



Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 04:17 PM EDT

PDB ID : 11TA / pdb_000011ta
EMDB ID : EMD-76028
Title : Cryo-EM structure of substrate engaged p97-Ufd1-NPL4-Faf1 complex (motor focused)
Authors : Liao, Z.; Arkinson, C.; Martin, A.
Deposited on : 2026-03-11
Resolution : 3.58 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

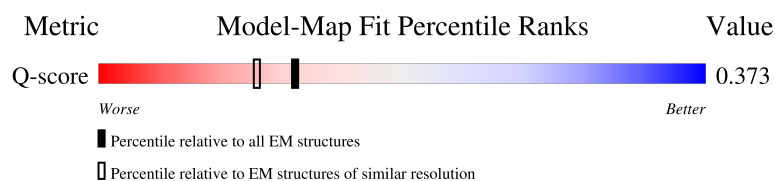
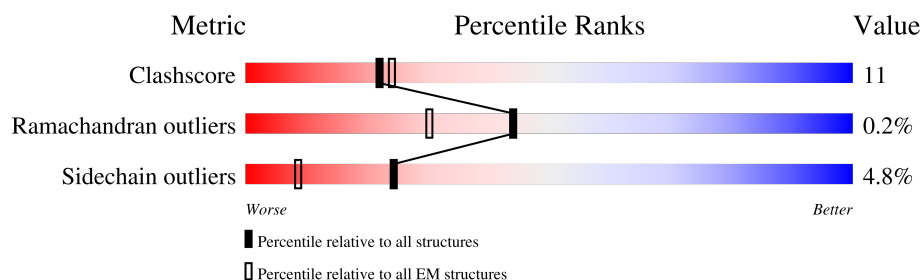
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 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	12629 (3.08 - 4.08)

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	G	611	
2	I	76	
2	K	76	
3	M	173	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	O	173	<div><div></div><div>21%42%18%40%</div></div>
4	P	313	<div><div></div><div>5%17%6%77%</div></div>
5	A	821	<div><div></div><div>64%23%•11%</div></div>
5	B	821	<div><div></div><div>45%20%•33%</div></div>
5	C	821	<div><div></div><div>•60%26%•13%</div></div>
5	D	821	<div><div></div><div>45%20%•34%</div></div>
5	E	821	<div><div></div><div>50%17%•32%</div></div>
5	F	821	<div><div></div><div>66%21%•11%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 37891 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 Nuclear protein localization protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	536	Total	C	N	O	S	0	0
			4273	2711	731	813	18		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	MET	-	initiating methionine	UNP Q8TAT6
G	-1	GLY	-	expression tag	UNP Q8TAT6
G	0	GLY	-	expression tag	UNP Q8TAT6
G	1	GLY	-	expression tag	UNP Q8TAT6

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	40	Total	C	N	O		0	0
			315	199	53	63			
2	K	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 3 is a protein called FAS-associated factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	122	Total	C	N	O	S	0	0
			1025	652	177	195	1		
3	O	104	Total	C	N	O		0	0
			861	553	144	164			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	478	PRO	-	expression tag	UNP Q9UNN5
M	479	LEU	-	expression tag	UNP Q9UNN5
M	480	GLY	-	expression tag	UNP Q9UNN5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
O	478	PRO	-	expression tag	UNP Q9UNN5
O	479	LEU	-	expression tag	UNP Q9UNN5
O	480	GLY	-	expression tag	UNP Q9UNN5

- Molecule 4 is a protein called Ubiquitin recognition factor in ER-associated degradation protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	P	71	Total	C	N	O	0	0
			549	351	104	94		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	308	HIS	-	expression tag	UNP Q92890
P	309	HIS	-	expression tag	UNP Q92890
P	310	HIS	-	expression tag	UNP Q92890
P	311	HIS	-	expression tag	UNP Q92890
P	312	HIS	-	expression tag	UNP Q92890
P	313	HIS	-	expression tag	UNP Q92890

- Molecule 5 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	731	Total	C	N	O	S	0	0
			5735	3609	1012	1084	30		
5	B	550	Total	C	N	O	S	0	0
			4271	2688	751	810	22		
5	C	717	Total	C	N	O	S	0	0
			5634	3541	994	1069	30		
5	D	541	Total	C	N	O	S	0	0
			4217	2648	744	803	22		
5	E	556	Total	C	N	O	S	0	0
			4356	2738	765	831	22		
5	F	729	Total	C	N	O	S	0	0
			5716	3596	1005	1085	30		

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	807	VAL	-	expression tag	UNP P55072
A	808	ASP	-	expression tag	UNP P55072

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	809	LYS	-	expression tag	UNP P55072
A	810	LEU	-	expression tag	UNP P55072
A	811	ALA	-	expression tag	UNP P55072
A	812	ALA	-	expression tag	UNP P55072
A	813	ALA	-	expression tag	UNP P55072
A	814	LEU	-	expression tag	UNP P55072
A	815	GLU	-	expression tag	UNP P55072
A	816	HIS	-	expression tag	UNP P55072
A	817	HIS	-	expression tag	UNP P55072
A	818	HIS	-	expression tag	UNP P55072
A	819	HIS	-	expression tag	UNP P55072
A	820	HIS	-	expression tag	UNP P55072
A	821	HIS	-	expression tag	UNP P55072
B	807	VAL	-	expression tag	UNP P55072
B	808	ASP	-	expression tag	UNP P55072
B	809	LYS	-	expression tag	UNP P55072
B	810	LEU	-	expression tag	UNP P55072
B	811	ALA	-	expression tag	UNP P55072
B	812	ALA	-	expression tag	UNP P55072
B	813	ALA	-	expression tag	UNP P55072
B	814	LEU	-	expression tag	UNP P55072
B	815	GLU	-	expression tag	UNP P55072
B	816	HIS	-	expression tag	UNP P55072
B	817	HIS	-	expression tag	UNP P55072
B	818	HIS	-	expression tag	UNP P55072
B	819	HIS	-	expression tag	UNP P55072
B	820	HIS	-	expression tag	UNP P55072
B	821	HIS	-	expression tag	UNP P55072
C	807	VAL	-	expression tag	UNP P55072
C	808	ASP	-	expression tag	UNP P55072
C	809	LYS	-	expression tag	UNP P55072
C	810	LEU	-	expression tag	UNP P55072
C	811	ALA	-	expression tag	UNP P55072
C	812	ALA	-	expression tag	UNP P55072
C	813	ALA	-	expression tag	UNP P55072
C	814	LEU	-	expression tag	UNP P55072
C	815	GLU	-	expression tag	UNP P55072
C	816	HIS	-	expression tag	UNP P55072
C	817	HIS	-	expression tag	UNP P55072
C	818	HIS	-	expression tag	UNP P55072
C	819	HIS	-	expression tag	UNP P55072
C	820	HIS	-	expression tag	UNP P55072

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	821	HIS	-	expression tag	UNP P55072
D	807	VAL	-	expression tag	UNP P55072
D	808	ASP	-	expression tag	UNP P55072
D	809	LYS	-	expression tag	UNP P55072
D	810	LEU	-	expression tag	UNP P55072
D	811	ALA	-	expression tag	UNP P55072
D	812	ALA	-	expression tag	UNP P55072
D	813	ALA	-	expression tag	UNP P55072
D	814	LEU	-	expression tag	UNP P55072
D	815	GLU	-	expression tag	UNP P55072
D	816	HIS	-	expression tag	UNP P55072
D	817	HIS	-	expression tag	UNP P55072
D	818	HIS	-	expression tag	UNP P55072
D	819	HIS	-	expression tag	UNP P55072
D	820	HIS	-	expression tag	UNP P55072
D	821	HIS	-	expression tag	UNP P55072
E	807	VAL	-	expression tag	UNP P55072
E	808	ASP	-	expression tag	UNP P55072
E	809	LYS	-	expression tag	UNP P55072
E	810	LEU	-	expression tag	UNP P55072
E	811	ALA	-	expression tag	UNP P55072
E	812	ALA	-	expression tag	UNP P55072
E	813	ALA	-	expression tag	UNP P55072
E	814	LEU	-	expression tag	UNP P55072
E	815	GLU	-	expression tag	UNP P55072
E	816	HIS	-	expression tag	UNP P55072
E	817	HIS	-	expression tag	UNP P55072
E	818	HIS	-	expression tag	UNP P55072
E	819	HIS	-	expression tag	UNP P55072
E	820	HIS	-	expression tag	UNP P55072
E	821	HIS	-	expression tag	UNP P55072
F	807	VAL	-	expression tag	UNP P55072
F	808	ASP	-	expression tag	UNP P55072
F	809	LYS	-	expression tag	UNP P55072
F	810	LEU	-	expression tag	UNP P55072
F	811	ALA	-	expression tag	UNP P55072
F	812	ALA	-	expression tag	UNP P55072
F	813	ALA	-	expression tag	UNP P55072
F	814	LEU	-	expression tag	UNP P55072
F	815	GLU	-	expression tag	UNP P55072
F	816	HIS	-	expression tag	UNP P55072
F	817	HIS	-	expression tag	UNP P55072

Continued on next page...

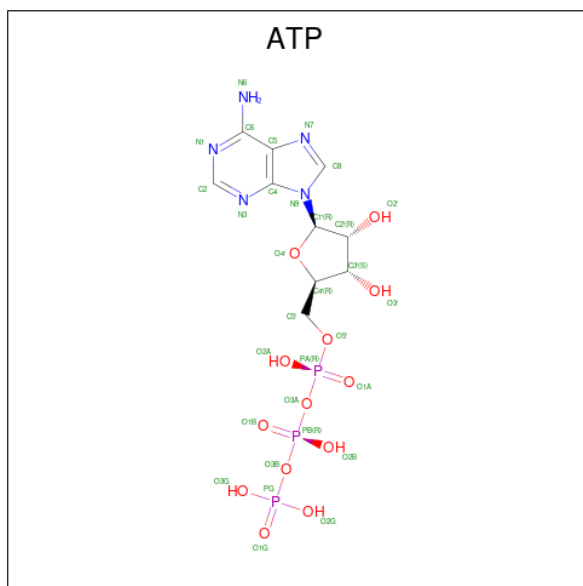
Continued from previous page...

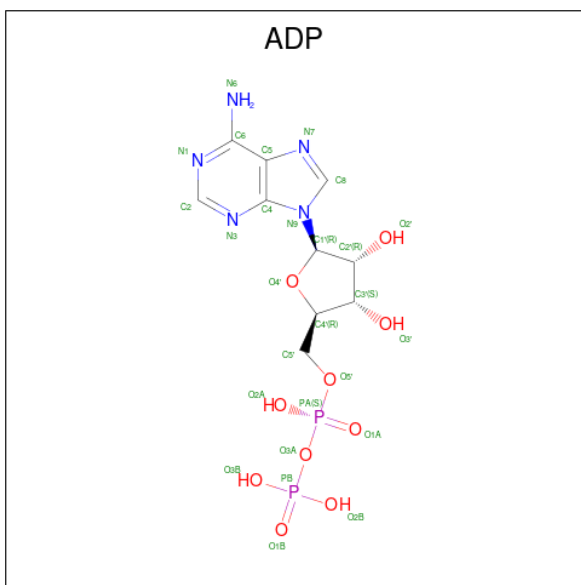
Chain	Residue	Modelled	Actual	Comment	Reference
F	818	HIS	-	expression tag	UNP P55072
F	819	HIS	-	expression tag	UNP P55072
F	820	HIS	-	expression tag	UNP P55072
F	821	HIS	-	expression tag	UNP P55072

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	G	2	Total	Zn	0
			2	2	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

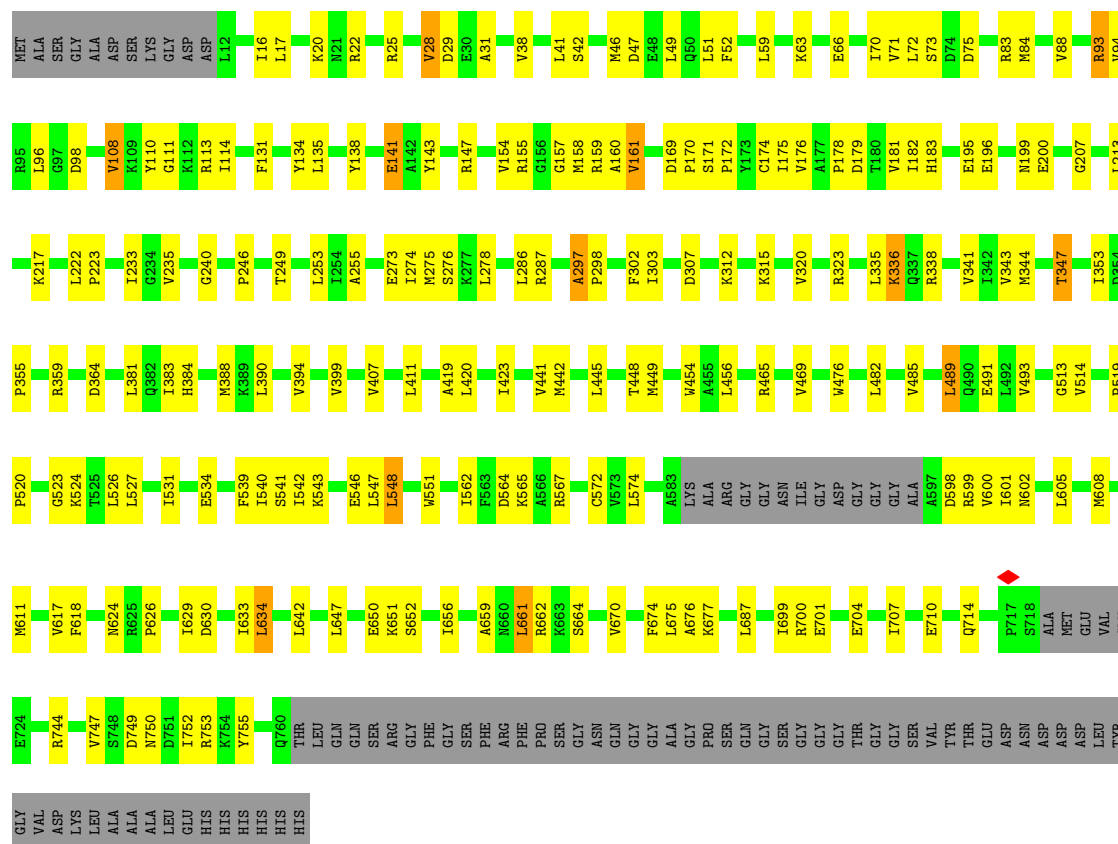




Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total 27	C 10	N 5	O 10	P 2	0
8	B	1	Total 27	C 10	N 5	O 10	P 2	0
8	C	1	Total 27	C 10	N 5	O 10	P 2	0
8	D	1	Total 27	C 10	N 5	O 10	P 2	0
8	D	1	Total 27	C 10	N 5	O 10	P 2	0
8	E	1	Total 27	C 10	N 5	O 10	P 2	0
8	E	1	Total 27	C 10	N 5	O 10	P 2	0
8	F	1	Total 27	C 10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

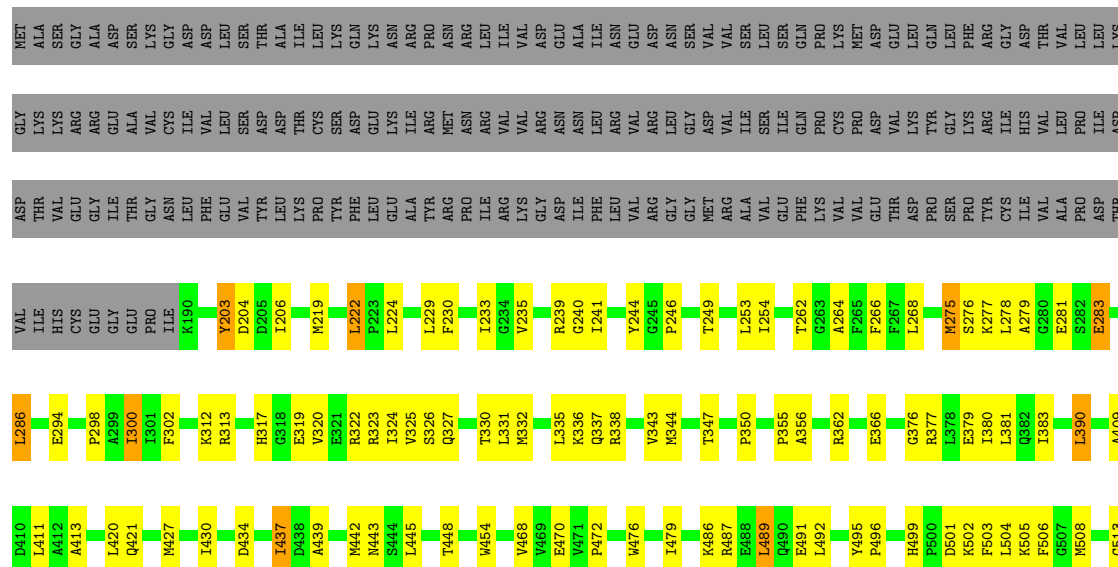
• Molecule 5: Transitional endoplasmic reticulum ATPase

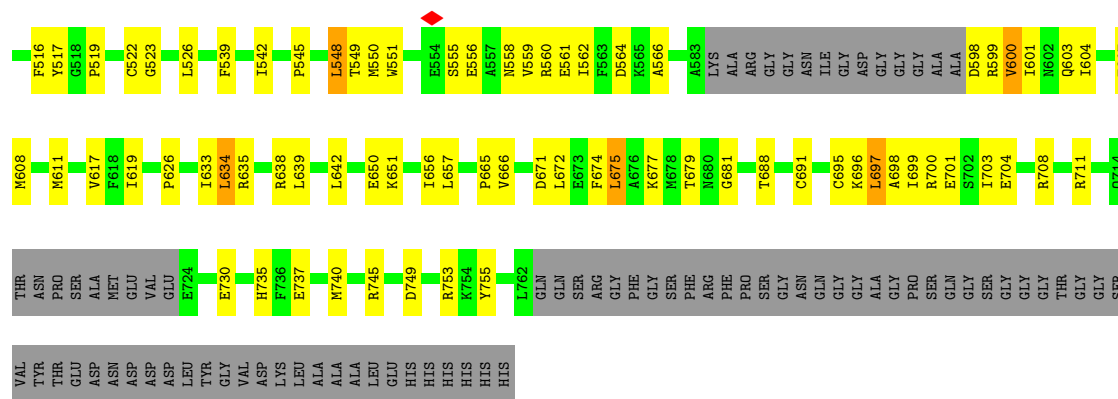
Chain A:  64% 23% 11%



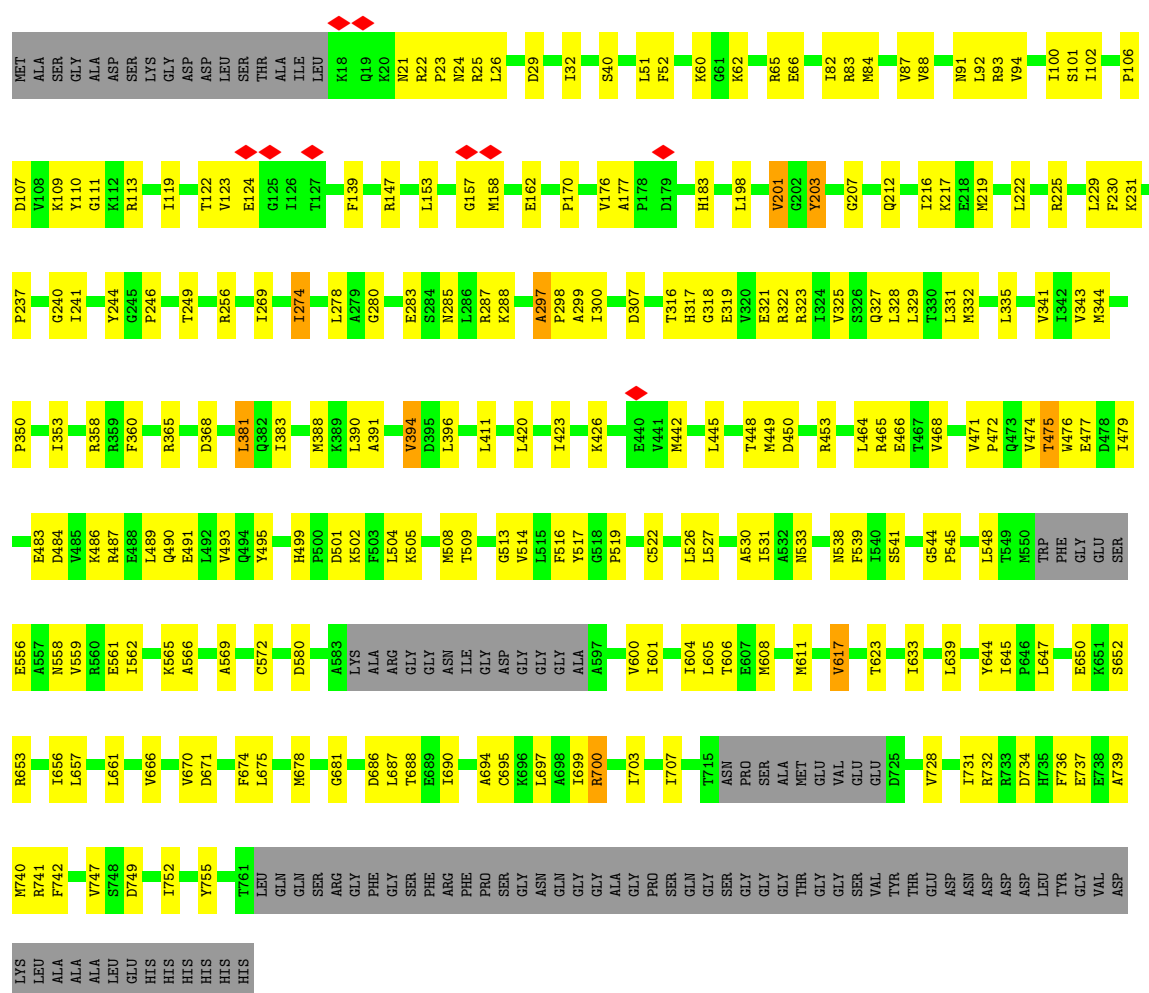
• Molecule 5: Transitional endoplasmic reticulum ATPase

Chain B:  45% 20% 33%



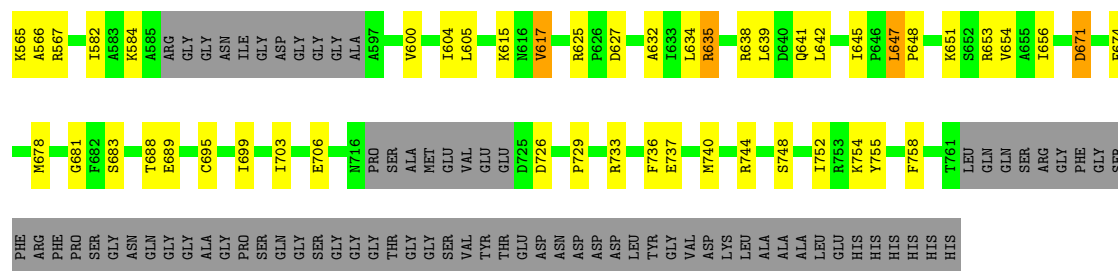


• Molecule 5: Transitional endoplasmic reticulum ATPase



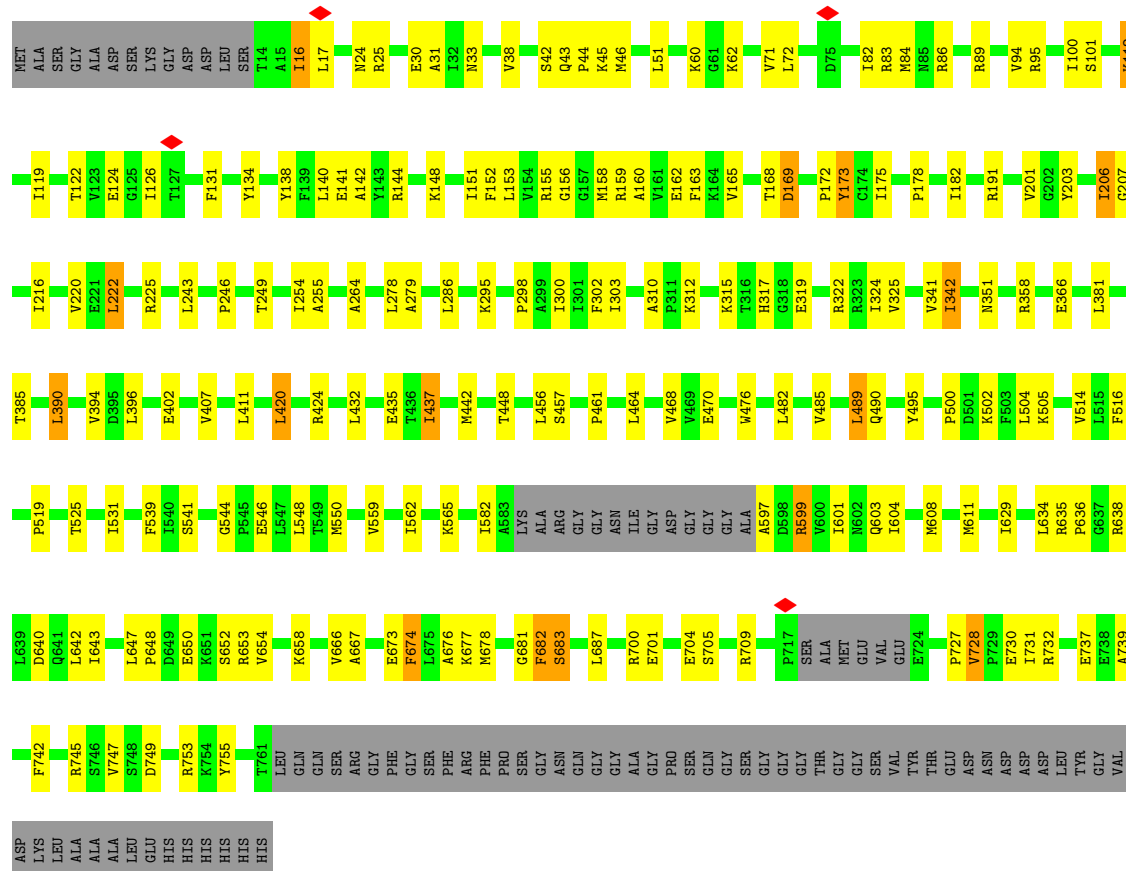
• Molecule 5: Transitional endoplasmic reticulum ATPase





• Molecule 5: Transitional endoplasmic reticulum ATPase

Chain F: 66% 21% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102875	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.332	Depositor
Minimum map value	-0.471	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.133	Depositor
Map size (Å)	378.24, 378.24, 378.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4775, 1.4775, 1.4775	Depositor

5 Model quality

5.1 Standard geometry

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

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	G	0.21	0/4372	0.32	0/5924
2	I	0.20	0/318	0.47	0/428
2	K	0.09	0/607	0.26	0/816
3	M	0.13	0/1046	0.33	0/1406
3	O	0.10	0/880	0.28	0/1187
4	P	0.12	0/560	0.30	0/744
5	A	0.26	0/5828	0.39	1/7873 (0.0%)
5	B	0.29	0/4340	0.39	0/5861
5	C	0.21	0/5722	0.36	0/7726
5	D	0.25	0/4280	0.41	0/5774
5	E	0.26	0/4426	0.37	0/5974
5	F	0.25	0/5809	0.36	0/7851
All	All	0.24	0/38188	0.37	1/51564 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	141	GLU	CA-CB-CG	5.04	124.19	114.10

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	G	4273	0	4189	82	0
2	I	315	0	329	15	0
2	K	601	0	629	15	0
3	M	1025	0	1023	33	0
3	O	861	0	865	21	0
4	P	549	0	572	13	0
5	A	5735	0	5804	137	0
5	B	4271	0	4266	124	0
5	C	5634	0	5702	175	0
5	D	4217	0	4241	107	0
5	E	4356	0	4385	84	0
5	F	5716	0	5765	123	0
6	G	2	0	0	0	0
7	A	31	0	12	3	0
7	B	31	0	12	1	0
7	C	31	0	12	3	0
8	A	27	0	12	1	0
8	B	27	0	12	3	0
8	C	27	0	12	2	0
8	D	54	0	24	1	0
8	E	54	0	24	3	0
8	F	54	0	24	4	0
All	All	37891	0	37914	870	0

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

All (870) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:469:ASN:HB3	1:G:494:GLN:HE21	1.42	0.84
5:C:653:ARG:HA	5:C:656:ILE:HD12	1.63	0.81
3:M:535:GLU:HA	3:M:538:ARG:HH21	1.47	0.80
5:C:423:ILE:HD11	5:D:229:LEU:HG	1.61	0.79
5:C:274:ILE:HD12	5:C:285:ASN:HB3	1.65	0.79
5:C:519:PRO:HG3	5:C:755:TYR:HB2	1.66	0.78
5:D:653:ARG:HE	5:D:682:PHE:HB2	1.49	0.77
5:C:661:LEU:HB2	5:C:666:VAL:HG21	1.66	0.77
5:C:51:LEU:HD12	5:C:52:PHE:H	1.51	0.76
1:G:520:PRO:HB2	1:G:522:GLN:HE22	1.51	0.76
5:E:726:ASP:HB3	5:E:729:PRO:HG3	1.68	0.75
5:B:319:GLU:HG3	5:B:323:ARG:HD3	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:131:PHE:HA	5:A:135:LEU:HB2	1.69	0.74
5:B:439:ALA:O	5:B:443:ASN:HB2	1.87	0.74
5:B:703:ILE:HD12	5:C:499:HIS:HD2	1.52	0.74
5:B:430:ILE:HG23	5:B:437:ILE:HD11	1.70	0.73
5:A:543:LYS:HB2	5:A:546:GLU:HG3	1.68	0.73
5:C:502:LYS:HA	5:C:505:LYS:HG2	1.70	0.72
5:A:84:MET:HE3	5:A:84:MET:HA	1.69	0.72
5:B:503:PHE:HB3	5:B:508:MET:HB3	1.72	0.72
1:G:504:ILE:HG12	1:G:528:LEU:HD11	1.70	0.72
5:D:297:ALA:HB1	5:D:298:PRO:HD2	1.71	0.72
5:D:219:MET:HE2	5:D:219:MET:HA	1.71	0.71
3:M:592:ALA:HB1	3:M:634:LEU:HB3	1.71	0.71
5:E:632:ALA:HA	5:E:635:ARG:HE	1.56	0.71
5:C:666:VAL:HG22	5:C:731:ILE:HD12	1.73	0.70
5:F:148:LYS:HE2	5:F:168:THR:H	1.55	0.70
5:D:659:ALA:HA	5:D:662:ARG:HE	1.56	0.69
1:G:424:VAL:HG23	1:G:440:ALA:HB3	1.74	0.69
2:K:44:ILE:HG23	2:K:68:HIS:HB3	1.75	0.69
5:D:381:LEU:HD21	5:D:411:LEU:HD12	1.74	0.69
5:C:318:GLY:HA2	5:C:322:ARG:HH11	1.58	0.69
5:E:492:LEU:HD11	5:E:641:GLN:HG2	1.75	0.68
5:C:526:LEU:HD21	8:C:902:ADP:H2'	1.74	0.68
5:B:335:LEU:O	5:B:338:ARG:HG2	1.94	0.68
5:D:475:THR:HG23	5:D:477:GLU:H	1.58	0.68
1:G:180:PHE:HA	5:C:288:LYS:HE3	1.76	0.67
1:G:242:ARG:HE	2:I:47:GLY:HA2	1.59	0.67
5:F:562:ILE:HD12	5:F:562:ILE:H	1.58	0.67
4:P:300:LEU:HB2	5:F:178:PRO:HA	1.75	0.67
5:B:634:LEU:HD23	5:B:642:LEU:HD21	1.75	0.67
5:E:524:LYS:HG2	5:E:645:ILE:HD12	1.74	0.67
1:G:234:ALA:O	1:G:238:LEU:HD12	1.93	0.67
5:A:240:GLY:HA2	5:A:343:VAL:O	1.94	0.67
5:E:695:CYS:O	5:E:699:ILE:HG12	1.95	0.67
5:A:572:CYS:HB3	5:A:617:VAL:HG23	1.77	0.67
5:A:656:ILE:HD11	5:A:687:LEU:HD12	1.76	0.67
5:A:602:ASN:HA	5:A:605:LEU:HD12	1.75	0.66
5:E:449:MET:HG3	5:E:453:ARG:HH21	1.61	0.66
5:F:124:GLU:HB2	5:F:159:ARG:HH22	1.58	0.66
5:E:438:ASP:HB2	5:E:441:VAL:HG12	1.76	0.66
5:C:318:GLY:HA2	5:C:322:ARG:HD3	1.77	0.65
5:F:312:LYS:HB2	5:F:315:LYS:HB2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:703:ILE:HD12	5:C:499:HIS:CD2	2.31	0.65
5:C:269:ILE:HD12	5:C:274:ILE:HD11	1.78	0.65
5:F:46:MET:HG2	5:F:51:LEU:HD22	1.77	0.65
3:M:575:LYS:HB3	3:M:641:GLN:HB2	1.79	0.65
5:A:41:LEU:HD21	5:A:46:MET:HB2	1.79	0.65
5:B:413:ALA:HB2	5:C:360:PHE:HB2	1.79	0.65
5:B:513:GLY:HA3	5:B:639:LEU:HA	1.78	0.64
5:A:312:LYS:HD3	5:A:355:PRO:HD3	1.80	0.64
5:F:489:LEU:HD21	5:F:531:ILE:HB	1.78	0.64
5:A:20:LYS:HB3	5:A:22:ARG:HG3	1.80	0.64
5:A:699:ILE:HD11	5:B:502:LYS:HB3	1.80	0.64
5:C:300:ILE:HD11	5:C:344:MET:HE2	1.79	0.64
5:E:752:ILE:HA	5:E:755:TYR:CZ	2.33	0.64
5:E:671:ASP:H	5:E:674:PHE:HE2	1.46	0.64
5:A:359:ARG:HH22	8:F:901:ADP:PB	2.20	0.64
5:A:493:VAL:HG22	5:A:618:PHE:CE2	2.33	0.63
5:F:122:THR:HG21	5:F:162:GLU:H	1.63	0.63
5:C:739:ALA:HA	5:C:742:PHE:CE2	2.33	0.63
1:G:495:ASN:HD21	1:G:503:THR:HG23	1.63	0.63
1:G:427:LYS:HB2	2:I:22:THR:HA	1.81	0.63
5:F:152:PHE:CE1	5:F:163:PHE:HB2	2.34	0.63
5:A:523:GLY:HA2	5:A:526:LEU:HD23	1.81	0.63
5:C:516:PHE:HB3	5:C:645:ILE:HD11	1.80	0.63
3:O:596:LEU:HB3	3:O:629:PRO:HA	1.81	0.62
5:D:524:LYS:HG2	5:D:645:ILE:HG13	1.81	0.62
5:C:381:LEU:HB3	5:C:396:LEU:HD12	1.81	0.62
5:A:31:ALA:HA	5:A:83:ARG:HB3	1.81	0.62
5:D:262:THR:HG23	5:D:264:ALA:H	1.64	0.62
5:B:233:ILE:HG23	5:B:235:VAL:HG13	1.80	0.62
3:O:550:ARG:O	3:O:554:ARG:HG2	1.99	0.62
5:E:567:ARG:HG3	5:E:615:LYS:HE3	1.81	0.62
5:F:682:PHE:HD1	5:F:745:ARG:HG2	1.64	0.62
5:C:671:ASP:HB2	5:C:674:PHE:HB3	1.81	0.61
5:E:207:GLY:H	8:E:901:ADP:HN62	1.48	0.61
3:M:579:ARG:HH21	3:M:583:GLY:HA2	1.65	0.61
5:B:336:LYS:O	5:B:336:LYS:HG3	1.99	0.61
2:I:36:ILE:HD11	2:I:42:ARG:HH12	1.66	0.60
3:M:591:LEU:HB3	3:M:594:ASN:HB2	1.82	0.60
5:B:551:TRP:HE1	5:B:599:ARG:HD3	1.65	0.60
1:G:514:VAL:HG13	1:G:522:GLN:HB3	1.84	0.60
5:B:206:ILE:HG12	5:B:253:LEU:HD21	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:430:ILE:HG22	5:D:432:LEU:H	1.66	0.60
5:D:390:LEU:HD11	5:D:394:VAL:HG11	1.83	0.60
5:E:674:PHE:HD1	5:E:678:MET:HE3	1.66	0.60
5:B:674:PHE:HE1	5:B:740:MET:HE1	1.66	0.60
5:D:276:SER:HB2	5:E:322:ARG:HB3	1.82	0.60
5:B:698:ALA:HA	5:B:735:HIS:CE1	2.36	0.60
2:I:33:LYS:HG3	2:I:42:ARG:HH22	1.66	0.60
5:F:278:LEU:HD12	5:F:279:ALA:H	1.67	0.60
5:D:216:ILE:HD11	5:D:243:LEU:HD21	1.83	0.60
5:D:275:MET:HE3	5:D:309:ILE:HA	1.84	0.60
5:E:513:GLY:HA3	5:E:639:LEU:HA	1.82	0.60
5:A:255:ALA:HB2	5:A:302:PHE:CZ	2.37	0.60
5:E:562:ILE:O	5:E:565:LYS:HB2	2.02	0.60
5:C:82:ILE:HG21	5:C:100:ILE:HD11	1.84	0.59
5:F:278:LEU:HD12	5:F:279:ALA:N	2.17	0.59
5:B:476:TRP:HZ2	5:B:486:LYS:HB2	1.66	0.59
5:C:464:LEU:HB2	5:C:465:ARG:HH11	1.67	0.59
1:G:299:ILE:HD11	1:G:514:VAL:HG11	1.84	0.59
5:C:230:PHE:CD2	5:C:237:PRO:HB3	2.37	0.59
3:O:577:ARG:HG2	3:O:587:GLU:HG2	1.84	0.59
5:A:31:ALA:HB2	5:A:84:MET:C	2.28	0.59
5:B:688:THR:HG21	8:B:902:ADP:H1'	1.85	0.59
5:E:424:ARG:HA	5:E:427:MET:HG3	1.85	0.59
5:E:432:LEU:HD13	5:F:222:LEU:HD22	1.85	0.59
1:G:322:LYS:HB2	1:G:324:THR:HG23	1.85	0.58
5:F:745:ARG:HH21	5:F:747:VAL:HG21	1.68	0.58
3:M:641:GLN:HB3	5:A:52:PHE:CD1	2.38	0.58
5:A:38:VAL:HA	5:A:70:ILE:H	1.67	0.58
5:A:551:TRP:HE1	5:A:599:ARG:HB2	1.68	0.58
5:B:262:THR:HG23	5:B:264:ALA:H	1.68	0.58
5:C:728:VAL:HG11	5:C:732:ARG:HD3	1.86	0.58
5:F:673:GLU:HA	5:F:676:ALA:HB3	1.84	0.58
5:C:122:THR:HG21	5:C:162:GLU:HB2	1.83	0.58
5:C:475:THR:HG23	5:C:477:GLU:HG2	1.85	0.58
5:B:489:LEU:HD11	5:B:516:PHE:HZ	1.69	0.58
3:O:561:LEU:HD22	3:O:588:ARG:HH12	1.69	0.58
5:E:547:LEU:HA	5:E:550:MET:HE3	1.85	0.58
5:D:651:LYS:HA	5:D:654:VAL:HB	1.86	0.58
1:G:527:LEU:HD23	1:G:543:TRP:HD1	1.69	0.57
3:O:579:ARG:HH12	5:F:175:ILE:HG21	1.68	0.57
5:D:517:TYR:HE2	5:D:759:ALA:HB2	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:629:ILE:HD11	5:A:633:ILE:HD11	1.85	0.57
5:E:656:ILE:HD12	8:E:902:ADP:HN62	1.69	0.57
5:F:207:GLY:H	8:F:901:ADP:N6	2.01	0.57
5:A:493:VAL:HG22	5:A:618:PHE:HE2	1.69	0.57
5:F:476:TRP:HZ3	5:F:490:GLN:HE21	1.51	0.57
5:E:336:LYS:HE3	5:E:337:GLN:H	1.68	0.57
5:B:523:GLY:HA2	5:B:526:LEU:HD13	1.87	0.57
5:C:51:LEU:HD12	5:C:52:PHE:N	2.18	0.57
5:C:244:TYR:CZ	5:C:368:ASP:HB3	2.40	0.57
5:C:548:LEU:HD12	5:D:602:ASN:HD21	1.69	0.57
1:G:277:PRO:HD2	1:G:290:ASP:HB2	1.86	0.57
5:C:111:GLY:HA2	5:C:170:PRO:HD2	1.87	0.57
5:A:336:LYS:HE3	5:A:338:ARG:HH21	1.70	0.57
5:D:757:MET:HA	5:D:760:GLN:HG2	1.87	0.57
5:D:686:ASP:O	5:D:690:ILE:HG12	2.05	0.57
5:D:567:ARG:HH22	5:D:611:MET:HA	1.70	0.56
5:F:739:ALA:HA	5:F:742:PHE:CE1	2.39	0.56
5:A:253:LEU:HD13	7:A:901:ATP:H2'	1.85	0.56
5:D:471:VAL:HG12	5:D:472:PRO:HD2	1.88	0.56
2:K:50:LEU:HD11	2:K:67:LEU:HD11	1.87	0.56
3:M:613:TYR:HD1	3:M:648:ALA:HA	1.70	0.56
3:O:595:LYS:HA	3:O:595:LYS:HE3	1.86	0.56
5:B:550:MET:SD	5:B:558:ASN:HB3	2.45	0.56
5:A:41:LEU:HD12	5:A:42:SER:H	1.70	0.56
5:A:420:LEU:HA	5:A:423:ILE:HD12	1.87	0.56
5:B:499:HIS:HB3	5:B:502:LYS:HG2	1.86	0.56
5:C:605:LEU:HA	5:C:608:MET:HE3	1.88	0.56
5:F:604:ILE:O	5:F:608:MET:HG3	2.05	0.56
5:B:633:ILE:HG23	5:B:639:LEU:HD13	1.87	0.56
5:C:26:LEU:HD13	5:C:82:ILE:HB	1.88	0.56
5:D:501:ASP:O	5:D:505:LYS:HG2	2.05	0.56
5:F:358:ARG:HD3	5:F:366:GLU:OE2	2.06	0.56
1:G:432:PHE:HB3	5:A:287:ARG:HH21	1.71	0.56
5:C:229:LEU:HD12	5:C:229:LEU:H	1.70	0.56
5:B:502:LYS:HA	5:B:505:LYS:HZ3	1.71	0.56
5:F:420:LEU:HD22	5:F:424:ARG:HH21	1.69	0.56
5:F:255:ALA:HB2	5:F:302:PHE:CZ	2.41	0.56
5:F:319:GLU:HA	5:F:322:ARG:HD2	1.88	0.56
4:P:227:ALA:HB3	4:P:247:SER:HB2	1.88	0.55
5:E:605:LEU:HD22	5:E:638:ARG:HH11	1.71	0.55
5:F:647:LEU:HD11	5:F:683:SER:HA	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:LYS:HE2	1:G:41:ASN:HD21	1.71	0.55
5:D:567:ARG:HD2	5:D:615:LYS:HG3	1.88	0.55
5:D:649:ASP:HA	5:D:680:ASN:HD21	1.70	0.55
5:A:233:ILE:HG23	5:A:235:VAL:HG12	1.88	0.55
5:A:297:ALA:HB3	5:A:298:PRO:HD3	1.88	0.55
1:G:230:ASN:HA	1:G:460:PRO:HB3	1.87	0.55
5:B:377:ARG:HG2	5:B:411:LEU:HD11	1.89	0.55
5:C:471:VAL:HG13	5:C:533:ASN:HA	1.89	0.55
5:C:526:LEU:HD12	5:C:526:LEU:H	1.72	0.55
5:F:546:GLU:O	5:F:550:MET:HG2	2.07	0.55
2:K:42:ARG:HH11	2:K:72:ARG:HG2	1.71	0.55
5:C:319:GLU:HB2	5:C:321:GLU:OE1	2.06	0.55
5:C:601:ILE:HA	5:C:604:ILE:HD12	1.89	0.55
5:B:650:GLU:O	5:B:651:LYS:HG2	2.07	0.55
5:D:697:LEU:HA	5:D:700:ARG:HG2	1.89	0.55
5:C:316:THR:HG23	5:C:318:GLY:H	1.72	0.55
5:F:155:ARG:HD2	5:F:160:ALA:HB2	1.88	0.55
1:G:242:ARG:HG2	2:I:48:LYS:H	1.72	0.55
5:C:445:LEU:HD22	5:D:233:ILE:HD11	1.89	0.55
1:G:107:GLU:HG3	1:G:356:ARG:HG3	1.90	0.54
5:E:556:GLU:O	5:E:559:VAL:HG12	2.06	0.54
1:G:249:PHE:HE2	1:G:276:PRO:HG2	1.72	0.54
5:C:207:GLY:H	7:C:901:ATP:HN62	1.53	0.54
5:D:519:PRO:N	5:D:520:PRO:HD2	2.22	0.54
5:F:683:SER:O	5:F:687:LEU:HD22	2.07	0.54
1:G:15:VAL:HB	5:C:106:PRO:HB2	1.89	0.54
5:B:434:ASP:H	5:C:225:ARG:HH22	1.53	0.54
5:A:111:GLY:C	5:A:176:VAL:HG13	2.32	0.54
5:A:626:PRO:O	5:A:629:ILE:HG22	2.07	0.54
5:C:604:ILE:HG22	5:C:608:MET:HE2	1.89	0.54
5:E:548:LEU:HD21	5:E:582:ILE:HA	1.88	0.54
5:F:220:VAL:HG13	5:F:342:ILE:HD13	1.90	0.54
5:C:66:GLU:HB2	5:C:147:ARG:HH12	1.73	0.54
5:B:600:VAL:O	5:B:604:ILE:HG12	2.08	0.54
5:B:526:LEU:HD11	8:B:902:ADP:H3'	1.90	0.54
5:C:153:LEU:HG	5:C:162:GLU:HG3	1.90	0.54
5:C:486:LYS:O	5:C:490:GLN:HG2	2.08	0.54
5:C:297:ALA:HB1	5:C:298:PRO:HD2	1.90	0.54
5:E:566:ALA:HB1	5:E:617:VAL:HG21	1.90	0.54
1:G:529:LEU:HA	1:G:532:VAL:HG12	1.90	0.54
5:C:566:ALA:HB1	5:C:617:VAL:HG21	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:482:LEU:HB3	5:F:485:VAL:HG12	1.90	0.54
5:B:277:LYS:HE3	5:B:279:ALA:HB3	1.89	0.53
5:C:246:PRO:HD2	5:C:249:THR:HG21	1.88	0.53
5:E:627:ASP:HB3	5:E:758:PHE:HZ	1.73	0.53
1:G:8:ARG:HD3	5:C:52:PHE:HD2	1.73	0.53
5:A:158:MET:HE3	5:A:158:MET:H	1.72	0.53
2:K:45:PHE:HB2	2:K:67:LEU:HD13	1.91	0.53
3:O:554:ARG:HH11	3:O:607:GLY:HA2	1.72	0.53
5:D:489:LEU:HD21	5:D:516:PHE:HZ	1.73	0.53
5:B:421:GLN:HG3	5:B:454:TRP:CD1	2.43	0.53
5:E:287:ARG:HG2	5:E:331:LEU:HD11	1.89	0.53
1:G:12:PRO:HA	5:C:110:TYR:HB2	1.91	0.53
5:B:283:GLU:HG2	5:B:323:ARG:O	2.09	0.53
5:C:657:LEU:HG	5:C:687:LEU:HD12	1.89	0.53
5:C:737:GLU:O	5:C:741:ARG:HG2	2.09	0.53
5:D:385:THR:HG22	5:D:388:MET:HE3	1.91	0.53
5:A:169:ASP:HB3	5:A:170:PRO:HD3	1.90	0.53
5:E:262:THR:HG23	5:E:264:ALA:H	1.73	0.53
5:A:445:LEU:HD13	5:B:233:ILE:HD12	1.90	0.53
5:C:219:MET:SD	5:C:241:ILE:HG12	2.49	0.53
5:E:240:GLY:HA3	5:E:363:PHE:HA	1.90	0.53
5:F:46:MET:HB3	5:F:51:LEU:HB3	1.91	0.53
5:A:469:VAL:HG22	5:A:540:ILE:HG12	1.90	0.53
5:A:564:ASP:HA	5:A:567:ARG:HG3	1.91	0.53
5:C:519:PRO:HB3	5:C:755:TYR:HD2	1.74	0.53
5:A:634:LEU:HD11	5:A:642:LEU:HD11	1.90	0.53
2:K:40:GLN:HA	2:K:72:ARG:HD2	1.91	0.52
1:G:449:ILE:HD11	2:I:30:ILE:HG12	1.91	0.52
5:C:109:LYS:HB2	5:C:170:PRO:HG3	1.91	0.52
5:C:472:PRO:HB2	5:C:474:VAL:HG22	1.91	0.52
5:A:390:LEU:HD21	5:A:394:VAL:HG21	1.90	0.52
5:C:60:LYS:HE2	5:C:101:SER:HB3	1.91	0.52
5:E:390:LEU:HD22	5:E:394:VAL:HG21	1.91	0.52
4:P:274:SER:O	4:P:276:PRO:HD3	2.09	0.52
5:C:695:CYS:O	5:C:699:ILE:HG12	2.10	0.52
5:C:611:MET:C	5:C:611:MET:HE3	2.35	0.52
3:O:591:LEU:HD12	3:O:591:LEU:H	1.74	0.52
5:F:89:ARG:HH21	5:F:95:ARG:HH12	1.58	0.52
5:F:131:PHE:HE1	5:F:182:ILE:HD12	1.75	0.52
5:F:246:PRO:HD2	5:F:249:THR:HG21	1.92	0.52
5:F:82:ILE:HG23	5:F:84:MET:HE2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:540:ILE:HG21	5:A:562:ILE:HD11	1.91	0.52
5:B:545:PRO:O	5:B:549:THR:HG23	2.10	0.52
5:D:520:PRO:HB2	5:D:522:CYS:SG	2.50	0.52
3:M:578:ILE:HG22	3:M:586:LEU:HB2	1.93	0.52
5:C:686:ASP:O	5:C:690:ILE:HG12	2.10	0.52
5:D:445:LEU:HB3	5:E:233:ILE:HD13	1.91	0.52
1:G:238:LEU:HD21	1:G:380:VAL:HG11	1.92	0.51
5:B:332:MET:HG2	5:B:362:ARG:HA	1.92	0.51
5:B:519:PRO:HA	5:B:755:TYR:HE2	1.75	0.51
5:C:449:MET:HG3	5:C:453:ARG:HE	1.74	0.51
5:D:317:HIS:H	5:D:321:GLU:HG3	1.75	0.51
5:F:381:LEU:HD21	5:F:411:LEU:HD22	1.92	0.51
5:A:629:ILE:HD12	5:A:630:ASP:H	1.75	0.51
5:E:647:LEU:HD13	5:E:648:PRO:HD2	1.92	0.51
1:G:514:VAL:HG12	1:G:515:THR:HG23	1.91	0.51
5:B:275:MET:HE1	5:C:323:ARG:HG2	1.93	0.51
5:C:513:GLY:HA3	5:C:639:LEU:HA	1.93	0.51
5:C:633:ILE:HG23	5:C:639:LEU:HD13	1.93	0.51
5:C:670:VAL:HB	5:C:675:LEU:HD11	1.93	0.51
5:E:547:LEU:HD13	5:E:582:ILE:HD11	1.92	0.51
5:F:437:ILE:HD11	5:F:442:MET:SD	2.51	0.51
5:A:493:VAL:HG21	5:A:531:ILE:HG12	1.92	0.51
5:A:347:THR:HG21	5:A:353:ILE:HD11	1.93	0.51
5:C:426:LYS:HD3	5:C:445:LEU:HG	1.91	0.51
5:F:216:ILE:HD11	5:F:243:LEU:HD21	1.92	0.51
2:K:23:ILE:HD11	2:K:52:ASP:HA	1.92	0.51
5:B:379:GLU:O	5:B:383:ILE:HG22	2.09	0.51
5:C:559:VAL:O	5:C:562:ILE:HG22	2.11	0.51
5:C:572:CYS:HB3	5:C:617:VAL:HG23	1.91	0.51
5:E:378:LEU:O	5:E:382:GLN:HG2	2.11	0.51
4:P:251:PRO:HA	4:P:254:ILE:HG12	1.93	0.51
5:C:84:MET:HE3	5:C:84:MET:HA	1.92	0.51
5:F:544:GLY:O	5:F:548:LEU:HG	2.11	0.51
3:O:624:VAL:HA	3:O:627:LEU:HD23	1.93	0.51
5:C:274:ILE:HG23	5:C:285:ASN:HB2	1.93	0.51
5:D:304:ASP:OD2	5:D:305:GLU:HG3	2.11	0.51
5:F:51:LEU:HD11	5:F:71:VAL:HG11	1.93	0.51
1:G:129:LEU:HB3	1:G:140:HIS:CE1	2.46	0.50
2:K:61:ILE:HD11	2:K:65:SER:HB2	1.93	0.50
5:D:423:ILE:HD11	5:E:233:ILE:HG21	1.92	0.50
5:F:674:PHE:HZ	5:F:737:GLU:HG3	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:624:VAL:HG21	3:M:644:LEU:HD13	1.93	0.50
5:D:547:LEU:HD11	5:D:582:ILE:HG23	1.92	0.50
5:F:636:PRO:HA	5:F:640:ASP:HB2	1.92	0.50
3:O:613:TYR:HB3	3:O:646:LEU:HD22	1.92	0.50
5:D:567:ARG:NH1	5:D:612:SER:H	2.08	0.50
5:D:736:PHE:O	5:D:740:MET:HE2	2.11	0.50
5:A:71:VAL:HG22	5:A:72:LEU:HG	1.93	0.50
5:B:244:TYR:CD2	5:B:350:PRO:HG3	2.46	0.50
5:B:421:GLN:HG3	5:B:454:TRP:NE1	2.27	0.50
5:C:212:GLN:HG2	5:C:368:ASP:O	2.12	0.50
5:E:201:VAL:HG23	5:E:201:VAL:O	2.12	0.50
5:F:119:ILE:HG22	5:F:162:GLU:HB2	1.94	0.50
3:M:573:VAL:HG22	3:M:591:LEU:HA	1.93	0.50
5:A:749:ASP:HA	5:A:752:ILE:HD12	1.93	0.50
5:E:491:GLU:HA	5:E:495:TYR:CD1	2.46	0.50
5:F:140:LEU:O	5:F:141:GLU:HG3	2.12	0.50
1:G:295:VAL:O	1:G:298:GLU:HG2	2.11	0.50
5:A:335:LEU:HD22	5:A:341:VAL:HG11	1.92	0.50
5:C:420:LEU:O	5:C:423:ILE:HG22	2.12	0.50
5:D:471:VAL:CG1	5:D:472:PRO:HD2	2.42	0.50
5:E:255:ALA:HB2	5:E:302:PHE:CZ	2.47	0.50
5:D:693:ARG:O	5:D:697:LEU:HD12	2.11	0.50
1:G:231:HIS:NE2	2:I:43:LEU:HD11	2.26	0.50
2:K:56:LEU:HB3	2:K:61:ILE:HG21	1.93	0.50
5:A:179:ASP:HA	5:A:182:ILE:HD11	1.94	0.50
5:B:241:ILE:O	5:B:344:MET:HA	2.11	0.50
5:B:671:ASP:OD1	5:B:674:PHE:HB2	2.12	0.50
5:C:517:TYR:CZ	5:C:644:TYR:HB2	2.46	0.50
5:C:491:GLU:HA	5:C:495:TYR:CE2	2.47	0.49
5:E:406:HIS:ND1	5:E:461:PRO:HB3	2.27	0.49
5:E:733:ARG:HA	5:E:736:PHE:CE2	2.47	0.49
5:F:402:GLU:HB3	5:F:456:LEU:HD21	1.93	0.49
5:F:634:LEU:HD11	5:F:642:LEU:HD21	1.93	0.49
5:B:708:ARG:HA	5:B:711:ARG:NE	2.27	0.49
1:G:458:LYS:HD2	2:I:41:GLN:HE22	1.77	0.49
5:A:38:VAL:HG22	5:A:73:SER:HB3	1.94	0.49
5:F:539:PHE:CE2	5:F:541:SER:HB2	2.47	0.49
1:G:182:ALA:HB2	5:C:288:LYS:HE2	1.94	0.49
4:P:231:SER:HB3	4:P:244:PRO:HD3	1.95	0.49
5:A:195:GLU:HA	5:A:199:ASN:HB2	1.94	0.49
5:B:239:ARG:HH22	5:B:337:GLN:HA	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:276:SER:HB3	5:C:280:GLY:HA2	1.95	0.49
5:B:381:LEU:HD21	5:B:411:LEU:HD22	1.94	0.49
5:B:635:ARG:HB2	5:B:638:ARG:HH11	1.77	0.49
5:C:321:GLU:O	5:C:325:VAL:HG12	2.12	0.49
5:C:483:GLU:O	5:C:486:LYS:HB3	2.13	0.49
3:M:618:THR:HG23	3:M:621:ARG:HH11	1.77	0.49
5:D:753:ARG:O	5:D:757:MET:HB3	2.11	0.49
2:K:4:PHE:O	2:K:66:THR:HA	2.13	0.49
1:G:311:ILE:HD13	1:G:370:ALA:HB3	1.95	0.49
5:B:749:ASP:O	5:B:753:ARG:HG3	2.13	0.49
5:C:694:ALA:HA	5:C:697:LEU:HD12	1.93	0.49
1:G:471:PHE:CD1	1:G:472:PRO:HD2	2.47	0.49
5:A:246:PRO:HD2	5:A:249:THR:HG21	1.94	0.49
5:C:84:MET:HE2	5:C:88:VAL:HB	1.95	0.49
5:F:673:GLU:O	5:F:677:LYS:HG2	2.12	0.49
5:A:28:VAL:HG12	5:A:96:LEU:HD23	1.95	0.48
5:B:224:LEU:HD22	5:B:298:PRO:HB3	1.95	0.48
5:B:501:ASP:O	5:B:504:LEU:HG	2.12	0.48
5:B:551:TRP:HE1	5:B:599:ARG:CD	2.26	0.48
5:B:566:ALA:HB1	5:B:617:VAL:HG21	1.93	0.48
5:C:653:ARG:NH2	5:C:681:GLY:H	2.11	0.48
5:F:749:ASP:O	5:F:753:ARG:HG2	2.13	0.48
2:K:1:MET:HB2	2:K:63:LYS:HD3	1.94	0.48
1:G:549:TRP:HA	1:G:552:ILE:HD12	1.94	0.48
5:C:476:TRP:HE3	5:C:479:ILE:HG21	1.78	0.48
5:D:693:ARG:HA	5:D:693:ARG:HH11	1.78	0.48
5:E:703:ILE:HA	5:E:706:GLU:CD	2.39	0.48
5:A:155:ARG:HB2	5:A:159:ARG:H	1.78	0.48
5:D:608:MET:HE1	5:D:619:ILE:HG21	1.96	0.48
1:G:259:HIS:CD2	1:G:262:ILE:HD12	2.49	0.48
5:A:94:VAL:HG13	5:A:98:ASP:HB2	1.95	0.48
5:B:322:ARG:C	5:B:324:ILE:H	2.20	0.48
5:D:223:PRO:HB2	5:D:340:HIS:CD2	2.49	0.48
5:F:559:VAL:HG11	5:F:603:GLN:HB3	1.95	0.48
3:O:603:VAL:HG21	3:O:615:LEU:HD11	1.95	0.48
5:A:20:LYS:H	5:A:25:ARG:NH1	2.12	0.48
5:A:394:VAL:HA	5:A:449:MET:HB2	1.95	0.48
5:C:40:SER:HB2	5:C:83:ARG:HB2	1.96	0.48
5:C:647:LEU:HD21	5:C:752:ILE:HG12	1.95	0.48
5:E:526:LEU:HD11	8:E:902:ADP:H5'2	1.94	0.48
5:E:625:ARG:HH22	5:E:754:LYS:NZ	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:273:GLU:HA	5:B:330:THR:HG21	1.94	0.48
5:A:222:LEU:HD12	5:F:432:LEU:HD12	1.95	0.48
5:E:241:ILE:O	5:E:344:MET:HA	2.14	0.48
5:F:51:LEU:HD11	5:F:71:VAL:HG21	1.96	0.48
5:A:701:GLU:O	5:A:704:GLU:HG3	2.14	0.48
5:B:603:GLN:O	5:B:607:GLU:HG2	2.14	0.48
5:E:529:LYS:HD3	5:E:529:LYS:HA	1.52	0.48
1:G:50:ARG:HG3	1:G:76:PHE:CE2	2.48	0.48
5:A:312:LYS:HB2	5:A:315:LYS:CE	2.44	0.48
5:A:661:LEU:HB2	5:A:664:SER:HB3	1.96	0.48
5:C:732:ARG:HE	5:C:734:ASP:HB2	1.79	0.48
5:E:266:PHE:HE1	5:E:268:LEU:HB2	1.79	0.48
1:G:10:GLN:HB2	1:G:15:VAL:HG22	1.96	0.47
1:G:254:GLY:HA3	1:G:269:GLU:O	2.14	0.47
1:G:404:LYS:HE3	4:P:260:ASN:HA	1.95	0.47
5:A:47:ASP:HA	5:A:51:LEU:HG	1.96	0.47
5:A:143:TYR:HD1	5:A:175:ILE:HD13	1.79	0.47
5:B:472:PRO:HD3	5:B:539:PHE:HB3	1.96	0.47
5:B:699:ILE:O	5:B:703:ILE:HG12	2.14	0.47
5:D:198:LEU:HD21	5:E:336:LYS:HZ2	1.79	0.47
5:D:574:LEU:HD23	5:D:575:PHE:N	2.29	0.47
5:F:525:THR:HG22	8:F:902:ADP:O2A	2.14	0.47
1:G:131:ARG:HE	5:E:334:GLY:HA2	1.78	0.47
3:O:619:PHE:HB3	5:F:72:LEU:HD11	1.97	0.47
5:A:16:ILE:HG22	5:A:17:LEU:HD23	1.96	0.47
5:C:240:GLY:C	5:C:241:ILE:HG13	2.39	0.47
5:C:527:LEU:O	5:C:531:ILE:HG22	2.14	0.47
5:F:112:LYS:HE3	5:F:169:ASP:OD1	2.14	0.47
5:A:567:ARG:HH12	5:F:464:LEU:HD13	1.80	0.47
5:C:350:PRO:HA	5:C:353:ILE:HD13	1.95	0.47
5:F:31:ALA:HA	5:F:83:ARG:HG2	1.95	0.47
5:F:206:ILE:HD12	5:F:254:ILE:HG12	1.96	0.47
5:E:388:MET:HE1	5:E:415:CYS:HB3	1.96	0.47
5:F:264:ALA:HB1	5:F:298:PRO:O	2.13	0.47
5:F:539:PHE:HE2	5:F:541:SER:HB2	1.79	0.47
1:G:302:LYS:HD2	1:G:302:LYS:HA	1.67	0.47
5:B:219:MET:HE3	5:B:241:ILE:HG12	1.97	0.47
5:D:524:LYS:HA	5:D:527:LEU:HG	1.95	0.47
5:E:201:VAL:O	5:E:257:ALA:HA	2.13	0.47
5:F:126:ILE:HD11	5:F:159:ARG:HD3	1.97	0.47
1:G:500:PHE:O	1:G:504:ILE:HG22	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:695:CYS:SG	5:C:508:MET:HG2	2.55	0.47
5:C:87:VAL:HG22	5:C:153:LEU:HD13	1.96	0.47
5:D:663:LYS:HD2	5:D:663:LYS:HA	1.65	0.47
5:A:29:ASP:HB3	5:A:83:ARG:HG2	1.96	0.47
5:B:442:MET:HA	5:B:445:LEU:HD23	1.97	0.47
5:C:580:ASP:HB3	5:C:623:THR:OG1	2.14	0.47
5:C:697:LEU:HB3	5:C:700:ARG:HH21	1.79	0.47
5:D:491:GLU:HA	5:D:495:TYR:CD2	2.50	0.47
5:D:492:LEU:HD23	5:D:493:VAL:HG23	1.96	0.47
5:D:541:SER:C	5:D:542:ILE:HD13	2.39	0.47
5:D:703:ILE:HG12	5:E:502:LYS:HD3	1.97	0.47
5:E:244:TYR:HA	5:E:347:THR:O	2.14	0.47
5:F:31:ALA:HA	5:F:83:ARG:CG	2.45	0.47
1:G:161:HIS:HE1	1:G:450:ILE:HG12	1.79	0.47
3:M:609:PRO:HD2	3:M:612:GLU:HB2	1.97	0.47
3:M:614:LYS:HZ2	3:M:649:LYS:HA	1.80	0.47
3:O:566:LYS:HB2	3:O:566:LYS:HE2	1.58	0.47
5:A:113:ARG:N	5:A:169:ASP:HB2	2.29	0.47
5:C:219:MET:HE2	5:C:365:ARG:HD3	1.95	0.47
5:C:493:VAL:HG11	5:C:531:ILE:HD11	1.96	0.47
5:C:538:ASN:ND2	5:C:569:ALA:HB1	2.29	0.47
3:M:615:LEU:HD12	3:M:645:PHE:O	2.15	0.47
5:D:219:MET:SD	5:D:238:PRO:HG2	2.54	0.47
5:D:543:LYS:HB3	5:D:543:LYS:HE2	1.82	0.47
5:B:327:GLN:O	5:B:331:LEU:HD12	2.14	0.47
5:C:110:TYR:HD1	5:C:177:ALA:HB2	1.80	0.47
5:C:325:VAL:O	5:C:329:LEU:HG	2.15	0.47
5:D:243:LEU:HD23	5:D:367:VAL:HB	1.96	0.47
5:A:519:PRO:HG3	5:A:755:TYR:HD2	1.80	0.46
5:F:642:LEU:O	5:F:643:ILE:HD13	2.16	0.46
3:M:639:PHE:CG	3:M:640:PRO:HA	2.51	0.46
5:B:665:PRO:HB2	5:B:730:GLU:HB2	1.96	0.46
5:D:489:LEU:HB3	5:D:531:ILE:HG21	1.97	0.46
5:D:559:VAL:O	5:D:562:ILE:HG13	2.15	0.46
5:F:24:ASN:HB2	5:F:25:ARG:NH1	2.31	0.46
1:G:241:TRP:CE2	1:G:315:LEU:HB2	2.51	0.46
5:A:141:GLU:CD	5:A:141:GLU:O	2.57	0.46
5:B:505:LYS:HG3	5:B:506:PHE:CD1	2.51	0.46
5:C:110:TYR:CD1	5:C:177:ALA:HB2	2.51	0.46
5:C:300:ILE:HD11	5:C:344:MET:CE	2.46	0.46
5:D:244:TYR:CZ	5:D:368:ASP:HB2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:246:PRO:HD2	5:E:249:THR:HG21	1.96	0.46
5:B:496:PRO:HA	5:B:503:PHE:HE2	1.80	0.46
5:C:92:LEU:HB2	5:C:94:VAL:HG22	1.98	0.46
5:E:653:ARG:NH2	5:E:681:GLY:H	2.14	0.46
5:F:310:ALA:HA	5:F:325:VAL:HG22	1.97	0.46
2:K:19:PRO:HA	2:K:56:LEU:HB2	1.98	0.46
5:A:42:SER:HA	5:A:75:ASP:HA	1.97	0.46
5:A:476:TRP:HZ3	5:A:531:ILE:HA	1.81	0.46
5:B:302:PHE:HA	5:B:344:MET:O	2.16	0.46
5:C:65:ARG:HA	5:C:65:ARG:HD3	1.61	0.46
5:C:487:ARG:HA	5:C:490:GLN:HG2	1.98	0.46
5:C:565:LYS:HE2	5:C:565:LYS:HB2	1.69	0.46
5:F:516:PHE:HD1	5:F:643:ILE:HB	1.80	0.46
1:G:155:LEU:HD21	1:G:262:ILE:HG23	1.97	0.46
1:G:177:LYS:HD2	1:G:177:LYS:HA	1.59	0.46
4:P:238:LYS:HD3	4:P:238:LYS:HA	1.67	0.46
5:A:520:PRO:HG3	5:A:624:ASN:HD22	1.81	0.46
5:B:275:MET:HE2	5:B:275:MET:HB3	1.71	0.46
5:C:65:ARG:NH2	5:C:93:ARG:HH21	2.13	0.46
5:D:577:ASP:HB3	5:D:578:GLU:OE1	2.16	0.46
5:D:695:CYS:SG	5:E:508:MET:HE2	2.56	0.46
5:F:381:LEU:HB3	5:F:396:LEU:HD12	1.98	0.46
5:A:489:LEU:HD12	5:A:527:LEU:HD12	1.97	0.46
5:A:611:MET:O	5:A:611:MET:HE3	2.16	0.46
5:B:604:ILE:HG22	5:B:608:MET:HE2	1.98	0.46
5:B:701:GLU:O	5:B:704:GLU:HG3	2.15	0.46
5:E:500:PRO:HA	5:E:503:PHE:HD2	1.81	0.46
2:I:31:GLN:O	2:I:31:GLN:HG2	2.15	0.45
5:A:66:GLU:O	5:A:147:ARG:HD3	2.16	0.45
5:B:222:LEU:HD12	5:B:230:PHE:HE1	1.80	0.45
5:C:526:LEU:HD11	8:C:902:ADP:H5'2	1.98	0.45
5:F:728:VAL:HG12	5:F:732:ARG:HE	1.81	0.45
5:A:84:MET:HB3	5:A:88:VAL:HB	1.97	0.45
5:B:312:LYS:HG3	5:B:355:PRO:HD3	1.97	0.45
5:B:336:LYS:HG2	5:B:338:ARG:HD3	1.98	0.45
5:B:519:PRO:HG2	5:B:522:CYS:SG	2.55	0.45
5:D:206:ILE:HD13	5:D:254:ILE:HG12	1.98	0.45
1:G:231:HIS:CD2	2:I:43:LEU:HD11	2.52	0.45
5:C:21:ASN:HB2	5:C:25:ARG:HH21	1.80	0.45
5:C:288:LYS:HD2	5:C:288:LYS:C	2.42	0.45
5:D:499:HIS:HB2	5:D:502:LYS:HG2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:635:ARG:HD3	5:F:636:PRO:HD2	1.98	0.45
1:G:142:VAL:HG12	1:G:143:PRO:HD2	1.98	0.45
5:A:547:LEU:HD13	5:A:600:VAL:HG21	1.99	0.45
5:C:611:MET:HE3	5:C:611:MET:O	2.16	0.45
5:E:357:LEU:HD22	5:E:363:PHE:CD2	2.50	0.45
3:M:597:GLN:HA	3:M:600:PHE:HB2	1.98	0.45
5:B:294:GLU:CD	5:B:338:ARG:HG3	2.42	0.45
5:B:513:GLY:HA2	5:B:619:ILE:O	2.16	0.45
5:C:558:ASN:O	5:C:561:GLU:HB3	2.16	0.45
5:E:651:LYS:HE3	5:E:651:LYS:HB3	1.84	0.45
1:G:303:LEU:HA	1:G:533:ARG:HD3	1.98	0.45
5:A:336:LYS:NZ	5:A:336:LYS:H	2.15	0.45
5:A:110:TYR:HA	5:A:175:ILE:O	2.17	0.45
5:B:286:LEU:HD12	5:B:286:LEU:HA	1.81	0.45
5:B:555:SER:O	5:B:556:GLU:HG2	2.17	0.45
5:B:675:LEU:HD12	5:B:679:THR:HG23	1.99	0.45
5:C:212:GLN:O	5:C:216:ILE:HG22	2.16	0.45
5:F:286:LEU:HD12	5:F:286:LEU:HA	1.72	0.45
5:F:468:VAL:HG22	5:F:470:GLU:OE1	2.17	0.45
3:O:596:LEU:O	3:O:599:VAL:HG22	2.16	0.45
5:B:491:GLU:HA	5:B:495:TYR:CD1	2.51	0.45
5:D:377:ARG:CZ	5:D:404:HIS:HA	2.47	0.45
5:D:523:GLY:HA2	8:D:902:ADP:H5'2	1.98	0.45
5:D:613:THR:O	5:D:614:LYS:HD2	2.17	0.45
5:F:148:LYS:HE2	5:F:168:THR:N	2.28	0.45
5:F:461:PRO:HG2	5:F:464:LEU:HD11	1.98	0.45
5:A:134:TYR:CE2	5:A:155:ARG:HG2	2.52	0.45
5:B:639:LEU:H	5:B:639:LEU:HD12	1.80	0.45
5:C:740:MET:HG2	5:C:741:ARG:HH21	1.81	0.45
5:E:736:PHE:HB3	5:E:740:MET:HE1	1.99	0.45
5:A:399:VAL:HG13	5:A:456:LEU:HD12	1.99	0.45
5:F:72:LEU:HD23	5:F:72:LEU:HA	1.84	0.45
5:F:667:ALA:HB2	5:F:730:GLU:HG3	1.99	0.45
1:G:441:ARG:HD3	1:G:441:ARG:HA	1.61	0.44
3:M:576:LEU:HD13	3:M:576:LEU:HA	1.84	0.44
5:B:278:LEU:HD22	5:C:278:LEU:HD13	1.98	0.44
5:B:672:LEU:HD12	5:B:672:LEU:HA	1.71	0.44
5:C:732:ARG:HH21	5:C:734:ASP:HB2	1.82	0.44
5:D:671:ASP:HB3	5:D:674:PHE:HE1	1.81	0.44
3:M:595:LYS:HG2	3:M:597:GLN:H	1.82	0.44
5:A:320:VAL:HA	5:A:323:ARG:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:541:SER:O	5:A:542:ILE:HD13	2.17	0.44
5:C:60:LYS:HG2	5:C:66:GLU:HG3	1.99	0.44
5:C:283:GLU:HB2	5:C:287:ARG:CZ	2.48	0.44
5:D:508:MET:HE3	5:D:509:THR:H	1.81	0.44
1:G:297:ASP:OD1	1:G:297:ASP:C	2.61	0.44
3:O:603:VAL:HA	3:O:606:LYS:NZ	2.32	0.44
4:P:255:LYS:HB3	4:P:255:LYS:HE3	1.67	0.44
5:A:482:LEU:HB3	5:A:485:VAL:HB	1.99	0.44
5:B:332:MET:HE2	5:B:332:MET:HB2	1.84	0.44
5:C:219:MET:CE	5:C:365:ARG:HD3	2.47	0.44
5:D:244:TYR:OH	5:D:368:ASP:HB2	2.17	0.44
5:B:240:GLY:O	5:B:241:ILE:C	2.61	0.44
5:B:277:LYS:HE2	5:B:281:GLU:C	2.42	0.44
5:B:356:ALA:O	5:B:362:ARG:HD3	2.17	0.44
1:G:183:LEU:HD22	1:G:183:LEU:HA	1.79	0.44
5:A:113:ARG:H	5:A:169:ASP:HB2	1.83	0.44
5:A:629:ILE:HD12	5:A:630:ASP:N	2.33	0.44
5:C:24:ASN:HB2	5:C:102:ILE:O	2.18	0.44
5:D:312:LYS:HG3	5:D:355:PRO:HD3	1.98	0.44
5:D:442:MET:HA	5:D:445:LEU:HD12	1.99	0.44
5:D:601:ILE:HA	5:D:604:ILE:HG22	1.99	0.44
5:D:647:LEU:HD11	5:D:752:ILE:HD13	2.00	0.44
5:E:547:LEU:HD12	5:E:547:LEU:H	1.82	0.44
5:F:62:LYS:HG2	5:F:94:VAL:HG12	1.99	0.44
5:F:286:LEU:HD22	5:F:324:ILE:HD11	2.00	0.44
3:M:575:LYS:HD2	3:M:589:ARG:HD2	2.00	0.44
5:B:264:ALA:HB1	5:B:298:PRO:O	2.17	0.44
5:C:299:ALA:O	5:C:341:VAL:HA	2.17	0.44
5:D:264:ALA:HB1	5:D:298:PRO:O	2.18	0.44
5:D:406:HIS:CE1	5:D:461:PRO:HG3	2.53	0.44
5:E:216:ILE:HD11	5:E:243:LEU:HD21	1.98	0.44
5:E:733:ARG:HA	5:E:736:PHE:CD2	2.53	0.44
5:F:138:TYR:CD1	5:F:138:TYR:C	2.96	0.44
3:M:639:PHE:CD1	3:M:640:PRO:HA	2.53	0.44
5:B:492:LEU:O	5:B:492:LEU:HD23	2.18	0.44
5:D:332:MET:HE2	5:D:332:MET:HB3	1.86	0.44
5:E:307:ASP:OD2	5:E:307:ASP:C	2.60	0.44
1:G:197:HIS:CE1	1:G:208:CYS:SG	3.10	0.44
3:O:578:ILE:HG23	3:O:586:LEU:HB2	2.00	0.44
5:A:155:ARG:HB2	5:A:159:ARG:HA	1.99	0.44
5:C:29:ASP:HB3	5:C:83:ARG:HD3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:322:ARG:H	5:C:322:ARG:HG2	1.61	0.44
5:D:269:ILE:HG23	5:D:274:ILE:HD12	2.00	0.44
5:D:632:ALA:HB1	5:D:638:ARG:HH12	1.82	0.44
1:G:229:GLU:HG3	1:G:270:VAL:O	2.17	0.44
3:O:550:ARG:O	3:O:553:ILE:HG22	2.18	0.44
5:A:513:GLY:N	5:A:618:PHE:HE1	2.16	0.44
5:A:519:PRO:HG3	5:A:755:TYR:CD2	2.53	0.44
5:A:547:LEU:HD12	5:A:548:LEU:HD22	2.00	0.44
5:B:335:LEU:HD12	5:B:335:LEU:HA	1.81	0.44
5:D:674:PHE:O	5:D:678:MET:HG2	2.18	0.44
5:F:489:LEU:HD11	5:F:531:ILE:HG21	2.00	0.44
5:F:629:ILE:HD12	5:F:629:ILE:HA	1.90	0.44
1:G:161:HIS:CE1	1:G:450:ILE:HG12	2.53	0.43
3:M:546:GLN:O	3:M:550:ARG:HG2	2.18	0.43
3:O:565:PRO:HB2	3:O:569:ASN:OD1	2.18	0.43
5:A:700:ARG:HG3	5:B:487:ARG:HH22	1.81	0.43
5:C:119:ILE:O	5:C:123:VAL:HG22	2.18	0.43
5:D:694:ALA:HA	5:D:697:LEU:HD12	2.00	0.43
5:F:351:ASN:HA	5:F:358:ARG:HH22	1.82	0.43
5:B:517:TYR:HD2	5:B:626:PRO:HG3	1.83	0.43
5:C:231:LYS:HA	5:C:231:LYS:HD3	1.82	0.43
5:D:733:ARG:HA	5:D:736:PHE:HD2	1.83	0.43
5:F:158:MET:SD	5:F:159:ARG:HG3	2.58	0.43
5:F:597:ALA:HB3	5:F:599:ARG:HH11	1.82	0.43
5:A:539:PHE:CE2	5:A:541:SER:HB3	2.53	0.43
5:B:262:THR:HG21	5:B:300:ILE:HD11	1.99	0.43
5:B:504:LEU:HD12	5:B:505:LYS:N	2.34	0.43
5:C:230:PHE:HD2	5:C:237:PRO:HB3	1.84	0.43
5:C:388:MET:HE3	5:C:390:LEU:HD21	2.00	0.43
5:D:603:GLN:O	5:D:607:GLU:HG2	2.19	0.43
5:F:225:ARG:HA	5:F:225:ARG:HD2	1.83	0.43
1:G:242:ARG:NE	2:I:47:GLY:HA2	2.30	0.43
1:G:526:SER:O	1:G:529:LEU:HD12	2.18	0.43
5:B:548:LEU:HD22	5:B:548:LEU:HA	1.90	0.43
5:C:411:LEU:HD23	5:C:411:LEU:HA	1.76	0.43
5:C:740:MET:HG2	5:C:741:ARG:NH2	2.33	0.43
5:D:651:LYS:HA	5:D:651:LYS:HD2	1.65	0.43
5:F:142:ALA:HB1	5:F:144:ARG:HG3	2.00	0.43
5:F:411:LEU:HA	5:F:411:LEU:HD23	1.85	0.43
1:G:312:PHE:HZ	1:G:329:ARG:HH12	1.66	0.43
3:O:591:LEU:HB2	3:O:594:ASN:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:138:TYR:CE1	5:A:154:VAL:HG11	2.54	0.43
5:A:155:ARG:HB3	5:A:157:GLY:H	1.83	0.43
5:A:491:GLU:CD	5:F:700:ARG:HG3	2.43	0.43
5:C:198:LEU:HD23	5:C:198:LEU:HA	1.86	0.43
5:F:424:ARG:HE	5:F:424:ARG:HB2	1.48	0.43
1:G:48:ILE:HA	1:G:75:LEU:HD22	2.00	0.43
5:A:114:ILE:HD11	5:A:176:VAL:HB	2.01	0.43
5:A:441:VAL:HG23	5:A:442:MET:H	1.84	0.43
5:A:465:ARG:HE	5:A:465:ARG:HB2	1.67	0.43
5:B:326:SER:O	5:B:330:THR:HG23	2.19	0.43
5:C:219:MET:HE3	5:C:219:MET:HB2	1.75	0.43
5:C:671:ASP:O	5:C:675:LEU:HG	2.19	0.43
5:D:681:GLY:O	5:D:745:ARG:HG3	2.19	0.43
5:D:737:GLU:HA	5:D:740:MET:CE	2.49	0.43
5:D:759:ALA:HA	5:D:762:LEU:HD12	2.00	0.43
5:F:45:LYS:HD2	5:F:45:LYS:HA	1.79	0.43
1:G:426:TYR:HD1	1:G:440:ALA:HB2	1.83	0.43
3:M:575:LYS:O	3:M:641:GLN:HA	2.18	0.43
3:O:597:GLN:HA	3:O:600:PHE:HD2	1.84	0.43
5:A:46:MET:O	5:A:46:MET:SD	2.76	0.43
5:C:22:ARG:HD2	5:C:23:PRO:HD2	2.00	0.43
5:C:600:VAL:O	5:C:604:ILE:HG13	2.18	0.43
5:C:687:LEU:HA	5:C:690:ILE:HG12	2.01	0.43
5:D:655:ALA:HA	5:D:658:LYS:HE3	2.01	0.43
5:E:427:MET:HE3	5:E:427:MET:HB3	1.90	0.43
5:F:30:GLU:H	5:F:30:GLU:HG3	1.63	0.43
5:A:336:LYS:HE2	5:A:336:LYS:HB2	1.84	0.43
5:A:338:ARG:H	5:A:338:ARG:HG3	1.58	0.43
5:A:465:ARG:HH22	5:B:560:ARG:HD2	1.84	0.43
5:A:526:LEU:H	5:A:526:LEU:HD22	1.83	0.43
5:B:681:GLY:HA3	5:B:745:ARG:HH12	1.83	0.43
5:C:489:LEU:O	5:C:493:VAL:HG12	2.18	0.43
5:C:544:GLY:N	5:C:545:PRO:HD2	2.33	0.43
5:D:267:PHE:HB3	5:D:301:ILE:HG23	2.01	0.43
2:I:21:ASP:OD1	2:I:26:VAL:HG23	2.18	0.43
5:A:217:LYS:HE2	5:A:217:LYS:HB3	1.72	0.43
5:A:707:ILE:O	5:A:710:GLU:HG3	2.19	0.43
5:B:604:ILE:O	5:B:608:MET:HE3	2.17	0.43
5:C:203:TYR:CE2	5:C:217:LYS:HD3	2.54	0.43
5:C:562:ILE:HD12	5:C:562:ILE:HA	1.78	0.43
5:D:349:ARG:HG3	5:D:352:SER:HB3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:33:LYS:HE2	2:I:35:GLY:HA2	2.01	0.43
3:M:615:LEU:H	3:M:625:THR:HG23	1.83	0.43
5:A:659:ALA:O	5:A:662:ARG:HG2	2.19	0.43
5:A:674:PHE:HA	5:A:677:LYS:HE2	2.00	0.43
5:B:657:LEU:HG	5:B:672:LEU:HD11	2.00	0.43
5:F:134:TYR:HD1	5:F:156:GLY:HA3	1.84	0.43
1:G:114:LEU:HD23	1:G:114:LEU:HA	1.83	0.42
1:G:402:PRO:HG2	4:P:260:ASN:HB3	2.00	0.42
2:K:30:ILE:HD13	2:K:69:LEU:HD22	2.01	0.42
5:A:286:LEU:HD12	5:A:286:LEU:HA	1.74	0.42
5:A:423:ILE:HG12	5:B:229:LEU:HD21	2.00	0.42
5:A:675:LEU:HD12	5:A:676:ALA:N	2.34	0.42
5:C:442:MET:HA	5:C:442:MET:HE2	2.00	0.42
5:D:625:ARG:HE	5:D:628:ILE:HD12	1.84	0.42
5:D:708:ARG:O	5:D:712:GLU:HG2	2.18	0.42
5:F:396:LEU:HA	5:F:396:LEU:HD13	1.81	0.42
1:G:130:CYS:SG	1:G:141:CYS:HB2	2.60	0.42
4:P:228:PHE:CG	5:A:113:ARG:HD3	2.54	0.42
4:P:235:LEU:HB2	5:A:178:PRO:HG2	2.01	0.42
5:A:275:MET:O	5:B:323:ARG:HG2	2.19	0.42
5:B:598:ASP:HB2	5:B:599:ARG:H	1.65	0.42
5:D:318:GLY:HA2	5:D:322:ARG:NH2	2.34	0.42
5:F:654:VAL:HG22	5:F:676:ALA:HB1	2.02	0.42
5:A:383:ILE:HD11	7:A:901:ATP:H2	1.84	0.42
5:A:526:LEU:HD21	8:A:902:ADP:H5'2	2.01	0.42
5:A:565:LYS:HB2	5:A:565:LYS:HE2	1.85	0.42
5:A:651:LYS:HE3	5:A:651:LYS:HB3	1.79	0.42
5:B:696:LYS:NZ	5:C:491:GLU:HB3	2.34	0.42
5:C:390:LEU:HB3	5:C:394:VAL:HG21	2.01	0.42
5:D:231:LYS:HA	5:D:231:LYS:HD2	1.59	0.42
1:G:8:ARG:HG2	1:G:17:ARG:HG2	2.01	0.42
5:B:562:ILE:HD12	5:B:562:ILE:H	1.84	0.42
5:B:634:LEU:HD12	5:B:634:LEU:H	1.85	0.42
5:F:33:ASN:HB3	5:F:38:VAL:HG11	2.00	0.42
5:F:502:LYS:HA	5:F:505:LYS:HD3	2.00	0.42
5:F:519:PRO:CA	5:F:755:TYR:HE2	2.31	0.42
5:F:565:LYS:HB2	5:F:565:LYS:HE2	1.78	0.42
5:A:171:SER:OG	5:A:172:PRO:HD3	2.19	0.42
5:B:246:PRO:HD2	5:B:249:THR:HG21	2.01	0.42
5:B:656:ILE:HG23	8:B:902:ADP:C6	2.54	0.42
5:E:476:TRP:CZ2	5:E:486:LYS:HG3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:420:LEU:HD22	5:F:424:ARG:NH2	2.33	0.42
5:F:597:ALA:HB3	5:F:599:ARG:NH1	2.34	0.42
3:M:596:LEU:O	3:M:599:VAL:HG22	2.20	0.42
5:C:22:ARG:O	5:C:25:ARG:HG3	2.20	0.42
5:D:608:MET:HE2	5:D:608:MET:HB2	1.79	0.42
2:K:43:LEU:HB3	2:K:50:LEU:HD12	2.02	0.42
4:P:231:SER:H	5:A:183:HIS:CG	2.38	0.42
5:A:63:LYS:HD3	5:A:200:GLU:HA	2.01	0.42
5:A:650:GLU:C	5:A:652:SER:H	2.26	0.42
5:C:650:GLU:C	5:C:652:SER:H	2.27	0.42
5:E:196:GLU:O	5:E:200:GLU:HG2	2.19	0.42
5:E:528:ALA:O	5:E:531:ILE:HG22	2.20	0.42
5:F:60:LYS:HB3	5:F:101:SER:OG	2.19	0.42
5:A:524:LYS:H	5:A:524:LYS:HG3	1.60	0.42
5:C:62:LYS:HZ3	5:C:94:VAL:HG12	1.85	0.42
5:C:466:GLU:CD	5:C:466:GLU:N	2.78	0.42
5:E:332:MET:HB2	5:E:332:MET:HE2	1.63	0.42
5:E:748:SER:O	5:E:752:ILE:HG13	2.20	0.42
5:A:493:VAL:HG22	5:A:618:PHE:CD2	2.55	0.42
5:B:266:PHE:CE2	5:B:268:LEU:HB2	2.55	0.42
5:B:542:ILE:HD13	5:B:542:ILE:HA	1.93	0.42
5:C:65:ARG:HG3	5:C:93:ARG:HG3	2.02	0.42
5:C:739:ALA:HA	5:C:742:PHE:CD2	2.54	0.42
5:D:657:LEU:HD21	5:D:687:LEU:HD12	2.02	0.42
5:E:224:LEU:HD23	5:E:224:LEU:HA	1.81	0.42
5:E:584:LYS:HB2	5:E:584:LYS:HE2	1.85	0.42
5:F:635:ARG:HB3	5:F:638:ARG:HH11	1.84	0.42
3:M:554:ARG:HH21	3:M:609:PRO:HG3	1.84	0.42
3:O:551:GLU:O	3:O:555:LEU:HG	2.20	0.42
5:A:222:LEU:HB3	5:A:223:PRO:HD3	2.02	0.42
5:A:598:ASP:O	5:A:601:ILE:HG22	2.20	0.42
5:A:749:ASP:O	5:A:753:ARG:HG2	2.20	0.42
5:B:468:VAL:HG22	5:B:470:GLU:H	1.85	0.42
5:B:476:TRP:CZ2	5:B:486:LYS:HB2	2.51	0.42
5:C:113:ARG:HD3	5:C:183:HIS:CE1	2.55	0.42
5:C:448:THR:HG23	5:C:450:ASP:H	1.84	0.42
5:F:134:TYR:CD1	5:F:156:GLY:HA3	2.55	0.42
1:G:161:HIS:CE1	1:G:450:ILE:HG23	2.55	0.41
1:G:522:GLN:CD	1:G:522:GLN:H	2.27	0.41
3:M:577:ARG:O	3:M:643:THR:HA	2.19	0.41
3:M:636:VAL:C	3:M:637:LYS:HG3	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:155:ARG:CG	5:A:161:VAL:HB	2.50	0.41
5:A:213:LEU:HD12	5:A:213:LEU:HA	1.81	0.41
5:B:561:GLU:HA	5:B:564:ASP:OD2	2.20	0.41
5:E:464:LEU:HD12	5:E:464:LEU:HA	1.83	0.41
5:F:43:GLN:HA	5:F:46:MET:SD	2.60	0.41
5:F:658:LYS:HB2	5:F:658:LYS:HE3	1.62	0.41
5:C:474:VAL:O	5:C:530:ALA:HA	2.20	0.41
5:D:275:MET:CE	5:D:309:ILE:HG12	2.50	0.41
5:D:757:MET:O	5:D:761:THR:HG23	2.19	0.41
5:E:476:TRP:HH2	5:E:490:GLN:HG3	1.85	0.41
5:F:191:ARG:HD2	5:F:191:ARG:HA	1.68	0.41
5:F:647:LEU:HD12	5:F:648:PRO:HD2	2.01	0.41
1:G:6:ILE:H	1:G:71:HIS:CE1	2.38	0.41
3:M:554:ARG:NH1	3:M:607:GLY:HA2	2.35	0.41
5:A:93:ARG:CZ	5:A:196:GLU:HA	2.50	0.41
5:A:388:MET:HE1	5:A:419:ALA:HB2	2.01	0.41
5:A:476:TRP:HE3	5:A:534:GLU:HG3	1.86	0.41
5:A:744:ARG:H	5:A:744:ARG:HG2	1.68	0.41
5:F:705:SER:CB	5:F:727:PRO:HG2	2.51	0.41
1:G:207:LYS:HE3	1:G:207:LYS:HB2	1.82	0.41
5:B:203:TYR:HD1	5:B:203:TYR:HA	1.63	0.41
5:B:700:ARG:HH11	5:C:491:GLU:CD	2.29	0.41
5:C:391:ALA:O	5:C:394:VAL:HG23	2.20	0.41
5:D:658:LYS:O	5:D:662:ARG:HG3	2.20	0.41
5:E:482:LEU:HB3	5:E:485:VAL:HB	2.01	0.41
1:G:414:GLU:H	1:G:414:GLU:HG2	1.68	0.41
2:I:33:LYS:HG2	2:I:35:GLY:H	1.86	0.41
3:M:576:LEU:HD12	3:M:644:LEU:HG	2.02	0.41
3:M:606:LYS:HD3	3:M:606:LYS:HA	1.93	0.41
5:A:307:ASP:OD1	5:A:347:THR:HB	2.20	0.41
5:C:350:PRO:HB2	5:C:358:ARG:NH2	2.36	0.41
5:C:657:LEU:HD23	5:C:657:LEU:HA	1.83	0.41
5:D:244:TYR:CD2	5:D:350:PRO:HG3	2.55	0.41
5:F:650:GLU:C	5:F:652:SER:H	2.28	0.41
1:G:8:ARG:O	1:G:74:LEU:HA	2.20	0.41
1:G:560:GLY:HA2	2:K:73:LEU:H	1.85	0.41
2:I:15:LEU:HD23	2:I:15:LEU:HA	1.87	0.41
5:A:155:ARG:HD2	5:A:160:ALA:O	2.21	0.41
5:C:83:ARG:HD3	5:C:83:ARG:HA	1.87	0.41
5:D:565:LYS:O	5:D:568:GLN:HG3	2.20	0.41
5:E:336:LYS:HE3	5:E:337:GLN:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:543:LYS:HB3	5:E:545:PRO:HD2	2.02	0.41
5:F:42:SER:OG	5:F:44:PRO:HD2	2.20	0.41
5:F:437:ILE:HD13	5:F:437:ILE:H	1.85	0.41
1:G:488:LEU:HD13	1:G:509:LEU:HD11	2.03	0.41
1:G:520:PRO:HB2	1:G:522:GLN:NE2	2.28	0.41
5:A:20:LYS:H	5:A:25:ARG:HH12	1.67	0.41
5:B:390:LEU:H	5:B:390:LEU:HD12	1.86	0.41
5:E:600:VAL:O	5:E:604:ILE:HG12	2.20	0.41
5:F:207:GLY:H	8:F:901:ADP:HN61	1.68	0.41
5:F:701:GLU:O	5:F:704:GLU:HG3	2.20	0.41
1:G:430:ASP:HB3	1:G:436:ILE:CD1	2.50	0.41
5:B:737:GLU:HA	5:B:740:MET:HE2	2.02	0.41
5:C:88:VAL:HA	5:C:91:ASN:HB2	2.02	0.41
5:C:139:PHE:CG	5:C:176:VAL:HG11	2.56	0.41
5:C:201:VAL:HG21	5:C:256:ARG:HH12	1.86	0.41
5:C:327:GLN:HG3	5:C:331:LEU:HD12	2.02	0.41
5:C:335:LEU:HD23	5:C:335:LEU:HA	1.90	0.41
5:C:383:ILE:HD11	7:C:901:ATP:C2	2.56	0.41
5:C:442:MET:HE1	5:D:229:LEU:HD13	2.03	0.41
5:C:538:ASN:HD22	5:C:569:ALA:HB1	1.85	0.41
5:C:539:PHE:CZ	5:C:541:SER:HB3	2.56	0.41
5:E:615:LYS:HD2	5:E:615:LYS:HA	1.89	0.41
5:F:86:ARG:HD3	5:F:86:ARG:HA	1.81	0.41
1:G:30:LEU:HD12	1:G:58:ALA:HB2	2.03	0.41
1:G:232:THR:HG21	1:G:466:ILE:HG12	2.02	0.41
5:A:540:ILE:HB	5:A:574:LEU:HD12	2.03	0.41
5:B:262:THR:HG23	5:B:264:ALA:N	2.34	0.41
5:B:376:GLY:O	5:B:380:ILE:HG12	2.21	0.41
5:C:157:GLY:O	5:C:158:MET:HB3	2.20	0.41
5:C:501:ASP:O	5:C:504:LEU:HG	2.21	0.41
5:C:670:VAL:HG11	5:C:736:PHE:HD2	1.85	0.41
5:D:286:LEU:HD22	5:D:324:ILE:HD11	2.02	0.41
5:F:172:PRO:HB2	5:F:173:TYR:CE2	2.56	0.41
5:F:653:ARG:NH1	5:F:681:GLY:H	2.18	0.41
3:M:536:GLN:CD	3:M:536:GLN:N	2.79	0.41
5:A:108:VAL:HG23	5:A:174:CYS:HA	2.02	0.41
5:C:674:PHE:O	5:C:678:MET:HE2	2.21	0.41
5:D:491:GLU:HG3	5:D:495:TYR:CE2	2.56	0.41
5:D:658:LYS:HE3	5:D:658:LYS:HB3	1.83	0.41
5:F:138:TYR:HE2	5:F:152:PHE:CD2	2.38	0.41
5:F:220:VAL:HG22	5:F:342:ILE:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:VAL:HG22	1:G:183:LEU:HD23	2.02	0.40
5:C:703:ILE:O	5:C:707:ILE:HG12	2.20	0.40
5:D:316:THR:HB	5:D:321:GLU:HG3	2.02	0.40
5:F:94:VAL:HG11	5:F:100:ILE:HD11	2.02	0.40
5:F:385:THR:HB	5:F:390:LEU:HD11	2.03	0.40
3:M:577:ARG:HE	3:M:587:GLU:CD	2.29	0.40
5:B:409:ALA:HB2	7:B:901:ATP:H5'1	2.03	0.40
5:B:427:MET:HE3	5:C:222:LEU:HD11	2.02	0.40
5:C:307:ASP:OD1	5:C:307:ASP:C	2.64	0.40
5:C:420:LEU:HD23	5:C:420:LEU:HA	1.87	0.40
5:E:189:ILE:HD12	5:E:192:GLU:H	1.86	0.40
5:E:244:TYR:CZ	5:E:368:ASP:HB2	2.56	0.40
5:E:703:ILE:HD13	5:F:495:TYR:CE1	2.56	0.40
5:E:736:PHE:O	5:E:737:GLU:HB2	2.22	0.40
5:F:516:PHE:CD1	5:F:643:ILE:HB	2.56	0.40
1:G:464:PHE:CE2	1:G:507:PHE:HB2	2.55	0.40
5:B:697:LEU:O	5:B:700:ARG:HG2	2.22	0.40
5:C:539:PHE:CE2	5:C:541:SER:HB3	2.57	0.40
5:E:479:ILE:HD13	5:E:479:ILE:HA	1.93	0.40
5:F:582:ILE:HG21	5:F:601:ILE:HD11	2.01	0.40
1:G:144:LEU:HA	1:G:144:LEU:HD23	1.85	0.40
1:G:179:LYS:HB2	1:G:179:LYS:HE3	1.84	0.40
1:G:555:LEU:HD21	2:K:44:ILE:HG21	2.04	0.40
5:A:207:GLY:H	7:A:901:ATP:HN62	1.69	0.40
5:A:381:LEU:HD21	5:A:411:LEU:HD22	2.02	0.40
5:B:476:TRP:O	5:B:479:ILE:HG12	2.21	0.40
5:B:697:LEU:HA	5:B:700:ARG:HG2	2.03	0.40
5:C:93:ARG:HH12	5:C:198:LEU:HD23	1.87	0.40
5:C:749:ASP:HA	5:C:752:ILE:HD12	2.03	0.40
5:D:267:PHE:CE2	5:D:289:ALA:HA	2.56	0.40
5:D:402:GLU:CD	5:D:453:ARG:HH12	2.28	0.40
5:E:558:ASN:O	5:E:561:GLU:HB3	2.22	0.40
5:F:500:PRO:O	5:F:504:LEU:HD23	2.22	0.40
3:M:600:PHE:O	3:M:603:VAL:HG12	2.21	0.40
4:P:228:PHE:HB3	4:P:245:SER:O	2.22	0.40
7:C:901:ATP:H5'1	5:D:359:ARG:NH1	2.36	0.40
5:D:494:GLN:HE22	5:D:534:GLU:HB3	1.85	0.40
5:E:398:GLN:O	5:E:402:GLU:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	G	532/611 (87%)	502 (94%)	30 (6%)	0	100	100
2	I	38/76 (50%)	33 (87%)	5 (13%)	0	100	100
2	K	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
3	M	120/173 (69%)	115 (96%)	5 (4%)	0	100	100
3	O	102/173 (59%)	99 (97%)	3 (3%)	0	100	100
4	P	67/313 (21%)	58 (87%)	9 (13%)	0	100	100
5	A	725/821 (88%)	665 (92%)	58 (8%)	2 (0%)	36	65
5	B	544/821 (66%)	494 (91%)	50 (9%)	0	100	100
5	C	709/821 (86%)	664 (94%)	42 (6%)	3 (0%)	30	60
5	D	533/821 (65%)	492 (92%)	39 (7%)	2 (0%)	30	60
5	E	550/821 (67%)	508 (92%)	42 (8%)	0	100	100
5	F	723/821 (88%)	682 (94%)	40 (6%)	1 (0%)	48	79
All	All	4717/6348 (74%)	4384 (93%)	325 (7%)	8 (0%)	44	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	297	ALA
5	D	298	PRO
5	D	472	PRO
5	C	747	VAL
5	F	16	ILE
5	C	297	ALA
5	A	181	VAL
5	C	201	VAL

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	G	476/531 (90%)	455 (96%)	21 (4%)	25	51
2	I	36/68 (53%)	34 (94%)	2 (6%)	19	46
2	K	68/68 (100%)	67 (98%)	1 (2%)	57	70
3	M	113/155 (73%)	111 (98%)	2 (2%)	51	68
3	O	96/155 (62%)	96 (100%)	0	100	100
4	P	58/273 (21%)	55 (95%)	3 (5%)	21	48
5	A	625/690 (91%)	596 (95%)	29 (5%)	24	50
5	B	451/690 (65%)	420 (93%)	31 (7%)	14	41
5	C	615/690 (89%)	593 (96%)	22 (4%)	31	56
5	D	450/690 (65%)	433 (96%)	17 (4%)	29	55
5	E	468/690 (68%)	439 (94%)	29 (6%)	16	44
5	F	622/690 (90%)	584 (94%)	38 (6%)	17	44
All	All	4078/5390 (76%)	3883 (95%)	195 (5%)	24	49

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	105	VAL
1	G	140	HIS
1	G	141	CYS
1	G	142	VAL
1	G	149	GLU
1	G	152	LEU
1	G	168	ILE
1	G	180	PHE
1	G	183	LEU
1	G	198	LEU
1	G	204	ILE
1	G	224	ASP
1	G	305	LEU
1	G	311	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	357	LEU
1	G	368	VAL
1	G	421	VAL
1	G	437	THR
1	G	466	ILE
1	G	518	VAL
1	G	559	VAL
2	I	13	ILE
2	I	26	VAL
2	K	67	LEU
3	M	580	THR
3	M	588	ARG
4	P	240	LYS
4	P	258	ILE
4	P	277	LEU
5	A	28	VAL
5	A	49	LEU
5	A	59	LEU
5	A	93	ARG
5	A	108	VAL
5	A	161	VAL
5	A	274	ILE
5	A	276	SER
5	A	278	LEU
5	A	303	ILE
5	A	336	LYS
5	A	344	MET
5	A	347	THR
5	A	364	ASP
5	A	384	HIS
5	A	407	VAL
5	A	448	THR
5	A	454	TRP
5	A	489	LEU
5	A	514	VAL
5	A	548	LEU
5	A	608	MET
5	A	634	LEU
5	A	647	LEU
5	A	661	LEU
5	A	670	VAL
5	A	714	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	747	VAL
5	A	750	ASN
5	B	203	TYR
5	B	204	ASP
5	B	222	LEU
5	B	254	ILE
5	B	275	MET
5	B	283	GLU
5	B	286	LEU
5	B	300	ILE
5	B	313	ARG
5	B	317	HIS
5	B	320	VAL
5	B	325	VAL
5	B	343	VAL
5	B	347	THR
5	B	366	GLU
5	B	390	LEU
5	B	420	LEU
5	B	437	ILE
5	B	448	THR
5	B	489	LEU
5	B	548	LEU
5	B	559	VAL
5	B	600	VAL
5	B	601	ILE
5	B	611	MET
5	B	634	LEU
5	B	666	VAL
5	B	675	LEU
5	B	677	LYS
5	B	691	CYS
5	B	697	LEU
5	C	32	ILE
5	C	107	ASP
5	C	124	GLU
5	C	203	TYR
5	C	274	ILE
5	C	317	HIS
5	C	328	LEU
5	C	332	MET
5	C	343	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	381	LEU
5	C	394	VAL
5	C	468	VAL
5	C	475	THR
5	C	484	ASP
5	C	509	THR
5	C	514	VAL
5	C	522	CYS
5	C	556	GLU
5	C	606	THR
5	C	617	VAL
5	C	688	THR
5	C	700	ARG
5	D	195	GLU
5	D	206	ILE
5	D	300	ILE
5	D	342	ILE
5	D	343	VAL
5	D	358	ARG
5	D	445	LEU
5	D	450	ASP
5	D	492	LEU
5	D	514	VAL
5	D	550	MET
5	D	619	ILE
5	D	639	LEU
5	D	651	LYS
5	D	670	VAL
5	D	706	GLU
5	D	756	GLU
5	E	199	ASN
5	E	218	GLU
5	E	315	LYS
5	E	332	MET
5	E	406	HIS
5	E	407	VAL
5	E	420	LEU
5	E	429	LEU
5	E	468	VAL
5	E	469	VAL
5	E	476	TRP
5	E	497	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	514	VAL
5	E	517	TYR
5	E	527	LEU
5	E	529	LYS
5	E	538	ASN
5	E	542	ILE
5	E	617	VAL
5	E	634	LEU
5	E	635	ARG
5	E	642	LEU
5	E	647	LEU
5	E	654	VAL
5	E	671	ASP
5	E	683	SER
5	E	688	THR
5	E	689	GLU
5	E	744	ARG
5	F	16	ILE
5	F	17	LEU
5	F	112	LYS
5	F	151	ILE
5	F	153	LEU
5	F	165	VAL
5	F	169	ASP
5	F	173	TYR
5	F	201	VAL
5	F	203	TYR
5	F	206	ILE
5	F	222	LEU
5	F	295	LYS
5	F	300	ILE
5	F	303	ILE
5	F	317	HIS
5	F	341	VAL
5	F	342	ILE
5	F	390	LEU
5	F	394	VAL
5	F	407	VAL
5	F	420	LEU
5	F	435	GLU
5	F	437	ILE
5	F	448	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	457	SER
5	F	489	LEU
5	F	514	VAL
5	F	599	ARG
5	F	611	MET
5	F	666	VAL
5	F	674	PHE
5	F	678	MET
5	F	682	PHE
5	F	683	SER
5	F	709	ARG
5	F	728	VAL
5	F	731	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	154	HIS
1	G	161	HIS
1	G	225	ASN
1	G	246	ASN
1	G	282	GLN
1	G	283	ASN
1	G	379	GLN
1	G	494	GLN
1	G	522	GLN
5	A	348	ASN
5	A	351	ASN
5	A	533	ASN
5	A	680	ASN
5	A	714	GLN
5	B	348	ASN
5	B	735	HIS
5	C	115	HIS
5	C	327	GLN
5	C	351	ASN
5	C	499	HIS
5	D	602	ASN
5	D	603	GLN
5	D	735	HIS
5	D	760	GLN
5	E	317	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	460	ASN
5	E	660	ASN
5	E	680	ASN
5	F	317	HIS
5	F	387	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 14 ligands modelled in this entry, 2 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	$\# Z > 2$
7	ATP	B	901	-	32,33,33	0.93	2 (6%)	48,52,52	0.48	0
7	ATP	A	901	-	32,33,33	1.28	2 (6%)	48,52,52	0.37	0
8	ADP	E	902	-	28,29,29	1.36	4 (14%)	43,45,45	1.96	8 (18%)
8	ADP	D	901	-	28,29,29	1.35	5 (17%)	43,45,45	1.87	9 (20%)
8	ADP	C	902	-	28,29,29	1.39	4 (14%)	43,45,45	1.89	8 (18%)
8	ADP	A	902	-	28,29,29	1.36	4 (14%)	43,45,45	1.91	8 (18%)
8	ADP	F	902	-	28,29,29	1.36	4 (14%)	43,45,45	1.96	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ADP	B	902	-	28,29,29	1.39	5 (17%)	43,45,45	1.81	8 (18%)
7	ATP	C	901	-	32,33,33	1.27	2 (6%)	48,52,52	0.44	0
8	ADP	D	902	-	28,29,29	1.41	4 (14%)	43,45,45	1.91	8 (18%)
8	ADP	F	901	-	28,29,29	1.36	5 (17%)	43,45,45	1.77	9 (20%)
8	ADP	E	901	-	28,29,29	1.40	4 (14%)	43,45,45	1.88	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
7	ATP	B	901	-	-	6/22/38/38	0/3/3/3
7	ATP	A	901	-	-	3/22/38/38	0/3/3/3
8	ADP	E	902	-	-	2/16/32/32	0/3/3/3
8	ADP	D	901	-	-	4/16/32/32	0/3/3/3
8	ADP	C	902	-	-	4/16/32/32	0/3/3/3
8	ADP	A	902	-	-	1/16/32/32	0/3/3/3
8	ADP	F	902	-	-	5/16/32/32	0/3/3/3
8	ADP	B	902	-	-	2/16/32/32	0/3/3/3
7	ATP	C	901	-	-	6/22/38/38	0/3/3/3
8	ADP	D	902	-	-	3/16/32/32	0/3/3/3
8	ADP	F	901	-	-	7/16/32/32	0/3/3/3
8	ADP	E	901	-	-	3/16/32/32	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	901	ATP	PB-O3B	-5.23	1.53	1.59
7	A	901	ATP	PB-O3B	-4.90	1.54	1.59
8	C	902	ADP	C5-C4	4.79	1.47	1.39
7	A	901	ATP	PA-O3A	-4.72	1.54	1.59
8	D	902	ADP	C5-C4	4.70	1.47	1.39
8	B	902	ADP	C5-C4	4.63	1.47	1.39
8	A	902	ADP	C5-C4	4.55	1.47	1.39
8	E	902	ADP	C5-C4	4.54	1.47	1.39
8	F	902	ADP	C5-C4	4.53	1.47	1.39
7	C	901	ATP	PA-O3A	-4.27	1.54	1.59
8	E	901	ADP	C5-C4	4.27	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	901	ADP	C5-C4	4.00	1.46	1.39
8	F	901	ADP	C5-C4	3.93	1.46	1.39
7	B	901	ATP	PB-O3B	-3.34	1.55	1.59
8	E	901	ADP	C5-N7	-3.08	1.33	1.39
7	B	901	ATP	PA-O3A	-3.08	1.56	1.59
8	D	901	ADP	C5-N7	-2.93	1.33	1.39
8	F	901	ADP	C5-N7	-2.91	1.33	1.39
8	E	902	ADP	C5-N7	-2.68	1.34	1.39
8	C	902	ADP	C5-C6	2.67	1.48	1.41
8	B	902	ADP	C5-N7	-2.62	1.34	1.39
8	F	902	ADP	C5-N7	-2.59	1.34	1.39
8	D	902	ADP	C5-N7	-2.57	1.34	1.39
8	D	902	ADP	C5-C6	2.56	1.48	1.41
8	A	902	ADP	C5-N7	-2.53	1.34	1.39
8	A	902	ADP	C5-C6	2.52	1.48	1.41
8	B	902	ADP	C5-C6	2.47	1.47	1.41
8	C	902	ADP	C5-N7	-2.47	1.34	1.39
8	F	901	ADP	C4-N9	-2.43	1.32	1.37
8	E	902	ADP	C5-C6	2.41	1.47	1.41
8	F	902	ADP	C5-C6	2.38	1.47	1.41
8	D	901	ADP	C4-N9	-2.21	1.33	1.37
8	C	902	ADP	C8-N7	2.19	1.35	1.31
8	D	902	ADP	C8-N7	2.16	1.35	1.31
8	A	902	ADP	C8-N7	2.13	1.35	1.31
8	F	901	ADP	C5-C6	2.11	1.46	1.41
8	E	901	ADP	C5-C6	2.10	1.46	1.41
8	D	901	ADP	C5-C6	2.08	1.46	1.41
8	E	901	ADP	C4-N9	-2.08	1.33	1.37
8	B	902	ADP	C8-N7	2.07	1.35	1.31
8	D	901	ADP	C8-N7	2.04	1.35	1.31
8	F	902	ADP	C8-N7	2.03	1.35	1.31
8	B	902	ADP	C4-N9	-2.03	1.33	1.37
8	E	902	ADP	C8-N7	2.01	1.35	1.31
8	F	901	ADP	C8-N7	2.01	1.35	1.31

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	902	ADP	C5-C4-N3	-6.37	117.95	126.72
8	A	902	ADP	C5-C4-N3	-6.35	117.97	126.72
8	E	902	ADP	C5-C4-N3	-6.34	117.98	126.72
8	D	902	ADP	C5-C4-N3	-6.33	118.00	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	902	ADP	C5-C4-N3	-6.31	118.02	126.72
8	D	901	ADP	C5-C4-N3	-6.16	118.24	126.72
8	E	901	ADP	C5-C4-N3	-6.14	118.26	126.72
8	B	902	ADP	C5-C4-N3	-5.80	118.73	126.72
8	F	901	ADP	C5-C4-N3	-5.52	119.11	126.72
8	F	902	ADP	N3-C4-N9	5.44	136.41	127.17
8	E	902	ADP	N3-C4-N9	5.27	136.13	127.17
8	A	902	ADP	N3-C4-N9	5.19	136.00	127.17
8	D	902	ADP	N3-C4-N9	5.10	135.83	127.17
8	C	902	ADP	N3-C4-N9	5.05	135.75	127.17
8	D	901	ADP	N3-C4-N9	4.97	135.63	127.17
8	E	901	ADP	N3-C4-N9	4.92	135.53	127.17
8	B	902	ADP	N3-C4-N9	4.83	135.38	127.17
8	F	901	ADP	N3-C4-N9	4.41	134.66	127.17
8	F	902	ADP	C2-N3-C4	3.86	121.25	111.83
8	A	902	ADP	C2-N3-C4	3.85	121.24	111.83
8	C	902	ADP	C2-N3-C4	3.84	121.21	111.83
8	D	902	ADP	C2-N3-C4	3.80	121.11	111.83
8	E	902	ADP	C2-N3-C4	3.78	121.06	111.83
8	E	901	ADP	C2-N3-C4	3.76	121.01	111.83
8	D	901	ADP	C2-N3-C4	3.71	120.89	111.83
8	B	902	ADP	C2-N3-C4	3.52	120.42	111.83
8	F	901	ADP	C2-N3-C4	3.42	120.18	111.83
8	C	902	ADP	C4-C5-N7	-3.41	106.68	110.58
8	D	902	ADP	C4-C5-N7	-3.36	106.74	110.58
8	E	902	ADP	C4-C5-N7	-3.29	106.82	110.58
8	D	902	ADP	N3-C2-N1	-3.24	123.67	128.58
8	F	902	ADP	N3-C2-N1	-3.23	123.69	128.58
8	E	901	ADP	N3-C2-N1	-3.22	123.70	128.58
8	C	902	ADP	N3-C2-N1	-3.19	123.75	128.58
8	A	902	ADP	C4-C5-N7	-3.18	106.95	110.58
8	E	902	ADP	N3-C2-N1	-3.18	123.78	128.58
8	D	901	ADP	N3-C2-N1	-3.16	123.80	128.58
8	A	902	ADP	N3-C2-N1	-3.15	123.81	128.58
8	B	902	ADP	C4-C5-N7	-3.04	107.11	110.58
8	D	901	ADP	C4-C5-N7	-3.00	107.16	110.58
8	B	902	ADP	N3-C2-N1	-2.98	124.07	128.58
8	D	902	ADP	C3'-C2'-C1'	2.96	107.07	101.46
8	F	901	ADP	C4-C5-N7	-2.95	107.21	110.58
8	F	902	ADP	C4-C5-N7	-2.90	107.27	110.58
8	F	902	ADP	C3'-C2'-C1'	2.89	106.92	101.46
8	E	902	ADP	C3'-C2'-C1'	2.86	106.87	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	901	ADP	C4-C5-N7	-2.84	107.33	110.58
8	F	901	ADP	N3-C2-N1	-2.79	124.36	128.58
8	E	901	ADP	C3'-C2'-C1'	2.75	106.67	101.46
8	F	902	ADP	C4-N9-C8	2.70	108.58	105.74
8	E	902	ADP	C4-N9-C8	2.68	108.55	105.74
8	E	902	ADP	C5-N7-C8	2.65	107.62	103.45
8	B	902	ADP	C4-N9-C8	2.65	108.52	105.74
8	C	902	ADP	C3'-C2'-C1'	2.63	106.44	101.46
8	B	902	ADP	C3'-C2'-C1'	2.60	106.38	101.46
8	F	901	ADP	C4-N9-C8	2.58	108.44	105.74
8	D	901	ADP	C4-N9-C8	2.57	108.44	105.74
8	C	902	ADP	C5-N7-C8	2.53	107.42	103.45
8	D	902	ADP	C5-N7-C8	2.51	107.40	103.45
8	D	901	ADP	C3'-C2'-C1'	2.51	106.21	101.46
8	A	902	ADP	C4-N9-C8	2.46	108.32	105.74
8	D	902	ADP	C4-N9-C8	2.36	108.22	105.74
8	A	902	ADP	C5-N7-C8	2.36	107.16	103.45
8	F	901	ADP	C2'-C3'-C4'	2.34	107.12	102.61
8	F	902	ADP	C5-N7-C8	2.34	107.12	103.45
8	C	902	ADP	C4-N9-C8	2.32	108.18	105.74
8	A	902	ADP	C3'-C2'-C1'	2.31	105.83	101.46
8	D	901	ADP	C5-N7-C8	2.28	107.03	103.45
8	B	902	ADP	C5-N7-C8	2.27	107.02	103.45
8	F	901	ADP	C2'-C1'-N9	-2.25	107.72	113.30
8	E	901	ADP	C2'-C3'-C4'	2.24	106.93	102.61
8	F	901	ADP	C5-N7-C8	2.18	106.87	103.45
8	D	901	ADP	C2'-C1'-N9	-2.13	108.01	113.30
8	E	901	ADP	C5-N7-C8	2.08	106.73	103.45

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	901	ATP	C5'-O5'-PA-O3A
7	B	901	ATP	C5'-O5'-PA-O1A
7	B	901	ATP	C5'-O5'-PA-O2A
7	B	901	ATP	C5'-O5'-PA-O3A
7	C	901	ATP	C5'-O5'-PA-O1A
7	C	901	ATP	C5'-O5'-PA-O2A
7	C	901	ATP	C5'-O5'-PA-O3A
7	C	901	ATP	O4'-C4'-C5'-O5'
8	A	902	ADP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

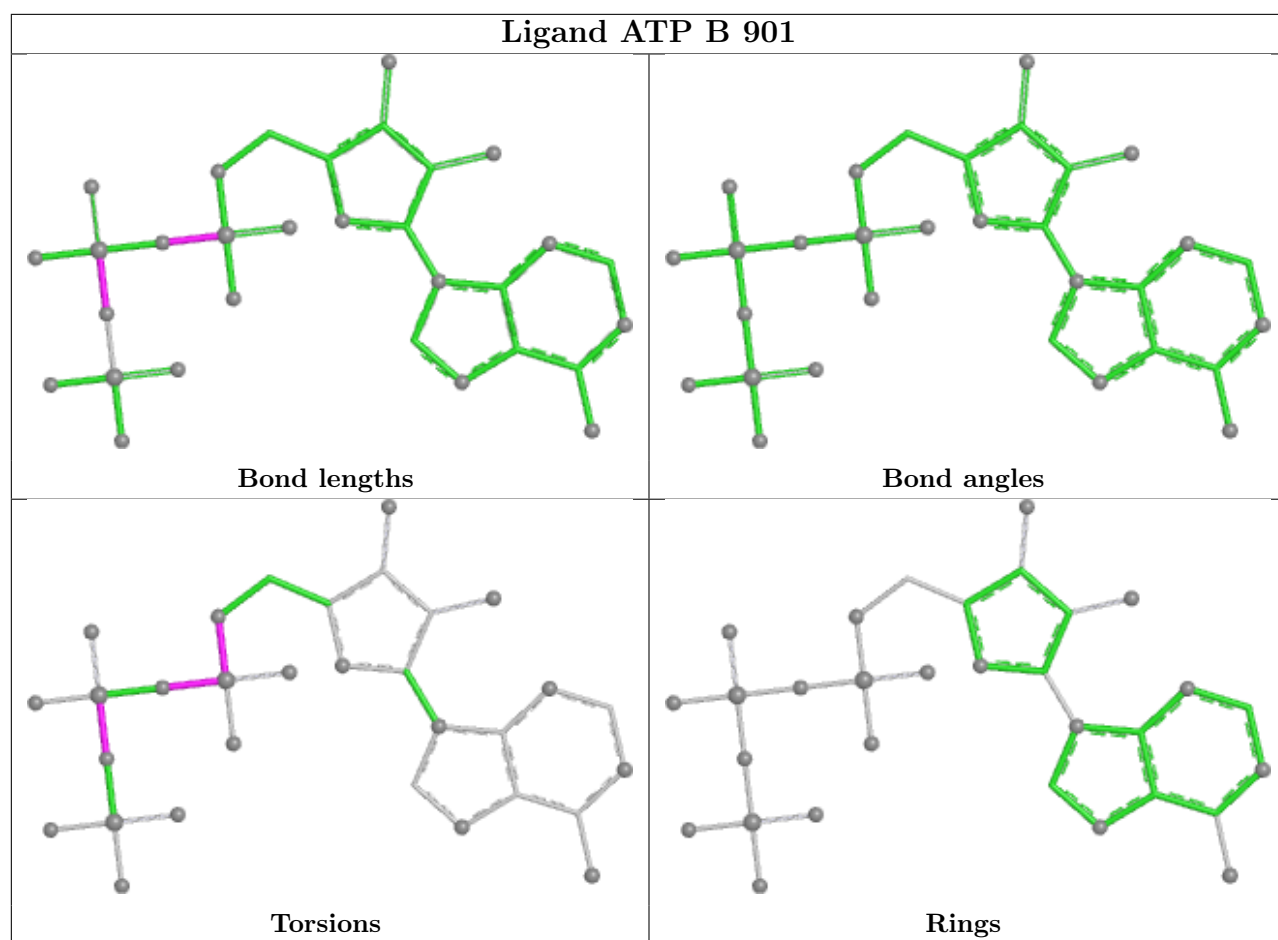
Mol	Chain	Res	Type	Atoms
8	B	902	ADP	C5'-O5'-PA-O2A
8	B	902	ADP	C5'-O5'-PA-O3A
8	C	902	ADP	C5'-O5'-PA-O3A
8	D	901	ADP	PA-O3A-PB-O3B
8	D	901	ADP	C5'-O5'-PA-O1A
8	D	901	ADP	O4'-C4'-C5'-O5'
8	D	901	ADP	C3'-C4'-C5'-O5'
8	D	902	ADP	C5'-O5'-PA-O3A
8	E	901	ADP	C5'-O5'-PA-O3A
8	E	902	ADP	C5'-O5'-PA-O1A
8	E	902	ADP	C5'-O5'-PA-O3A
8	F	901	ADP	C5'-O5'-PA-O1A
8	F	901	ADP	C5'-O5'-PA-O3A
8	F	902	ADP	C5'-O5'-PA-O1A
8	F	901	ADP	C3'-C4'-C5'-O5'
8	F	901	ADP	O4'-C4'-C5'-O5'
8	F	902	ADP	C3'-C4'-C5'-O5'
7	C	901	ATP	C3'-C4'-C5'-O5'
8	F	902	ADP	O4'-C4'-C5'-O5'
7	B	901	ATP	PB-O3A-PA-O5'
7	C	901	ATP	PB-O3B-PG-O3G
8	F	901	ADP	C2'-C1'-N9-C8
7	A	901	ATP	C5'-O5'-PA-O1A
8	C	902	ADP	C5'-O5'-PA-O1A
8	D	902	ADP	C5'-O5'-PA-O1A
8	E	901	ADP	C5'-O5'-PA-O1A
8	E	901	ADP	C3'-C4'-C5'-O5'
7	B	901	ATP	PG-O3B-PB-O2B
8	F	901	ADP	O4'-C1'-N9-C8
8	F	901	ADP	O4'-C1'-N9-C4
8	C	902	ADP	C2'-C1'-N9-C8
8	F	902	ADP	C2'-C1'-N9-C8
7	B	901	ATP	PB-O3A-PA-O1A
8	C	902	ADP	C2'-C1'-N9-C4
8	F	902	ADP	C2'-C1'-N9-C4
8	D	902	ADP	C2'-C1'-N9-C8
7	A	901	ATP	PB-O3A-PA-O2A

There are no ring outliers.

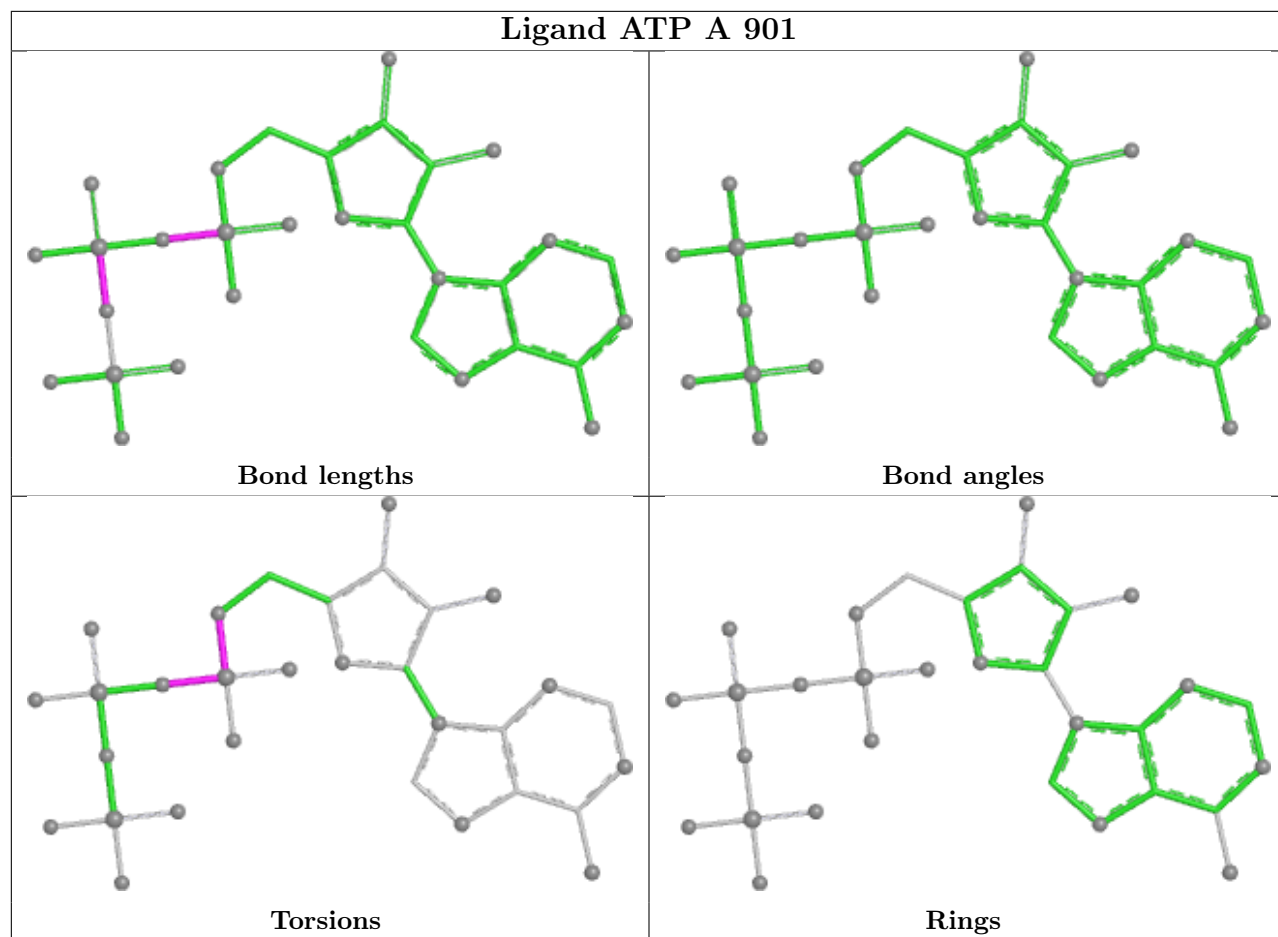
11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	901	ATP	1	0
7	A	901	ATP	3	0
8	E	902	ADP	2	0
8	C	902	ADP	2	0
8	A	902	ADP	1	0
8	F	902	ADP	1	0
8	B	902	ADP	3	0
7	C	901	ATP	3	0
8	D	902	ADP	1	0
8	F	901	ADP	3	0
8	E	901	ADP	1	0

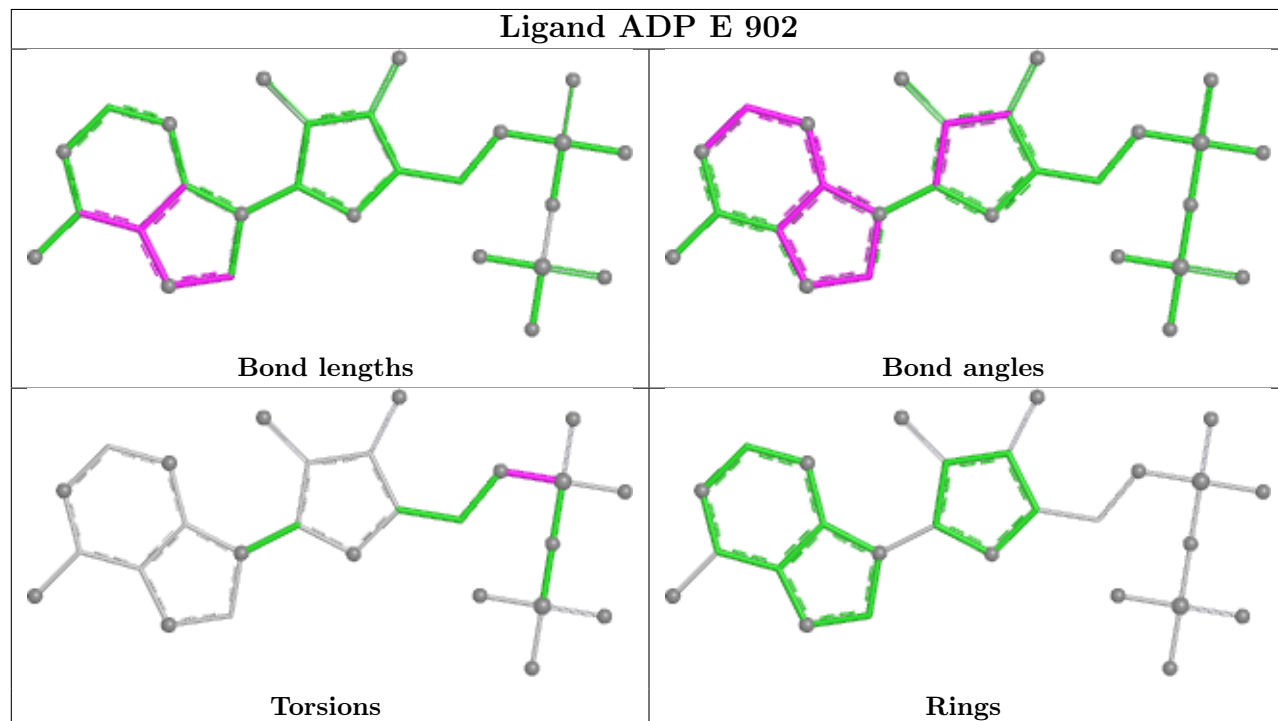
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

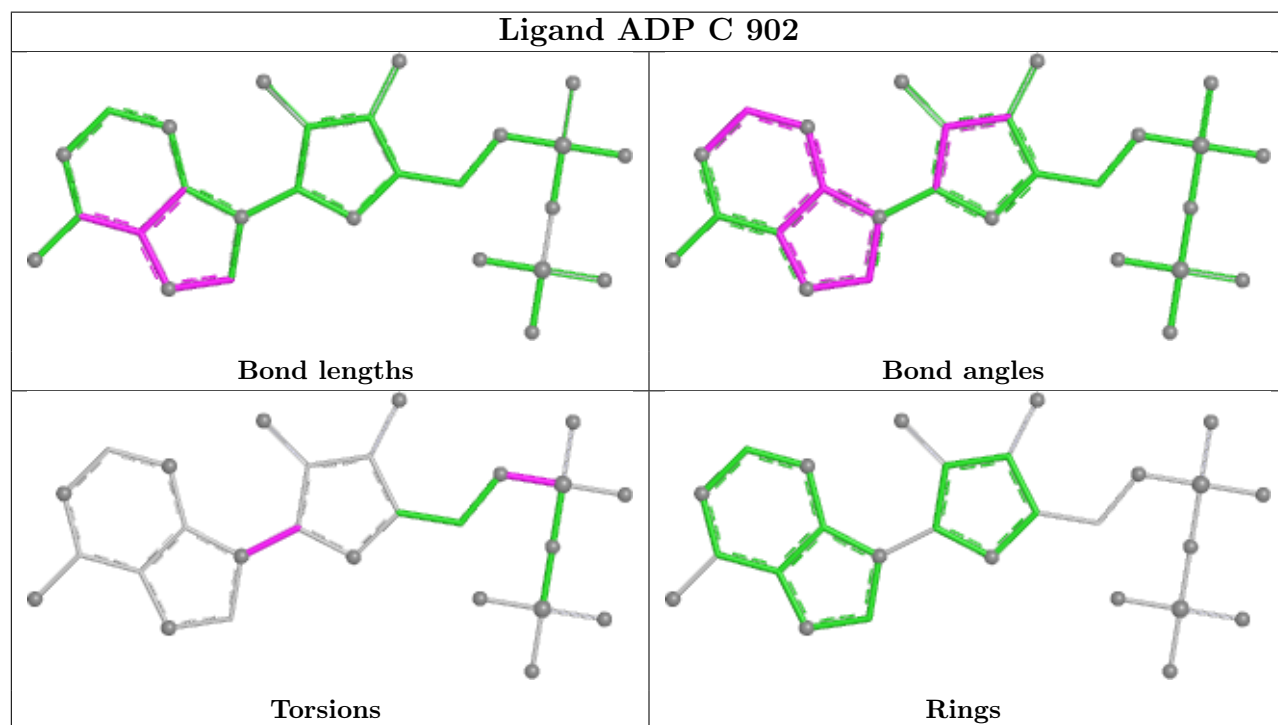
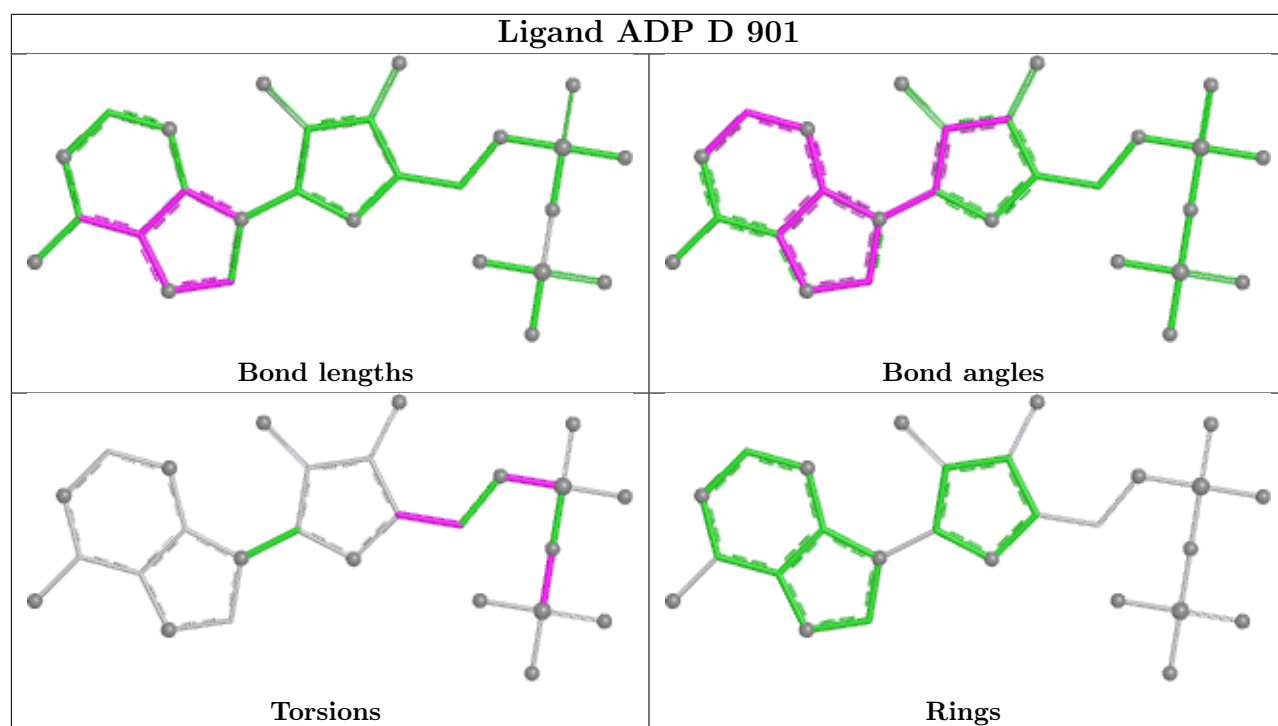


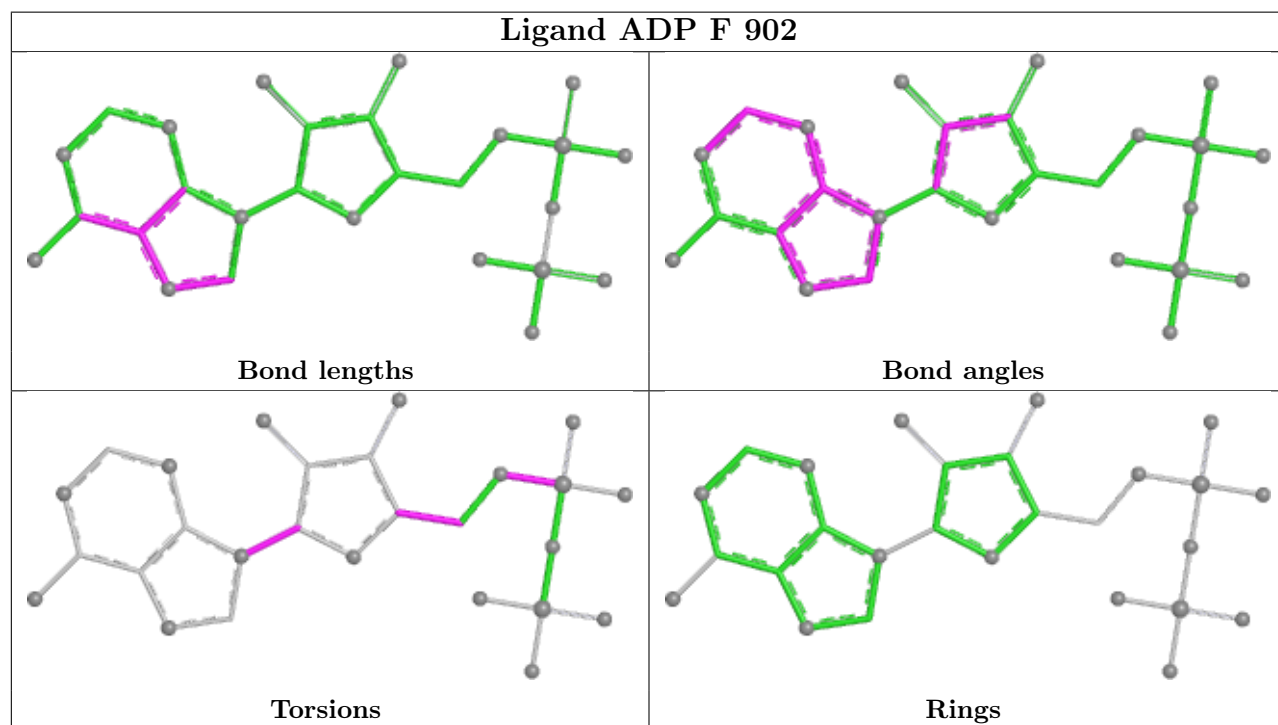
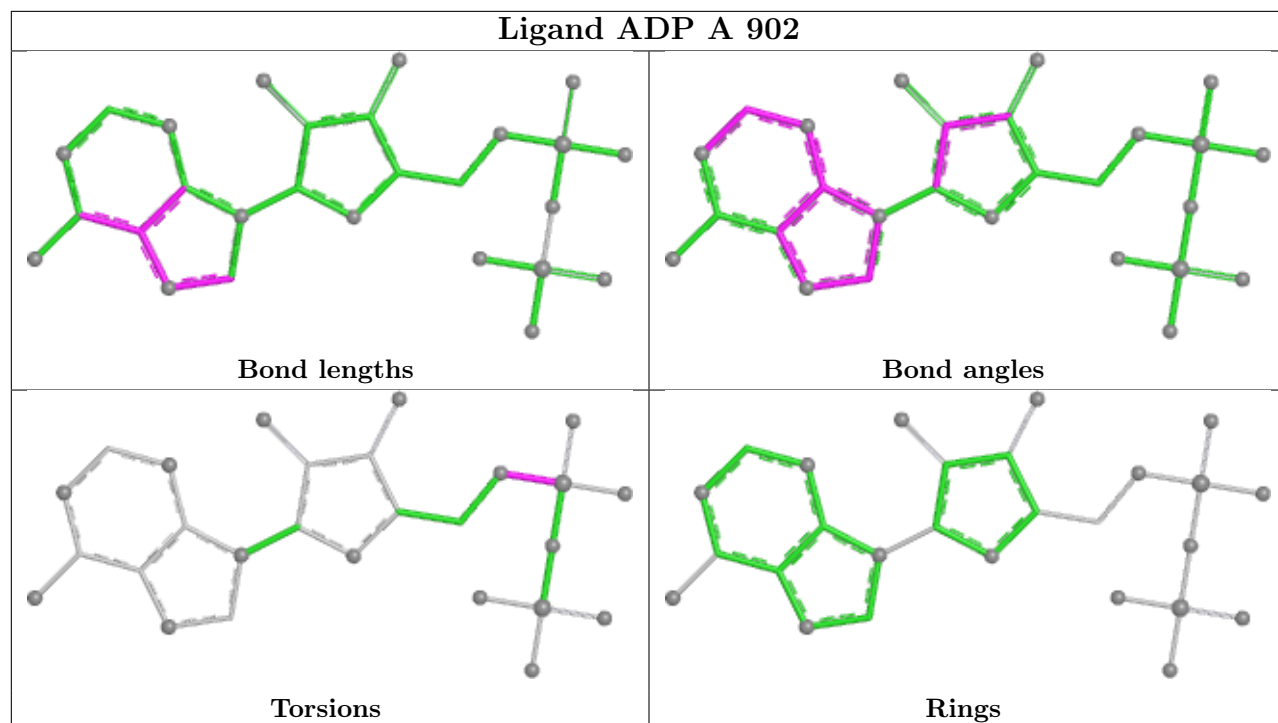
Ligand ATP A 901

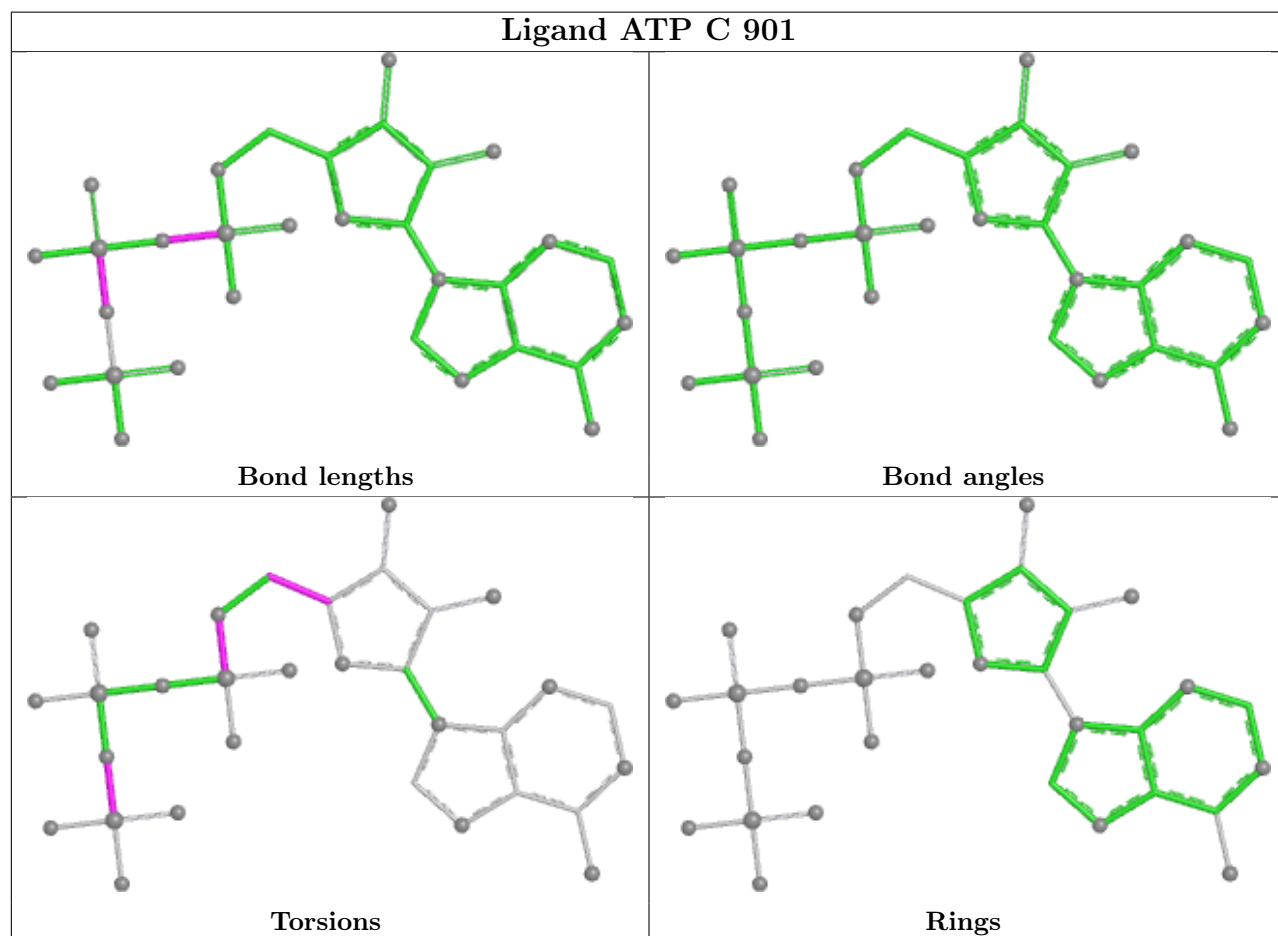
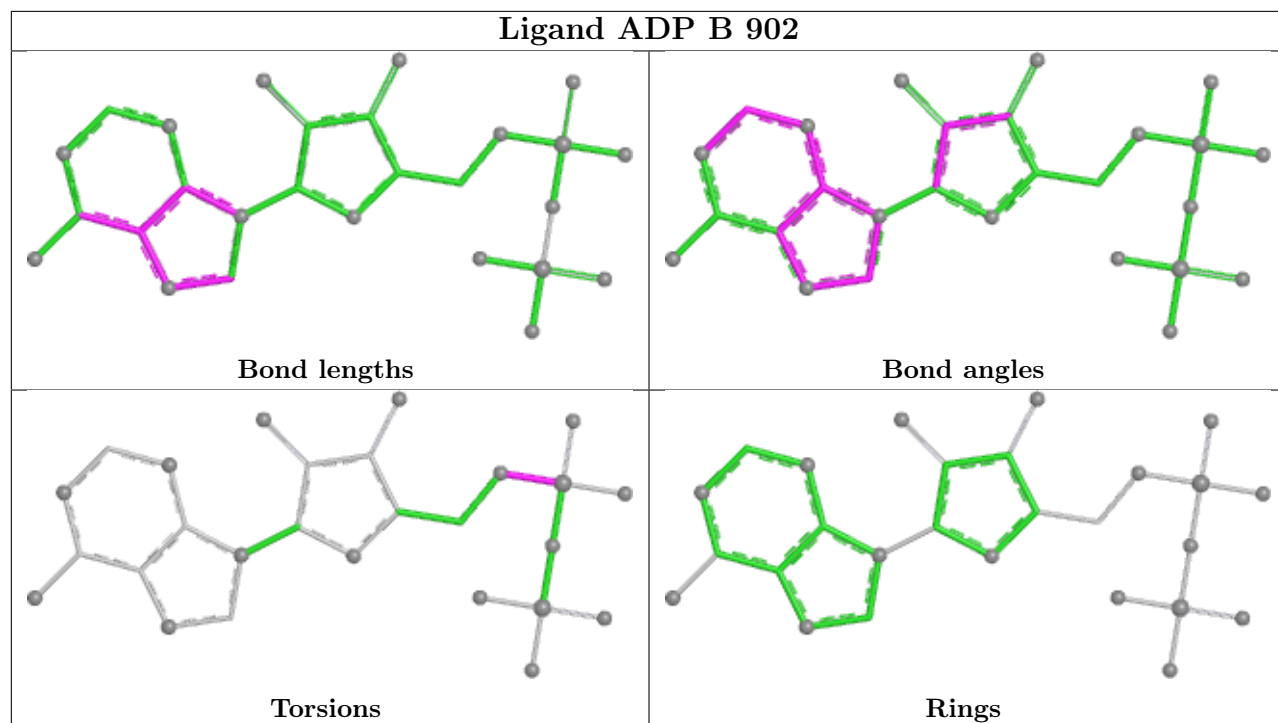


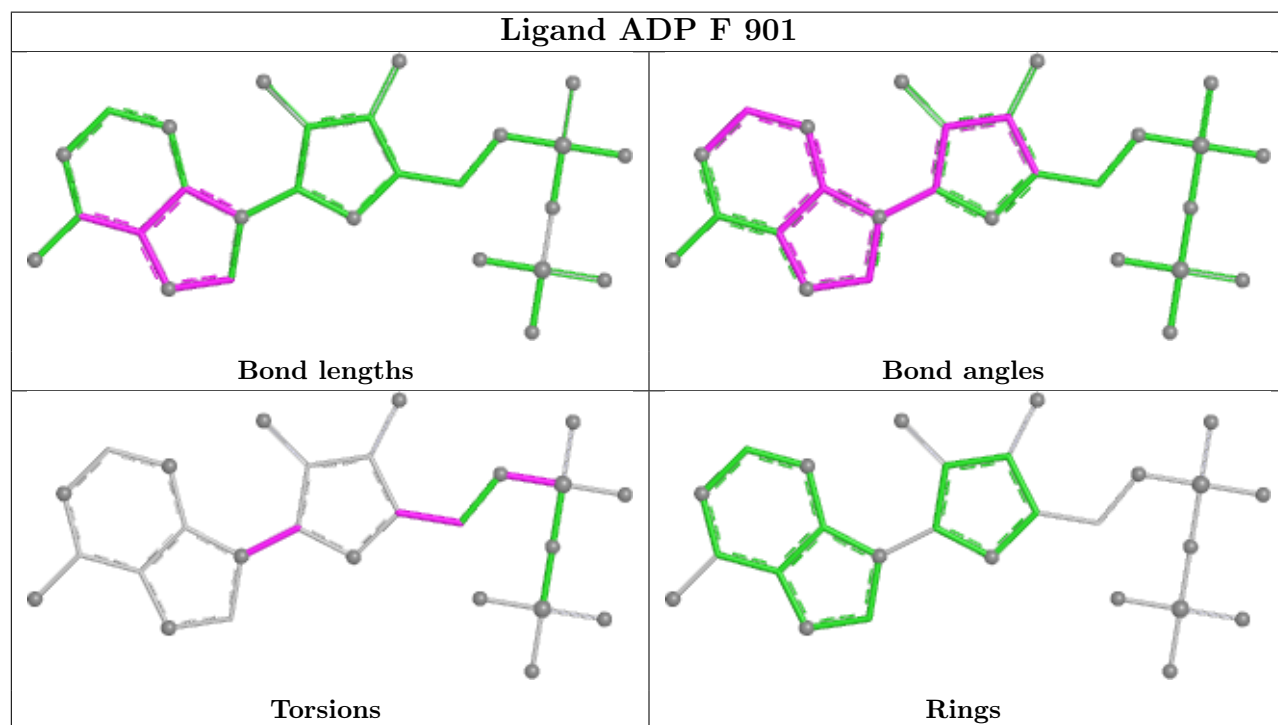
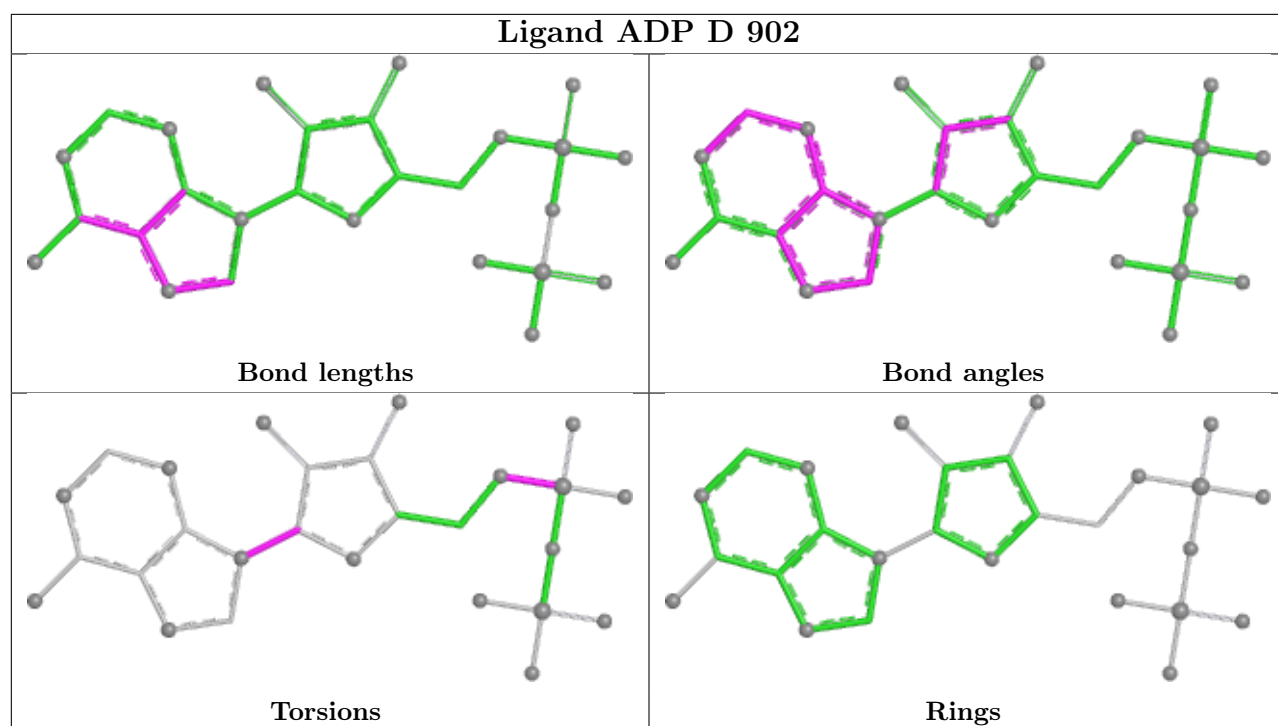
Ligand ADP E 902

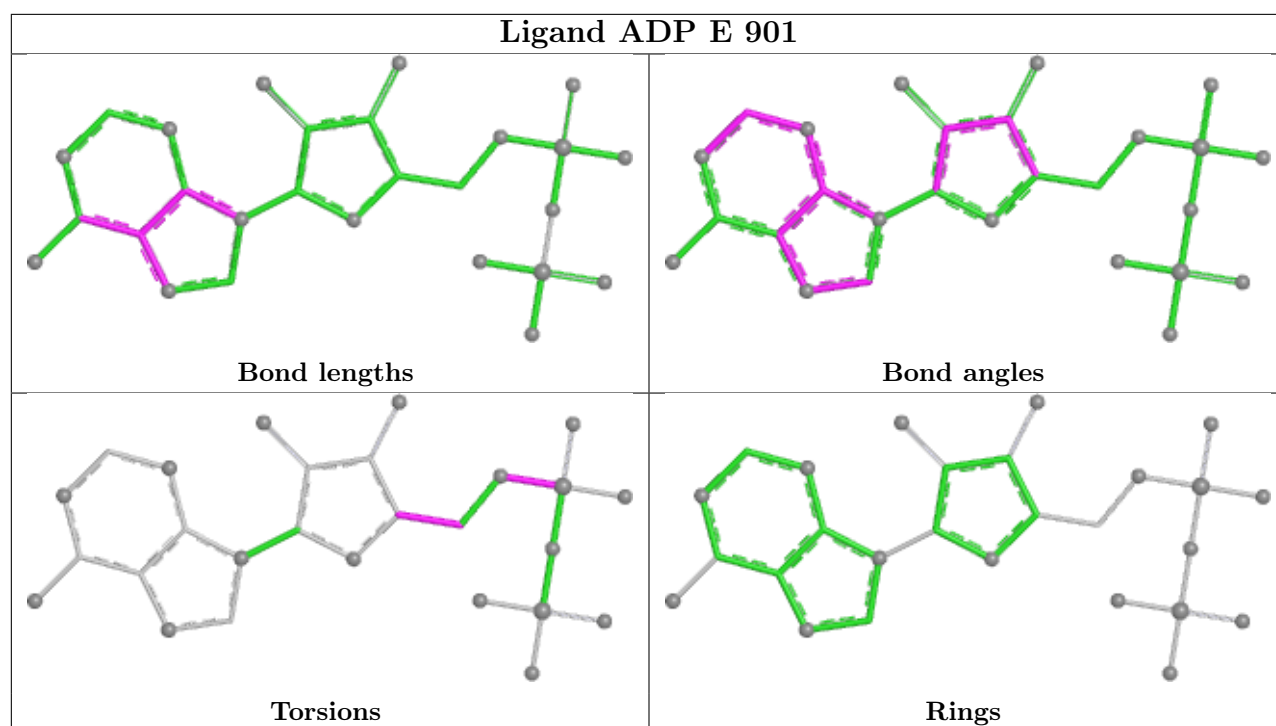












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

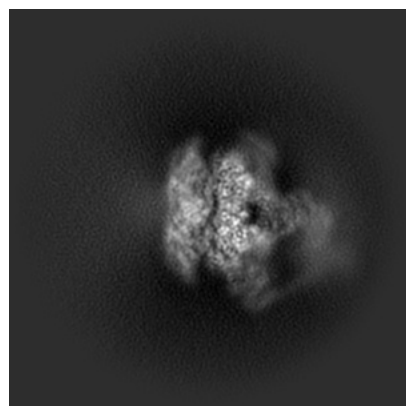
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-76028. These allow visual inspection of the internal detail of the map and identification of artifacts.

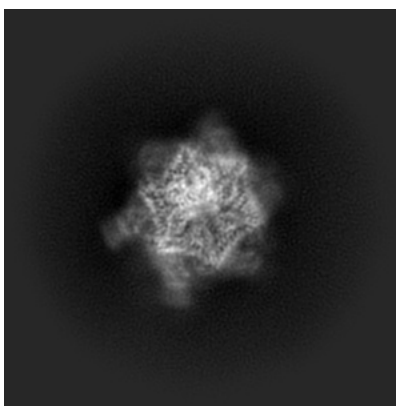
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

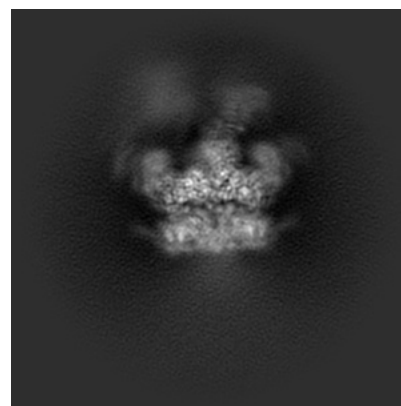
6.1.1 Primary map



X

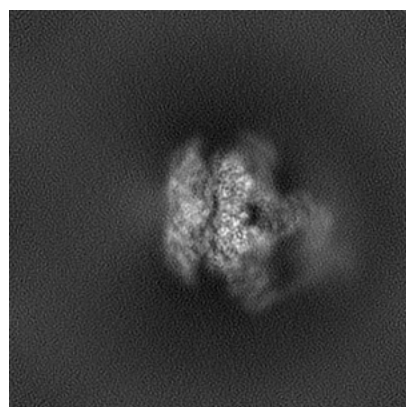


Y

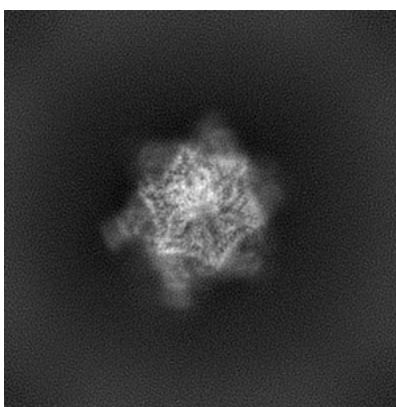


Z

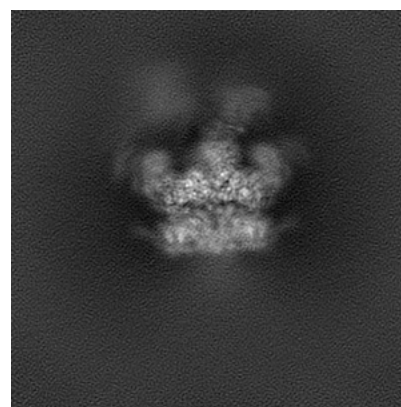
6.1.2 Raw map



X



Y

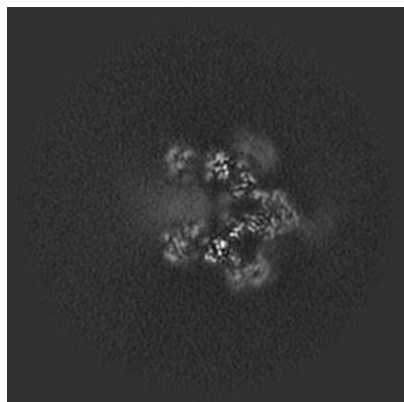


Z

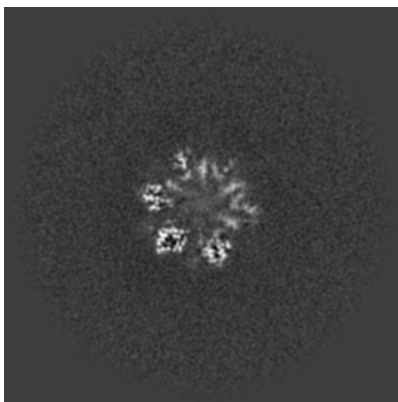
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

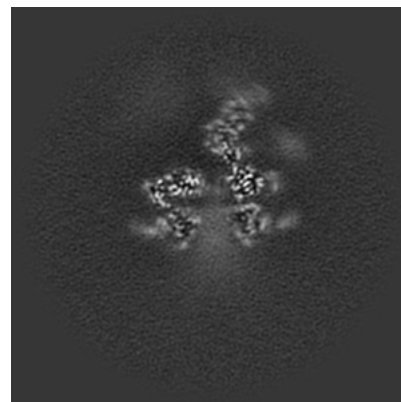
6.2.1 Primary map



X Index: 128

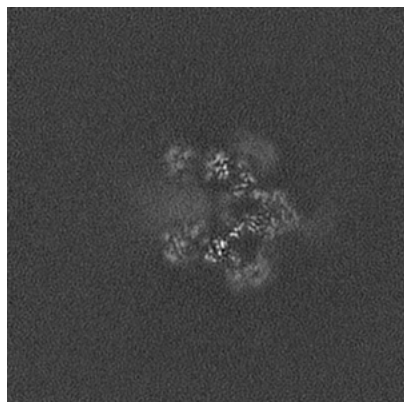


Y Index: 128

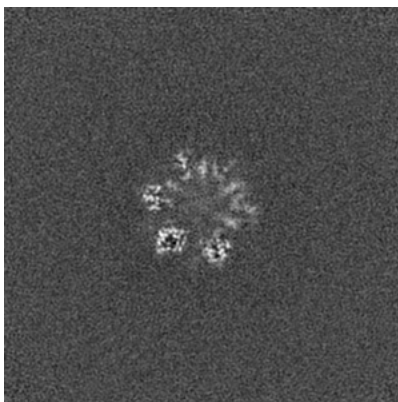


Z Index: 128

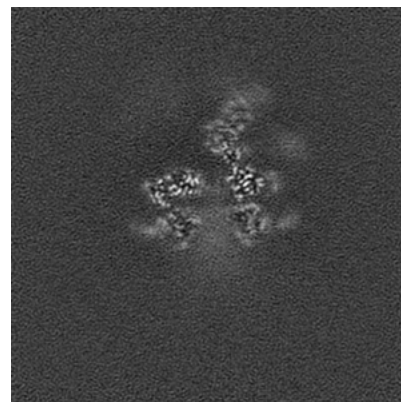
6.2.2 Raw map



X Index: 128



Y Index: 128

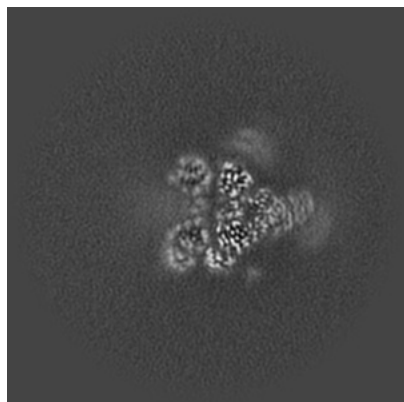


Z Index: 128

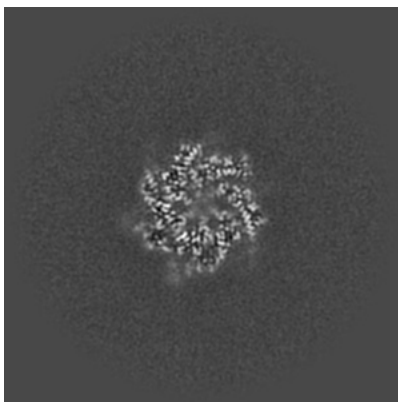
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

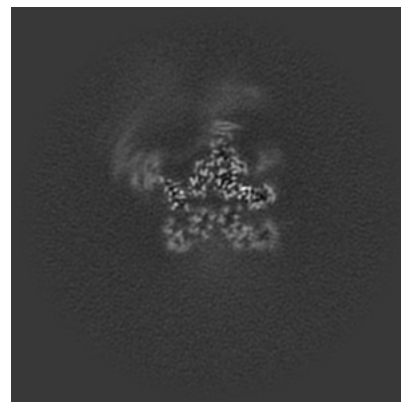
6.3.1 Primary map



X Index: 140

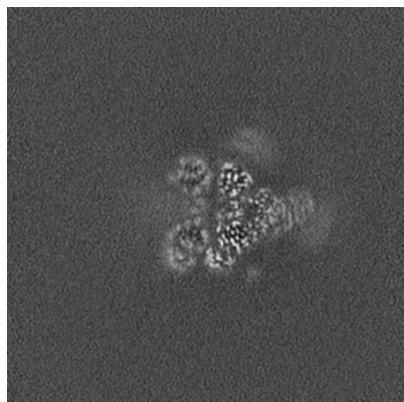


Y Index: 137

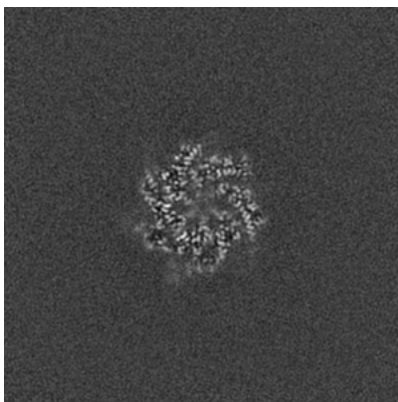


Z Index: 114

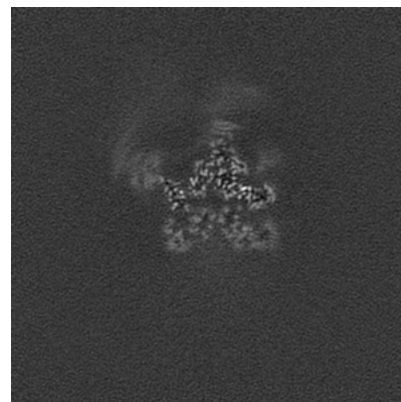
6.3.2 Raw map



X Index: 140



Y Index: 137

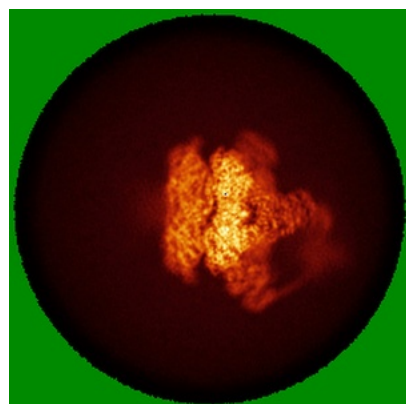


Z Index: 114

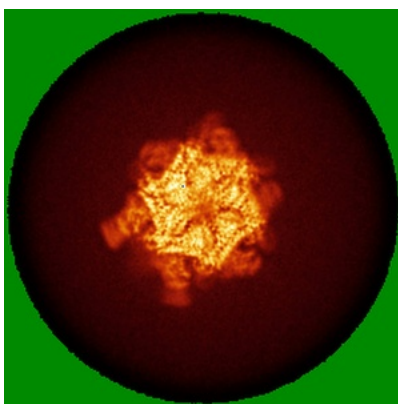
The images above show the largest variance slices of the map in three orthogonal directions.

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

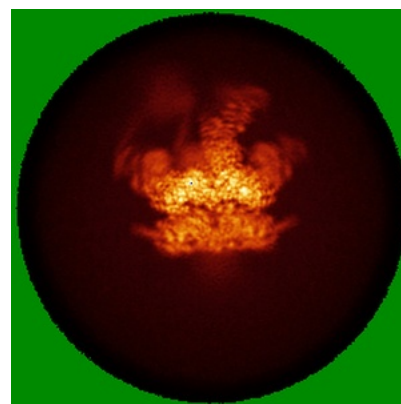
6.4.1 Primary map



X

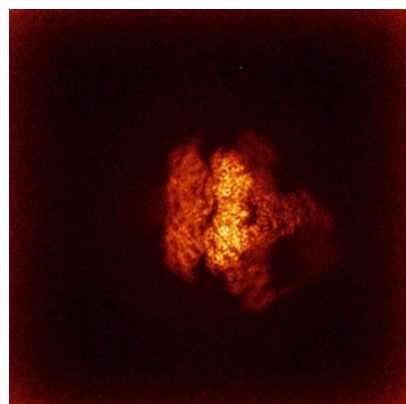


Y

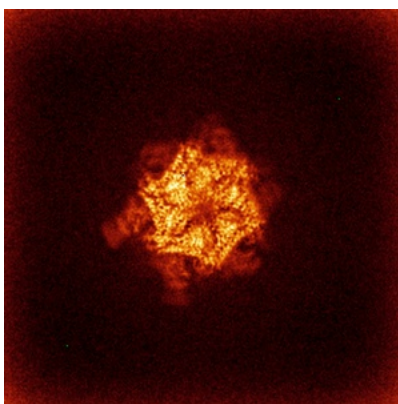


Z

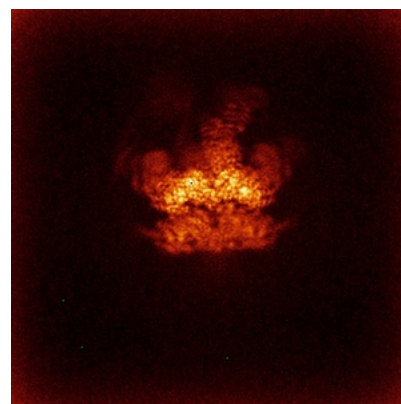
6.4.2 Raw map



X



Y

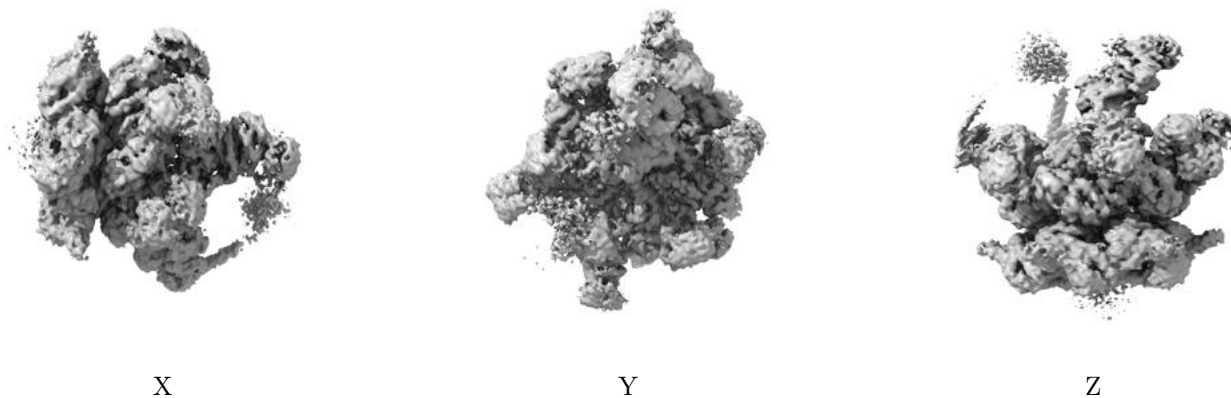


Z

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.

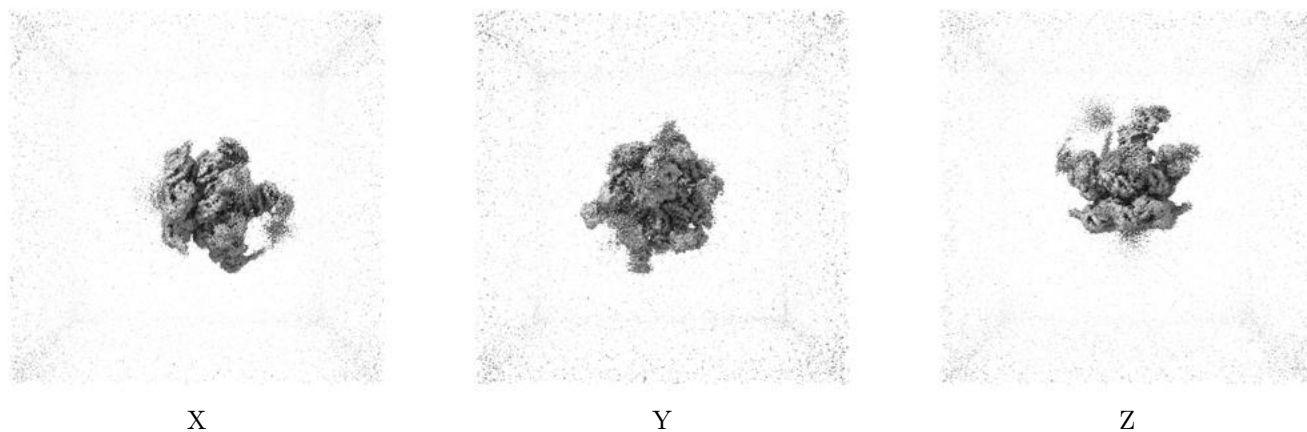
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.133. 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.

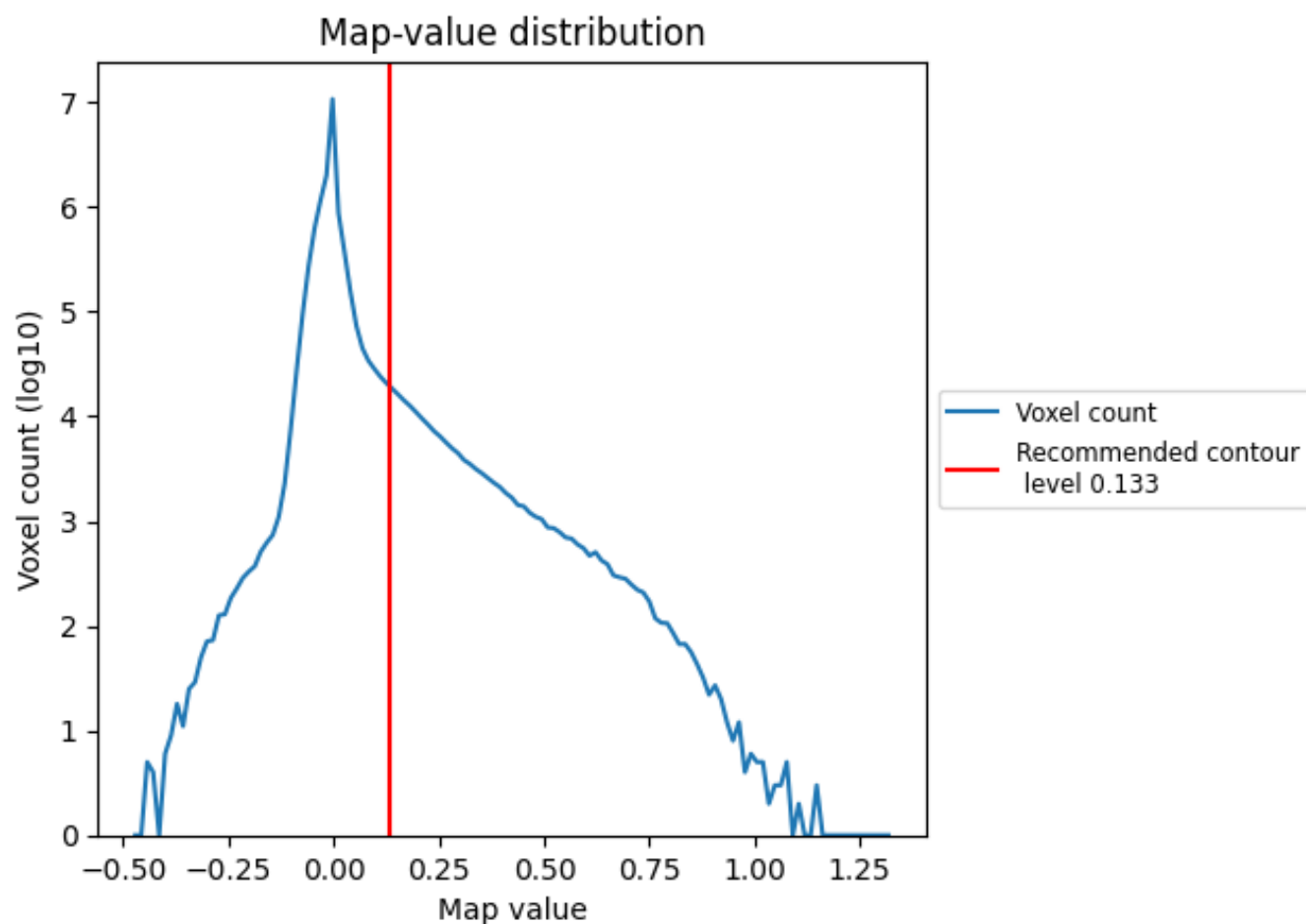
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

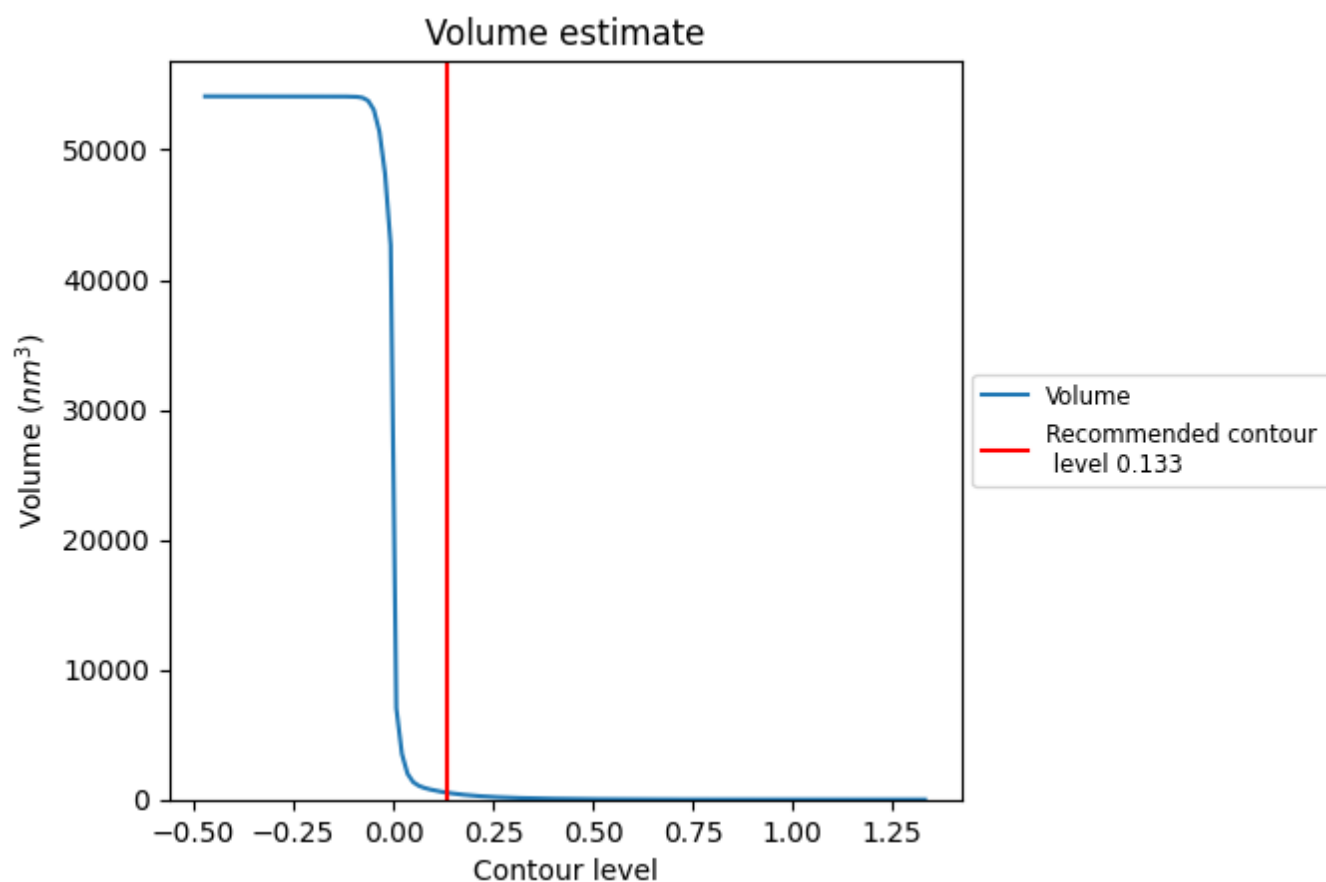
This section contains the results of statistical analysis of the map.

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.

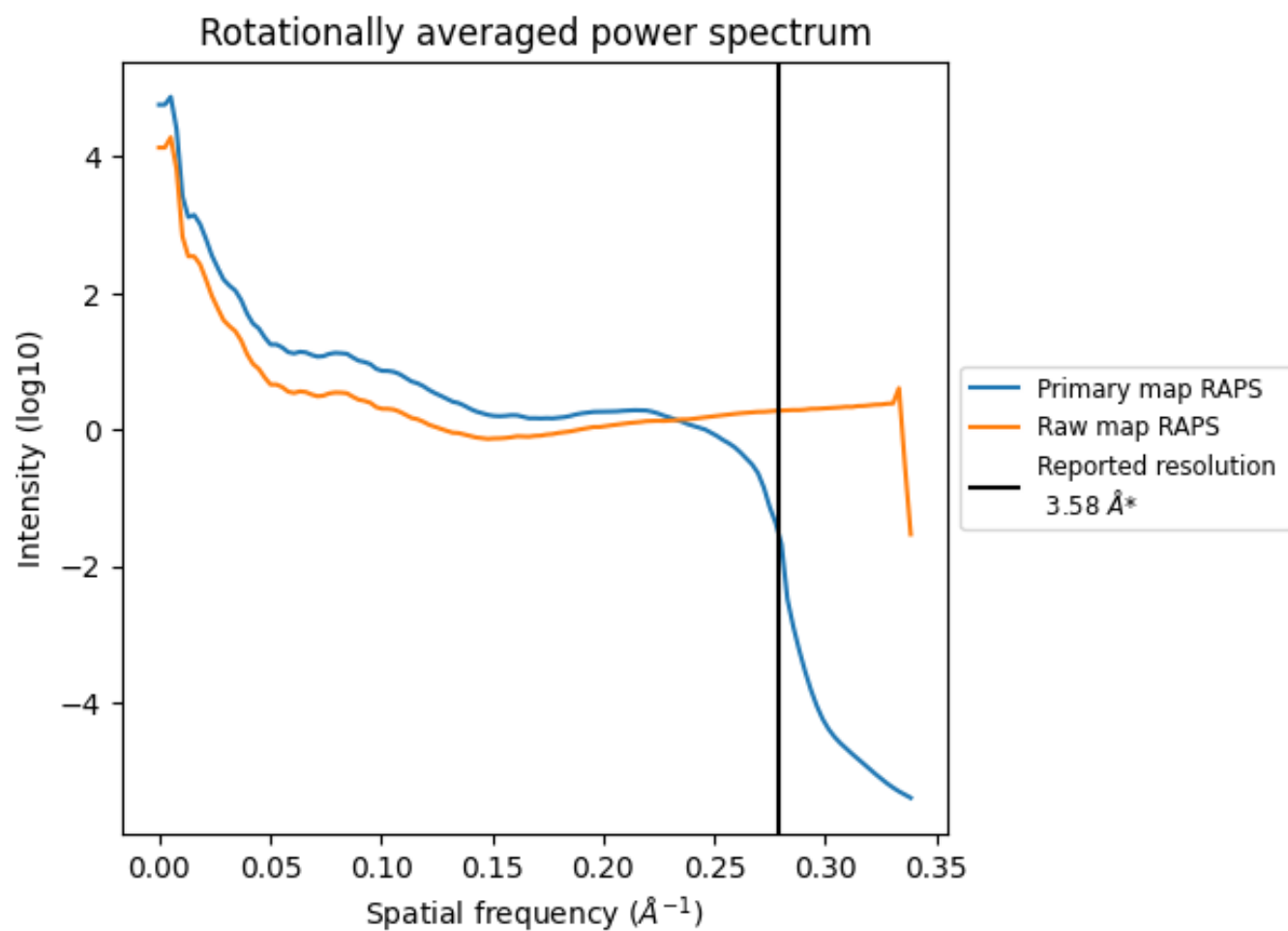
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 541 nm^3 ; this corresponds to an approximate mass of 489 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 ⓘ

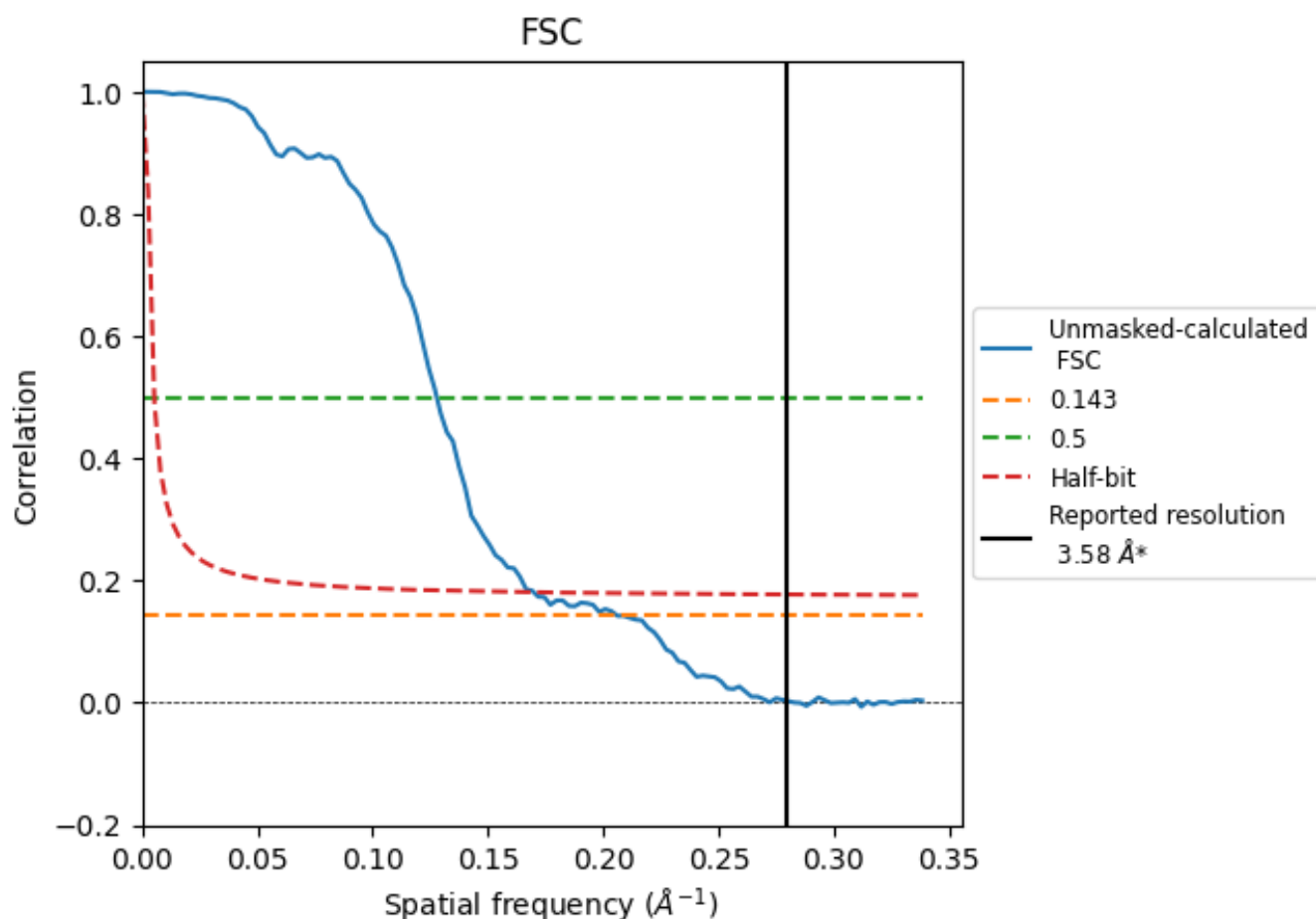


*Reported resolution corresponds to spatial frequency of 0.279 Å⁻¹

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 0.279 \AA^{-1}

8.2 Resolution estimates [i](#)

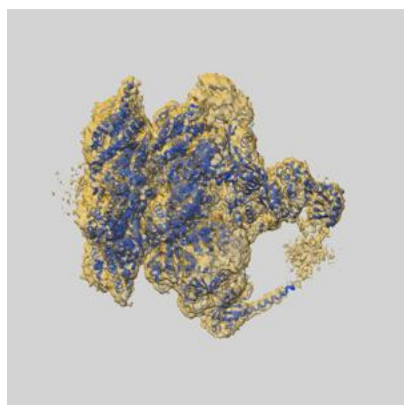
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.86	7.82	5.89

*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 4.86 differs from the reported value 3.58 by more than 10 %

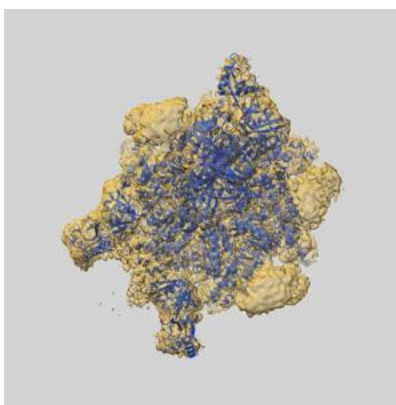
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-76028 and PDB model 11TA. Per-residue inclusion information can be found in section [3](#) on page [10](#).

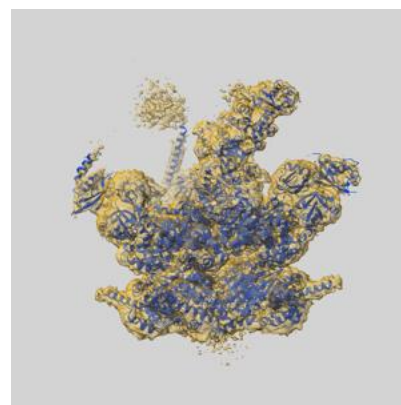
9.1 Map-model overlay [i](#)



X



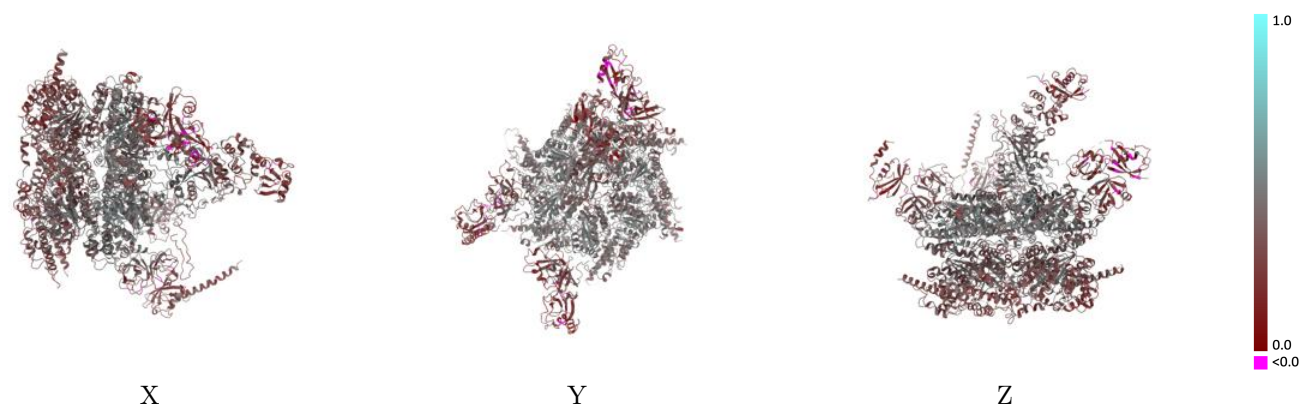
Y



Z

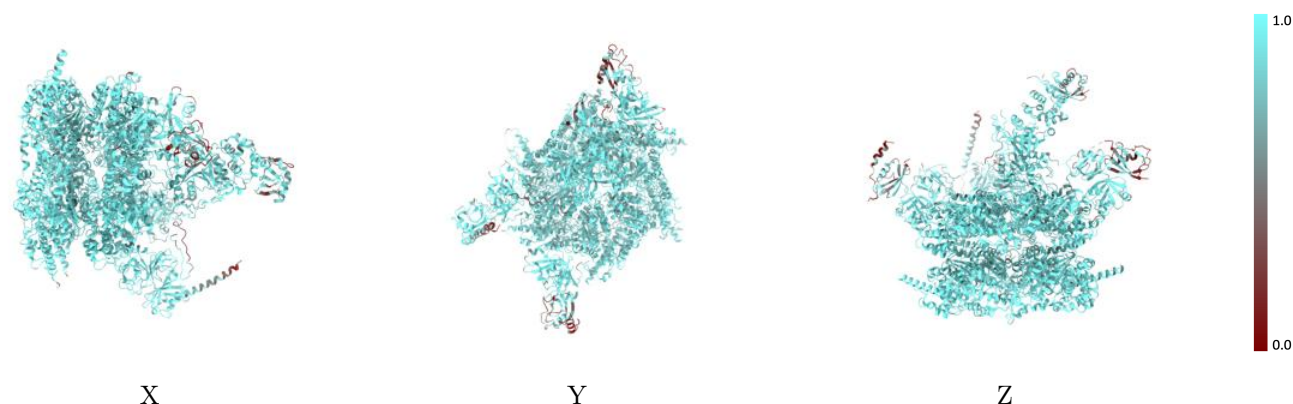
The images above show the 3D surface view of the map at the recommended contour level 0.133 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



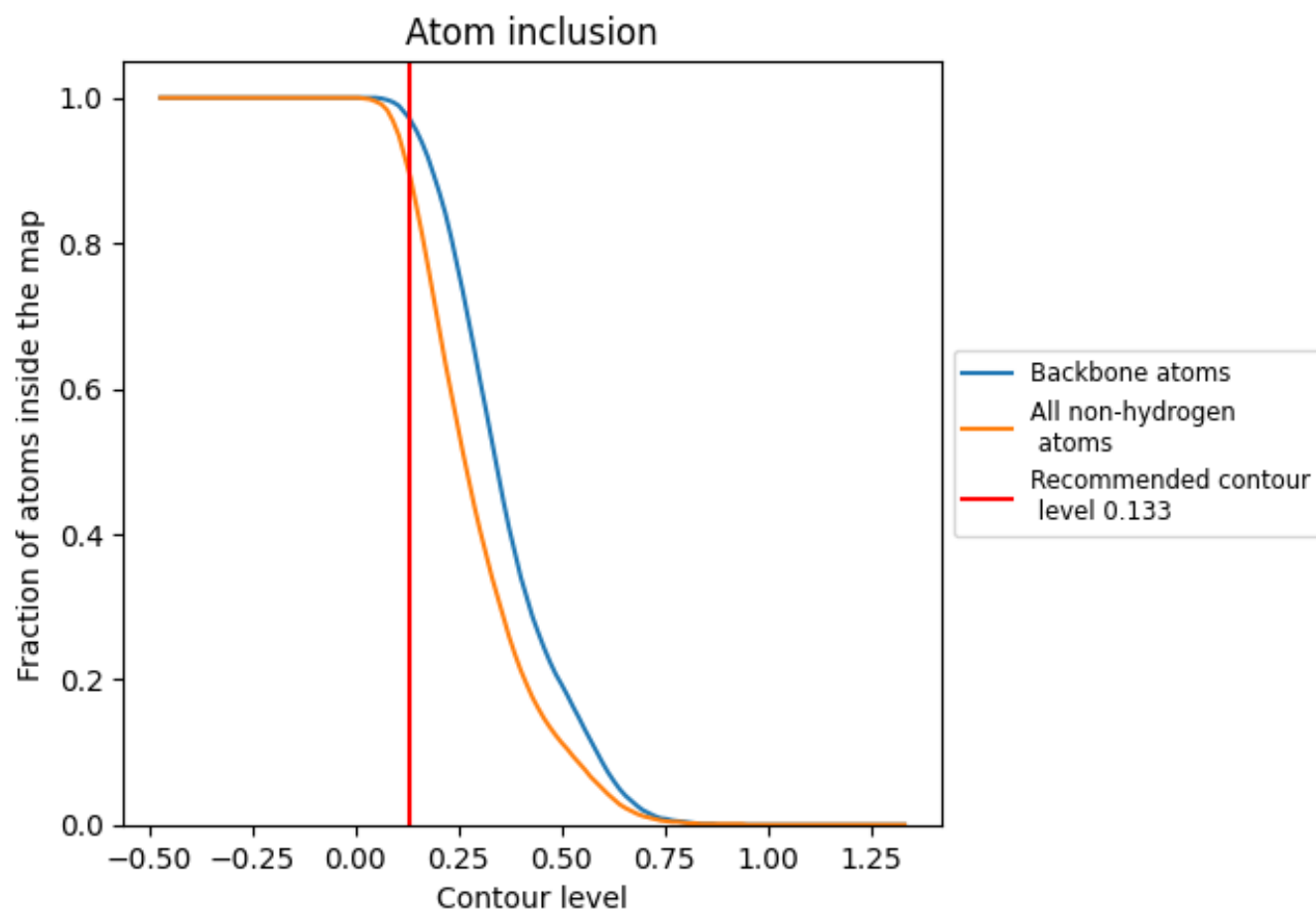
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.133).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 89% 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 (0.133) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8940	<div></div> 0.3730
A	<div></div> 0.9290	<div></div> 0.3910
B	<div></div> 0.9330	<div></div> 0.4090
C	<div></div> 0.9080	<div></div> 0.3520
D	<div></div> 0.9220	<div></div> 0.3810
E	<div></div> 0.9260	<div></div> 0.3950
F	<div></div> 0.9310	<div></div> 0.3790
G	<div></div> 0.8340	<div></div> 0.3750
I	<div></div> 0.8820	<div></div> 0.4000
K	<div></div> 0.6590	<div></div> 0.2520
M	<div></div> 0.8000	<div></div> 0.2660
O	<div></div> 0.5330	<div></div> 0.2130
P	<div></div> 0.7040	<div></div> 0.3400

