEU:HG	2.02	0.41
1:G:241:GLU:HB2	1:G:258:TYR:O	2.21	0.41
2:H:253:LEU:HD12	2:H:253:LEU:HA	1.77	0.41
2:H:1164:PHE:HZ	2:H:1259:VAL:HG23	1.85	0.41
1:A:75:PHE:HB3	1:A:163:MET:SD	2.61	0.41
1:A:238:ILE:HA	1:A:239:PRO:HD3	1.96	0.41
2:B:523:GLU:O	2:B:527:ARG:HG3	2.21	0.41
2:B:890:LYS:HB2	2:B:893:TYR:CE2	2.55	0.41
2:B:1102:LEU:HD23	2:B:1102:LEU:HA	1.76	0.41
2:B:1146:SER:HB3	2:B:1298:MET:HB2	2.02	0.41
2:B:1348:GLN:CG	2:B:1402:ARG:HB2	2.51	0.41
2:B:1394:ARG:HE	2:B:1415:LEU:HD11	1.86	0.41
1:C:86:PHE:HA	1:C:89:VAL:HG12	2.02	0.41
2:D:150:LYS:CB	2:D:176:VAL:HG22	2.44	0.41
2:D:414:ALA:HA	2:D:1208:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1144:SER:O	2:D:1147:THR:HG22	2.21	0.41
2:D:1552:LEU:HD23	2:D:1557:ILE:HG12	2.03	0.41
1:E:75:PHE:HB3	1:E:163:MET:SD	2.61	0.41
1:E:188:VAL:HG12	1:E:310:LEU:HD11	2.02	0.41
1:E:286:ILE:HG23	1:E:301:ARG:HG2	2.02	0.41
2:F:72:ASN:OD1	2:F:72:ASN:N	2.54	0.41
2:F:592:LEU:HD23	2:F:592:LEU:HA	1.89	0.41
2:F:888:THR:OG1	2:F:889:HIS:N	2.53	0.41
2:F:1348:GLN:CG	2:F:1402:ARG:HB2	2.51	0.41
2:F:1553:LYS:CE	2:F:1558:LEU:HB2	2.50	0.41
1:G:75:PHE:HB3	1:G:163:MET:SD	2.61	0.41
1:G:284:ILE:HA	1:G:302:THR:O	2.21	0.41
2:H:547:ASN:O	2:H:551:PRO:HG2	2.21	0.41
1:A:220:VAL:HB	1:A:233:LEU:HG	2.02	0.41
2:B:1164:PHE:HZ	2:B:1259:VAL:HG23	1.85	0.41
1:C:189:ILE:HD11	1:C:311:TRP:CE2	2.56	0.41
1:E:48:ASN:ND2	1:G:329:ASP:OD1	2.53	0.41
2:F:427:GLN:OE1	2:F:602:LYS:HD3	2.21	0.41
2:F:451:LEU:HD13	2:F:582:LEU:HD21	2.01	0.41
2:F:1226:LYS:O	2:F:1230:TYR:HD1	2.03	0.41
2:F:1376:GLY:O	2:F:1549:VAL:HA	2.21	0.41
2:F:1415:LEU:HA	2:F:1418:LEU:HD12	2.03	0.41
2:H:40:LEU:HD11	2:H:115:MET:HB2	2.03	0.41
2:H:423:ILE:HG13	2:H:424:ASP:N	2.36	0.41
2:H:489:LEU:HD21	2:H:602:LYS:HG2	2.03	0.41
2:H:707:GLN:HE21	2:H:899:TRP:CD1	2.39	0.41
2:H:1348:GLN:CG	2:H:1402:ARG:HB2	2.51	0.41
2:H:1521:GLN:O	2:H:1525:MET:HG2	2.20	0.41
1:A:148:ILE:HD12	1:A:148:ILE:HA	1.91	0.40
1:A:189:ILE:HD11	1:A:311:TRP:CE2	2.56	0.40
2:B:597:VAL:O	2:B:601:VAL:HG12	2.21	0.40
2:D:730:MET:HE3	2:D:730:MET:HB3	1.89	0.40
2:D:1376:GLY:O	2:D:1549:VAL:HA	2.21	0.40
2:F:246:ASP:OD1	2:F:247:LEU:N	2.49	0.40
2:F:423:ILE:HG13	2:F:424:ASP:N	2.36	0.40
1:G:188:VAL:HG12	1:G:310:LEU:HD11	2.02	0.40
2:H:857:PHE:HE2	2:H:886:LEU:HD21	1.85	0.40
2:H:1386:SER:OG	3:H:2502:ADP:O1A	2.36	0.40
1:A:284:ILE:HA	1:A:302:THR:O	2.21	0.40
2:B:417:ILE:O	2:B:420:LEU:HB3	2.20	0.40
2:B:894:LEU:HB2	2:B:895:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:ILE:HA	1:C:302:THR:O	2.21	0.40
1:C:286:ILE:HD12	1:C:301:ARG:HG2	2.02	0.40
2:D:544:ILE:HD12	2:D:591:PHE:CE2	2.56	0.40
2:D:618:GLU:HG2	2:D:619:ILE:H	1.87	0.40
2:D:1415:LEU:HA	2:D:1418:LEU:HD12	2.03	0.40
1:E:286:ILE:HD12	1:E:301:ARG:HG2	2.02	0.40
2:F:890:LYS:HB2	2:F:893:TYR:CE2	2.55	0.40
2:F:1211:LEU:HD13	2:F:1211:LEU:HA	1.91	0.40
2:H:72:ASN:OD1	2:H:72:ASN:N	2.54	0.40
2:H:1480:GLU:HB2	3:H:2501:ADP:C6	2.57	0.40
2:H:1552:LEU:HD23	2:H:1557:ILE:HG12	2.03	0.40
2:B:489:LEU:HD21	2:B:602:LYS:HG2	2.03	0.40
2:B:871:ALA:O	2:B:875:GLU:HB2	2.22	0.40
2:B:1480:GLU:HB2	3:B:2501:ADP:C6	2.57	0.40
1:C:209:MET:HB2	1:C:292:GLU:OE2	2.20	0.40
2:D:91:GLU:OE1	2:D:171:LEU:HD12	2.18	0.40
2:D:489:LEU:HD21	2:D:602:LYS:HG2	2.03	0.40
2:D:597:VAL:O	2:D:601:VAL:HG12	2.21	0.40
2:D:1386:SER:OG	3:D:2502:ADP:O1A	2.36	0.40
2:D:1486:GLN:O	2:D:1490:PHE:HD1	2.05	0.40
1:E:237:ASP:HB3	1:G:243:GLY:H	1.86	0.40
2:F:139:LEU:HD23	2:F:139:LEU:HA	1.94	0.40
2:F:489:LEU:HD21	2:F:602:LYS:HG2	2.03	0.40
1:A:237:ASP:HB3	1:C:243:GLY:H	1.86	0.40
1:A:243:GLY:H	1:G:237:ASP:HB3	1.86	0.40
2:B:414:ALA:HA	2:B:1208:VAL:HG11	2.03	0.40
1:C:75:PHE:HB3	1:C:163:MET:SD	2.61	0.40
1:C:125:ILE:HD12	1:C:125:ILE:HA	1.95	0.40
2:D:381:ILE:HG21	2:D:1242:THR:HG21	2.04	0.40
1:E:189:ILE:HD11	1:E:311:TRP:CE2	2.56	0.40
2:F:40:LEU:HD11	2:F:115:MET:HB2	2.03	0.40
2:F:618:GLU:HG2	2:F:619:ILE:H	1.87	0.40
1:G:136:ARG:H	1:G:136:ARG:HG2	1.73	0.40
2:H:1486:GLN:O	2:H:1490:PHE:HD1	2.05	0.40
1:A:209:MET:HE3	1:A:209:MET:HB3	1.86	0.40
2:B:485:GLN:NE2	2:B:598:ARG:HG3	2.37	0.40
2:B:685:PHE:O	2:B:732:LYS:HB3	2.22	0.40
2:D:131:ASN:OD1	2:D:131:ASN:N	2.43	0.40
2:D:707:GLN:HE21	2:D:899:TRP:CD1	2.39	0.40
2:F:523:GLU:O	2:F:527:ARG:HG3	2.21	0.40
2:F:544:ILE:HD12	2:F:591:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:547:ASN:O	2:F:551:PRO:HG2	2.21	0.40
1:G:189:ILE:HD11	1:G:311:TRP:CE2	2.56	0.40
1:G:261:ILE:H	1:G:261:ILE:HG13	1.61	0.40
2:H:523:GLU:O	2:H:527:ARG:HG3	2.21	0.40
2:H:618:GLU:HG2	2:H:619:ILE:H	1.87	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%)	305 (94%)	15 (5%)	3 (1%)	14	49
1	C	323/390 (83%)	305 (94%)	15 (5%)	3 (1%)	14	49
1	E	323/390 (83%)	305 (94%)	15 (5%)	3 (1%)	14	49
1	G	323/390 (83%)	305 (94%)	15 (5%)	3 (1%)	14	49
2	B	1300/1582 (82%)	1245 (96%)	51 (4%)	4 (0%)	36	71
2	D	1300/1582 (82%)	1245 (96%)	51 (4%)	4 (0%)	36	71
2	F	1300/1582 (82%)	1245 (96%)	51 (4%)	4 (0%)	36	71
2	H	1300/1582 (82%)	1245 (96%)	51 (4%)	4 (0%)	36	71
All	All	6492/7888 (82%)	6200 (96%)	264 (4%)	28 (0%)	31	67

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	54	ARG
2	B	197	PHE
2	B	199	LYS
1	C	50	ARG

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Mol	Chain	Res	Type
1	C	54	ARG
2	D	197	PHE
2	D	199	LYS
1	E	50	ARG
1	E	54	ARG
2	F	197	PHE
2	F	199	LYS
1	G	50	ARG
1	G	54	ARG
2	H	197	PHE
2	H	199	LYS
2	B	205	LYS
2	D	205	LYS
2	F	205	LYS
2	H	205	LYS
1	A	244	VAL
1	C	244	VAL
1	E	244	VAL
1	G	244	VAL
2	B	196	ILE
2	D	196	ILE
2	F	196	ILE
2	H	196	ILE

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	250/339 (74%)	216 (86%)	34 (14%)	3	15
1	C	250/339 (74%)	216 (86%)	34 (14%)	3	15
1	E	250/339 (74%)	216 (86%)	34 (14%)	3	15
1	G	250/339 (74%)	216 (86%)	34 (14%)	3	15
2	B	1095/1371 (80%)	1026 (94%)	69 (6%)	16	37
2	D	1095/1371 (80%)	1026 (94%)	69 (6%)	16	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	1095/1371 (80%)	1026 (94%)	69 (6%)	16	37
2	H	1095/1371 (80%)	1026 (94%)	69 (6%)	16	37
All	All	5380/6840 (79%)	4968 (92%)	412 (8%)	14	32

All (412) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	49	ILE
1	A	59	VAL
1	A	63	LEU
1	A	71	THR
1	A	81	CYS
1	A	88	MET
1	A	90	TRP
1	A	108	VAL
1	A	111	VAL
1	A	122	LEU
1	A	133	PHE
1	A	152	GLN
1	A	179	GLU
1	A	181	LEU
1	A	190	THR
1	A	204	ASP
1	A	205	LEU
1	A	219	VAL
1	A	236	VAL
1	A	238	ILE
1	A	249	ILE
1	A	252	VAL
1	A	256	ILE
1	A	261	ILE
1	A	287	LEU
1	A	290	VAL
1	A	294	THR
1	A	297	THR
1	A	298	THR
1	A	310	LEU
1	A	323	ASP
1	A	345	THR
1	A	349	LEU

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Mol	Chain	Res	Type
2	B	37	VAL
2	B	72	ASN
2	B	119	THR
2	B	121	VAL
2	B	167	LEU
2	B	190	ILE
2	B	193	ARG
2	B	204	VAL
2	B	218	LEU
2	B	222	VAL
2	B	229	THR
2	B	237	ILE
2	B	253	LEU
2	B	292	CYS
2	B	358	LEU
2	B	387	LEU
2	B	420	LEU
2	B	423	ILE
2	B	425	THR
2	B	429	MET
2	B	432	PHE
2	B	443	VAL
2	B	451	LEU
2	B	466	VAL
2	B	470	LEU
2	B	511	LEU
2	B	563	VAL
2	B	571	LEU
2	B	574	SER
2	B	614	LEU
2	B	682	ILE
2	B	689	THR
2	B	696	LEU
2	B	701	ILE
2	B	707	GLN
2	B	708	LEU
2	B	723	LEU
2	B	730	MET
2	B	737	VAL
2	B	770	VAL
2	B	850	VAL
2	B	861	ASP

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Mol	Chain	Res	Type
2	B	869	MET
2	B	891	LEU
2	B	892	GLN
2	B	894	LEU
2	B	1038	THR
2	B	1136	ILE
2	B	1204	PHE
2	B	1211	LEU
2	B	1227	LEU
2	B	1240	PHE
2	B	1251	ARG
2	B	1255	ILE
2	B	1258	CYS
2	B	1268	ILE
2	B	1270	ASN
2	B	1315	ILE
2	B	1378	CYS
2	B	1409	ASP
2	B	1417	THR
2	B	1424	ILE
2	B	1432	PHE
2	B	1509	THR
2	B	1522	LYS
2	B	1536	ILE
2	B	1551	VAL
2	B	1557	ILE
2	B	1566	LEU
1	C	36	VAL
1	C	49	ILE
1	C	59	VAL
1	C	63	LEU
1	C	71	THR
1	C	81	CYS
1	C	88	MET
1	C	90	TRP
1	C	108	VAL
1	C	111	VAL
1	C	122	LEU
1	C	133	PHE
1	C	152	GLN
1	C	179	GLU
1	C	181	LEU

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Mol	Chain	Res	Type
1	C	190	THR
1	C	204	ASP
1	C	205	LEU
1	C	219	VAL
1	C	236	VAL
1	C	238	ILE
1	C	249	ILE
1	C	252	VAL
1	C	256	ILE
1	C	261	ILE
1	C	287	LEU
1	C	290	VAL
1	C	294	THR
1	C	297	THR
1	C	298	THR
1	C	310	LEU
1	C	323	ASP
1	C	345	THR
1	C	349	LEU
2	D	37	VAL
2	D	72	ASN
2	D	119	THR
2	D	121	VAL
2	D	167	LEU
2	D	190	ILE
2	D	193	ARG
2	D	204	VAL
2	D	218	LEU
2	D	222	VAL
2	D	229	THR
2	D	237	ILE
2	D	253	LEU
2	D	292	CYS
2	D	358	LEU
2	D	387	LEU
2	D	420	LEU
2	D	423	ILE
2	D	425	THR
2	D	429	MET
2	D	432	PHE
2	D	443	VAL
2	D	451	LEU

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Mol	Chain	Res	Type
2	D	466	VAL
2	D	470	LEU
2	D	511	LEU
2	D	563	VAL
2	D	571	LEU
2	D	574	SER
2	D	614	LEU
2	D	682	ILE
2	D	689	THR
2	D	696	LEU
2	D	701	ILE
2	D	707	GLN
2	D	708	LEU
2	D	723	LEU
2	D	730	MET
2	D	737	VAL
2	D	770	VAL
2	D	850	VAL
2	D	861	ASP
2	D	869	MET
2	D	891	LEU
2	D	892	GLN
2	D	894	LEU
2	D	1038	THR
2	D	1136	ILE
2	D	1204	PHE
2	D	1211	LEU
2	D	1227	LEU
2	D	1240	PHE
2	D	1251	ARG
2	D	1255	ILE
2	D	1258	CYS
2	D	1268	ILE
2	D	1270	ASN
2	D	1315	ILE
2	D	1378	CYS
2	D	1409	ASP
2	D	1417	THR
2	D	1424	ILE
2	D	1432	PHE
2	D	1509	THR
2	D	1522	LYS

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Mol	Chain	Res	Type
2	D	1536	ILE
2	D	1551	VAL
2	D	1557	ILE
2	D	1566	LEU
1	E	36	VAL
1	E	49	ILE
1	E	59	VAL
1	E	63	LEU
1	E	71	THR
1	E	81	CYS
1	E	88	MET
1	E	90	TRP
1	E	108	VAL
1	E	111	VAL
1	E	122	LEU
1	E	133	PHE
1	E	152	GLN
1	E	179	GLU
1	E	181	LEU
1	E	190	THR
1	E	204	ASP
1	E	205	LEU
1	E	219	VAL
1	E	236	VAL
1	E	238	ILE
1	E	249	ILE
1	E	252	VAL
1	E	256	ILE
1	E	261	ILE
1	E	287	LEU
1	E	290	VAL
1	E	294	THR
1	E	297	THR
1	E	298	THR
1	E	310	LEU
1	E	323	ASP
1	E	345	THR
1	E	349	LEU
2	F	37	VAL
2	F	72	ASN
2	F	119	THR
2	F	121	VAL

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Mol	Chain	Res	Type
2	F	167	LEU
2	F	190	ILE
2	F	193	ARG
2	F	204	VAL
2	F	218	LEU
2	F	222	VAL
2	F	229	THR
2	F	237	ILE
2	F	253	LEU
2	F	292	CYS
2	F	358	LEU
2	F	387	LEU
2	F	420	LEU
2	F	423	ILE
2	F	425	THR
2	F	429	MET
2	F	432	PHE
2	F	443	VAL
2	F	451	LEU
2	F	466	VAL
2	F	470	LEU
2	F	511	LEU
2	F	563	VAL
2	F	571	LEU
2	F	574	SER
2	F	614	LEU
2	F	682	ILE
2	F	689	THR
2	F	696	LEU
2	F	701	ILE
2	F	707	GLN
2	F	708	LEU
2	F	723	LEU
2	F	730	MET
2	F	737	VAL
2	F	770	VAL
2	F	850	VAL
2	F	861	ASP
2	F	869	MET
2	F	891	LEU
2	F	892	GLN
2	F	894	LEU

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Mol	Chain	Res	Type
2	F	1038	THR
2	F	1136	ILE
2	F	1204	PHE
2	F	1211	LEU
2	F	1227	LEU
2	F	1240	PHE
2	F	1251	ARG
2	F	1255	ILE
2	F	1258	CYS
2	F	1268	ILE
2	F	1270	ASN
2	F	1315	ILE
2	F	1378	CYS
2	F	1409	ASP
2	F	1417	THR
2	F	1424	ILE
2	F	1432	PHE
2	F	1509	THR
2	F	1522	LYS
2	F	1536	ILE
2	F	1551	VAL
2	F	1557	ILE
2	F	1566	LEU
1	G	36	VAL
1	G	49	ILE
1	G	59	VAL
1	G	63	LEU
1	G	71	THR
1	G	81	CYS
1	G	88	MET
1	G	90	TRP
1	G	108	VAL
1	G	111	VAL
1	G	122	LEU
1	G	133	PHE
1	G	152	GLN
1	G	179	GLU
1	G	181	LEU
1	G	190	THR
1	G	204	ASP
1	G	205	LEU
1	G	219	VAL

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Mol	Chain	Res	Type
1	G	236	VAL
1	G	238	ILE
1	G	249	ILE
1	G	252	VAL
1	G	256	ILE
1	G	261	ILE
1	G	287	LEU
1	G	290	VAL
1	G	294	THR
1	G	297	THR
1	G	298	THR
1	G	310	LEU
1	G	323	ASP
1	G	345	THR
1	G	349	LEU
2	H	37	VAL
2	H	72	ASN
2	H	119	THR
2	H	121	VAL
2	H	167	LEU
2	H	190	ILE
2	H	193	ARG
2	H	204	VAL
2	H	218	LEU
2	H	222	VAL
2	H	229	THR
2	H	237	ILE
2	H	253	LEU
2	H	292	CYS
2	H	358	LEU
2	H	387	LEU
2	H	420	LEU
2	H	423	ILE
2	H	425	THR
2	H	429	MET
2	H	432	PHE
2	H	443	VAL
2	H	451	LEU
2	H	466	VAL
2	H	470	LEU
2	H	511	LEU
2	H	563	VAL

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Mol	Chain	Res	Type
2	H	571	LEU
2	H	574	SER
2	H	614	LEU
2	H	682	ILE
2	H	689	THR
2	H	696	LEU
2	H	701	ILE
2	H	707	GLN
2	H	708	LEU
2	H	723	LEU
2	H	730	MET
2	H	737	VAL
2	H	770	VAL
2	H	850	VAL
2	H	861	ASP
2	H	869	MET
2	H	891	LEU
2	H	892	GLN
2	H	894	LEU
2	H	1038	THR
2	H	1136	ILE
2	H	1204	PHE
2	H	1211	LEU
2	H	1227	LEU
2	H	1240	PHE
2	H	1251	ARG
2	H	1255	ILE
2	H	1258	CYS
2	H	1268	ILE
2	H	1270	ASN
2	H	1315	ILE
2	H	1378	CYS
2	H	1409	ASP
2	H	1417	THR
2	H	1424	ILE
2	H	1432	PHE
2	H	1509	THR
2	H	1522	LYS
2	H	1536	ILE
2	H	1551	VAL
2	H	1557	ILE
2	H	1566	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	48	ASN
1	A	128	GLN
1	A	173	GLN
1	A	216	HIS
1	A	234	HIS
1	A	259	HIS
2	B	223	ASN
2	B	416	GLN
2	B	707	GLN
2	B	863	HIS
2	B	1203	HIS
2	B	1518	ASN
1	C	46	HIS
1	C	48	ASN
1	C	128	GLN
1	C	173	GLN
1	C	216	HIS
1	C	234	HIS
1	C	259	HIS
2	D	223	ASN
2	D	416	GLN
2	D	863	HIS
2	D	1203	HIS
2	D	1518	ASN
1	E	46	HIS
1	E	48	ASN
1	E	128	GLN
1	E	173	GLN
1	E	216	HIS
1	E	234	HIS
2	F	223	ASN
2	F	416	GLN
2	F	707	GLN
2	F	863	HIS
2	F	1203	HIS
2	F	1373	GLN
2	F	1518	ASN
1	G	46	HIS
1	G	48	ASN
1	G	128	GLN

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Mol	Chain	Res	Type
1	G	173	GLN
1	G	216	HIS
1	G	234	HIS
1	G	259	HIS
2	H	223	ASN
2	H	416	GLN
2	H	707	GLN
2	H	863	HIS
2	H	1203	HIS
2	H	1518	ASN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ADP	D	2501	4	28,29,29	1.39	5 (17%)	43,45,45	1.80	9 (20%)
3	ADP	H	2501	4	28,29,29	1.39	5 (17%)	43,45,45	1.80	9 (20%)
3	ADP	H	2502	4	28,29,29	1.39	4 (14%)	43,45,45	1.78	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	401	-	28,29,29	1.42	4 (14%)	43,45,45	1.80	8 (18%)
3	ADP	B	2501	4	28,29,29	1.39	5 (17%)	43,45,45	1.80	9 (20%)
3	ADP	D	2502	4	28,29,29	1.39	4 (14%)	43,45,45	1.78	8 (18%)
3	ADP	C	401	-	28,29,29	1.42	4 (14%)	43,45,45	1.80	8 (18%)
3	ADP	E	401	-	28,29,29	1.42	4 (14%)	43,45,45	1.80	8 (18%)
3	ADP	B	2502	4	28,29,29	1.39	4 (14%)	43,45,45	1.78	8 (18%)
3	ADP	G	401	-	28,29,29	1.42	4 (14%)	43,45,45	1.80	8 (18%)
3	ADP	F	2501	4	28,29,29	1.39	5 (17%)	43,45,45	1.80	9 (20%)
3	ADP	F	2502	4	28,29,29	1.39	4 (14%)	43,45,45	1.78	8 (18%)

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	ADP	D	2501	4	-	1/16/32/32	0/3/3/3
3	ADP	H	2501	4	-	1/16/32/32	0/3/3/3
3	ADP	H	2502	4	-	4/16/32/32	0/3/3/3
3	ADP	A	401	-	-	5/16/32/32	0/3/3/3
3	ADP	B	2501	4	-	1/16/32/32	0/3/3/3
3	ADP	D	2502	4	-	4/16/32/32	0/3/3/3
3	ADP	C	401	-	-	5/16/32/32	0/3/3/3
3	ADP	E	401	-	-	5/16/32/32	0/3/3/3
3	ADP	B	2502	4	-	4/16/32/32	0/3/3/3
3	ADP	G	401	-	-	5/16/32/32	0/3/3/3
3	ADP	F	2501	4	-	1/16/32/32	0/3/3/3
3	ADP	F	2502	4	-	4/16/32/32	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ADP	C5-C4	4.68	1.47	1.39
3	C	401	ADP	C5-C4	4.68	1.47	1.39
3	E	401	ADP	C5-C4	4.68	1.47	1.39
3	G	401	ADP	C5-C4	4.68	1.47	1.39
3	B	2502	ADP	C5-C4	4.66	1.47	1.39
3	D	2502	ADP	C5-C4	4.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2502	ADP	C5-C4	4.66	1.47	1.39
3	H	2502	ADP	C5-C4	4.66	1.47	1.39
3	B	2501	ADP	C5-C4	4.55	1.47	1.39
3	D	2501	ADP	C5-C4	4.55	1.47	1.39
3	F	2501	ADP	C5-C4	4.55	1.47	1.39
3	H	2501	ADP	C5-C4	4.55	1.47	1.39
3	B	2501	ADP	C5-C6	2.71	1.48	1.41
3	D	2501	ADP	C5-C6	2.71	1.48	1.41
3	F	2501	ADP	C5-C6	2.71	1.48	1.41
3	H	2501	ADP	C5-C6	2.71	1.48	1.41
3	A	401	ADP	C5-C6	2.69	1.48	1.41
3	C	401	ADP	C5-C6	2.69	1.48	1.41
3	E	401	ADP	C5-C6	2.69	1.48	1.41
3	G	401	ADP	C5-C6	2.69	1.48	1.41
3	B	2502	ADP	C5-C6	2.61	1.48	1.41
3	D	2502	ADP	C5-C6	2.61	1.48	1.41
3	F	2502	ADP	C5-C6	2.61	1.48	1.41
3	H	2502	ADP	C5-C6	2.61	1.48	1.41
3	B	2502	ADP	C5-N7	-2.35	1.34	1.39
3	D	2502	ADP	C5-N7	-2.35	1.34	1.39
3	F	2502	ADP	C5-N7	-2.35	1.34	1.39
3	H	2502	ADP	C5-N7	-2.35	1.34	1.39
3	A	401	ADP	C5-N7	-2.30	1.34	1.39
3	C	401	ADP	C5-N7	-2.30	1.34	1.39
3	E	401	ADP	C5-N7	-2.30	1.34	1.39
3	G	401	ADP	C5-N7	-2.30	1.34	1.39
3	B	2501	ADP	C8-N7	2.28	1.36	1.31
3	D	2501	ADP	C8-N7	2.28	1.36	1.31
3	F	2501	ADP	C8-N7	2.28	1.36	1.31
3	H	2501	ADP	C8-N7	2.28	1.36	1.31
3	B	2502	ADP	C8-N7	2.25	1.36	1.31
3	D	2502	ADP	C8-N7	2.25	1.36	1.31
3	F	2502	ADP	C8-N7	2.25	1.36	1.31
3	H	2502	ADP	C8-N7	2.25	1.36	1.31
3	B	2501	ADP	C5-N7	-2.20	1.35	1.39
3	D	2501	ADP	C5-N7	-2.20	1.35	1.39
3	F	2501	ADP	C5-N7	-2.20	1.35	1.39
3	H	2501	ADP	C5-N7	-2.20	1.35	1.39
3	A	401	ADP	C8-N7	2.20	1.35	1.31
3	C	401	ADP	C8-N7	2.20	1.35	1.31
3	E	401	ADP	C8-N7	2.20	1.35	1.31
3	G	401	ADP	C8-N7	2.20	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2501	ADP	C4-N9	-2.01	1.33	1.37
3	D	2501	ADP	C4-N9	-2.01	1.33	1.37
3	F	2501	ADP	C4-N9	-2.01	1.33	1.37
3	H	2501	ADP	C4-N9	-2.01	1.33	1.37

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	C5-C4-N3	-5.92	118.57	126.72
3	C	401	ADP	C5-C4-N3	-5.92	118.57	126.72
3	E	401	ADP	C5-C4-N3	-5.92	118.57	126.72
3	G	401	ADP	C5-C4-N3	-5.92	118.57	126.72
3	B	2502	ADP	C5-C4-N3	-5.81	118.71	126.72
3	D	2502	ADP	C5-C4-N3	-5.81	118.71	126.72
3	F	2502	ADP	C5-C4-N3	-5.81	118.71	126.72
3	H	2502	ADP	C5-C4-N3	-5.81	118.71	126.72
3	B	2501	ADP	C5-C4-N3	-5.75	118.79	126.72
3	D	2501	ADP	C5-C4-N3	-5.75	118.79	126.72
3	F	2501	ADP	C5-C4-N3	-5.75	118.79	126.72
3	H	2501	ADP	C5-C4-N3	-5.75	118.79	126.72
3	A	401	ADP	N3-C4-N9	4.68	135.12	127.17
3	C	401	ADP	N3-C4-N9	4.68	135.12	127.17
3	E	401	ADP	N3-C4-N9	4.68	135.12	127.17
3	G	401	ADP	N3-C4-N9	4.68	135.12	127.17
3	B	2502	ADP	N3-C4-N9	4.68	135.12	127.17
3	D	2502	ADP	N3-C4-N9	4.68	135.12	127.17
3	F	2502	ADP	N3-C4-N9	4.68	135.12	127.17
3	H	2502	ADP	N3-C4-N9	4.68	135.12	127.17
3	B	2501	ADP	N3-C4-N9	4.50	134.82	127.17
3	D	2501	ADP	N3-C4-N9	4.50	134.82	127.17
3	F	2501	ADP	N3-C4-N9	4.50	134.82	127.17
3	H	2501	ADP	N3-C4-N9	4.50	134.82	127.17
3	B	2501	ADP	C2-N3-C4	3.74	120.97	111.83
3	D	2501	ADP	C2-N3-C4	3.74	120.97	111.83
3	F	2501	ADP	C2-N3-C4	3.74	120.97	111.83
3	H	2501	ADP	C2-N3-C4	3.74	120.97	111.83
3	B	2502	ADP	C2-N3-C4	3.69	120.85	111.83
3	D	2502	ADP	C2-N3-C4	3.69	120.85	111.83
3	F	2502	ADP	C2-N3-C4	3.69	120.85	111.83
3	H	2502	ADP	C2-N3-C4	3.69	120.85	111.83
3	A	401	ADP	C2-N3-C4	3.69	120.84	111.83
3	C	401	ADP	C2-N3-C4	3.69	120.84	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	ADP	C2-N3-C4	3.69	120.84	111.83
3	G	401	ADP	C2-N3-C4	3.69	120.84	111.83
3	A	401	ADP	C4-C5-N7	-3.42	106.67	110.58
3	C	401	ADP	C4-C5-N7	-3.42	106.67	110.58
3	E	401	ADP	C4-C5-N7	-3.42	106.67	110.58
3	G	401	ADP	C4-C5-N7	-3.42	106.67	110.58
3	B	2501	ADP	C4-C5-N7	-3.37	106.73	110.58
3	D	2501	ADP	C4-C5-N7	-3.37	106.73	110.58
3	F	2501	ADP	C4-C5-N7	-3.37	106.73	110.58
3	H	2501	ADP	C4-C5-N7	-3.37	106.73	110.58
3	B	2502	ADP	C4-C5-N7	-3.33	106.78	110.58
3	D	2502	ADP	C4-C5-N7	-3.33	106.78	110.58
3	F	2502	ADP	C4-C5-N7	-3.33	106.78	110.58
3	H	2502	ADP	C4-C5-N7	-3.33	106.78	110.58
3	B	2501	ADP	N3-C2-N1	-3.31	123.58	128.58
3	D	2501	ADP	N3-C2-N1	-3.31	123.58	128.58
3	F	2501	ADP	N3-C2-N1	-3.31	123.58	128.58
3	H	2501	ADP	N3-C2-N1	-3.31	123.58	128.58
3	B	2502	ADP	N3-C2-N1	-3.23	123.69	128.58
3	D	2502	ADP	N3-C2-N1	-3.23	123.69	128.58
3	F	2502	ADP	N3-C2-N1	-3.23	123.69	128.58
3	H	2502	ADP	N3-C2-N1	-3.23	123.69	128.58
3	A	401	ADP	N3-C2-N1	-3.19	123.75	128.58
3	C	401	ADP	N3-C2-N1	-3.19	123.75	128.58
3	E	401	ADP	N3-C2-N1	-3.19	123.75	128.58
3	G	401	ADP	N3-C2-N1	-3.19	123.75	128.58
3	B	2502	ADP	C4-N9-C8	2.64	108.51	105.74
3	D	2502	ADP	C4-N9-C8	2.64	108.51	105.74
3	F	2502	ADP	C4-N9-C8	2.64	108.51	105.74
3	H	2502	ADP	C4-N9-C8	2.64	108.51	105.74
3	B	2501	ADP	C4-N9-C8	2.62	108.49	105.74
3	D	2501	ADP	C4-N9-C8	2.62	108.49	105.74
3	F	2501	ADP	C4-N9-C8	2.62	108.49	105.74
3	H	2501	ADP	C4-N9-C8	2.62	108.49	105.74
3	B	2502	ADP	C5-N7-C8	2.51	107.39	103.45
3	D	2502	ADP	C5-N7-C8	2.51	107.39	103.45
3	F	2502	ADP	C5-N7-C8	2.51	107.39	103.45
3	H	2502	ADP	C5-N7-C8	2.51	107.39	103.45
3	A	401	ADP	C5-N7-C8	2.46	107.32	103.45
3	C	401	ADP	C5-N7-C8	2.46	107.32	103.45
3	E	401	ADP	C5-N7-C8	2.46	107.32	103.45
3	G	401	ADP	C5-N7-C8	2.46	107.32	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	C3'-C2'-C1'	2.45	106.09	101.46
3	C	401	ADP	C3'-C2'-C1'	2.45	106.09	101.46
3	E	401	ADP	C3'-C2'-C1'	2.45	106.09	101.46
3	G	401	ADP	C3'-C2'-C1'	2.45	106.09	101.46
3	A	401	ADP	C4-N9-C8	2.43	108.28	105.74
3	C	401	ADP	C4-N9-C8	2.43	108.28	105.74
3	E	401	ADP	C4-N9-C8	2.43	108.28	105.74
3	G	401	ADP	C4-N9-C8	2.43	108.28	105.74
3	B	2501	ADP	C5-N7-C8	2.42	107.25	103.45
3	D	2501	ADP	C5-N7-C8	2.42	107.25	103.45
3	F	2501	ADP	C5-N7-C8	2.42	107.25	103.45
3	H	2501	ADP	C5-N7-C8	2.42	107.25	103.45
3	B	2501	ADP	C3'-C2'-C1'	2.39	105.99	101.46
3	D	2501	ADP	C3'-C2'-C1'	2.39	105.99	101.46
3	F	2501	ADP	C3'-C2'-C1'	2.39	105.99	101.46
3	H	2501	ADP	C3'-C2'-C1'	2.39	105.99	101.46
3	B	2501	ADP	C6-C5-N7	2.13	136.20	132.09
3	D	2501	ADP	C6-C5-N7	2.13	136.20	132.09
3	F	2501	ADP	C6-C5-N7	2.13	136.20	132.09
3	H	2501	ADP	C6-C5-N7	2.13	136.20	132.09
3	B	2502	ADP	C6-C5-N7	2.03	136.00	132.09
3	D	2502	ADP	C6-C5-N7	2.03	136.00	132.09
3	F	2502	ADP	C6-C5-N7	2.03	136.00	132.09
3	H	2502	ADP	C6-C5-N7	2.03	136.00	132.09

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2502	ADP	C5'-O5'-PA-O3A
3	B	2502	ADP	O4'-C4'-C5'-O5'
3	D	2502	ADP	C5'-O5'-PA-O3A
3	D	2502	ADP	O4'-C4'-C5'-O5'
3	F	2502	ADP	C5'-O5'-PA-O3A
3	F	2502	ADP	O4'-C4'-C5'-O5'
3	H	2502	ADP	C5'-O5'-PA-O3A
3	H	2502	ADP	O4'-C4'-C5'-O5'
3	B	2502	ADP	C3'-C4'-C5'-O5'
3	D	2502	ADP	C3'-C4'-C5'-O5'
3	F	2502	ADP	C3'-C4'-C5'-O5'
3	H	2502	ADP	C3'-C4'-C5'-O5'
3	A	401	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	C	401	ADP	O4'-C4'-C5'-O5'
3	E	401	ADP	O4'-C4'-C5'-O5'
3	G	401	ADP	O4'-C4'-C5'-O5'
3	A	401	ADP	PB-O3A-PA-O1A
3	C	401	ADP	PB-O3A-PA-O1A
3	E	401	ADP	PB-O3A-PA-O1A
3	G	401	ADP	PB-O3A-PA-O1A
3	B	2501	ADP	C5'-O5'-PA-O1A
3	B	2502	ADP	C5'-O5'-PA-O2A
3	D	2501	ADP	C5'-O5'-PA-O1A
3	D	2502	ADP	C5'-O5'-PA-O2A
3	F	2501	ADP	C5'-O5'-PA-O1A
3	F	2502	ADP	C5'-O5'-PA-O2A
3	H	2501	ADP	C5'-O5'-PA-O1A
3	H	2502	ADP	C5'-O5'-PA-O2A
3	A	401	ADP	PB-O3A-PA-O2A
3	C	401	ADP	PB-O3A-PA-O2A
3	E	401	ADP	PB-O3A-PA-O2A
3	G	401	ADP	PB-O3A-PA-O2A
3	A	401	ADP	C3'-C4'-C5'-O5'
3	C	401	ADP	C3'-C4'-C5'-O5'
3	E	401	ADP	C3'-C4'-C5'-O5'
3	G	401	ADP	C3'-C4'-C5'-O5'
3	A	401	ADP	C2'-C1'-N9-C8
3	C	401	ADP	C2'-C1'-N9-C8
3	E	401	ADP	C2'-C1'-N9-C8
3	G	401	ADP	C2'-C1'-N9-C8

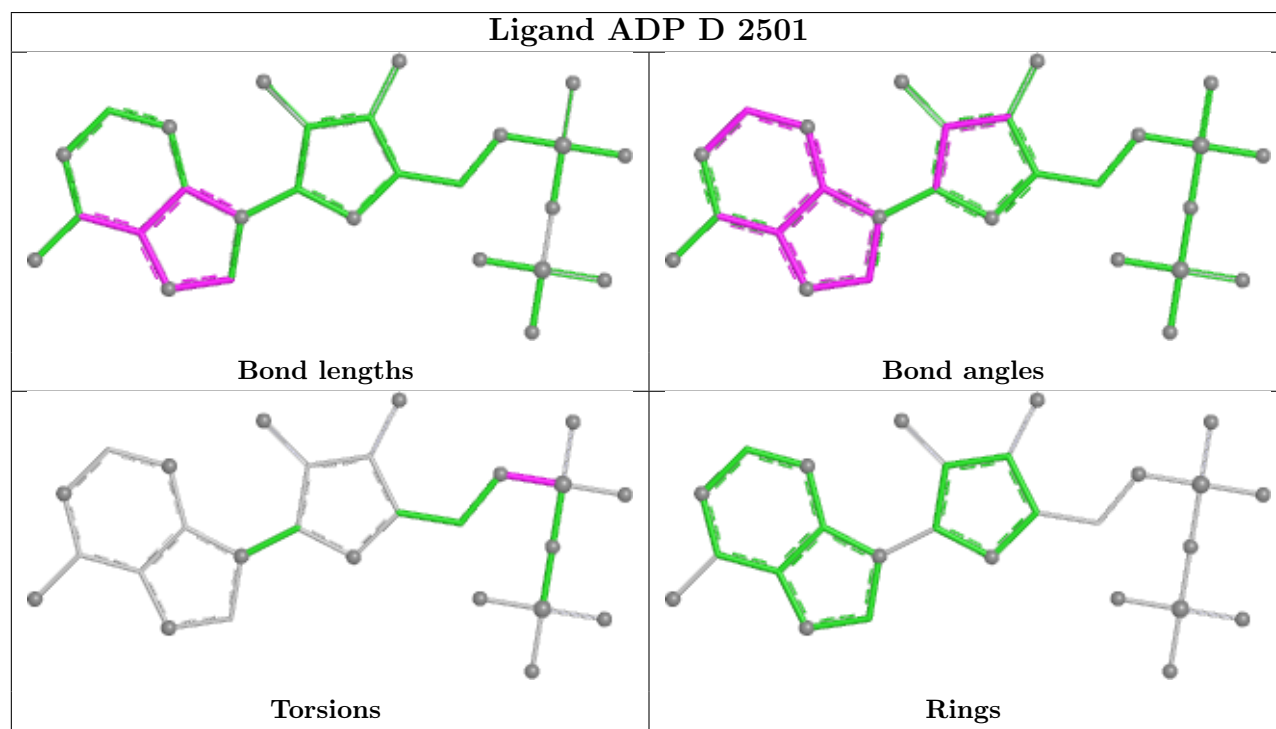
There are no ring outliers.

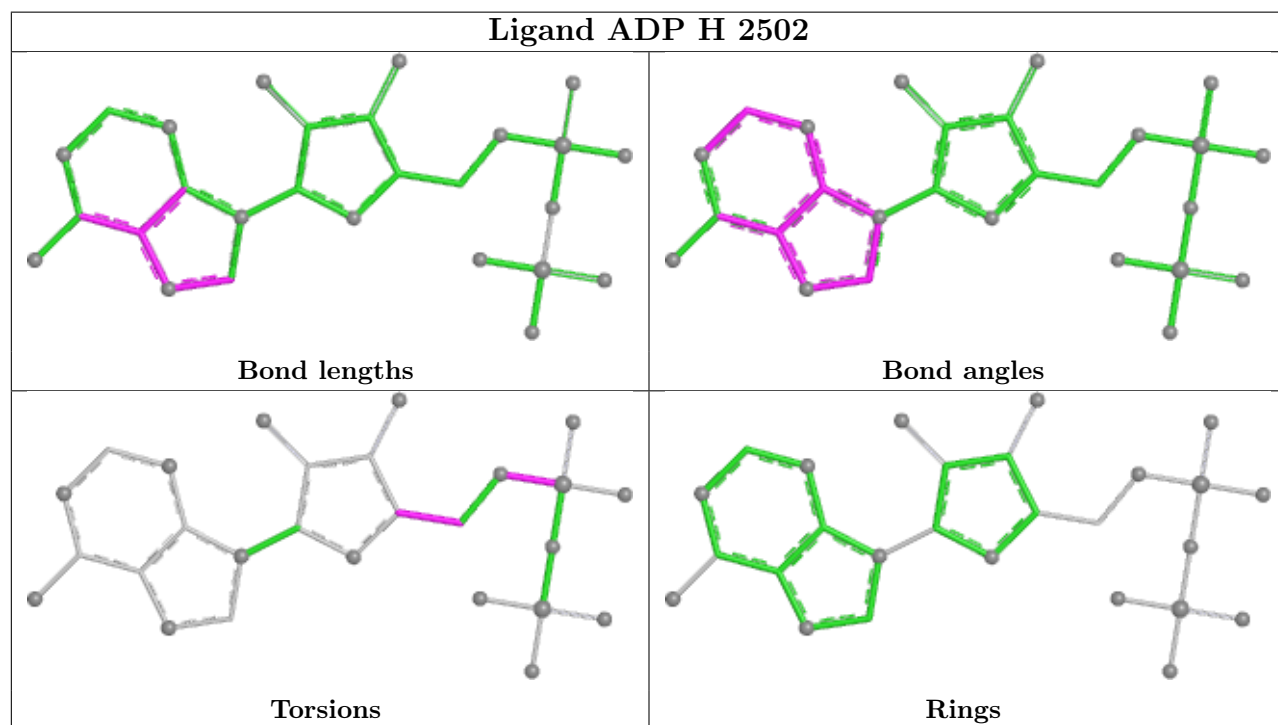
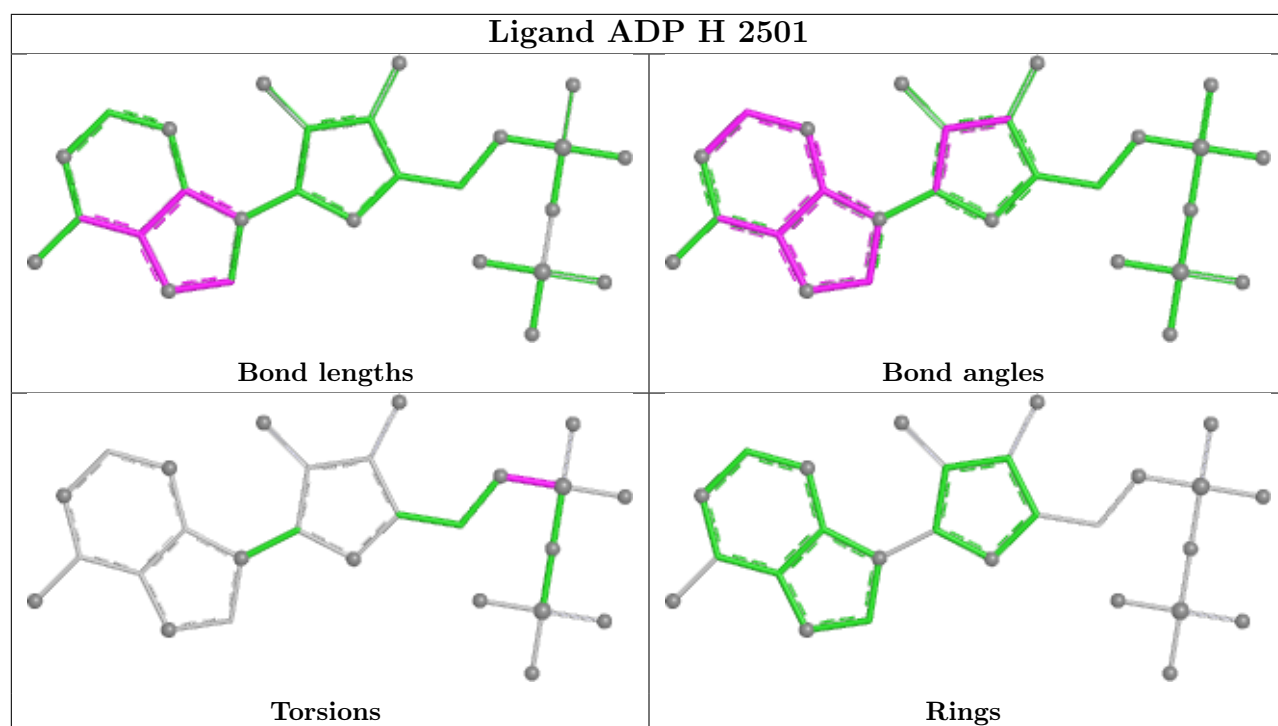
8 monomers are involved in 17 short contacts:

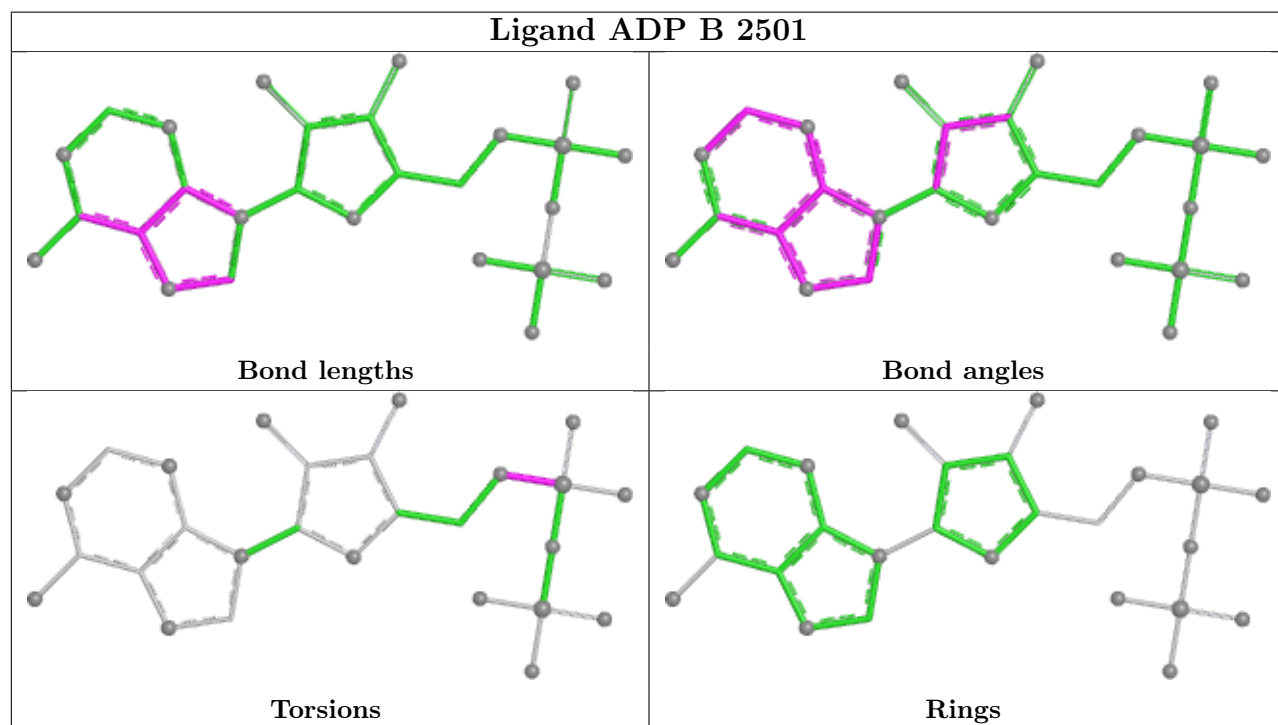
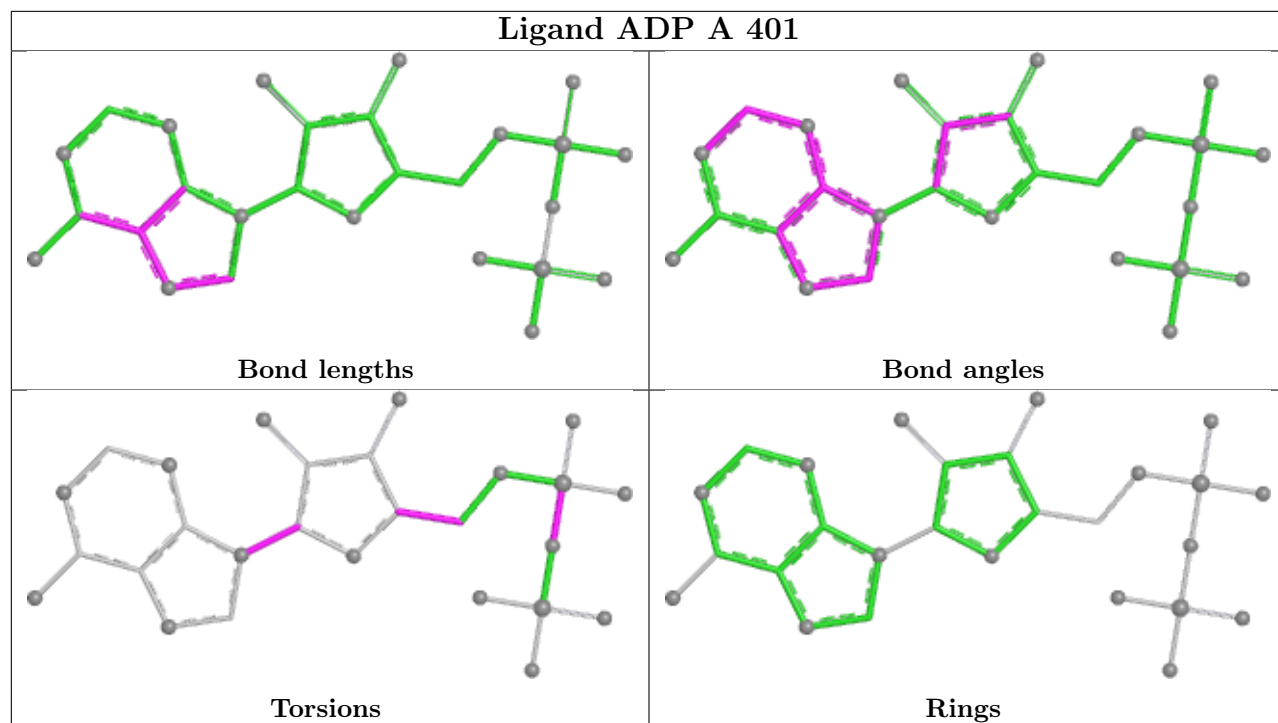
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2501	ADP	1	0
3	H	2501	ADP	2	0
3	H	2502	ADP	3	0
3	B	2501	ADP	2	0
3	D	2502	ADP	3	0
3	B	2502	ADP	3	0
3	F	2501	ADP	1	0
3	F	2502	ADP	2	0

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

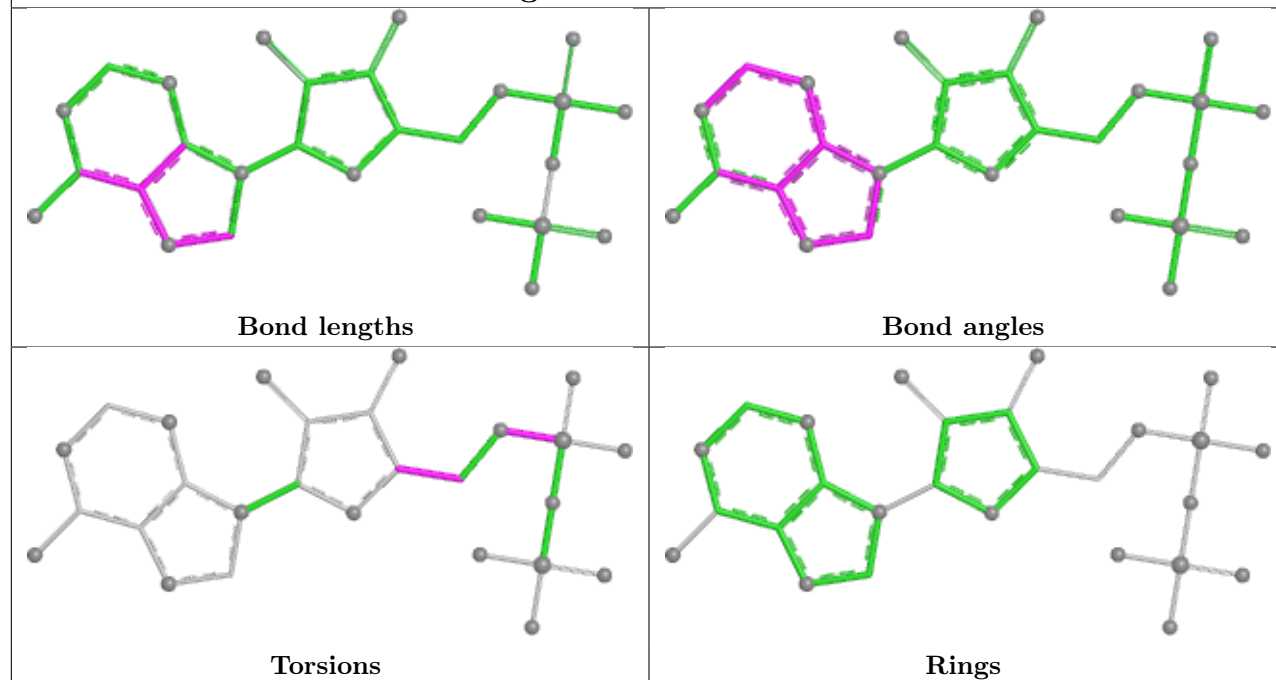
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



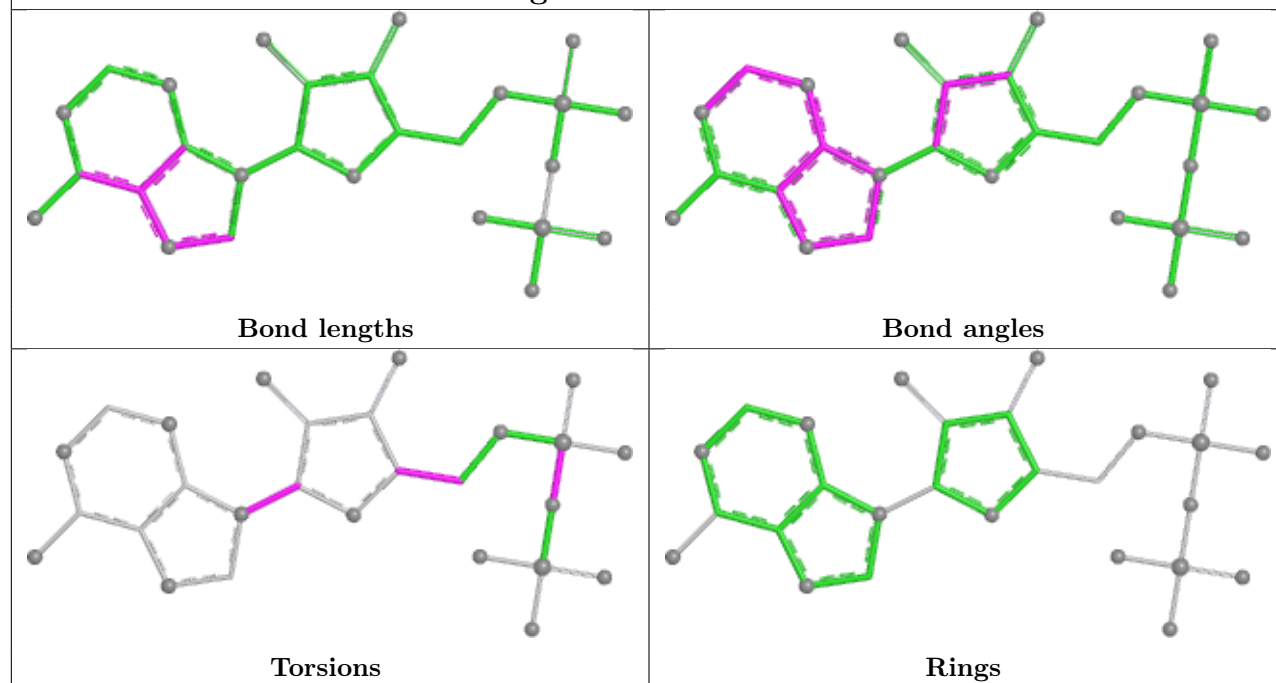


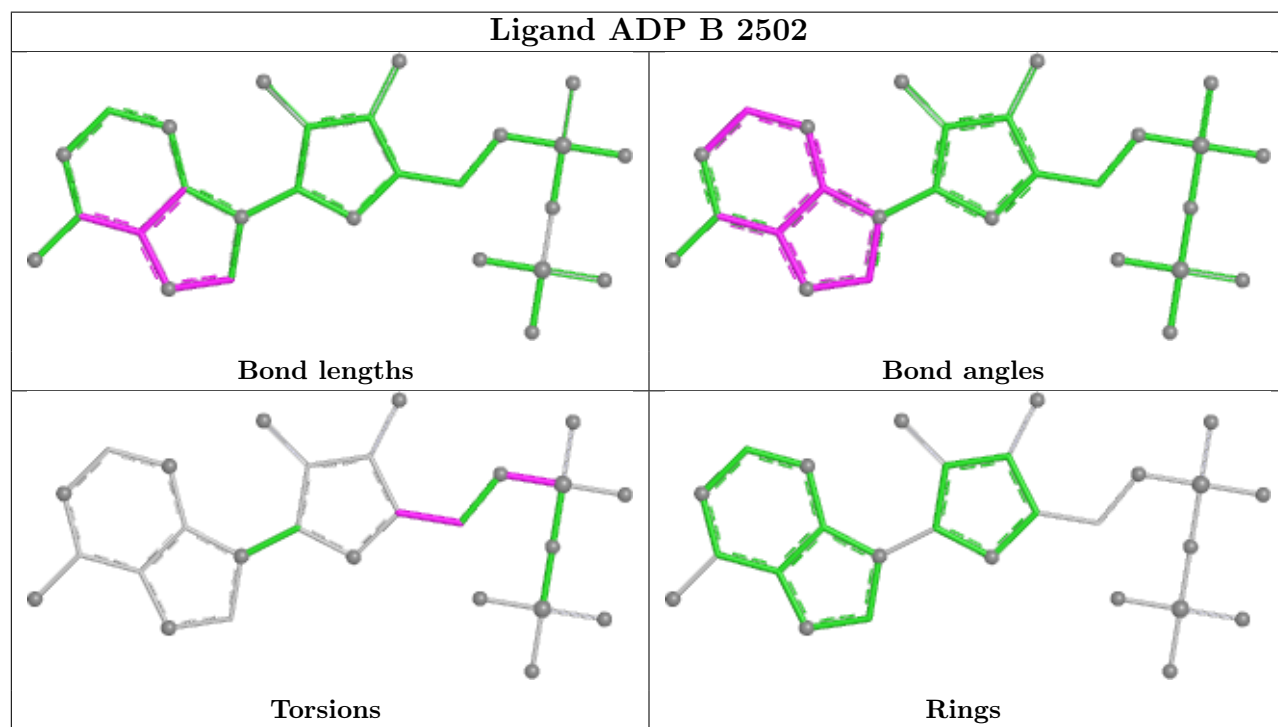
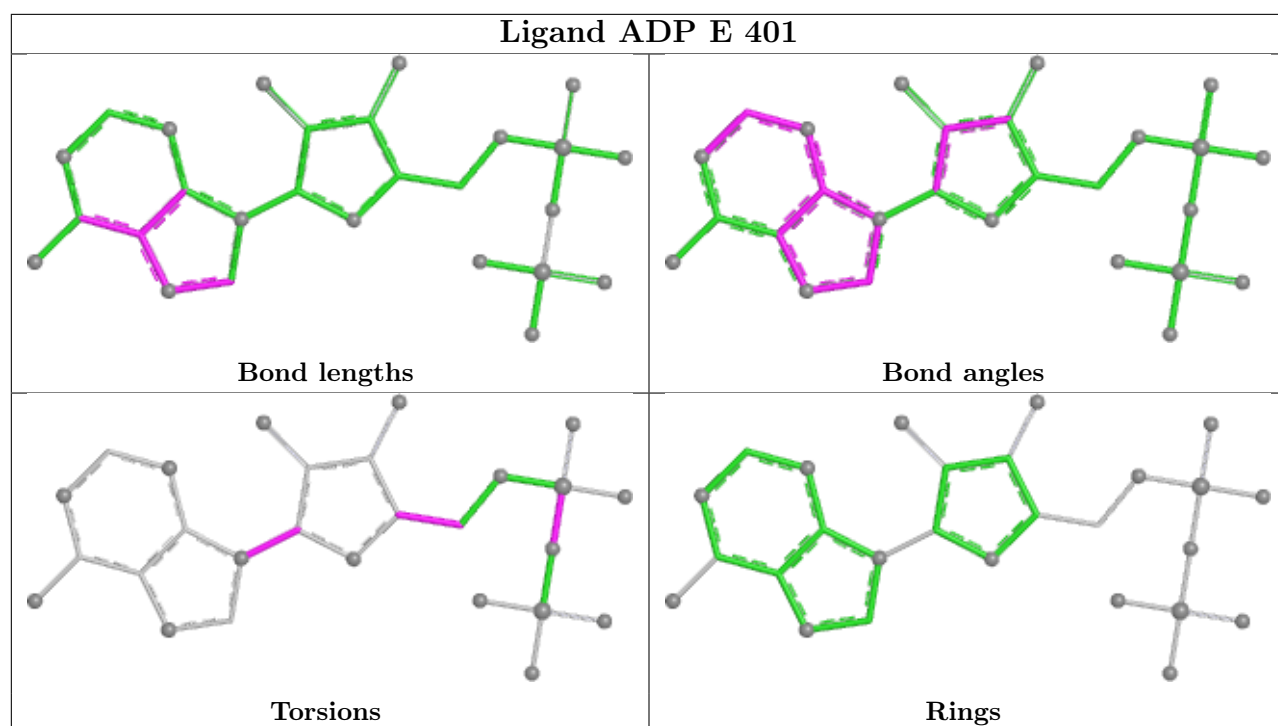


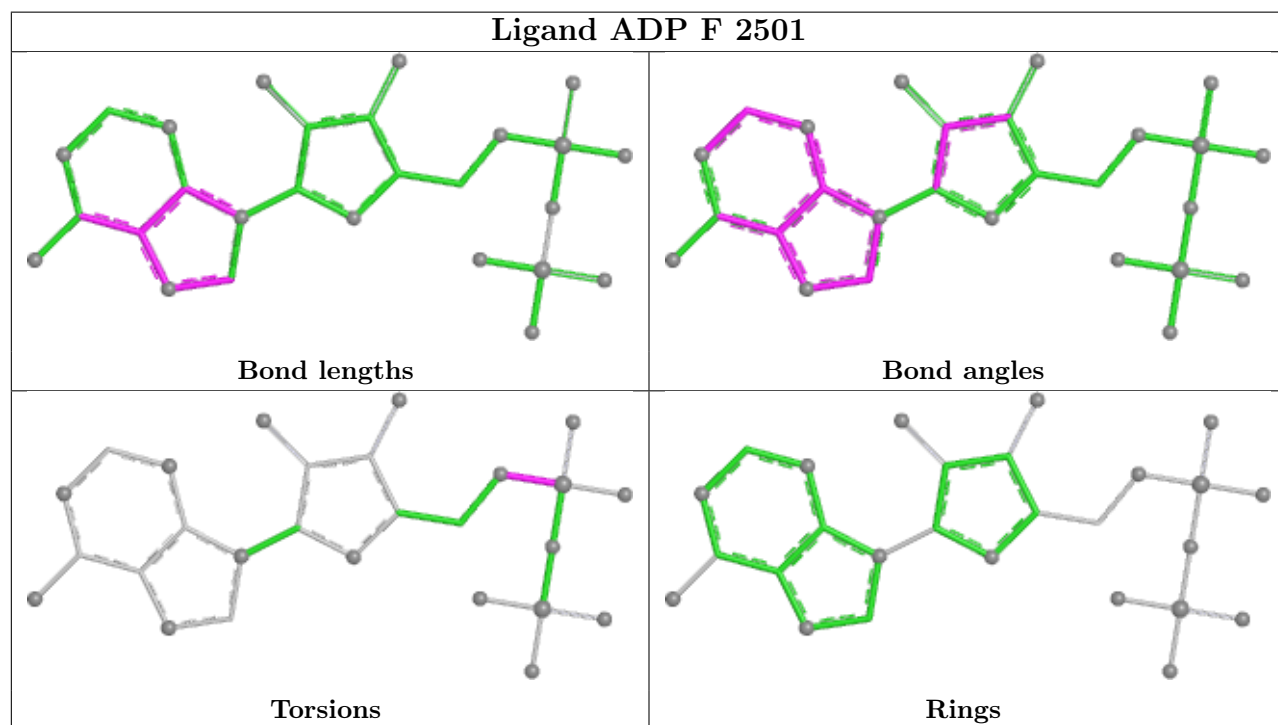
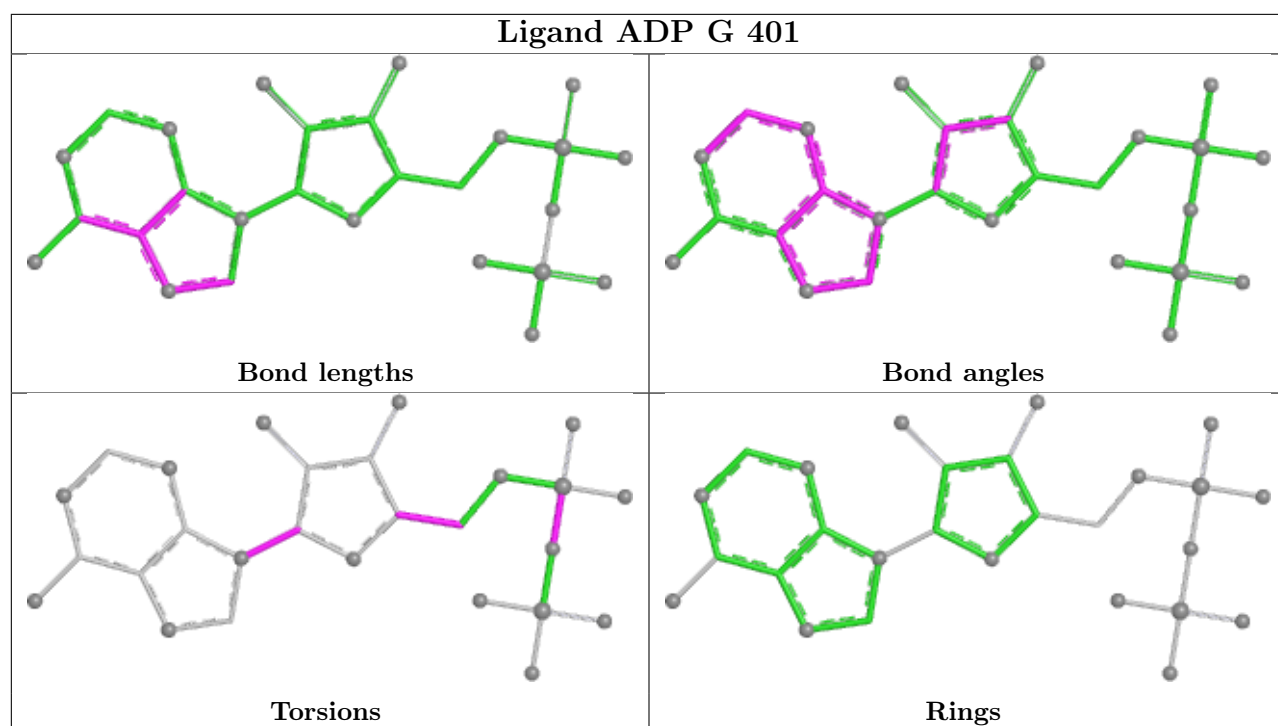
Ligand ADP D 2502

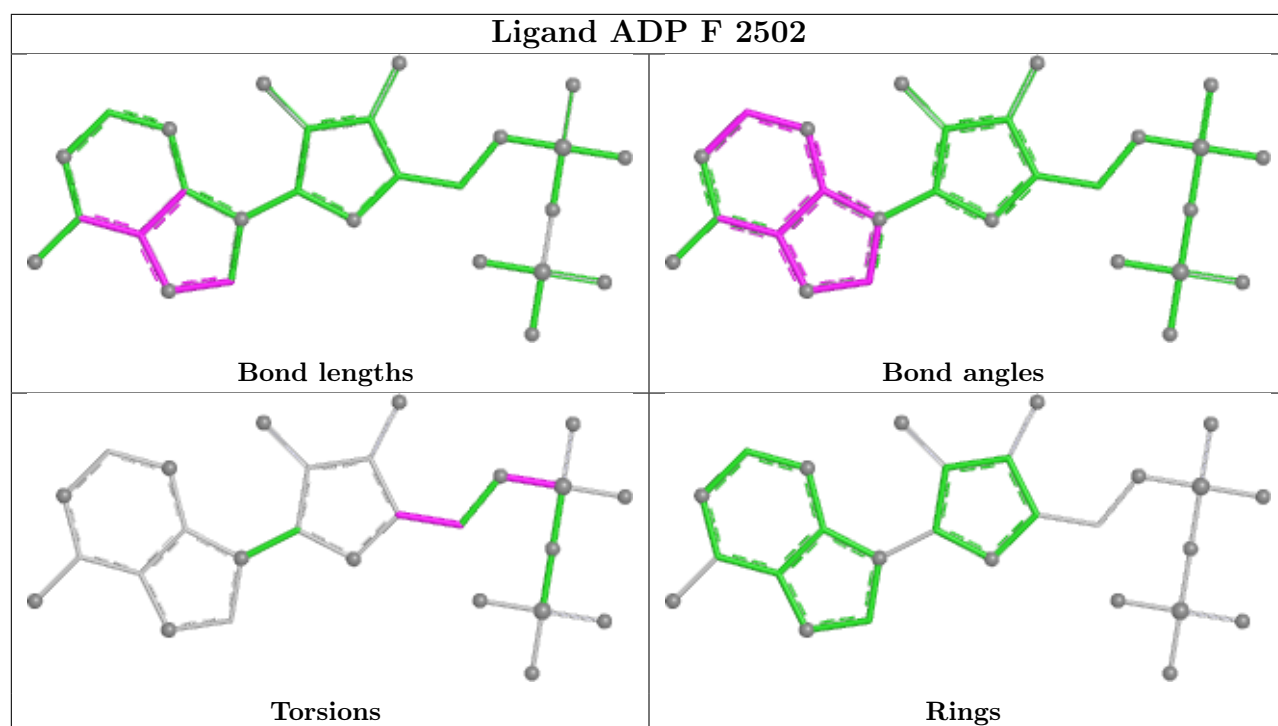


Ligand ADP C 401









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.

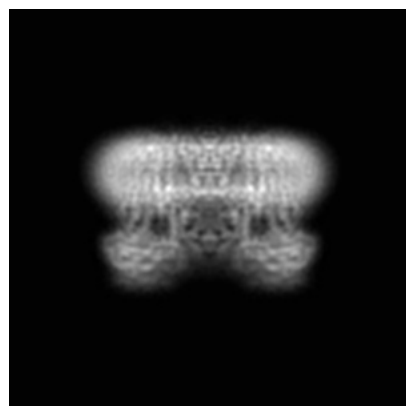
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6851. These allow visual inspection of the internal detail of the map and identification of artifacts.

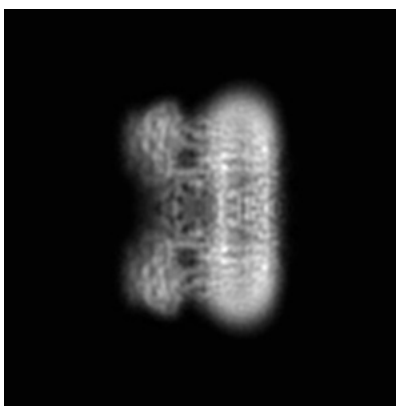
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

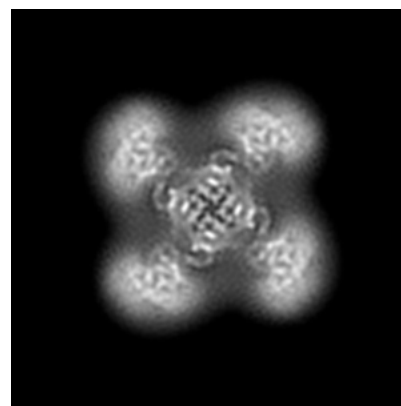
6.1.1 Primary map



X

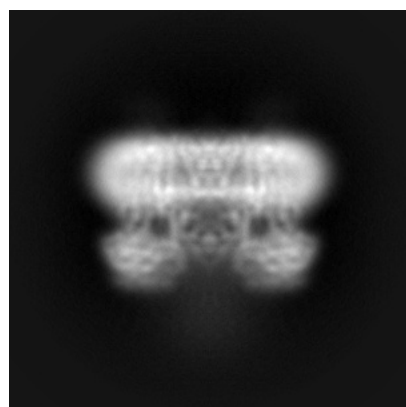


Y

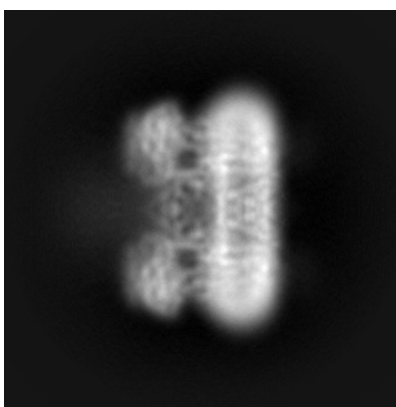


Z

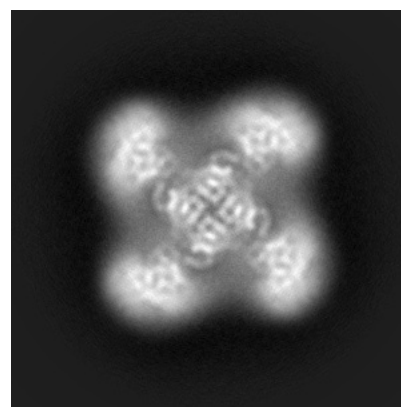
6.1.2 Raw map



X



Y



Z

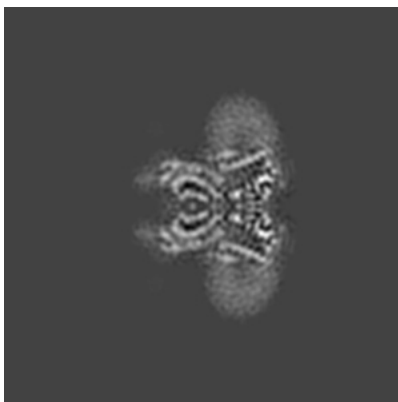
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

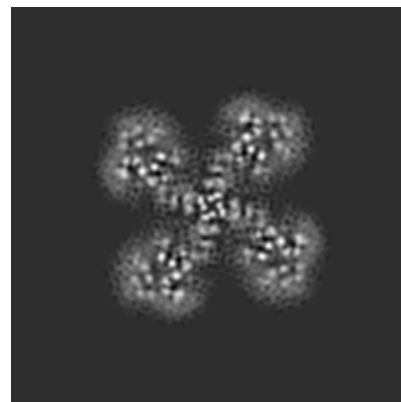
6.2.1 Primary map



X Index: 156

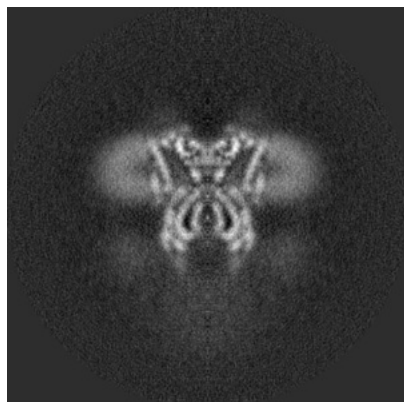


Y Index: 156

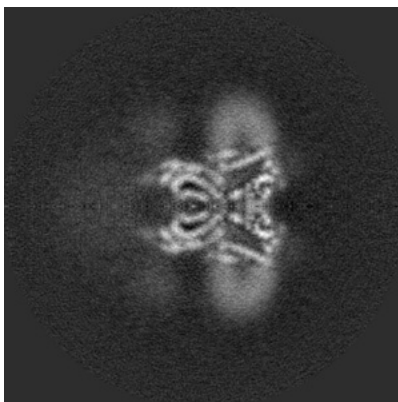


Z Index: 156

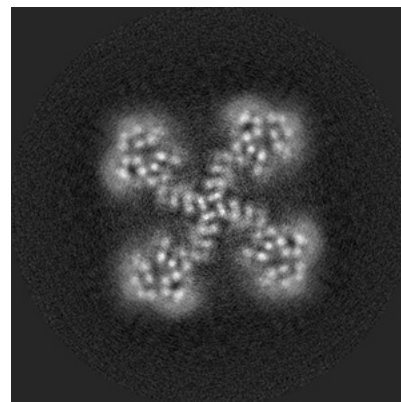
6.2.2 Raw map



X Index: 156



Y Index: 156



Z Index: 156

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

6.3 Largest variance slices [i](#)

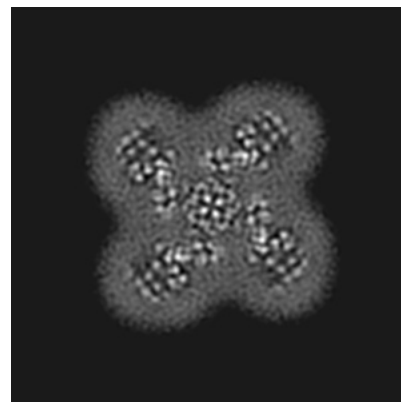
6.3.1 Primary map



X Index: 196

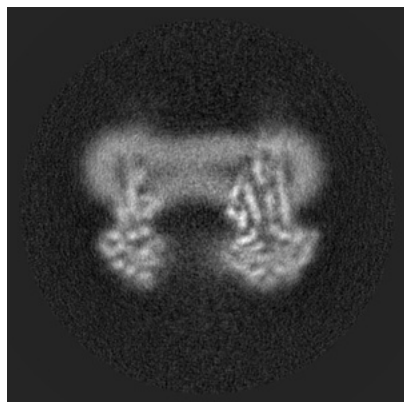


Y Index: 116

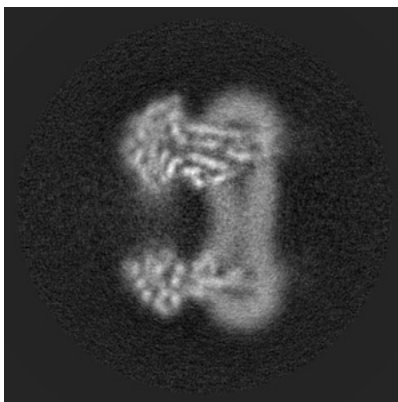


Z Index: 170

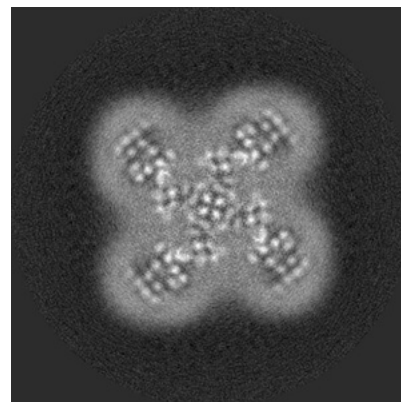
6.3.2 Raw map



X Index: 98



Y Index: 214

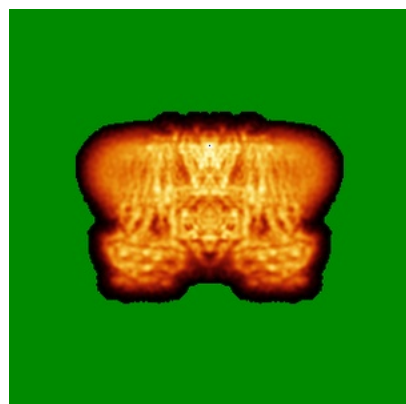


Z Index: 170

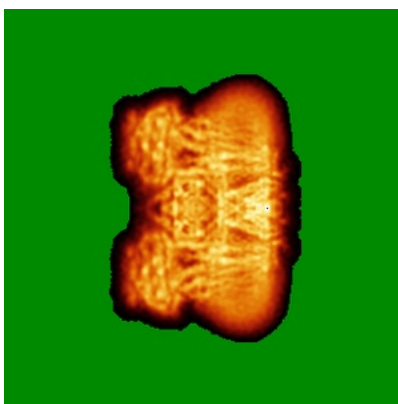
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

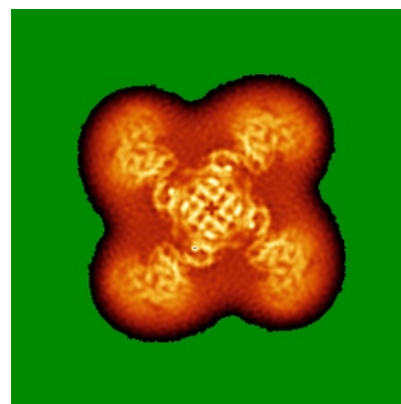
6.4.1 Primary map



X

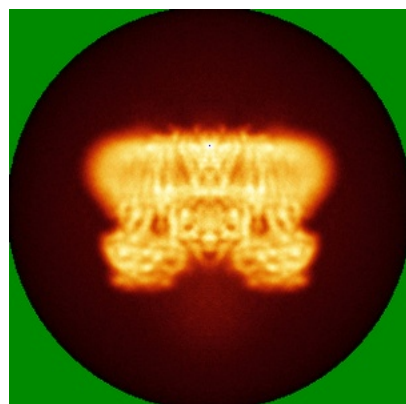


Y

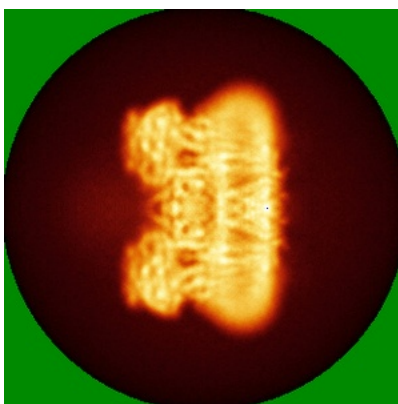


Z

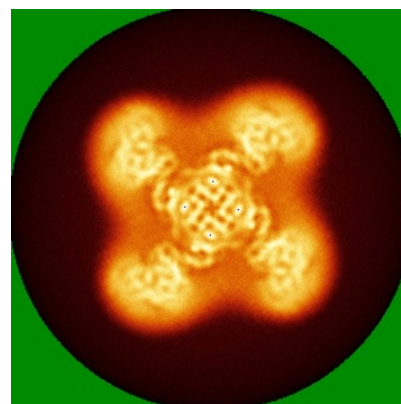
6.4.2 Raw map



X



Y

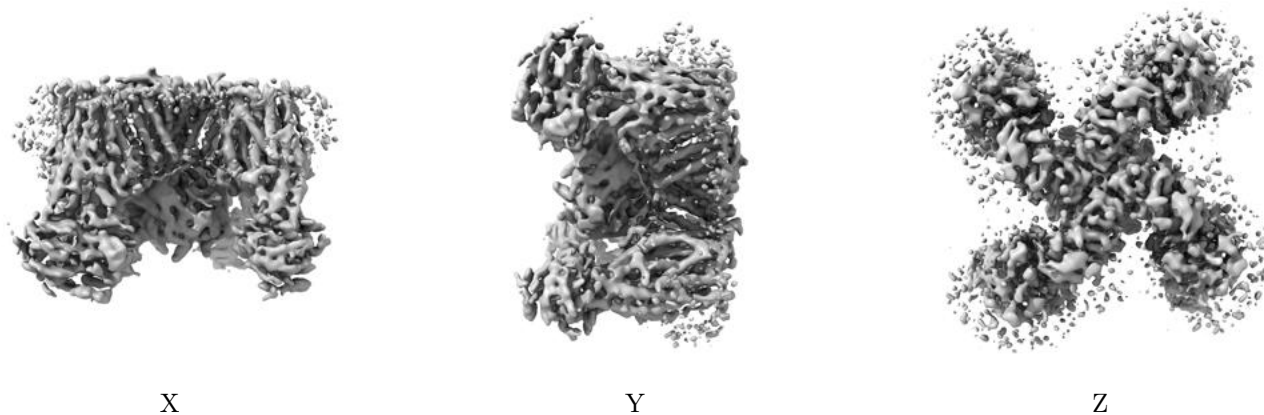


Z

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

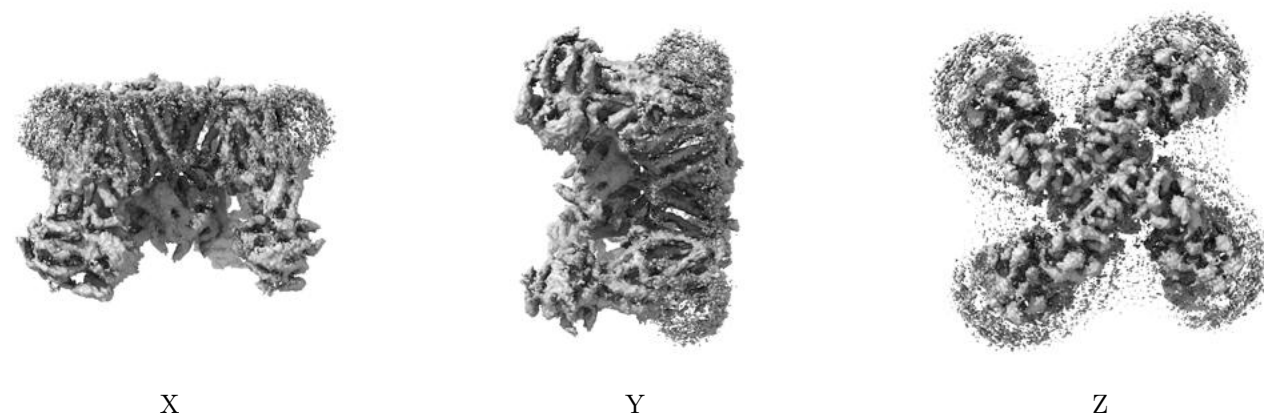
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

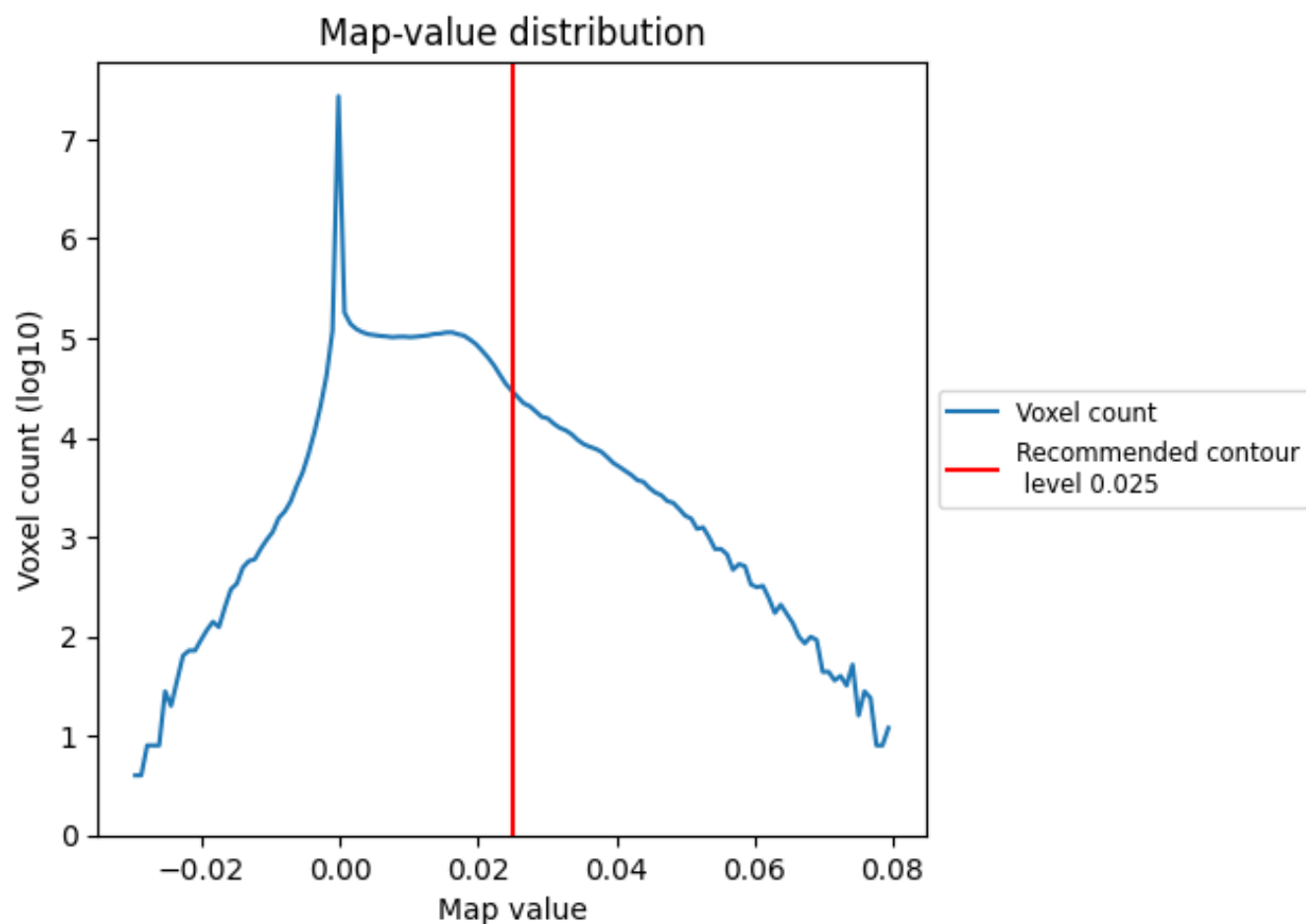
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

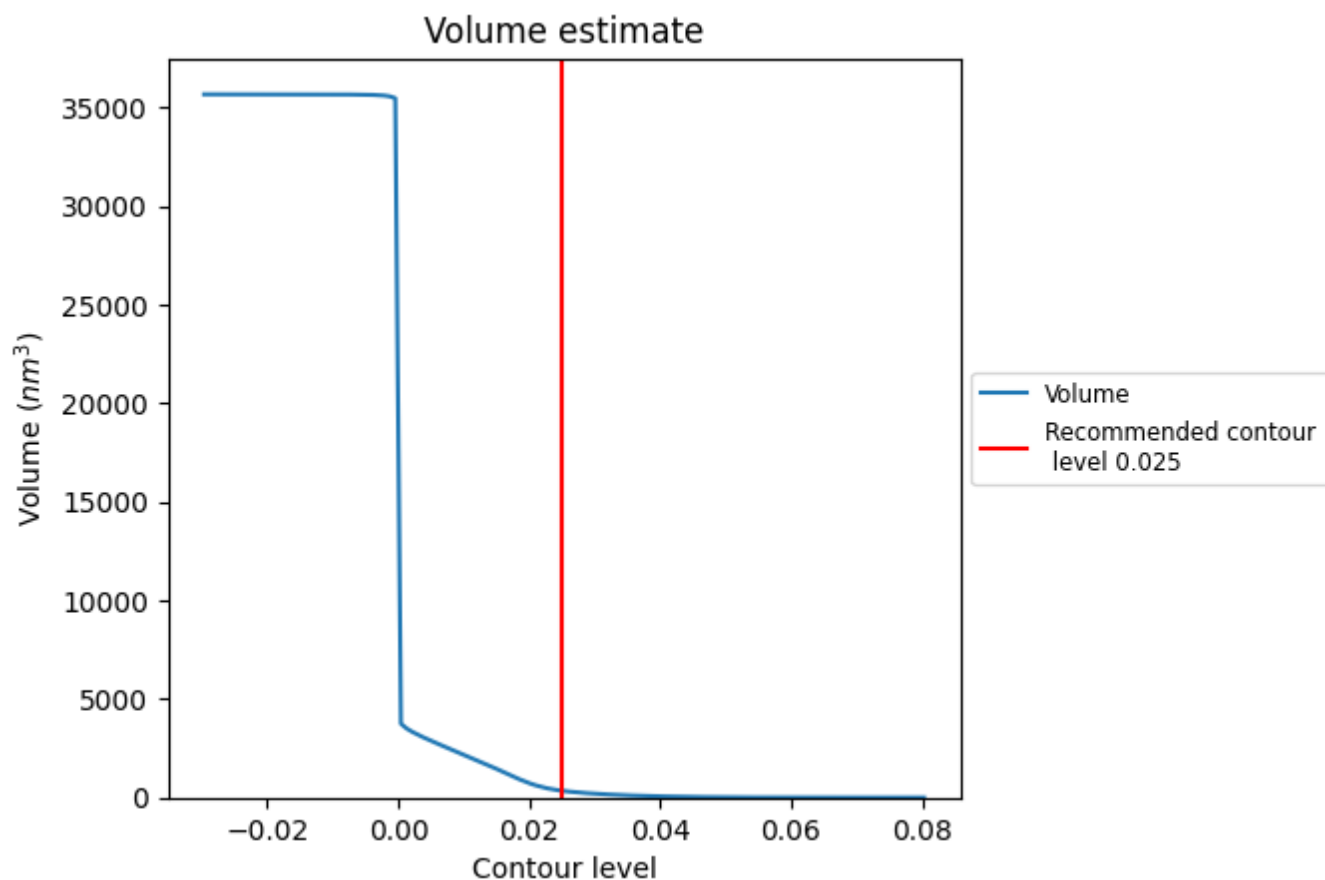
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

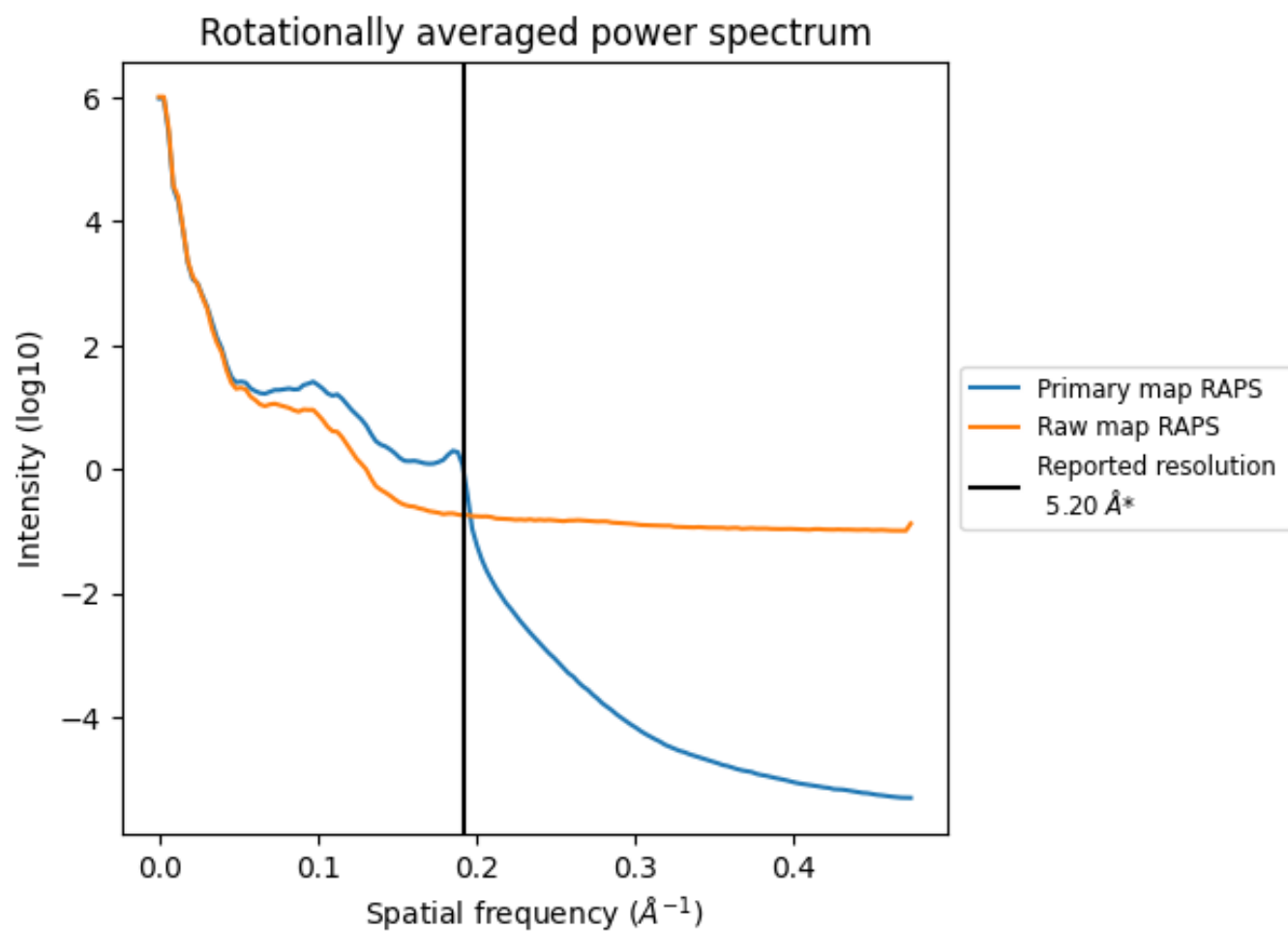
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 347 nm³; this corresponds to an approximate mass of 314 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

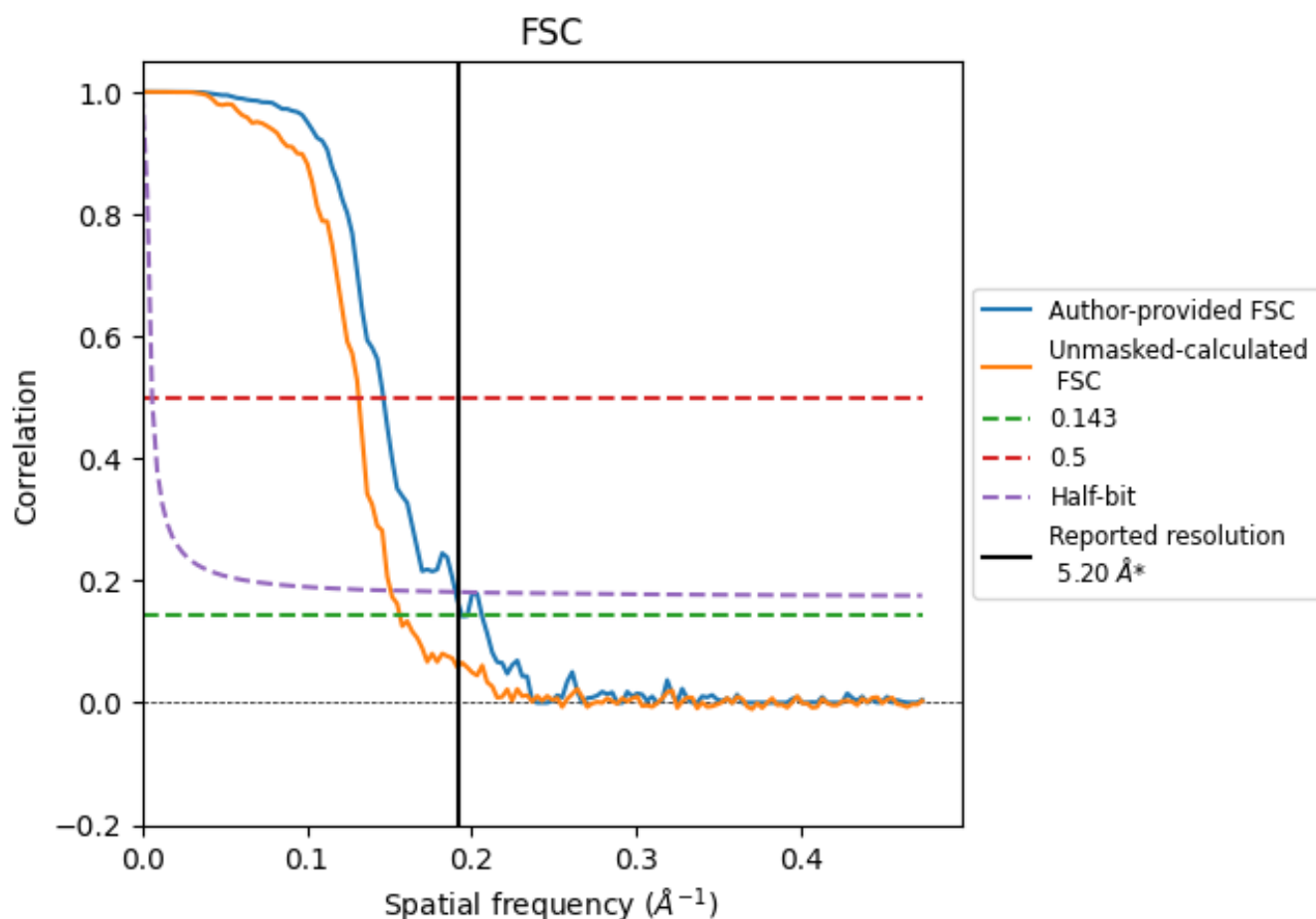


*Reported resolution corresponds to spatial frequency of 0.192 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.192 Å⁻¹

8.2 Resolution estimates [i](#)

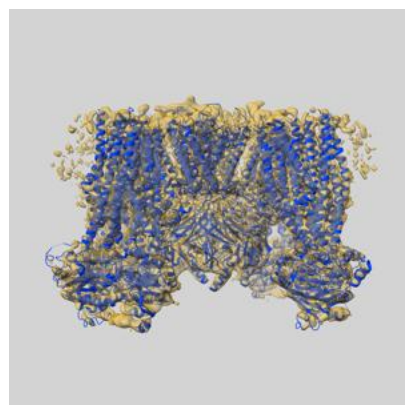
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.20	-	-
Author-provided FSC curve	5.15	6.83	5.25
Unmasked-calculated*	6.39	7.60	6.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.39 differs from the reported value 5.2 by more than 10 %

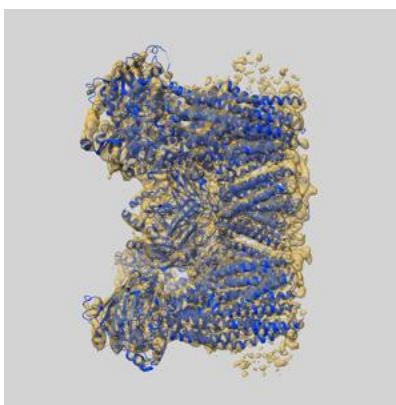
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6851 and PDB model 5YWB. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

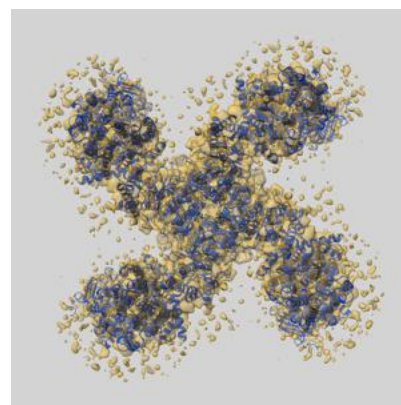
9.1 Map-model overlay [i](#)



X



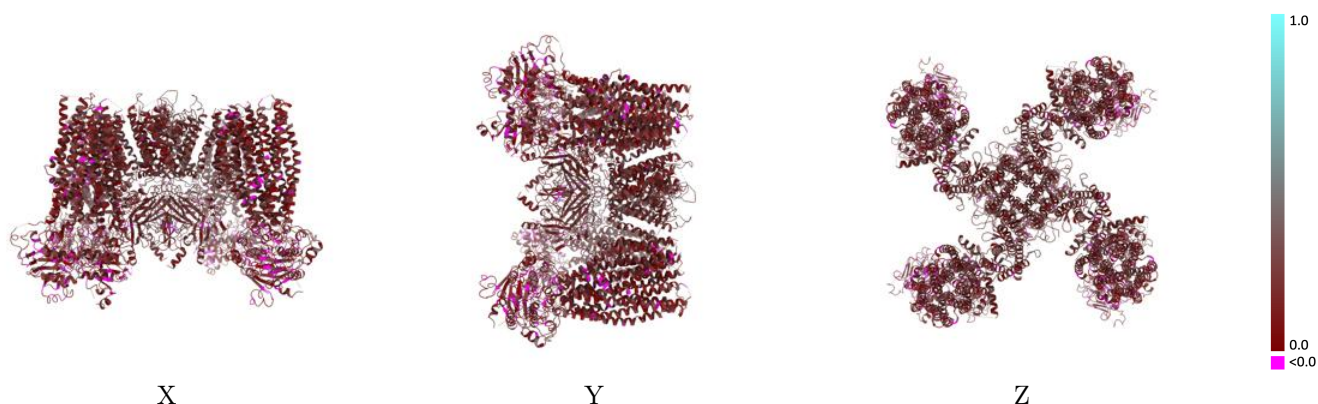
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

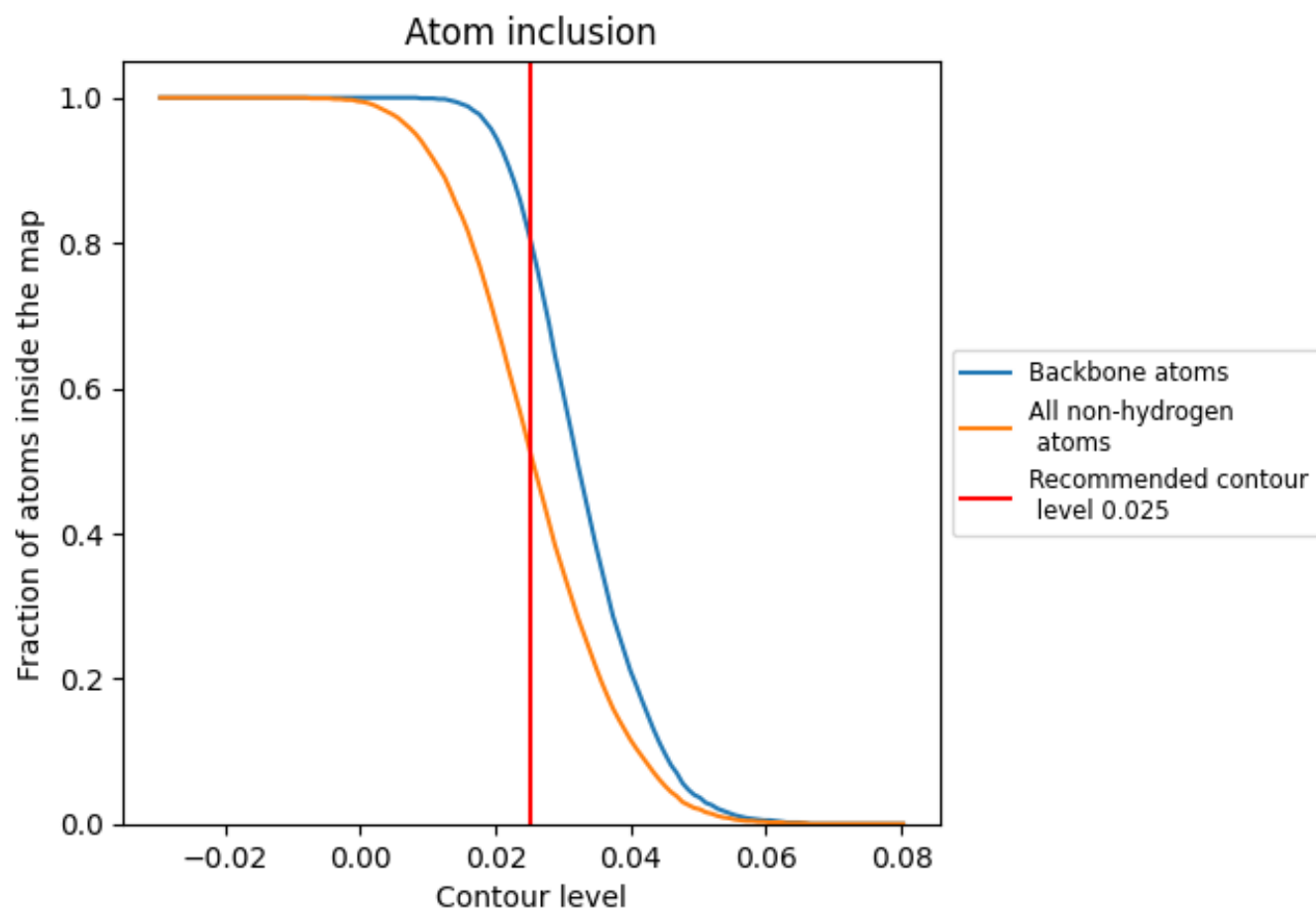


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5160	0.1930
A	0.6260	0.2330
B	0.4890	0.1840
C	0.6260	0.2350
D	0.4890	0.1830
E	0.6260	0.2340
F	0.4890	0.1830
G	0.6260	0.2320
H	0.4890	0.1830

1.0

0.0

<0.0