



## Full wwPDB EM Validation Report ⓘ

Sep 29, 2025 – 03:18 PM EDT

PDB ID : 9PBA / pdb\_00009pba  
EMDB ID : EMD-71475  
Title : 21bin20S complex (NSF-alphaSNAP-2:1 syntaxin-1a:SNAP-25), non-hydrolyzing, class 9  
Authors : White, K.I.; Brunger, A.T.  
Deposited on : 2025-06-26  
Resolution : 3.47 Å(reported)  
Based on initial model : 6MDM

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

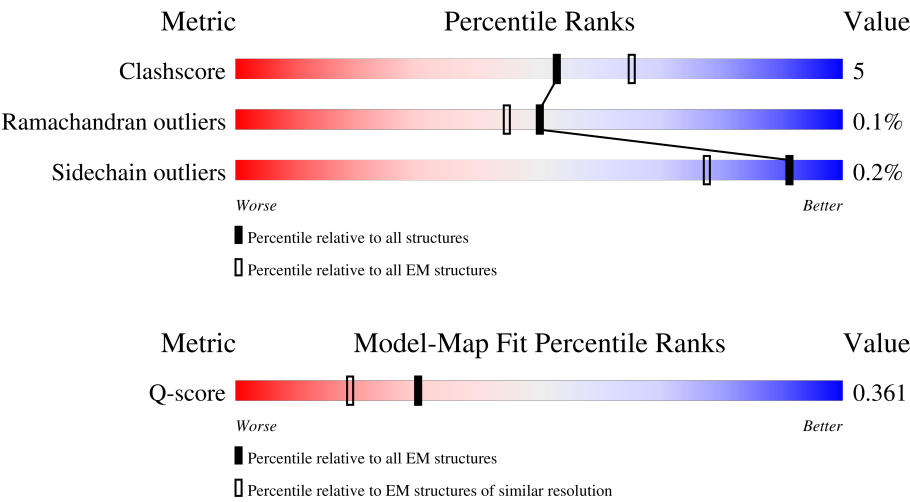
EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB 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) : 2.46

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.47 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13733 ( 2.97 - 3.97 )

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  $\geq 3$ , 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	747	<div><div></div><div>63%8%30%</div></div>
1	B	747	<div><div>21%</div><div>85%12%</div><div>.</div></div>
1	C	747	<div><div>22%</div><div>88%9%</div><div>.</div></div>
1	D	747	<div><div>23%</div><div>86%11%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	E	747	
1	F	747	
2	G	267	
2	H	267	
3	I	222	
4	J	296	
4	K	296	
4	L	296	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 81890 atoms, of which 40938 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 Vesicle-fusing ATPase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	525	Total	C	H	N	O	S	11	0
			8534	2651	4340	748	773	22		
1	B	726	Total	C	H	N	O	S	6	0
			11600	3618	5878	1000	1073	31		
1	C	726	Total	C	H	N	O	S	4	0
			11513	3599	5824	990	1069	31		
1	D	726	Total	C	H	N	O	S	4	0
			11532	3600	5837	994	1070	31		
1	E	726	Total	C	H	N	O	S	4	0
			11534	3608	5832	993	1070	31		
1	F	511	Total	C	H	N	O	S	2	0
			8128	2537	4128	696	747	20		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P18708
A	-1	ALA	-	expression tag	UNP P18708
A	0	HIS	-	expression tag	UNP P18708
B	-2	GLY	-	expression tag	UNP P18708
B	-1	ALA	-	expression tag	UNP P18708
B	0	HIS	-	expression tag	UNP P18708
C	-2	GLY	-	expression tag	UNP P18708
C	-1	ALA	-	expression tag	UNP P18708
C	0	HIS	-	expression tag	UNP P18708
D	-2	GLY	-	expression tag	UNP P18708
D	-1	ALA	-	expression tag	UNP P18708
D	0	HIS	-	expression tag	UNP P18708
E	-2	GLY	-	expression tag	UNP P18708
E	-1	ALA	-	expression tag	UNP P18708
E	0	HIS	-	expression tag	UNP P18708
F	-2	GLY	-	expression tag	UNP P18708
F	-1	ALA	-	expression tag	UNP P18708
F	0	HIS	-	expression tag	UNP P18708

- Molecule 2 is a protein called Syntaxin-1A.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	G	63	Total	C	H	N	O	S	0	0
			1022	320	505	89	103	5		
2	H	72	Total	C	H	N	O	S	0	0
			1162	362	576	100	119	5		

- Molecule 3 is a protein called Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	I	155	Total	C	H	N	O	S	24	0
			2819	845	1384	266	309	15		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-15	MET	-	expression tag	UNP P60881
I	-14	GLY	-	expression tag	UNP P60881
I	-13	SER	-	expression tag	UNP P60881
I	-12	SER	-	expression tag	UNP P60881
I	-11	HIS	-	expression tag	UNP P60881
I	-10	HIS	-	expression tag	UNP P60881
I	-9	HIS	-	expression tag	UNP P60881
I	-8	HIS	-	expression tag	UNP P60881
I	-7	HIS	-	expression tag	UNP P60881
I	-6	HIS	-	expression tag	UNP P60881
I	-5	SER	-	expression tag	UNP P60881
I	-4	GLN	-	expression tag	UNP P60881
I	-3	ASP	-	expression tag	UNP P60881
I	-2	PRO	-	expression tag	UNP P60881
I	-1	ASN	-	expression tag	UNP P60881
I	0	SER	-	expression tag	UNP P60881
I	85	ALA	CYS	conflict	UNP P60881
I	88	ALA	CYS	conflict	UNP P60881
I	90	ALA	CYS	conflict	UNP P60881
I	92	ALA	CYS	conflict	UNP P60881

- Molecule 4 is a protein called Alpha-soluble NSF attachment protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	J	287	Total	C	H	N	O	S	0	0
			4467	1424	2212	375	438	18		

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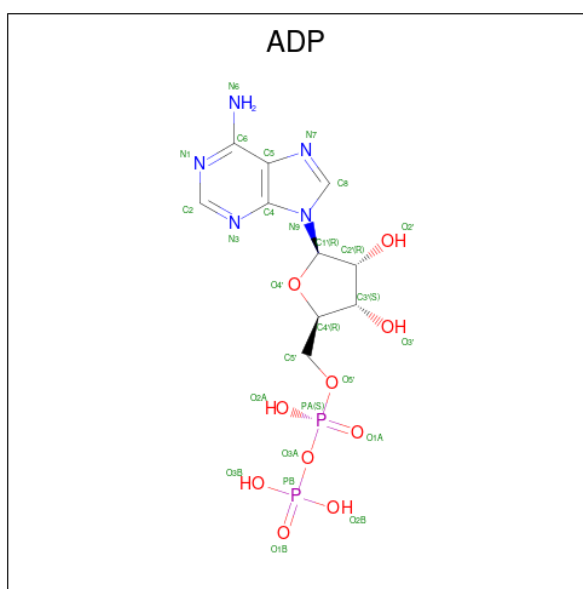
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Mol	Chain	Residues	Atoms						AltConf	Trace
4	K	276	Total	C	H	N	O	S	0	0
			4319	1373	2142	363	423	18		
4	L	275	Total	C	H	N	O	S	0	0
			4305	1368	2136	362	421	18		

There are 3 discrepancies between the modelled and reference sequences:

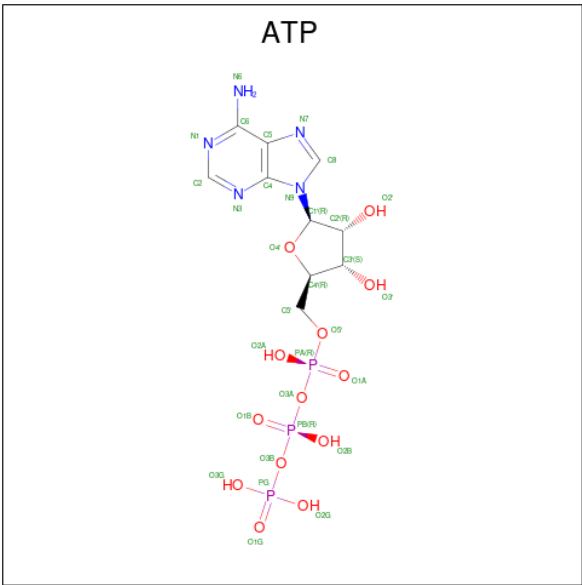
Chain	Residue	Modelled	Actual	Comment	Reference
J	0	GLY	-	expression tag	UNP P54921
K	0	GLY	-	expression tag	UNP P54921
L	0	GLY	-	expression tag	UNP P54921

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	105	Total	O	0
			105	105	

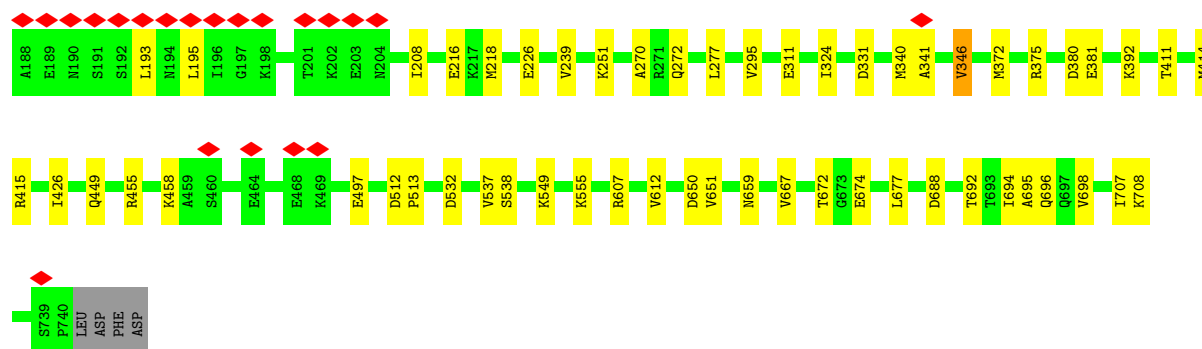
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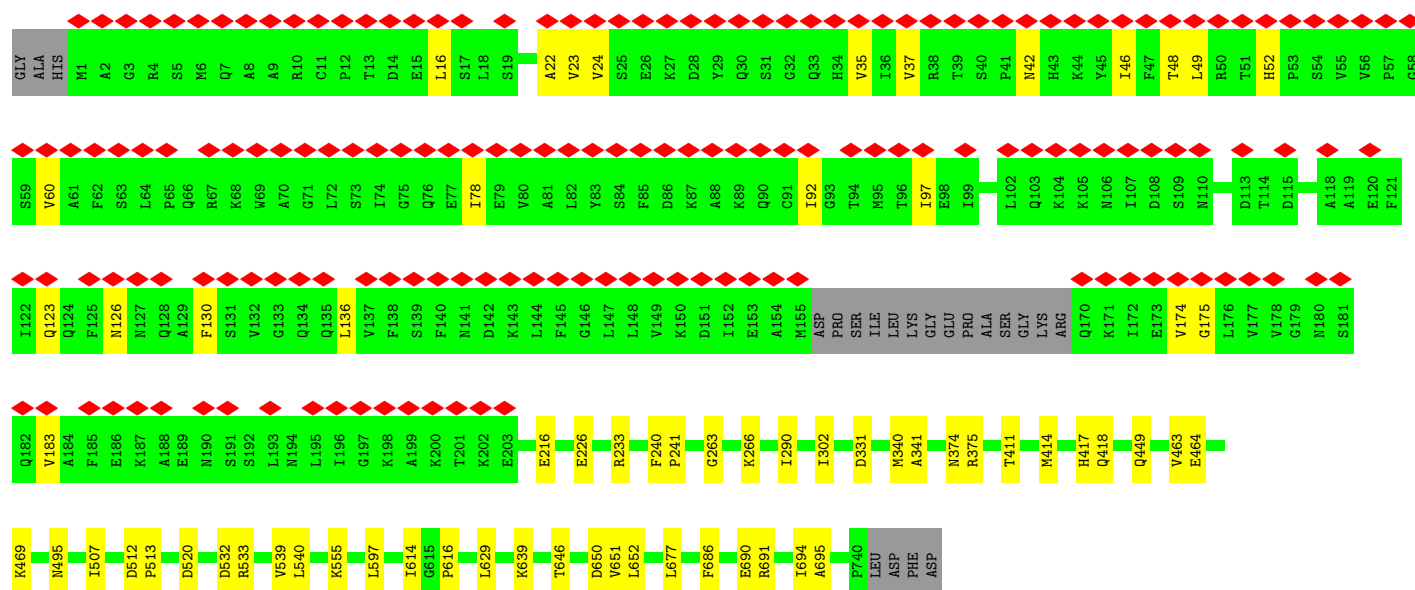
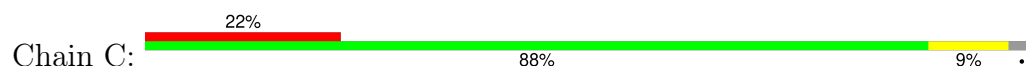
Mol	Chain	Residues	Atoms		AltConf
7	B	105	Total 105	O 105	0
7	C	102	Total 102	O 102	0
7	D	82	Total 82	O 82	0
7	E	33	Total 33	O 33	0
7	F	16	Total 16	O 16	0



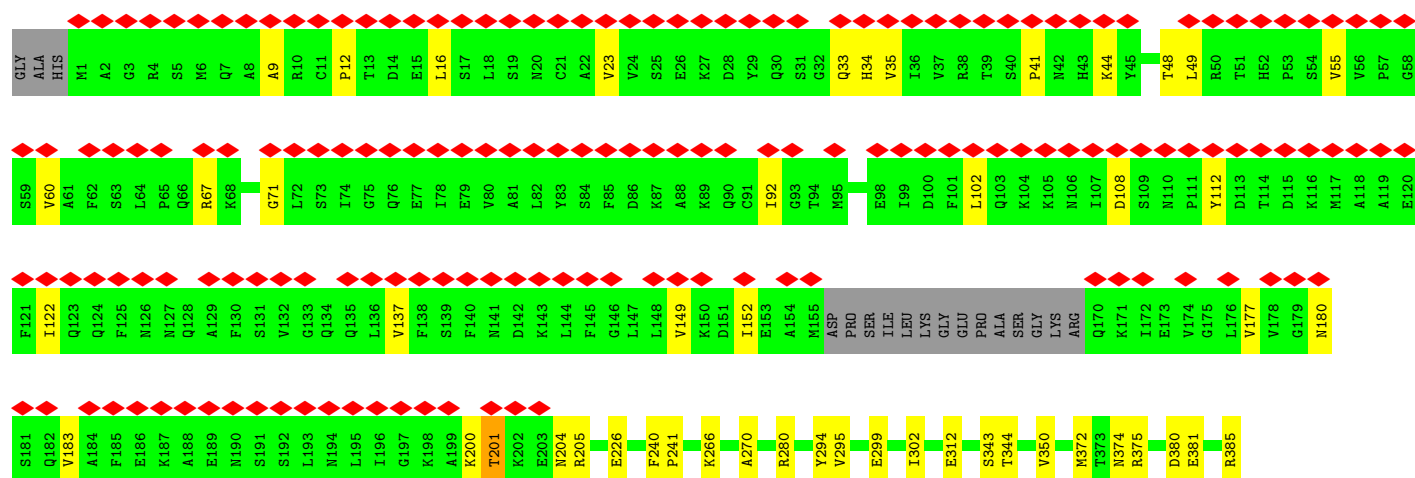
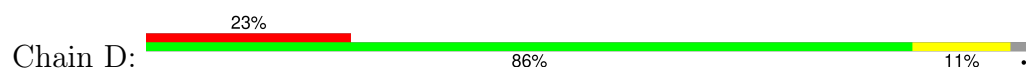


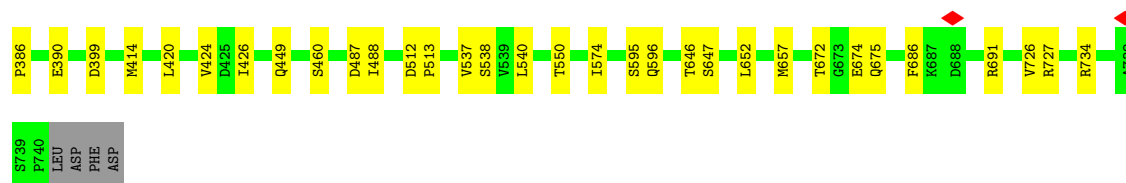


• Molecule 1: Vesicle-fusing ATPase

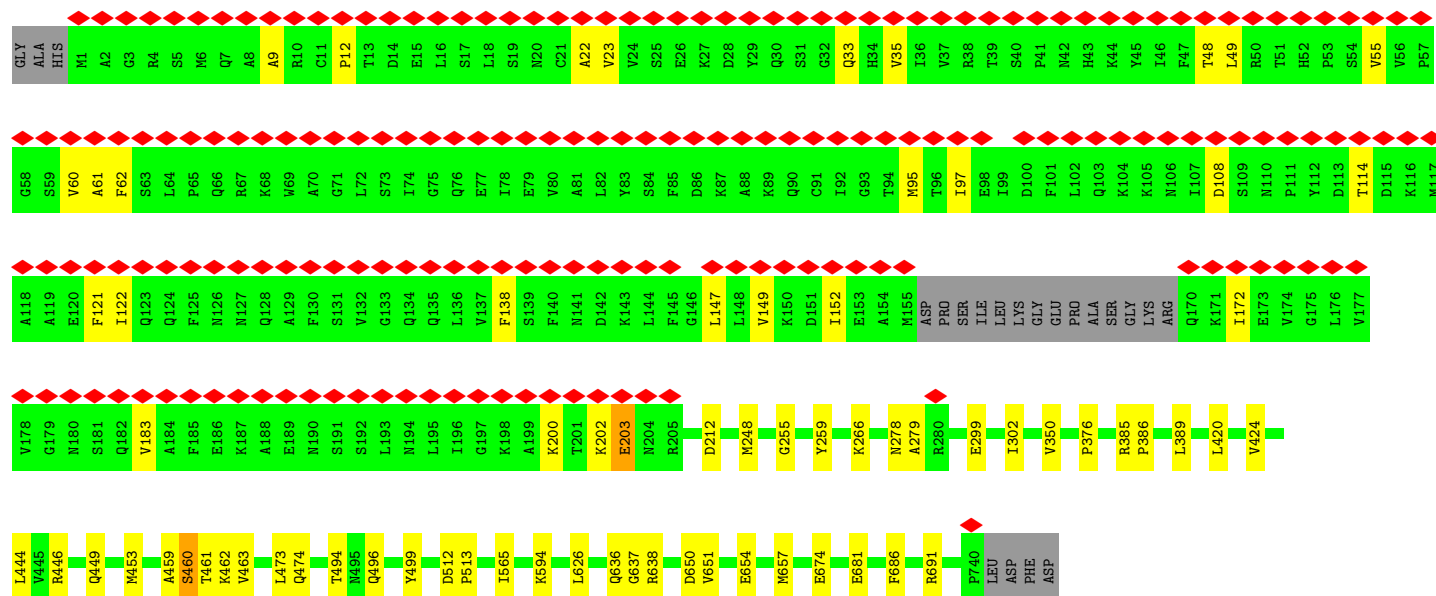
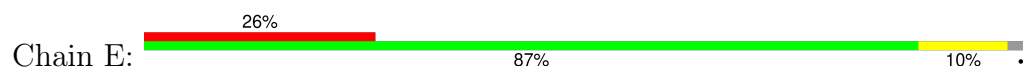


• Molecule 1: Vesicle-fusing ATPase

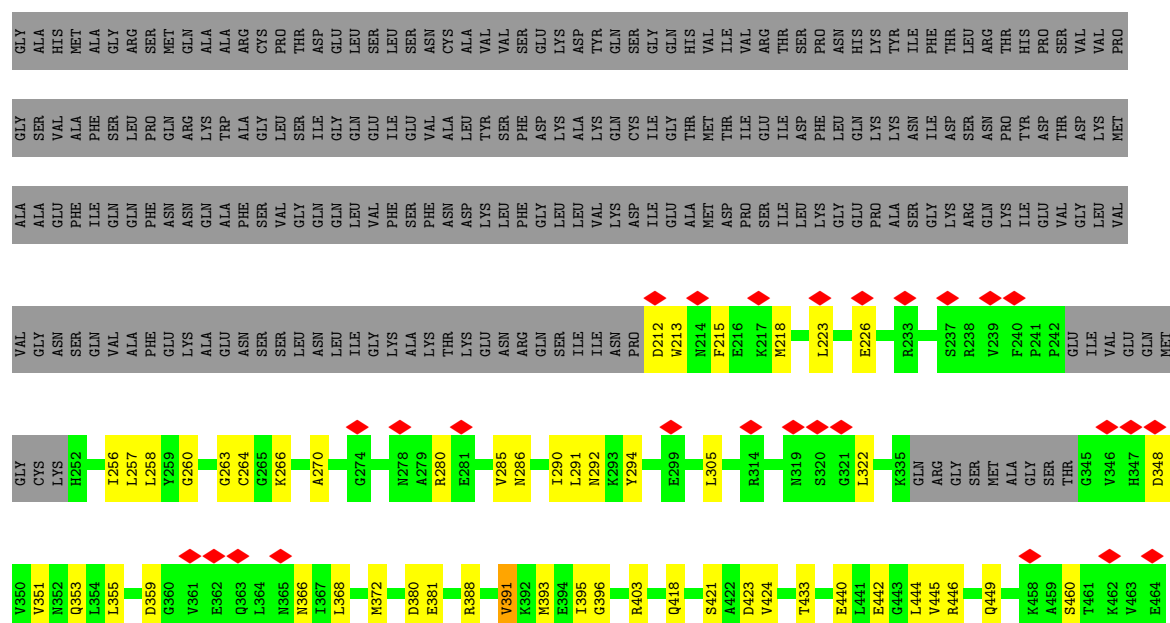


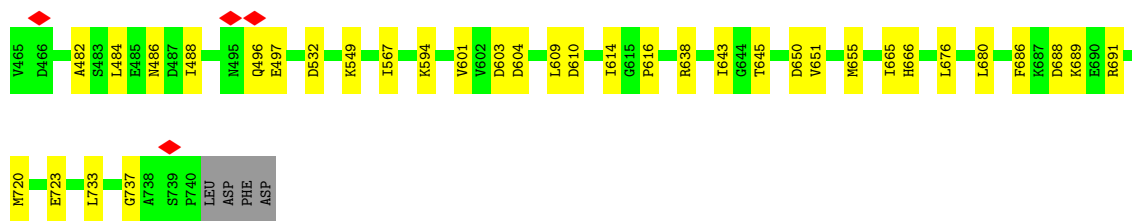


• Molecule 1: Vesicle-fusing ATPase

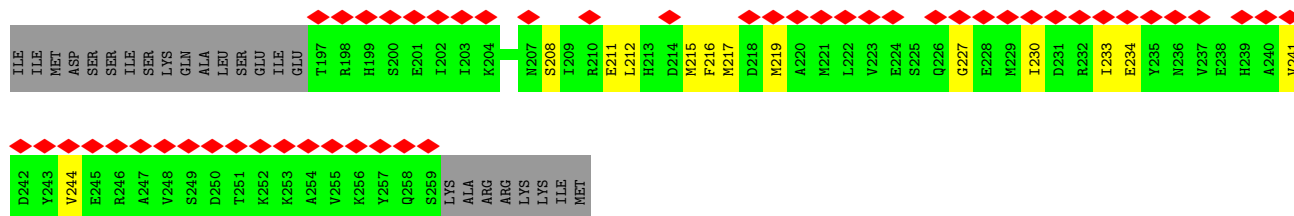
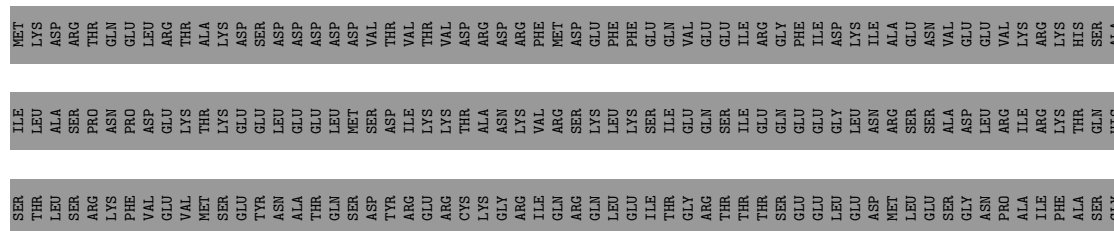


• Molecule 1: Vesicle-fusing ATPase

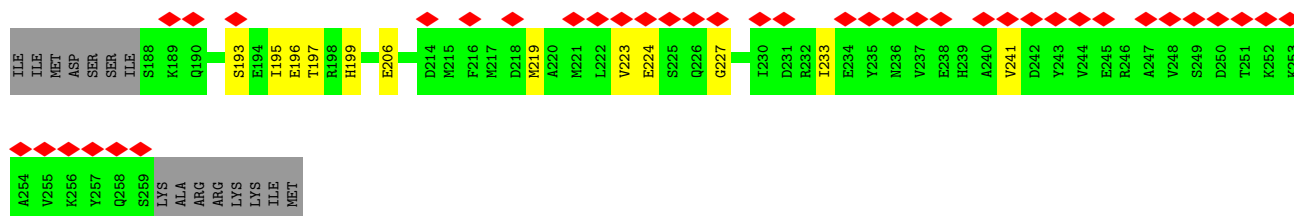
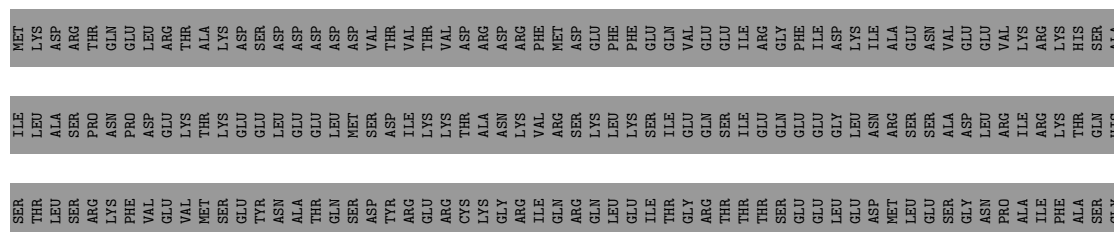




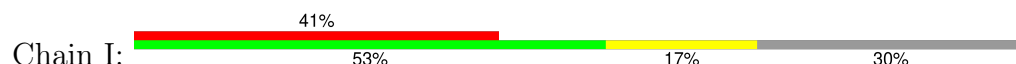
• Molecule 2: Syntaxin-1A

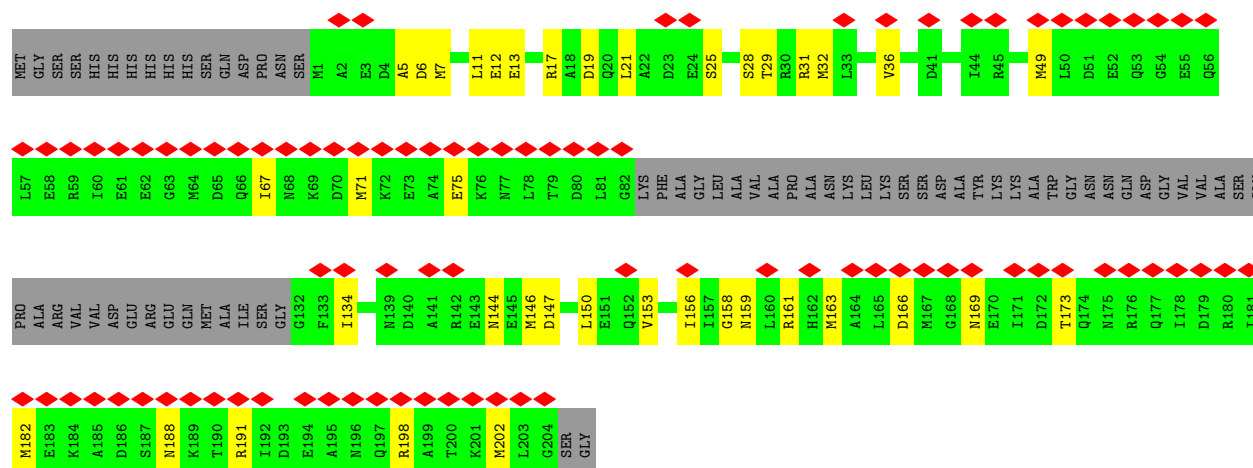


• Molecule 2: Syntaxin-1A

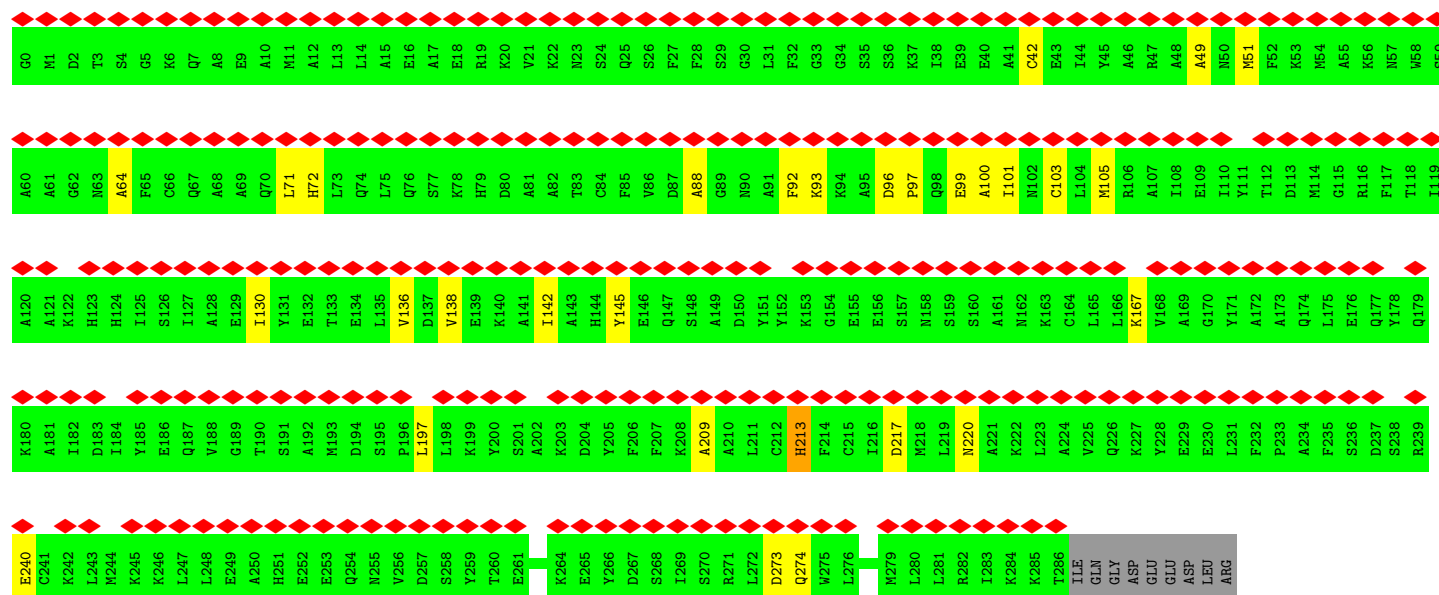
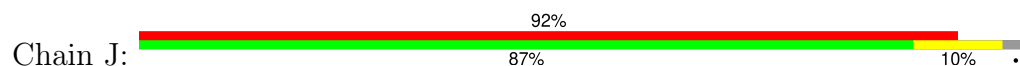


• Molecule 3: Synaptosomal-associated protein 25

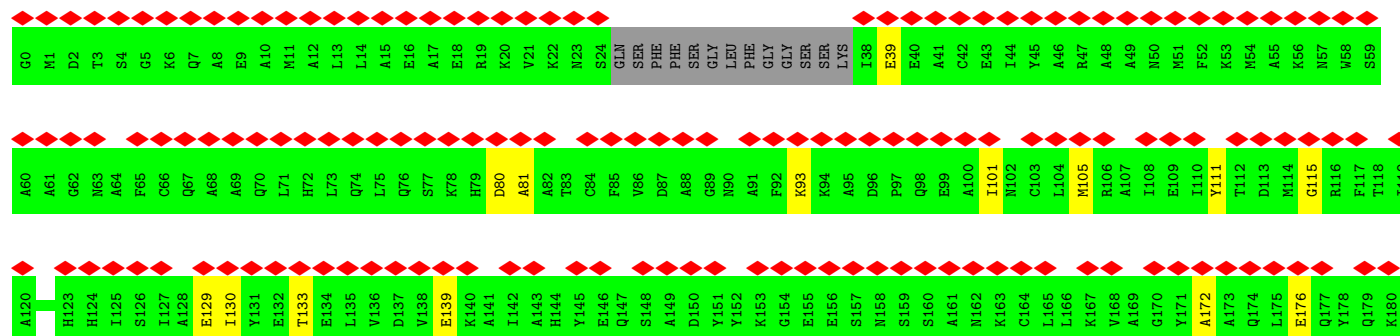
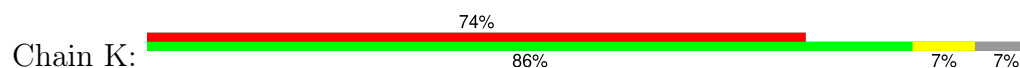


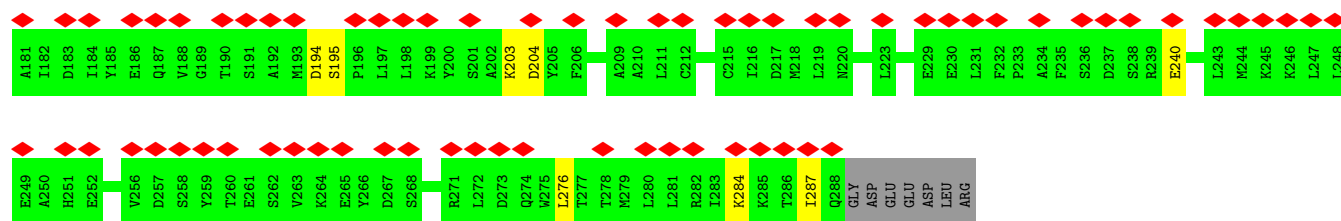


• Molecule 4: Alpha-soluble NSF attachment protein

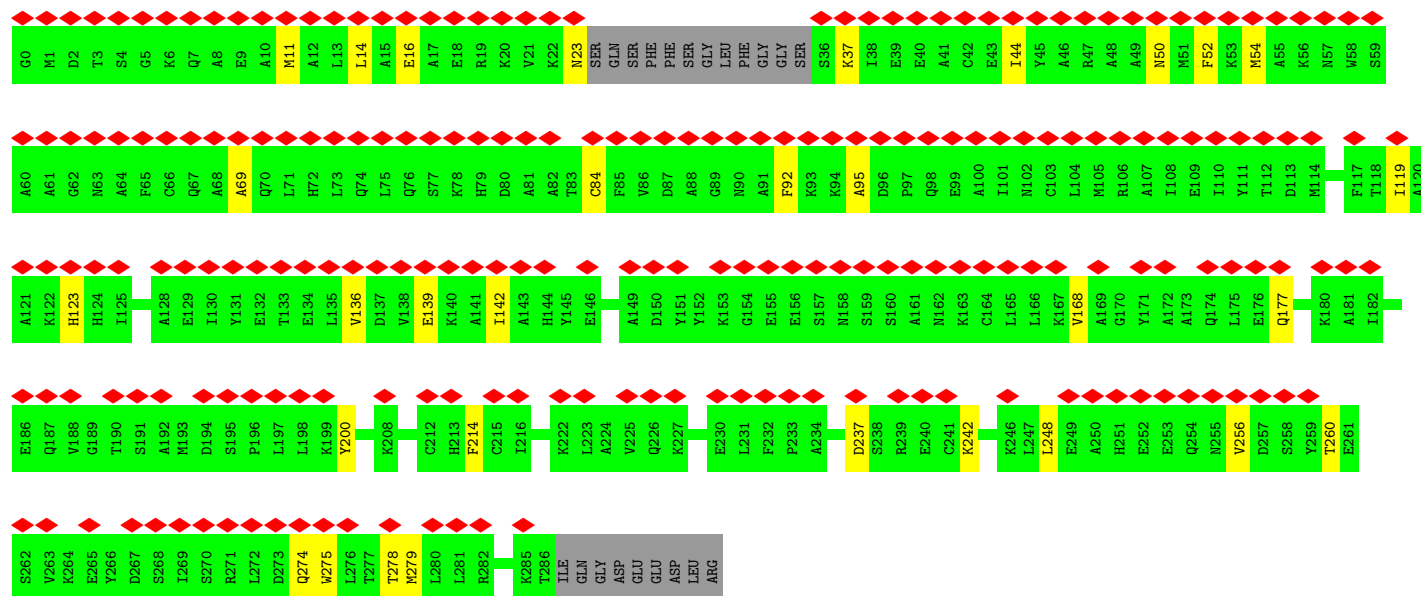
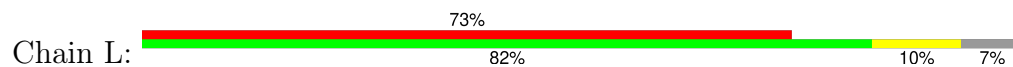


• Molecule 4: Alpha-soluble NSF attachment protein





• Molecule 4: Alpha-soluble NSF attachment protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	230804	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 ( $e^-/\text{\AA}^2$ )	31.560, 36.760, 35.480	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.484	Depositor
Minimum map value	-2.502	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.3	Depositor
Map size ( $\text{\AA}$ )	322.224, 322.224, 322.224	wwPDB
Map dimensions	294, 294, 294	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.096, 1.096, 1.096	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 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	A	0.19	0/4276	0.35	0/5757
1	B	0.18	0/5810	0.36	0/7824
1	C	0.12	0/5783	0.29	0/7793
1	D	0.12	0/5783	0.29	0/7790
1	E	0.14	0/5793	0.30	0/7807
1	F	0.13	0/4069	0.29	0/5482
2	G	0.16	0/523	0.33	0/700
2	H	0.16	0/592	0.32	0/792
3	I	0.16	0/1435	0.27	0/1910
4	J	0.18	0/2295	0.33	0/3084
4	K	0.08	0/2213	0.20	0/2975
4	L	0.09	0/2205	0.21	0/2963
All	All	0.14	0/40777	0.30	0/54877

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4194	4340	4317	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5722	5878	5876	73	0
1	C	5689	5824	5820	47	0
1	D	5695	5837	5838	52	0
1	E	5702	5832	5831	50	0
1	F	4000	4128	4118	57	0
2	G	517	505	505	14	0
2	H	586	576	575	13	0
3	I	1435	1384	1386	37	0
4	J	2255	2212	2212	22	0
4	K	2177	2142	2142	14	0
4	L	2169	2136	2136	21	0
5	A	27	12	12	0	0
6	A	31	12	12	0	0
6	B	62	24	24	1	0
6	C	62	24	24	1	0
6	D	62	24	24	0	0
6	E	62	24	24	1	0
6	F	62	24	24	1	0
7	A	105	0	0	2	0
7	B	105	0	0	5	0
7	C	102	0	0	3	0
7	D	82	0	0	1	0
7	E	33	0	0	0	0
7	F	16	0	0	0	0
All	All	40952	40938	40900	418	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 5.

All (418) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:GLU:OE1	1:C:464:GLU:N	2.11	0.83
2:G:212:LEU:HD21	3:I:161:ARG:HE	1.45	0.82
1:E:299:GLU:N	1:E:299:GLU:OE1	2.15	0.80
3:I:36:VAL:HG21	3:I:153:VAL:HG13	1.64	0.78
1:D:414:MET:SD	1:D:449:GLN:NE2	2.57	0.77
1:B:674:GLU:OE2	1:B:674:GLU:N	2.19	0.76
1:B:414:MET:SD	1:B:449:GLN:NE2	2.59	0.76
1:B:39:THR:HG22	1:B:78:ILE:HG22	1.69	0.74
1:B:497:GLU:OE1	1:B:497:GLU:N	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:594:LYS:O	1:E:638:ARG:NH1	2.21	0.73
1:D:299:GLU:N	1:D:299:GLU:OE1	2.21	0.72
1:D:674:GLU:N	1:D:674:GLU:OE1	2.22	0.71
1:D:390:GLU:OE2	1:E:446:ARG:NH1	2.22	0.71
1:A:233:ARG:NH2	1:A:390:GLU:OE2	2.23	0.71
1:B:411:THR:O	1:B:415:ARG:NH1	2.24	0.71
1:B:392:LYS:NZ	7:B:901:HOH:O	2.22	0.70
1:E:9:ALA:N	1:E:60:VAL:O	2.25	0.69
1:A:243:GLU:N	1:A:243:GLU:OE1	2.26	0.69
1:B:331:ASP:OD2	1:B:375[B]:ARG:NH1	2.25	0.69
1:B:549:LYS:HG2	1:B:667:VAL:HG21	1.75	0.68
3:I:11[A]:LEU:HD13	3:I:12[A]:GLU:N	2.08	0.68
1:A:380:ASP:OD1	1:A:381:GLU:N	2.27	0.68
1:D:385:ARG:NH1	1:D:386:PRO:O	2.27	0.68
1:A:226:GLU:N	1:A:226:GLU:OE1	2.26	0.68
1:C:233:ARG:NH1	7:C:903:HOH:O	2.26	0.67
1:C:414:MET:SD	1:C:449:GLN:NE2	2.66	0.67
4:K:172:ALA:O	4:K:176:GLU:N	2.27	0.67
1:C:216:GLU:N	1:C:216:GLU:OE1	2.26	0.67
1:C:418:GLN:N	1:C:418:GLN:OE1	2.27	0.66
1:B:15:GLU:OE1	1:C:42:ASN:ND2	2.29	0.66
1:B:92:ILE:HG22	1:B:95:MET:HE2	1.77	0.66
1:B:251:LYS:NZ	7:B:904:HOH:O	2.28	0.66
1:D:226:GLU:N	1:D:226:GLU:OE1	2.29	0.66
2:H:206:GLU:OE2	3:I:31:ARG:NE	2.29	0.65
1:B:208:ILE:O	1:B:208:ILE:HG22	1.95	0.65
1:B:226:GLU:N	1:B:226:GLU:OE1	2.30	0.64
1:E:255:GLY:HA3	1:E:389:LEU:HD23	1.78	0.64
2:H:196:GLU:OE2	3:I:17[B]:ARG:NH2	2.30	0.64
1:B:555:LYS:NZ	7:B:905:HOH:O	2.29	0.64
3:I:75:GLU:OE1	3:I:191:ARG:NH2	2.31	0.64
1:D:35:VAL:HG13	1:D:49:LEU:HD11	1.79	0.64
1:F:226:GLU:N	1:F:226:GLU:OE1	2.30	0.64
1:B:6:MET:HE1	1:B:60:VAL:HG23	1.80	0.63
3:I:169:ASN:O	3:I:173:THR:HG23	1.97	0.63
2:G:211:GLU:O	2:G:215:MET:HE2	1.99	0.63
4:K:139:GLU:N	4:K:139:GLU:OE1	2.30	0.63
1:E:674:GLU:OE1	1:E:674:GLU:N	2.31	0.63
1:F:256:ILE:HD12	1:F:368:LEU:HD11	1.81	0.63
1:E:636:GLN:OE1	1:E:637:GLY:N	2.31	0.62
1:B:426:ILE:O	1:B:426:ILE:HG22	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:ASN:ND2	7:C:905:HOH:O	2.30	0.62
1:B:24:VAL:HG12	1:B:60:VAL:HG22	1.81	0.62
1:B:455:ARG:O	1:B:458:LYS:NZ	2.32	0.61
1:B:659:ASN:ND2	7:B:907:HOH:O	2.32	0.61
1:B:6:MET:CE	1:B:60:VAL:HG23	2.31	0.60
1:D:266:LYS:NZ	1:D:374:ASN:OD1	2.34	0.60
4:L:92:PHE:O	4:L:95:ALA:N	2.34	0.60
1:C:226:GLU:OE1	1:C:226:GLU:N	2.33	0.60
1:D:302:ILE:HD11	1:D:350:VAL:HG13	1.82	0.60
1:D:343:SER:O	1:D:344:THR:OG1	2.13	0.60
2:G:233:ILE:HG12	3:I:182:MET:HE1	1.82	0.60
1:B:607:ARG:NH2	7:B:908:HOH:O	2.34	0.60
1:D:12:PRO:HD2	1:D:23:VAL:HG11	1.84	0.59
1:E:97:ILE:HG21	1:E:147:LEU:HD22	1.83	0.59
1:F:380:ASP:OD1	1:F:381:GLU:N	2.36	0.59
1:F:723:GLU:N	1:F:723:GLU:OE1	2.34	0.59
1:F:482:ALA:O	1:F:486:ASN:ND2	2.35	0.59
4:L:139:GLU:OE1	4:L:139:GLU:N	2.34	0.59
1:F:532:ASP:OD1	1:F:532:ASP:N	2.34	0.58
2:H:224:GLU:HA	3:I:49:MET:HE1	1.85	0.58
4:J:240:GLU:OE1	4:J:240:GLU:N	2.35	0.58
1:C:686:PHE:O	1:C:691:ARG:NH2	2.36	0.58
4:K:80:ASP:OD1	4:K:81:ALA:N	2.37	0.58
4:L:274:GLN:OE1	4:L:278:THR:OG1	2.22	0.58
1:A:208:ILE:O	1:A:278:ASN:ND2	2.37	0.58
1:D:295:VAL:HG23	3:I:11[A]:LEU:O	2.04	0.57
1:D:67:ARG:O	1:D:71:GLY:N	2.37	0.57
4:K:39:GLU:OE1	4:K:39:GLU:N	2.36	0.57
4:J:93:LYS:HE2	4:J:130:ILE:HD11	1.85	0.57
1:A:214:ASN:OD1	1:A:215:PHE:N	2.38	0.57
1:F:292:ASN:OD1	1:F:294:TYR:N	2.38	0.57
1:A:605:ILE:HG22	1:A:605:ILE:O	2.05	0.57
1:B:24:VAL:HG11	1:B:49:LEU:HD13	1.86	0.57
1:A:210:ASN:ND2	1:A:278:ASN:OD1	2.36	0.56
1:F:218:MET:SD	1:F:218:MET:N	2.73	0.56
1:D:399:ASP:OD1	1:D:399:ASP:N	2.38	0.56
1:B:380:ASP:OD1	1:B:381:GLU:N	2.35	0.56
2:H:219:MET:O	2:H:223:VAL:HG23	2.06	0.56
4:L:275:TRP:CZ2	4:L:279:MET:HE1	2.40	0.56
1:F:280:ARG:NH1	1:F:322:LEU:O	2.39	0.56
1:B:216:GLU:OE1	1:B:216:GLU:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:420:LEU:HD21	1:E:424:VAL:HG21	1.87	0.56
1:F:257:LEU:C	1:F:258:LEU:HD12	2.30	0.56
1:F:440:GLU:N	1:F:440:GLU:OE1	2.38	0.56
1:C:629:LEU:HD13	1:D:574:ILE:HD13	1.88	0.56
1:B:62:PHE:O	1:B:67:ARG:NE	2.37	0.55
1:E:35:VAL:HG13	1:E:49:LEU:HD11	1.87	0.55
1:E:122:ILE:HD11	1:E:183:VAL:HG23	1.87	0.55
1:F:496:GLN:NE2	1:F:497:GLU:O	2.40	0.55
1:D:204:ASN:OD1	1:D:205:ARG:N	2.39	0.55
1:F:484:LEU:HD23	1:F:484:LEU:O	2.07	0.55
2:H:241:VAL:HA	3:I:67:ILE:HD11	1.89	0.55
1:C:123:GLN:O	1:C:126:ASN:ND2	2.39	0.55
1:F:601:VAL:HG12	1:F:643:ILE:HB	1.89	0.55
1:B:277:LEU:HD12	1:B:324:ILE:HD11	1.89	0.54
1:D:686:PHE:O	1:D:691:ARG:NH1	2.41	0.54
1:E:473:LEU:HD23	1:E:474:GLN:N	2.22	0.54
4:K:93:LYS:HG3	4:K:130:ILE:HD12	1.88	0.54
1:A:292:ASN:OD1	1:A:293:LYS:N	2.39	0.54
1:F:488:ILE:HG22	1:F:488:ILE:O	2.08	0.54
1:B:16:LEU:HD13	1:B:23:VAL:CG1	2.38	0.54
1:C:331:ASP:OD1	1:C:375[A]:ARG:NH2	2.41	0.54
4:J:273:ASP:OD1	4:J:274:GLN:N	2.41	0.54
1:E:95:MET:SD	1:E:183:VAL:HG22	2.48	0.54
1:E:463:VAL:HG23	1:E:463:VAL:O	2.08	0.53
1:F:212:ASP:OD1	1:F:213:TRP:N	2.42	0.53
4:K:101:ILE:HG22	4:K:105:MET:HE3	1.90	0.53
1:F:594:LYS:O	1:F:638:ARG:NH1	2.42	0.53
1:B:208:ILE:O	1:B:208:ILE:CG2	2.57	0.53
1:D:280:ARG:NH2	1:D:312:GLU:OE2	2.41	0.53
1:B:99:ILE:HD13	1:B:117:MET:HE1	1.90	0.53
1:C:22:ALA:N	1:C:48:THR:O	2.42	0.53
4:J:49:ALA:HB2	4:J:64:ALA:HB3	1.90	0.53
1:F:445:VAL:HG12	1:F:449:GLN:OE1	2.09	0.52
2:G:233:ILE:CG1	3:I:182:MET:HE1	2.39	0.52
1:C:614:ILE:O	1:C:616:PRO:HA	2.09	0.52
1:D:647:SER:O	1:D:647:SER:OG	2.28	0.52
1:E:686:PHE:O	1:E:691:ARG:NH2	2.42	0.52
1:D:102:LEU:HD22	1:D:137:VAL:HG11	1.90	0.52
1:E:385:ARG:NH1	1:E:386:PRO:O	2.43	0.52
4:K:284:LYS:O	4:K:287:ILE:HG22	2.10	0.52
1:F:609:LEU:HD12	1:F:609:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:720:MET:HA	1:F:720:MET:HE2	1.92	0.51
4:J:145:TYR:OH	4:J:167:LYS:NZ	2.43	0.51
1:E:459:ALA:O	1:E:460:SER:CB	2.59	0.51
1:C:677:LEU:HD21	1:C:695:ALA:HB2	1.93	0.51
1:E:149:VAL:HG11	1:E:152:ILE:HD11	1.92	0.51
2:G:230:ILE:HA	2:G:233:ILE:HG22	1.93	0.51
1:B:95:MET:HE3	1:B:182:GLN:O	2.12	0.51
4:K:240:GLU:N	4:K:240:GLU:OE1	2.44	0.51
1:B:311:GLU:C	1:B:311:GLU:OE1	2.53	0.50
1:C:263:GLY:N	6:C:801:ATP:O2B	2.43	0.50
1:E:202:LYS:O	1:E:203:GLU:HB2	2.11	0.50
1:B:99:ILE:HG21	1:B:117:MET:HE1	1.93	0.50
1:F:650:ASP:OD1	1:F:651:VAL:N	2.45	0.50
1:F:614:ILE:O	1:F:616:PRO:HA	2.10	0.50
2:G:212:LEU:HD21	3:I:161:ARG:NE	2.21	0.50
1:F:391:VAL:HG12	1:F:393:MET:SD	2.51	0.50
1:F:686:PHE:O	1:F:691:ARG:NE	2.45	0.50
4:L:23:ASN:O	4:L:37:LYS:NZ	2.34	0.50
1:D:652:LEU:HD22	1:D:657:MET:HE3	1.94	0.50
1:E:626:LEU:HD23	1:E:657:MET:HE1	1.94	0.50
1:A:694:ILE:O	1:A:698:VAL:HG22	2.11	0.50
1:B:122:ILE:O	1:B:126:ASN:N	2.44	0.50
1:B:35:VAL:HG11	1:B:49:LEU:HD11	1.94	0.49
1:A:709:LYS:NZ	7:A:902:HOH:O	2.24	0.49
1:B:16:LEU:HD11	1:B:52:HIS:CD2	2.47	0.49
1:A:388:ARG:NH2	6:B:801:ATP:O3G	2.46	0.49
1:F:442:GLU:OE1	1:F:446:ARG:NH1	2.46	0.49
4:J:209:ALA:O	4:J:213:HIS:N	2.45	0.49
1:B:696:GLN:CD	1:B:696:GLN:C	2.80	0.49
1:E:266:LYS:NZ	6:E:801:ATP:O1B	2.45	0.49
1:A:331:ASP:OD1	1:A:373:THR:OG1	2.31	0.49
1:F:285:VAL:HG22	1:F:286:ASN:H	1.76	0.49
4:J:93:LYS:N	4:J:100:ALA:HB2	2.27	0.49
1:C:266:LYS:NZ	1:C:374:ASN:OD1	2.45	0.49
1:A:512:ASP:N	1:A:513:PRO:CD	2.76	0.49
1:B:92:ILE:CG2	1:B:95:MET:HE2	2.42	0.49
3:I:28:SER:O	3:I:32:MET:HG2	2.12	0.49
1:B:270:ALA:CB	1:B:372:MET:HE2	2.43	0.49
1:D:550:THR:HG22	1:D:550:THR:O	2.13	0.49
1:C:411:THR:HG22	1:C:411:THR:O	2.13	0.48
1:D:149:VAL:HG11	1:D:152:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:101:ILE:HG22	4:K:105:MET:CE	2.43	0.48
1:B:30:GLN:N	1:B:33:GLN:OE1	2.41	0.48
1:C:97:ILE:HD12	1:C:183:VAL:CG1	2.42	0.48
1:E:108:ASP:OD1	1:E:108:ASP:N	2.46	0.48
1:B:694:ILE:O	1:B:698:VAL:HG12	2.13	0.48
1:E:248:MET:HE3	1:E:248:MET:HA	1.95	0.48
3:I:198:ARG:NH1	3:I:202:MET:SD	2.87	0.48
1:C:37:VAL:HG11	1:C:78:ILE:HD12	1.94	0.48
1:E:33:GLN:HB2	1:E:49:LEU:HD12	1.94	0.48
3:I:32:MET:O	3:I:36:VAL:HG23	2.13	0.48
1:E:449:GLN:O	1:E:453:MET:HG3	2.14	0.48
3:I:36:VAL:HG12	3:I:156:ILE:HG21	1.96	0.48
1:D:380:ASP:OD1	1:D:381:GLU:N	2.46	0.48
1:B:677:LEU:HD21	1:B:695:ALA:CB	2.43	0.48
4:J:88:ALA:O	4:J:92:PHE:CD2	2.66	0.48
1:A:517:VAL:HG11	1:A:552:LEU:HD23	1.96	0.48
1:A:650:ASP:OD1	1:A:651:VAL:N	2.45	0.48
1:B:95:MET:HE1	1:B:181:SER:HB3	1.96	0.47
1:D:420:LEU:HD11	1:D:424:VAL:HG11	1.95	0.47
1:E:302:ILE:HD11	1:E:350:VAL:HG13	1.96	0.47
1:F:223:LEU:HD11	1:F:395:ILE:HG23	1.94	0.47
3:I:25:SER:OG	3:I:146:MET:SD	2.72	0.47
1:A:413:ARG:HD3	1:A:413:ARG:C	2.40	0.47
4:J:93:LYS:HA	4:J:97:PRO:HB3	1.96	0.47
1:A:715:GLU:C	1:A:715:GLU:OE1	2.58	0.47
1:E:278:ASN:O	1:E:279:ALA:HB3	2.15	0.47
4:J:42:CYS:HB2	4:J:71:LEU:HD23	1.97	0.47
1:B:537:VAL:HG12	1:B:538:SER:H	1.79	0.47
1:C:290:ILE:HD13	1:C:302:ILE:HD11	1.97	0.47
1:D:240:PHE:CD2	1:D:241:PRO:HD2	2.49	0.47
2:G:208:SER:O	2:G:212:LEU:HD23	2.14	0.47
4:L:142:ILE:HG23	4:L:168:VAL:HG23	1.95	0.47
1:A:657:MET:O	1:A:657:MET:HG3	2.14	0.47
1:D:302:ILE:CD1	1:D:350:VAL:HG13	2.44	0.47
1:E:22:ALA:N	1:E:48:THR:O	2.48	0.47
1:E:202:LYS:O	1:E:203:GLU:CB	2.63	0.47
1:F:348:ASP:O	1:F:351:VAL:HG12	2.14	0.47
2:H:227:GLY:HA3	3:I:49:MET:HE3	1.96	0.47
1:E:496:GLN:NE2	1:E:565:ILE:O	2.48	0.47
1:A:271[A]:ARG:NH1	7:A:908:HOH:O	2.48	0.46
1:C:463:VAL:HG23	1:C:463:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:LYS:O	1:C:469:LYS:HG2	2.14	0.46
1:D:23:VAL:HG12	1:D:55:VAL:HG21	1.96	0.46
4:L:14:LEU:HD12	4:L:52:PHE:CE2	2.50	0.46
1:B:340:MET:O	1:B:341:ALA:HB3	2.15	0.46
1:B:672:THR:HG22	1:B:674:GLU:OE2	2.15	0.46
1:C:650:ASP:OD1	1:C:651:VAL:N	2.48	0.46
1:F:421:SER:O	1:F:424:VAL:HG22	2.15	0.46
1:C:16:LEU:HD13	1:C:23:VAL:CG1	2.45	0.46
1:C:24:VAL:HG11	1:C:49:LEU:HD22	1.97	0.46
1:A:423:ASP:OD1	1:A:424:VAL:N	2.48	0.46
4:L:16:GLU:OE1	4:L:44:ILE:HD11	2.16	0.46
1:A:705:ILE:HD11	1:A:709:LYS:CG	2.46	0.46
1:C:16:LEU:HD11	1:C:52:HIS:CD2	2.51	0.46
1:A:646:THR:HG21	1:A:652:LEU:HD12	1.97	0.46
1:B:127:ASN:N	1:B:177:VAL:O	2.49	0.46
1:F:270:ALA:HB2	1:F:372:MET:HE1	1.97	0.46
1:A:698:VAL:O	1:A:698:VAL:HG23	2.16	0.46
1:D:41:PRO:O	1:D:44:LYS:NZ	2.48	0.46
1:D:294:TYR:CE1	3:I:11[A]:LEU:HD12	2.50	0.46
1:F:359:ASP:O	1:F:359:ASP:OD2	2.34	0.46
1:F:403:ARG:NH2	1:F:433:THR:O	2.49	0.46
1:F:549:LYS:N	6:F:802:ATP:O2B	2.50	0.45
4:L:177:GLN:N	4:L:177:GLN:OE1	2.49	0.45
1:B:97:ILE:HD12	1:B:183:VAL:HG11	1.99	0.45
1:F:444:LEU:HB2	1:F:488:ILE:HG21	1.98	0.45
1:F:676:LEU:O	1:F:680:LEU:HD22	2.16	0.45
3:I:144:ASN:O	3:I:147:ASP:OD1	2.32	0.45
1:A:285:VAL:HG12	1:A:286:ASN:N	2.31	0.45
1:B:295:VAL:HG23	3:I:7[A]:MET:O	2.17	0.45
1:E:33:GLN:CB	1:E:49:LEU:HD12	2.47	0.45
3:I:21[A]:LEU:H	3:I:21[A]:LEU:HD22	1.81	0.45
2:H:227:GLY:HA3	3:I:49:MET:CE	2.46	0.45
1:F:651:VAL:HG12	1:F:655:MET:HE3	1.98	0.45
1:A:425:ASP:OD1	1:A:426:ILE:N	2.50	0.45
1:A:499:TYR:OH	1:A:565:ILE:HG21	2.17	0.45
1:D:9:ALA:N	1:D:60:VAL:O	2.49	0.45
1:D:33:GLN:HB2	1:D:49:LEU:HD12	1.98	0.45
1:A:418:GLN:C	1:A:419:LEU:HD12	2.41	0.45
1:C:16:LEU:HD13	1:C:23:VAL:HG11	1.98	0.45
1:D:657:MET:O	1:D:657:MET:HG3	2.16	0.45
1:B:34:HIS:NE2	1:B:176:LEU:HD13	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:182:MET:HE2	3:I:182:MET:HA	1.99	0.45
1:B:92:ILE:HG21	1:B:95:MET:HB3	1.99	0.45
1:B:667:VAL:HG23	1:B:667:VAL:O	2.17	0.45
1:B:218:MET:O	1:B:272:GLN:NE2	2.50	0.45
2:G:234:GLU:HB2	2:H:233:ILE:HD11	1.98	0.45
3:I:166:ASP:OD2	4:J:197:LEU:HD23	2.17	0.45
1:B:532:ASP:OD1	1:B:532:ASP:N	2.49	0.44
1:C:507:ILE:HD12	1:C:555[B]:LYS:HG3	1.99	0.44
4:L:119:ILE:O	4:L:123:HIS:ND1	2.47	0.44
1:F:355:LEU:HD11	1:F:388:ARG:CZ	2.47	0.44
2:G:212:LEU:HD12	2:G:216:PHE:HE2	1.81	0.44
2:H:195:ILE:HG23	2:H:199:HIS:CE1	2.52	0.44
3:I:134:ILE:HD12	3:I:147:ASP:HB3	1.99	0.44
4:J:42:CYS:HG	4:J:72:HIS:CE1	2.33	0.44
1:E:654:GLU:OE1	1:E:654:GLU:O	2.36	0.44
1:C:97:ILE:HD12	1:C:183:VAL:HG11	1.99	0.44
1:D:537:VAL:HG12	1:D:538:SER:N	2.33	0.44
1:E:444:LEU:O	1:E:444:LEU:HD23	2.17	0.44
1:E:494:THR:HG22	1:E:496:GLN:H	1.83	0.44
1:B:537:VAL:HG12	1:B:538:SER:N	2.32	0.44
2:H:193:SER:O	2:H:197:THR:HG23	2.17	0.44
3:I:5[A]:ALA:O	3:I:6[A]:ASP:CG	2.61	0.44
1:A:255:GLY:CA	1:A:369:VAL:O	2.66	0.44
1:D:270:ALA:CB	1:D:372:MET:HE1	2.48	0.44
1:D:487:ASP:O	1:D:488:ILE:C	2.60	0.44
1:E:35:VAL:CG1	1:E:49:LEU:HD11	2.47	0.44
1:A:659:ASN:OD1	1:A:659:ASN:C	2.61	0.44
1:B:125:PHE:CE1	1:B:136:LEU:HD12	2.52	0.44
1:B:187:LYS:N	1:B:195:LEU:HD12	2.33	0.44
2:G:212:LEU:CD2	3:I:161:ARG:HE	2.23	0.44
2:G:217:MET:HE2	4:L:200:TYR:HB2	2.00	0.44
1:A:499:TYR:N	1:A:499:TYR:CD1	2.86	0.44
3:I:29:THR:HG21	3:I:146:MET:HG2	1.99	0.44
3:I:71:MET:SD	3:I:188:ASN:ND2	2.82	0.44
1:C:690:GLU:O	1:C:694:ILE:HD12	2.17	0.43
1:D:34:HIS:CD2	1:D:48:THR:HG23	2.53	0.43
2:H:195:ILE:O	2:H:199:HIS:ND1	2.48	0.43
4:J:92:PHE:CD2	4:J:99:GLU:HB3	2.53	0.43
1:E:152:ILE:HG22	1:E:172:ILE:HD11	1.99	0.43
4:K:111:TYR:O	4:K:115:GLY:N	2.52	0.43
4:L:11:MET:HE2	4:L:52:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:PHE:CE2	1:C:136:LEU:HD13	2.54	0.43
1:D:180:ASN:OD1	1:D:180:ASN:N	2.51	0.43
1:D:512:ASP:N	1:D:513:PRO:CD	2.81	0.43
4:L:275:TRP:CH2	4:L:279:MET:HE1	2.53	0.43
1:C:520:ASP:OD2	7:C:901:HOH:O	2.21	0.43
3:I:158:GLY:O	3:I:161:ARG:HB3	2.18	0.43
1:C:646:THR:HG21	1:C:652:LEU:HD22	2.00	0.43
1:F:263:GLY:O	1:F:264:CYS:C	2.61	0.43
1:B:16:LEU:HD13	1:B:23:VAL:HG11	2.00	0.43
1:B:650:ASP:OD1	1:B:651:VAL:N	2.50	0.43
1:E:114:THR:HG21	1:E:200:LYS:HG3	2.00	0.43
3:I:36:VAL:HG21	3:I:153:VAL:CG1	2.42	0.43
4:K:129:GLU:O	4:K:133:THR:HG22	2.19	0.43
3:I:29:THR:HG22	3:I:150:LEU:HD11	2.00	0.43
1:C:597:LEU:HD23	1:C:639:LYS:HB2	2.00	0.43
1:D:16:LEU:HD13	1:D:23:VAL:HG22	2.01	0.43
1:D:540:LEU:HD11	1:D:646:THR:HG22	2.00	0.43
1:F:395:ILE:HG22	1:F:396:GLY:N	2.34	0.43
1:F:418:GLN:O	1:F:418:GLN:HG2	2.19	0.43
4:K:194:ASP:OD1	4:K:195:SER:N	2.51	0.43
1:E:121:PHE:CD1	1:E:183:VAL:HG21	2.54	0.43
1:E:444:LEU:HD23	1:E:444:LEU:C	2.43	0.43
1:E:461:THR:OG1	1:E:462:LYS:N	2.51	0.43
1:A:456:HIS:HB2	1:A:473:LEU:HD13	2.01	0.42
1:D:672:THR:OG1	1:D:675:GLN:OE1	2.27	0.42
1:B:512:ASP:N	1:B:513:PRO:HD2	2.34	0.42
1:C:92:ILE:HD11	1:C:175:GLY:C	2.44	0.42
1:E:138:PHE:HB2	1:E:147:LEU:HD11	1.99	0.42
2:G:241:VAL:HA	2:G:244:VAL:HG12	2.01	0.42
4:L:237:ASP:O	4:L:242:LYS:NZ	2.49	0.42
1:B:125:PHE:CZ	1:B:136:LEU:HD12	2.54	0.42
1:F:285:VAL:HG21	1:F:305:LEU:HD11	2.01	0.42
1:D:734:ARG:NE	1:D:734:ARG:HA	2.34	0.42
1:E:212:ASP:C	1:E:212:ASP:OD1	2.63	0.42
4:L:256:VAL:HG12	4:L:260:THR:OG1	2.19	0.42
1:D:200:LYS:O	1:D:201:THR:HG23	2.19	0.42
2:H:206:GLU:HB2	3:I:32:MET:HE1	2.00	0.42
4:J:136:VAL:HG12	4:J:136:VAL:O	2.20	0.42
1:B:35:VAL:HG21	1:B:49:LEU:HD21	2.00	0.42
1:B:612:VAL:O	1:B:612:VAL:HG13	2.19	0.42
1:F:260:GLY:O	1:F:266:LYS:NZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:688:ASP:OD1	1:F:689:LYS:NZ	2.52	0.42
4:J:97:PRO:O	4:J:100:ALA:HB3	2.20	0.42
1:A:346:VAL:HG22	1:A:346:VAL:O	2.19	0.42
2:G:219:MET:HB3	2:H:219:MET:HE1	2.02	0.42
4:L:14:LEU:HD23	4:L:14:LEU:O	2.20	0.42
1:E:259:TYR:CG	1:E:376:PRO:HG3	2.55	0.42
1:F:290:ILE:O	1:F:291:LEU:HG	2.19	0.42
1:F:418:GLN:O	1:F:418:GLN:CG	2.67	0.42
4:K:276:LEU:H	4:K:276:LEU:HD22	1.84	0.42
1:A:255:GLY:HA2	1:A:369:VAL:O	2.20	0.42
1:A:308:ASP:N	1:A:308:ASP:OD1	2.53	0.42
1:D:595:SER:OG	1:D:596:GLN:N	2.52	0.42
1:E:23:VAL:HB	1:E:61:ALA:HB3	2.02	0.42
1:E:512:ASP:N	1:E:513:PRO:CD	2.83	0.42
1:E:681:GLU:OE1	1:E:691:ARG:NE	2.53	0.42
1:F:349:THR:O	1:F:353:GLN:HG3	2.20	0.42
1:F:423:ASP:OD1	1:F:423:ASP:N	2.53	0.42
1:B:183:VAL:HG11	1:B:185:PHE:CZ	2.55	0.41
1:B:688:ASP:O	1:B:692:THR:HG23	2.20	0.41
1:C:46:ILE:HD13	1:C:174:VAL:HG21	2.01	0.41
1:C:340:MET:O	1:C:341:ALA:HB3	2.20	0.41
1:C:417:HIS:C	1:C:418:GLN:OE1	2.63	0.41
1:E:23:VAL:HG12	1:E:55:VAL:HG21	2.00	0.41
1:F:366:ASN:OD1	1:F:366:ASN:N	2.52	0.41
1:A:537:VAL:HG12	1:A:538:SER:N	2.36	0.41
1:A:720:MET:HE3	1:A:720:MET:O	2.19	0.41
1:C:512:ASP:N	1:C:513:PRO:CD	2.82	0.41
1:E:650:ASP:OD1	1:E:651:VAL:N	2.52	0.41
1:F:355:LEU:HD11	1:F:388:ARG:CD	2.51	0.41
4:J:138:VAL:HG12	4:J:142:ILE:HG12	2.02	0.41
1:B:707:ILE:HG23	1:B:708:LYS:N	2.35	0.41
4:L:136:VAL:HG12	4:L:136:VAL:O	2.20	0.41
1:A:681:GLU:OE1	1:A:691:ARG:NE	2.53	0.41
1:B:23:VAL:HG12	1:B:55:VAL:HG21	2.02	0.41
1:B:121:PHE:CD2	1:B:125:PHE:CD2	3.08	0.41
2:G:227:GLY:O	2:G:230:ILE:HG22	2.21	0.41
4:J:99:GLU:O	4:J:103:CYS:SG	2.75	0.41
1:A:259:TYR:HA	1:A:373:THR:O	2.19	0.41
1:A:274:GLY:HA2	1:A:324:ILE:CD1	2.50	0.41
1:D:375[B]:ARG:NH2	7:D:908:HOH:O	2.53	0.41
1:F:733:LEU:O	1:F:737:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:159:ASN:O	3:I:163:MET:HG2	2.21	0.41
1:C:411:THR:O	1:C:411:THR:CG2	2.68	0.41
1:C:532:ASP:OD1	1:C:533:ARG:N	2.53	0.41
1:B:18:LEU:HD13	1:B:139:SER:CB	2.50	0.41
1:D:108:ASP:OD2	1:D:112:TYR:OH	2.33	0.41
1:C:240:PHE:CD2	1:C:241:PRO:HD2	2.56	0.41
4:J:101:ILE:O	4:J:105:MET:HG2	2.21	0.41
1:C:24:VAL:HG12	1:C:60:VAL:HG13	2.03	0.41
1:C:174:VAL:HG22	1:C:175:GLY:N	2.36	0.41
1:D:122:ILE:HD11	1:D:183:VAL:CG2	2.51	0.41
1:D:726:VAL:HG13	1:D:727:ARG:N	2.36	0.41
1:E:60:VAL:HG11	1:E:62:PHE:CZ	2.56	0.41
1:F:215:PHE:O	1:F:215:PHE:CG	2.74	0.41
1:F:567:ILE:HG23	1:F:601:VAL:HG23	2.03	0.41
1:F:609:LEU:O	1:F:610:ASP:C	2.64	0.41
4:J:51:MET:HE2	4:J:51:MET:CA	2.51	0.41
4:J:92:PHE:O	4:J:96:ASP:C	2.63	0.41
4:L:69:ALA:HB2	4:L:84:CYS:HB3	2.03	0.41
1:B:239:VAL:HG22	1:B:239:VAL:O	2.21	0.41
1:D:294:TYR:CD1	3:I:11[A]:LEU:HD12	2.56	0.41
4:J:217:ASP:OD2	4:J:217:ASP:C	2.63	0.41
4:L:50:ASN:O	4:L:54:MET:HG2	2.21	0.41
1:A:331:ASP:OD2	1:A:331:ASP:C	2.64	0.40
1:C:35:VAL:HG21	1:C:49:LEU:HD21	2.03	0.40
1:F:665:ILE:HG22	1:F:666:HIS:N	2.36	0.40
1:B:193:LEU:HD21	1:B:195:LEU:HD21	2.03	0.40
1:B:346:VAL:HG12	1:B:346:VAL:O	2.21	0.40
1:E:12:PRO:HD2	1:E:23:VAL:HG11	2.03	0.40
1:F:676:LEU:O	1:F:680:LEU:CD2	2.69	0.40
1:B:177:VAL:HG13	1:B:181:SER:CB	2.51	0.40
1:C:539:VAL:HG22	1:C:540:LEU:N	2.37	0.40
4:K:203:LYS:O	4:K:204:ASP:C	2.65	0.40
4:L:11:MET:HE2	4:L:52:PHE:CE1	2.57	0.40
1:D:426:ILE:O	1:D:426:ILE:HG22	2.20	0.40
1:F:264:CYS:HB2	1:F:395:ILE:HG21	2.03	0.40
1:B:178:VAL:HG23	1:B:180:ASN:OD1	2.21	0.40
1:D:92:ILE:HD12	1:D:177:VAL:HG23	2.02	0.40
1:F:603:ASP:HA	1:F:645:THR:OG1	2.21	0.40
4:J:213:HIS:NE2	4:J:220:ASN:OD1	2.54	0.40
4:L:214:PHE:CE2	4:L:248:LEU:HD13	2.56	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	A	532/747 (71%)	512 (96%)	20 (4%)	0	100	100
1	B	729/747 (98%)	705 (97%)	23 (3%)	1 (0%)	48	79
1	C	726/747 (97%)	708 (98%)	18 (2%)	0	100	100
1	D	726/747 (97%)	705 (97%)	20 (3%)	1 (0%)	48	79
1	E	726/747 (97%)	703 (97%)	21 (3%)	2 (0%)	37	69
1	F	507/747 (68%)	488 (96%)	18 (4%)	1 (0%)	44	76
2	G	61/267 (23%)	61 (100%)	0	0	100	100
2	H	70/267 (26%)	70 (100%)	0	0	100	100
3	I	174/222 (78%)	172 (99%)	2 (1%)	0	100	100
4	J	285/296 (96%)	279 (98%)	6 (2%)	0	100	100
4	K	272/296 (92%)	269 (99%)	3 (1%)	0	100	100
4	L	271/296 (92%)	263 (97%)	8 (3%)	0	100	100
All	All	5079/6126 (83%)	4935 (97%)	139 (3%)	5 (0%)	50	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	460	SER
1	E	460	SER
1	E	203	GLU
1	F	460	SER
1	B	346	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	A	460/638 (72%)	460 (100%)	0	100	100
1	B	629/638 (99%)	629 (100%)	0	100	100
1	C	625/638 (98%)	625 (100%)	0	100	100
1	D	626/638 (98%)	625 (100%)	1 (0%)	92	96
1	E	626/638 (98%)	625 (100%)	1 (0%)	92	96
1	F	439/638 (69%)	437 (100%)	2 (0%)	86	92
2	G	58/245 (24%)	58 (100%)	0	100	100
2	H	66/245 (27%)	66 (100%)	0	100	100
3	I	155/187 (83%)	151 (97%)	4 (3%)	41	66
4	J	235/243 (97%)	234 (100%)	1 (0%)	89	94
4	K	227/243 (93%)	227 (100%)	0	100	100
4	L	226/243 (93%)	226 (100%)	0	100	100
All	All	4372/5234 (84%)	4363 (100%)	9 (0%)	91	96

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	201	THR
1	E	499	TYR
1	F	391	VAL
1	F	604	ASP
3	I	13[A]	GLU
3	I	13[B]	GLU
3	I	19[A]	ASP
3	I	19[B]	ASP
4	J	213	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	HIS
1	A	474	GLN
1	B	124	GLN
1	B	128	GLN
1	B	272	GLN

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Mol	Chain	Res	Type
1	B	319	ASN
1	C	52	HIS
1	C	106	ASN
1	C	456	HIS
1	C	486	ASN
1	C	495	ASN
1	D	214	ASN
1	E	33	GLN
1	E	204	ASN
1	E	247	GLN
1	E	408	HIS
1	F	214	ASN
1	F	418	GLN
1	F	486	ASN
1	F	530	ASN
1	F	666	HIS
1	F	685	ASN
2	H	207	ASN
2	H	213	HIS
4	J	174	GLN
4	L	144	HIS

### 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](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	ATP	B	801	-	28,33,33	0.72	0	34,52,52	0.93	1 (2%)
5	ADP	A	801	-	24,29,29	0.90	0	29,45,45	1.26	2 (6%)
6	ATP	C	802	-	28,33,33	0.72	0	34,52,52	0.91	1 (2%)
6	ATP	A	802	-	28,33,33	0.87	1 (3%)	34,52,52	0.81	1 (2%)
6	ATP	D	802	-	28,33,33	0.92	1 (3%)	34,52,52	0.79	1 (2%)
6	ATP	E	802	-	28,33,33	0.66	0	34,52,52	0.94	1 (2%)
6	ATP	C	801	-	28,33,33	0.72	0	34,52,52	1.04	4 (11%)
6	ATP	F	801	-	28,33,33	0.65	0	34,52,52	0.96	1 (2%)
6	ATP	F	802	-	28,33,33	0.63	0	34,52,52	0.88	1 (2%)
6	ATP	B	802	-	28,33,33	0.72	0	34,52,52	0.90	1 (2%)
6	ATP	E	801	-	28,33,33	0.70	0	34,52,52	0.96	1 (2%)
6	ATP	D	801	-	28,33,33	0.67	0	34,52,52	0.90	1 (2%)

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
6	ATP	B	801	-	-	2/18/38/38	0/3/3/3
5	ADP	A	801	-	-	2/12/32/32	0/3/3/3
6	ATP	C	802	-	-	6/18/38/38	0/3/3/3
6	ATP	A	802	-	-	1/18/38/38	0/3/3/3
6	ATP	D	802	-	-	5/18/38/38	0/3/3/3
6	ATP	E	802	-	-	5/18/38/38	0/3/3/3
6	ATP	C	801	-	-	5/18/38/38	0/3/3/3
6	ATP	F	801	-	-	5/18/38/38	0/3/3/3
6	ATP	F	802	-	-	2/18/38/38	0/3/3/3
6	ATP	B	802	-	-	4/18/38/38	0/3/3/3
6	ATP	E	801	-	-	4/18/38/38	0/3/3/3
6	ATP	D	801	-	-	7/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	802	ATP	C1'-N9	-2.46	1.43	1.49
6	D	802	ATP	C1'-N9	-2.04	1.44	1.49

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	801	ADP	N3-C2-N1	-4.00	123.24	128.67
5	A	801	ADP	C4-C5-N7	-2.51	106.69	109.34
6	B	801	ATP	C5-C6-N6	2.36	123.90	120.31
6	B	802	ATP	C5-C6-N6	2.35	123.90	120.31
6	D	801	ATP	C5-C6-N6	2.35	123.89	120.31
6	C	801	ATP	C5-C6-N6	2.35	123.89	120.31
6	E	802	ATP	C5-C6-N6	2.34	123.88	120.31
6	A	802	ATP	C5-C6-N6	2.34	123.87	120.31
6	C	802	ATP	C5-C6-N6	2.33	123.87	120.31
6	F	802	ATP	C5-C6-N6	2.33	123.86	120.31
6	E	801	ATP	C5-C6-N6	2.31	123.83	120.31
6	F	801	ATP	C5-C6-N6	2.29	123.80	120.31
6	C	801	ATP	C4'-O4'-C1'	-2.28	107.84	109.92
6	C	801	ATP	O3'-C3'-C2'	-2.12	105.01	111.82
6	C	801	ATP	O4'-C4'-C3'	-2.08	101.03	105.15
6	D	802	ATP	C5-C6-N6	2.07	123.47	120.31

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	801	ATP	PB-O3B-PG-O2G
6	B	802	ATP	C5'-O5'-PA-O1A
6	B	802	ATP	C5'-O5'-PA-O3A
6	C	801	ATP	C5'-O5'-PA-O1A
6	C	801	ATP	C5'-O5'-PA-O2A
6	C	801	ATP	C5'-O5'-PA-O3A
6	C	801	ATP	O4'-C4'-C5'-O5'
6	C	802	ATP	PB-O3B-PG-O2G
6	C	802	ATP	C5'-O5'-PA-O2A
6	C	802	ATP	C5'-O5'-PA-O3A
6	D	801	ATP	C5'-O5'-PA-O2A
6	D	801	ATP	C5'-O5'-PA-O3A
6	E	802	ATP	C5'-O5'-PA-O1A
6	E	802	ATP	C5'-O5'-PA-O2A
6	E	802	ATP	C5'-O5'-PA-O3A

*Continued on next page...*



*Continued from previous page...*

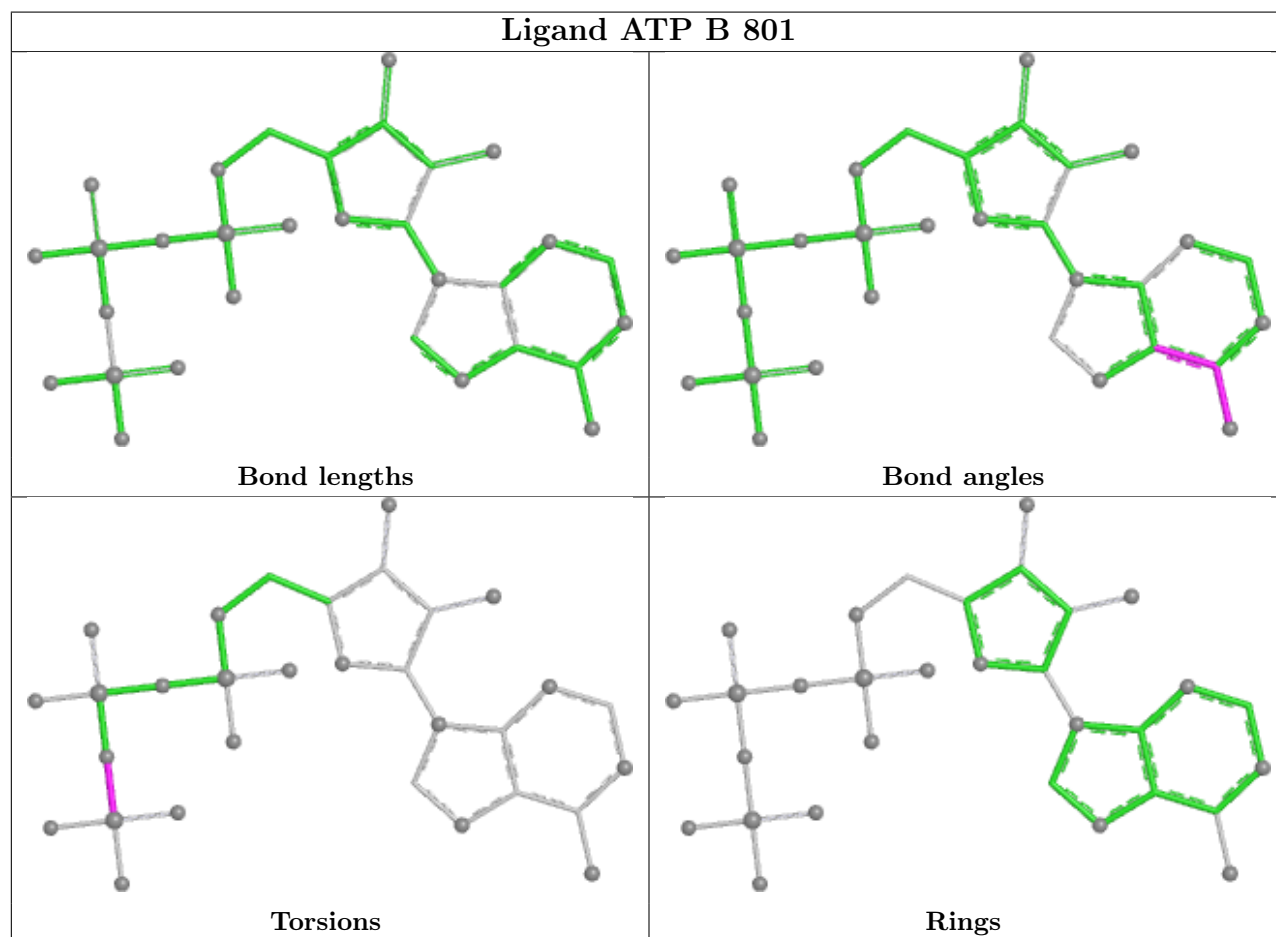
Mol	Chain	Res	Type	Atoms
6	B	802	ATP	C3'-C4'-C5'-O5'
6	C	801	ATP	C3'-C4'-C5'-O5'
6	E	802	ATP	C3'-C4'-C5'-O5'
6	F	801	ATP	C3'-C4'-C5'-O5'
6	B	802	ATP	O4'-C4'-C5'-O5'
6	E	802	ATP	O4'-C4'-C5'-O5'
6	F	801	ATP	O4'-C4'-C5'-O5'
6	C	802	ATP	C3'-C4'-C5'-O5'
6	D	801	ATP	O4'-C4'-C5'-O5'
6	D	801	ATP	C3'-C4'-C5'-O5'
6	C	802	ATP	O4'-C4'-C5'-O5'
6	F	802	ATP	C3'-C4'-C5'-O5'
6	F	802	ATP	O4'-C4'-C5'-O5'
6	F	801	ATP	C4'-C5'-O5'-PA
6	D	802	ATP	O4'-C4'-C5'-O5'
6	D	802	ATP	PA-O3A-PB-O2B
6	C	802	ATP	C5'-O5'-PA-O1A
6	D	801	ATP	C5'-O5'-PA-O1A
6	E	801	ATP	C5'-O5'-PA-O1A
6	D	802	ATP	C3'-C4'-C5'-O5'
5	A	801	ADP	C3'-C4'-C5'-O5'
6	D	802	ATP	PA-O3A-PB-O1B
5	A	801	ADP	O4'-C4'-C5'-O5'
6	B	801	ATP	PB-O3B-PG-O3G
6	A	802	ATP	O4'-C4'-C5'-O5'
6	D	801	ATP	PG-O3B-PB-O1B
6	D	801	ATP	PG-O3B-PB-O2B
6	F	801	ATP	PG-O3B-PB-O1B
6	F	801	ATP	PG-O3B-PB-O2B
6	D	802	ATP	PB-O3B-PG-O1G
6	E	801	ATP	O4'-C4'-C5'-O5'
6	E	801	ATP	PA-O3A-PB-O1B
6	E	801	ATP	PA-O3A-PB-O2B

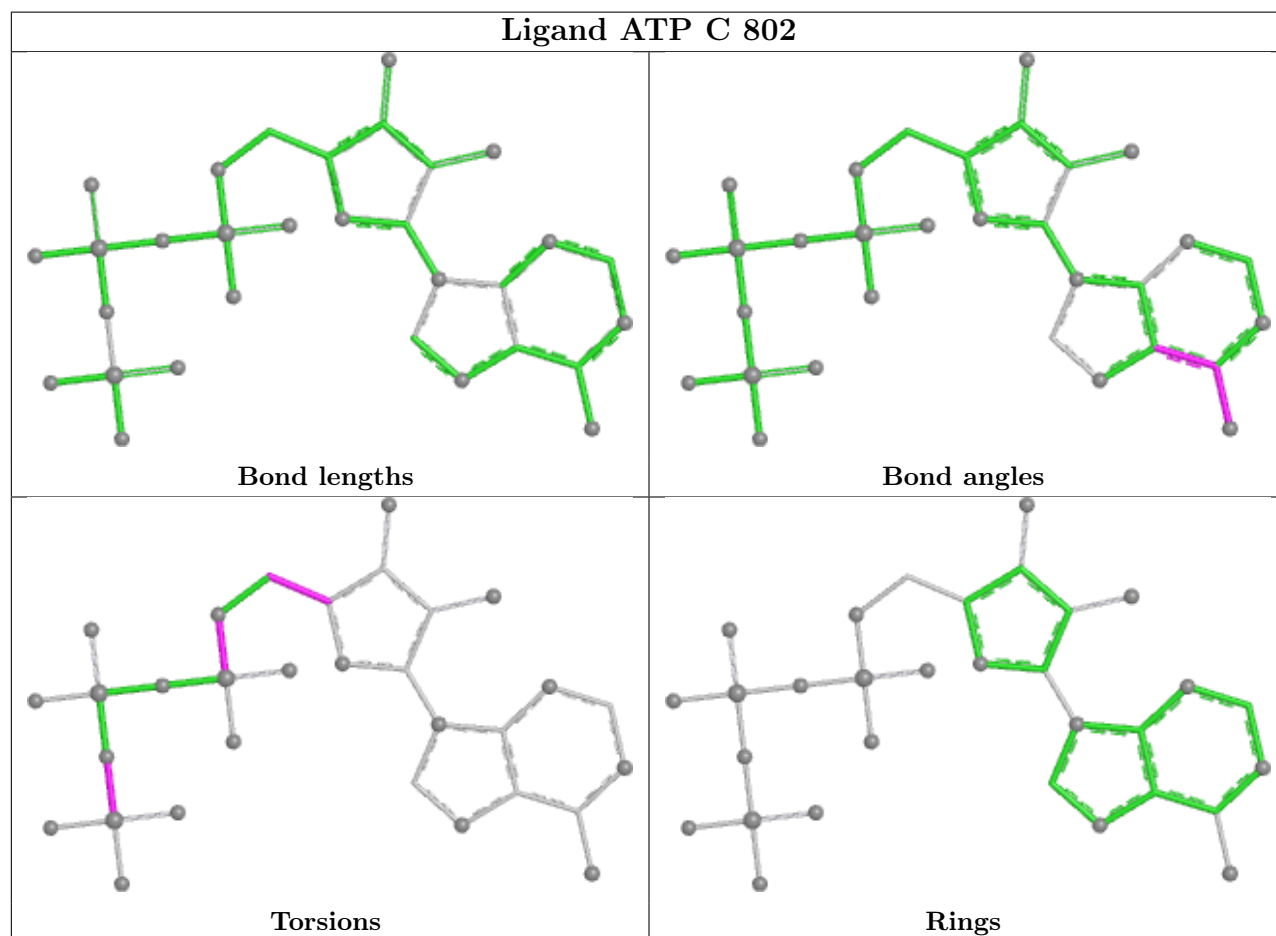
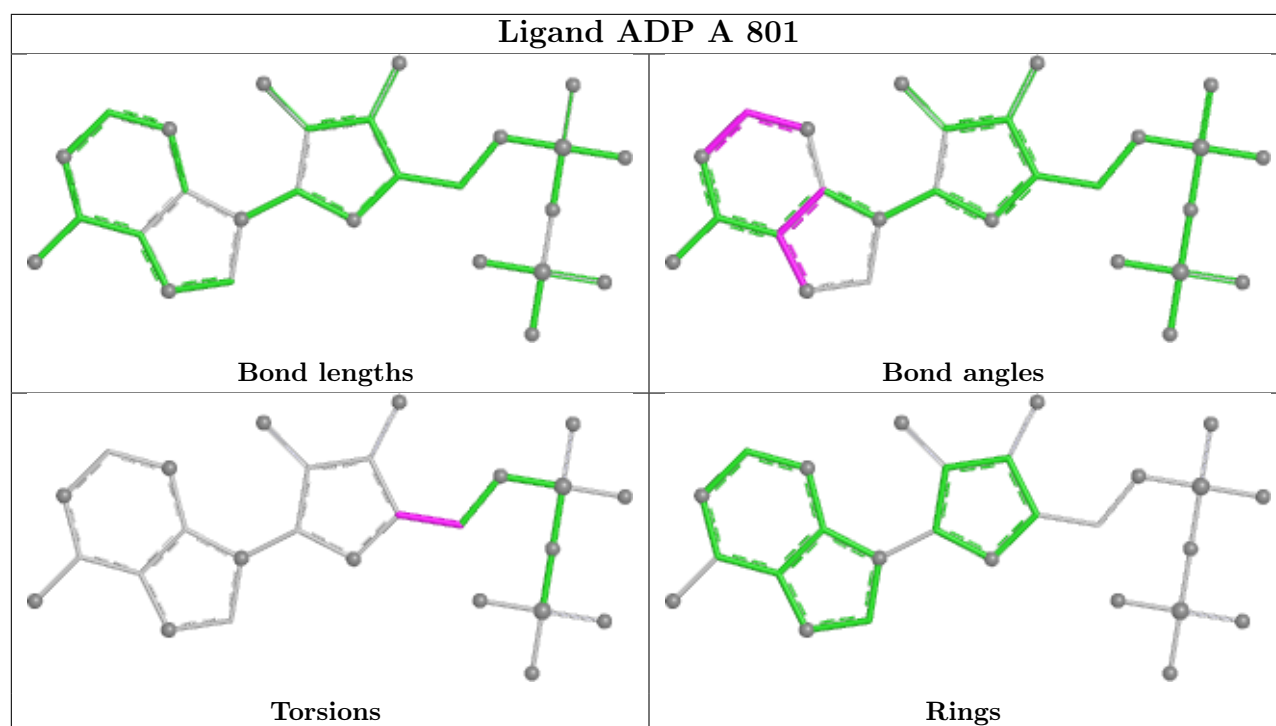
There are no ring outliers.

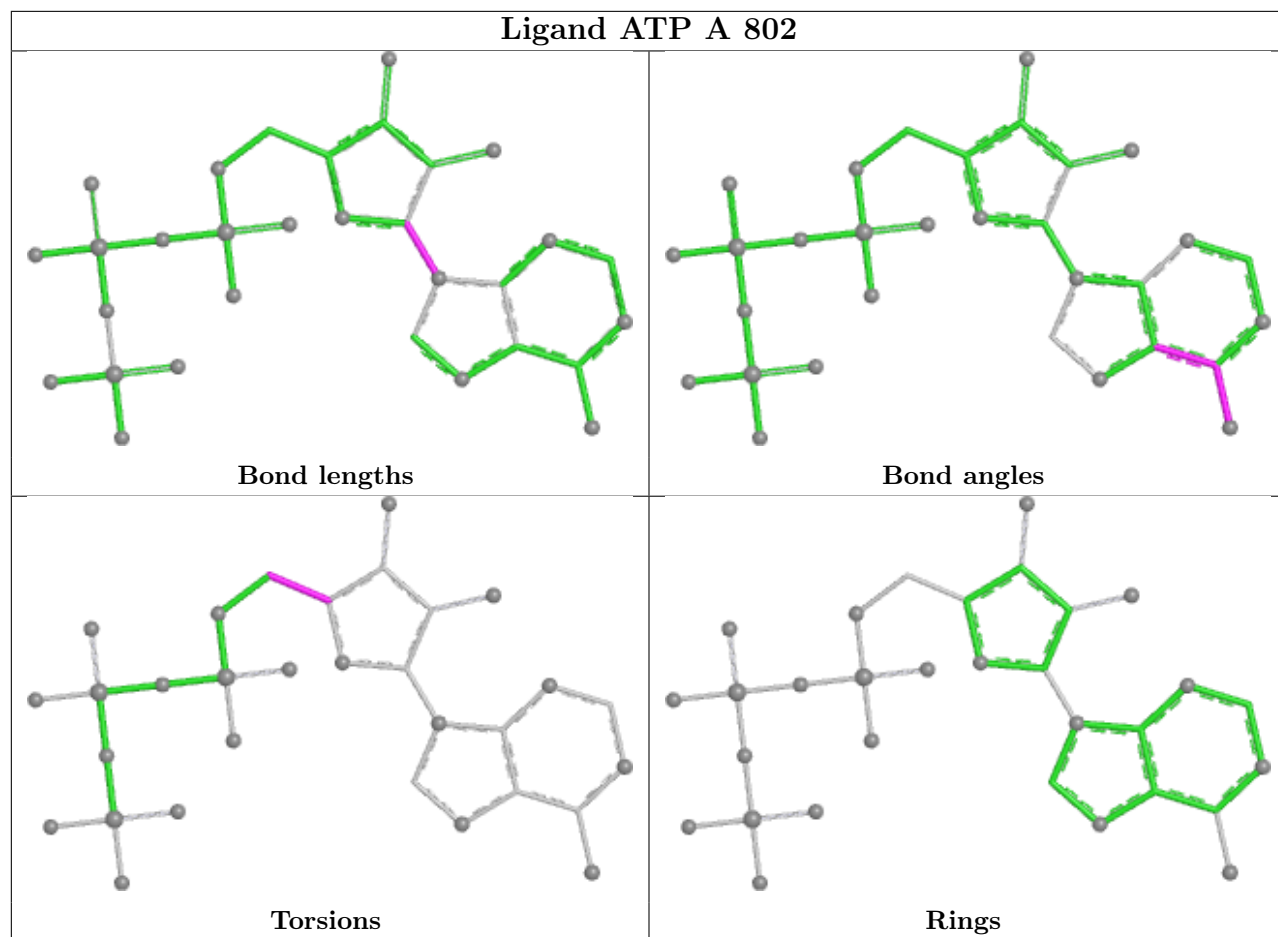
4 monomers are involved in 4 short contacts:

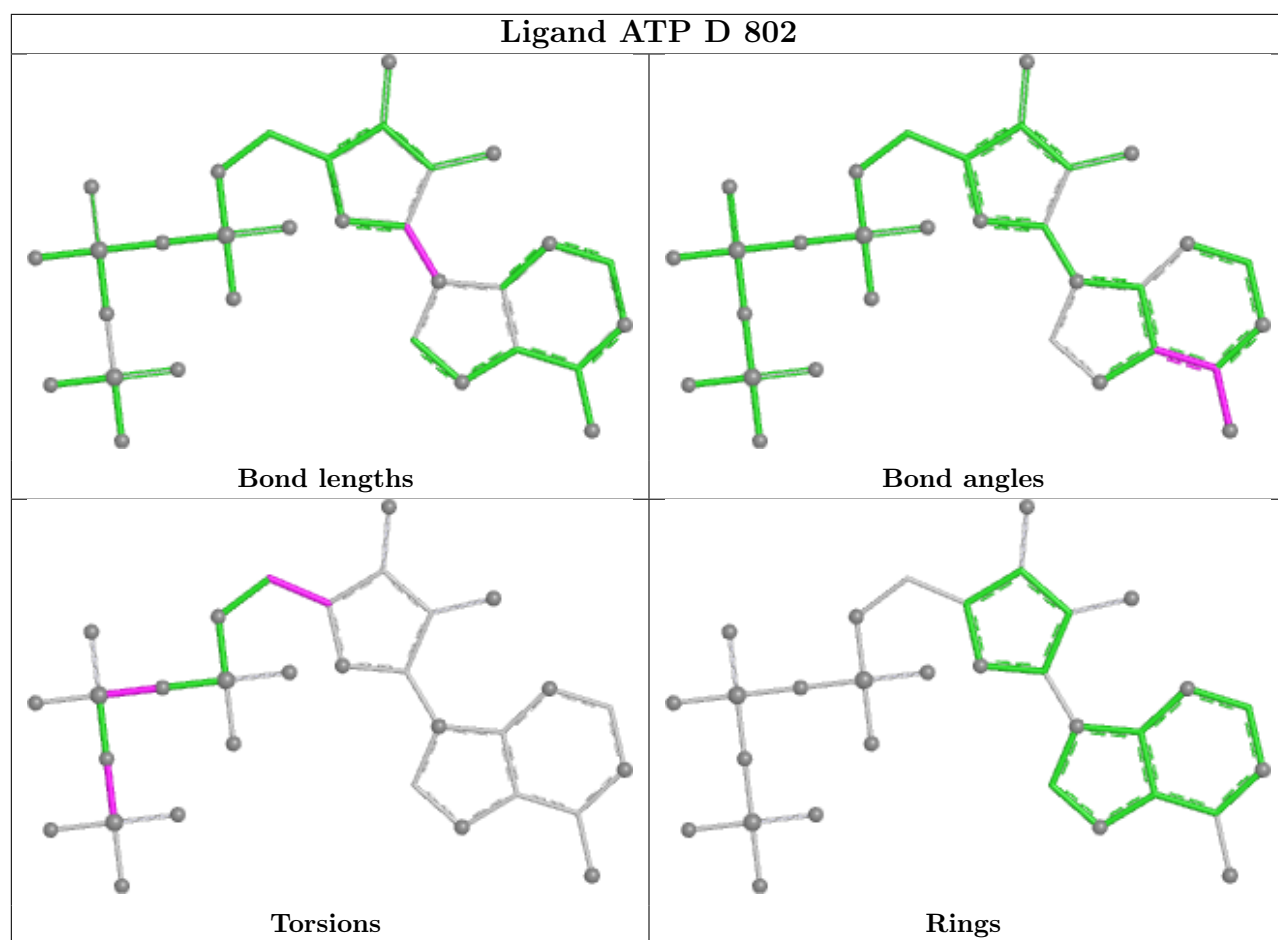
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	801	ATP	1	0
6	C	801	ATP	1	0
6	F	802	ATP	1	0
6	E	801	ATP	1	0

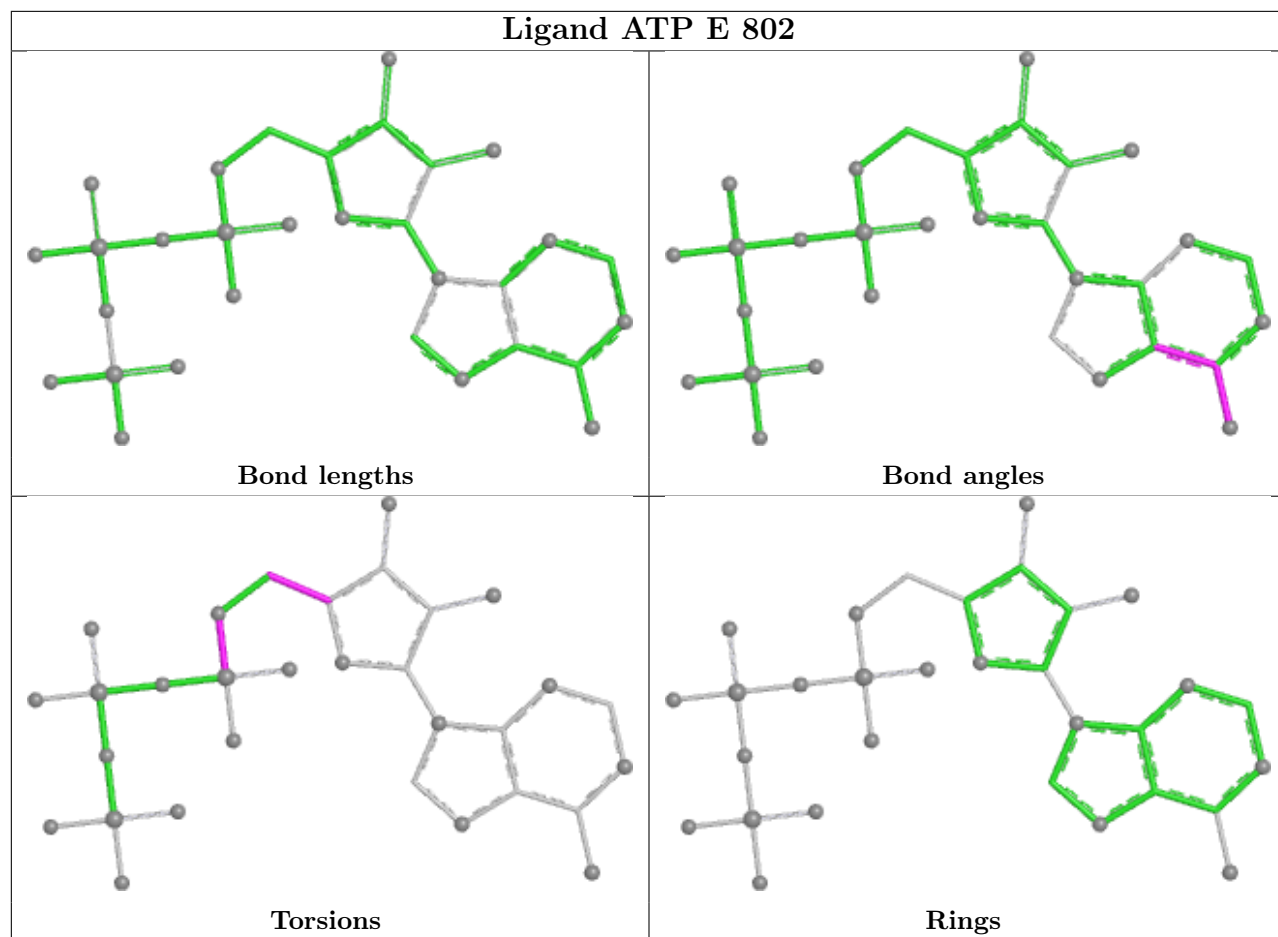
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

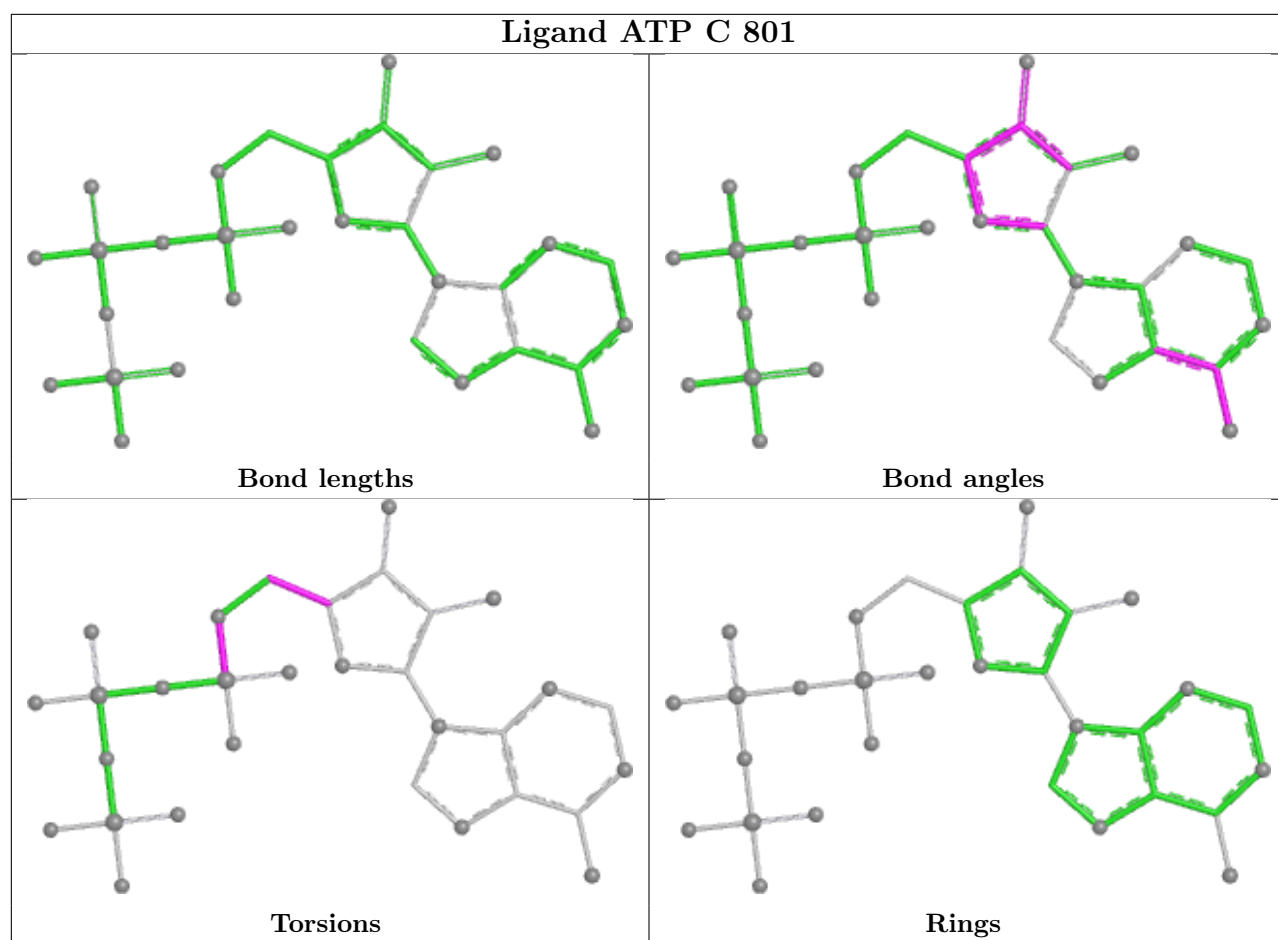


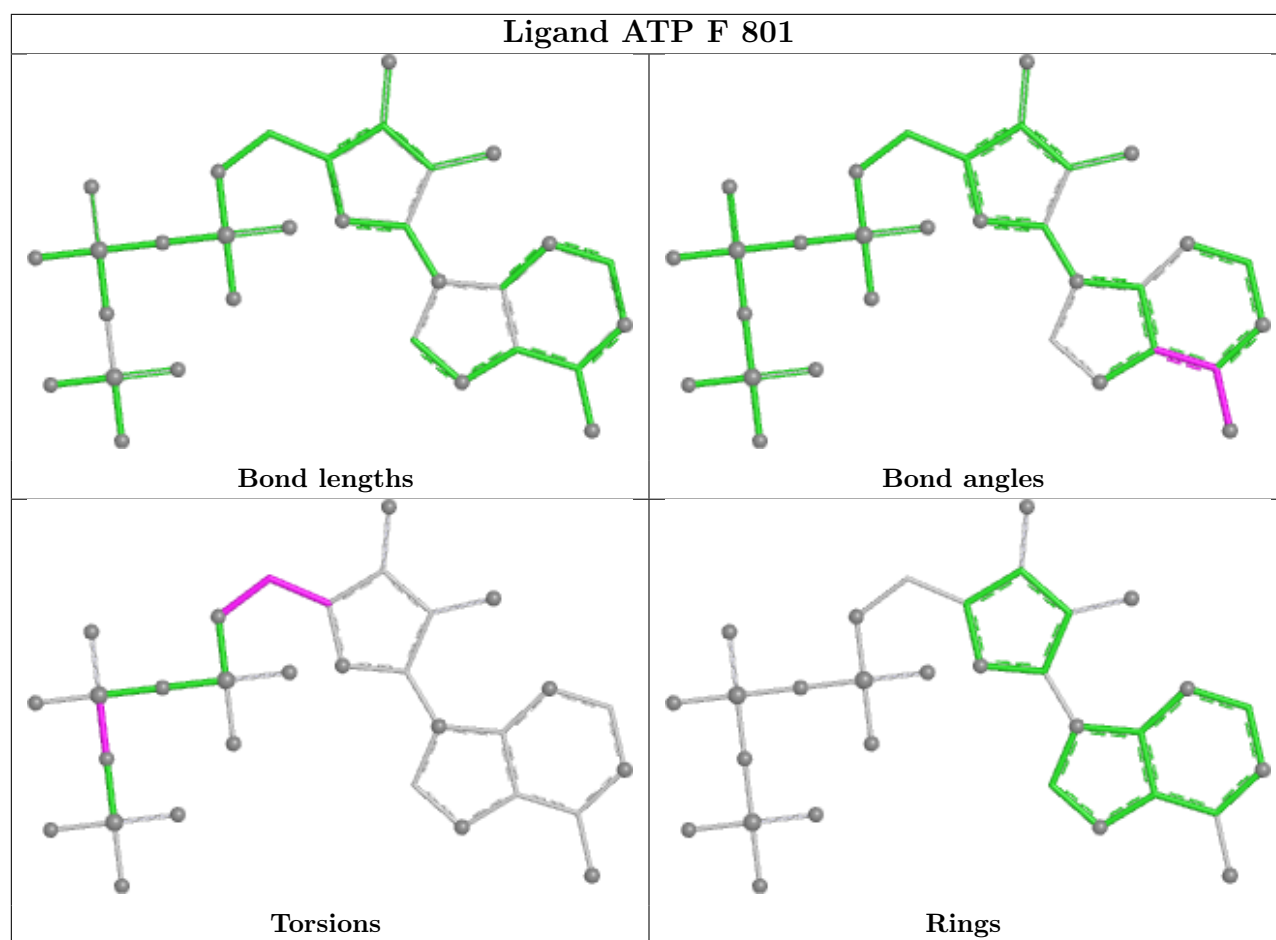




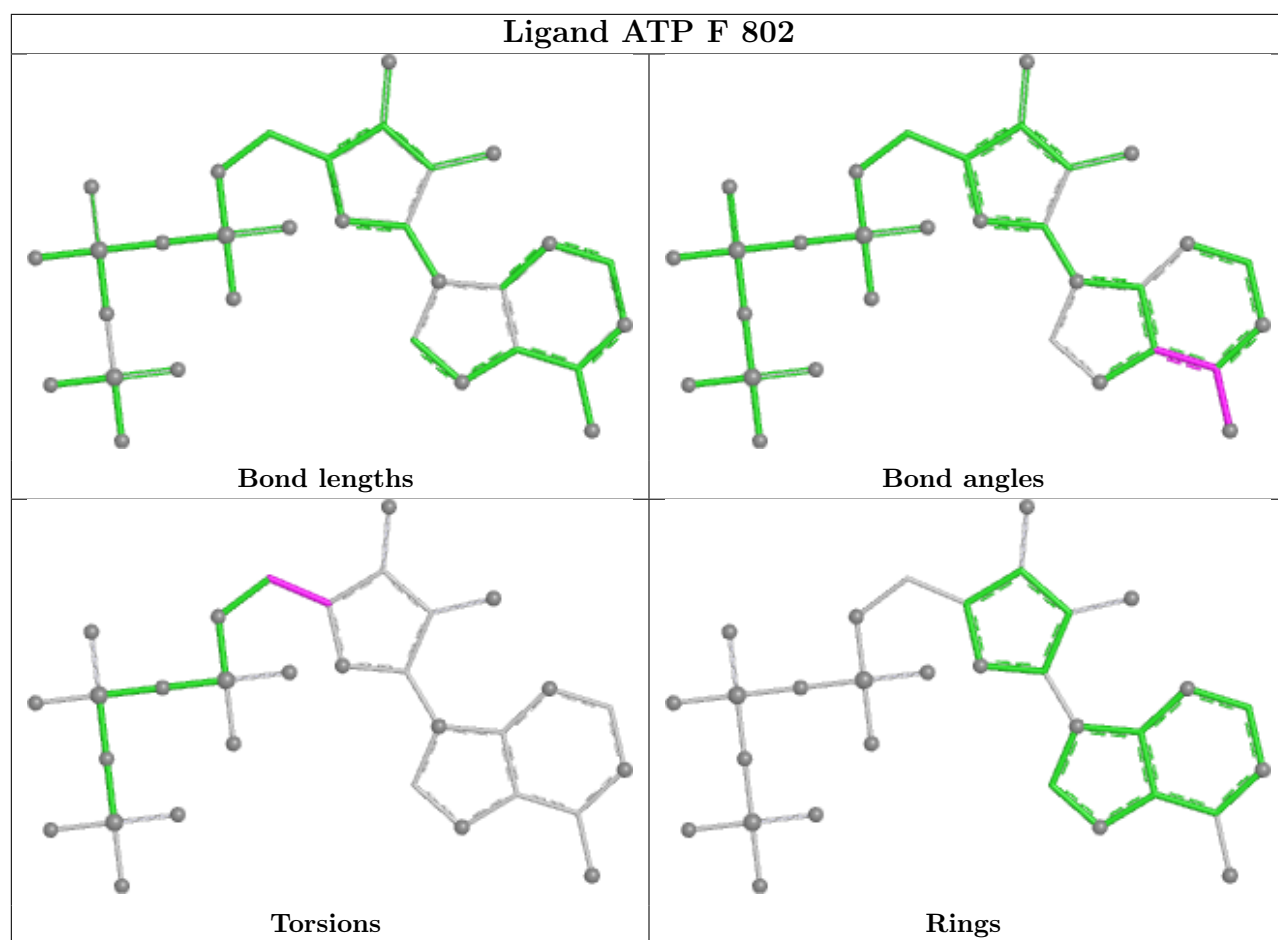


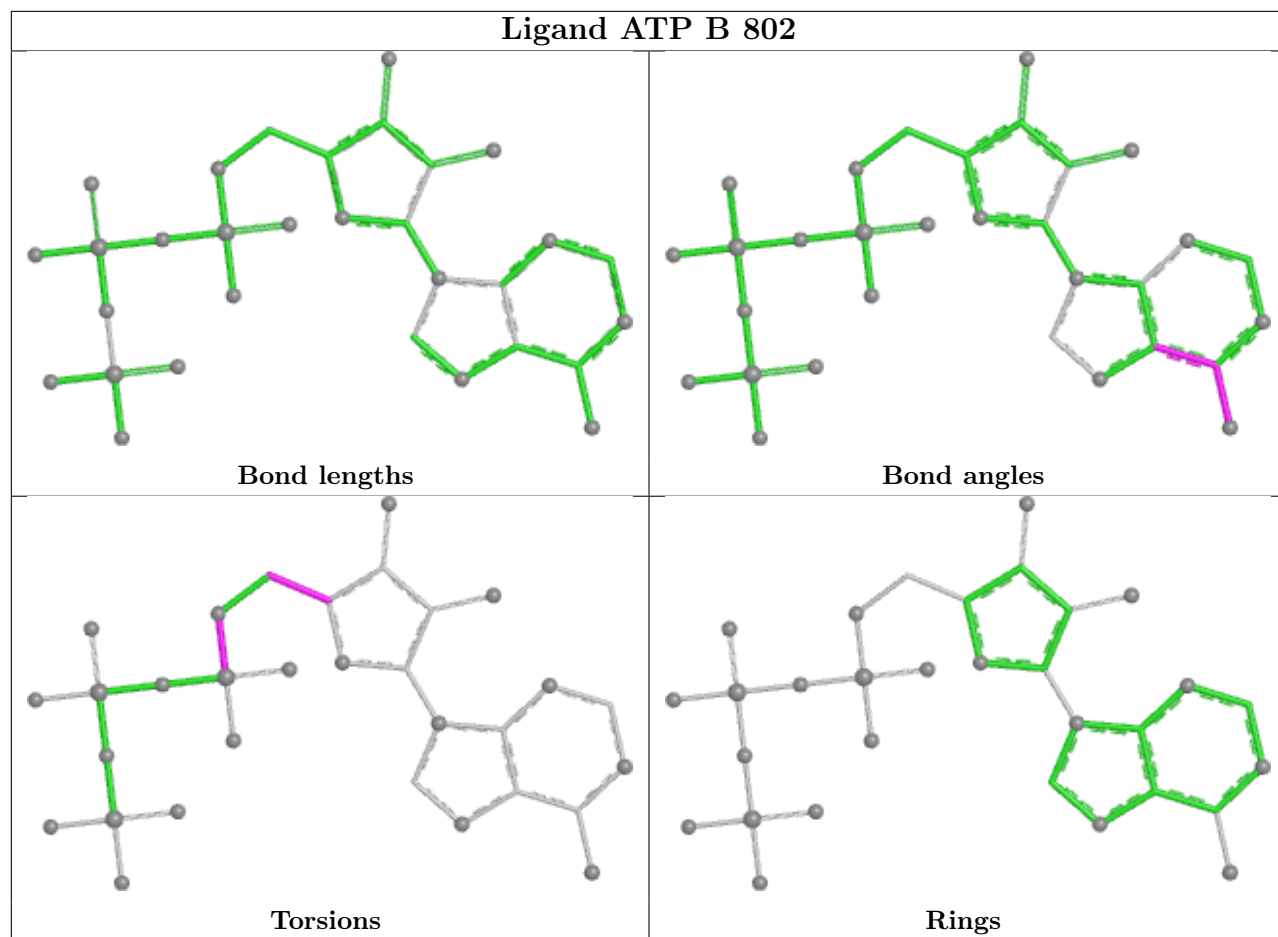


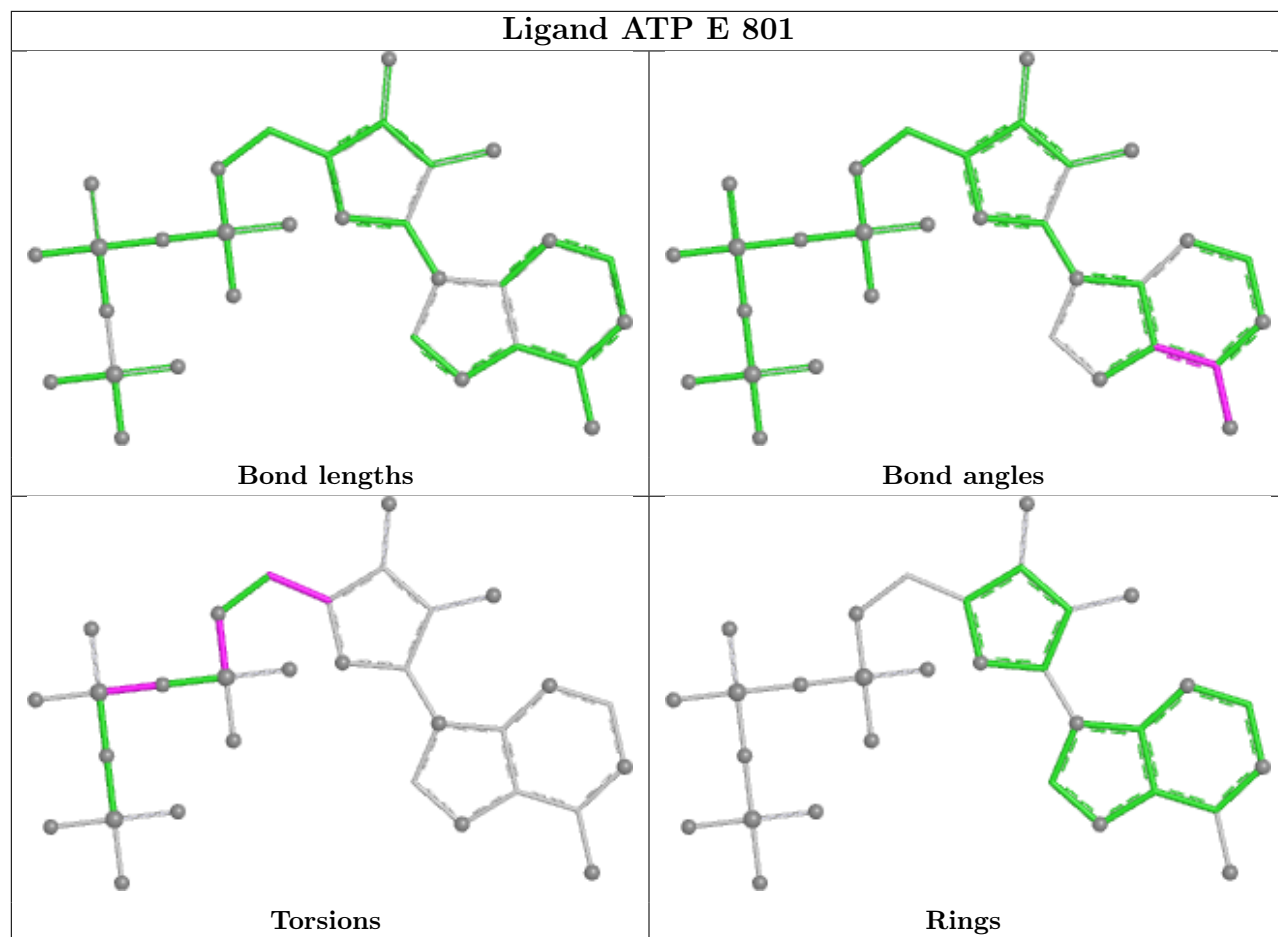


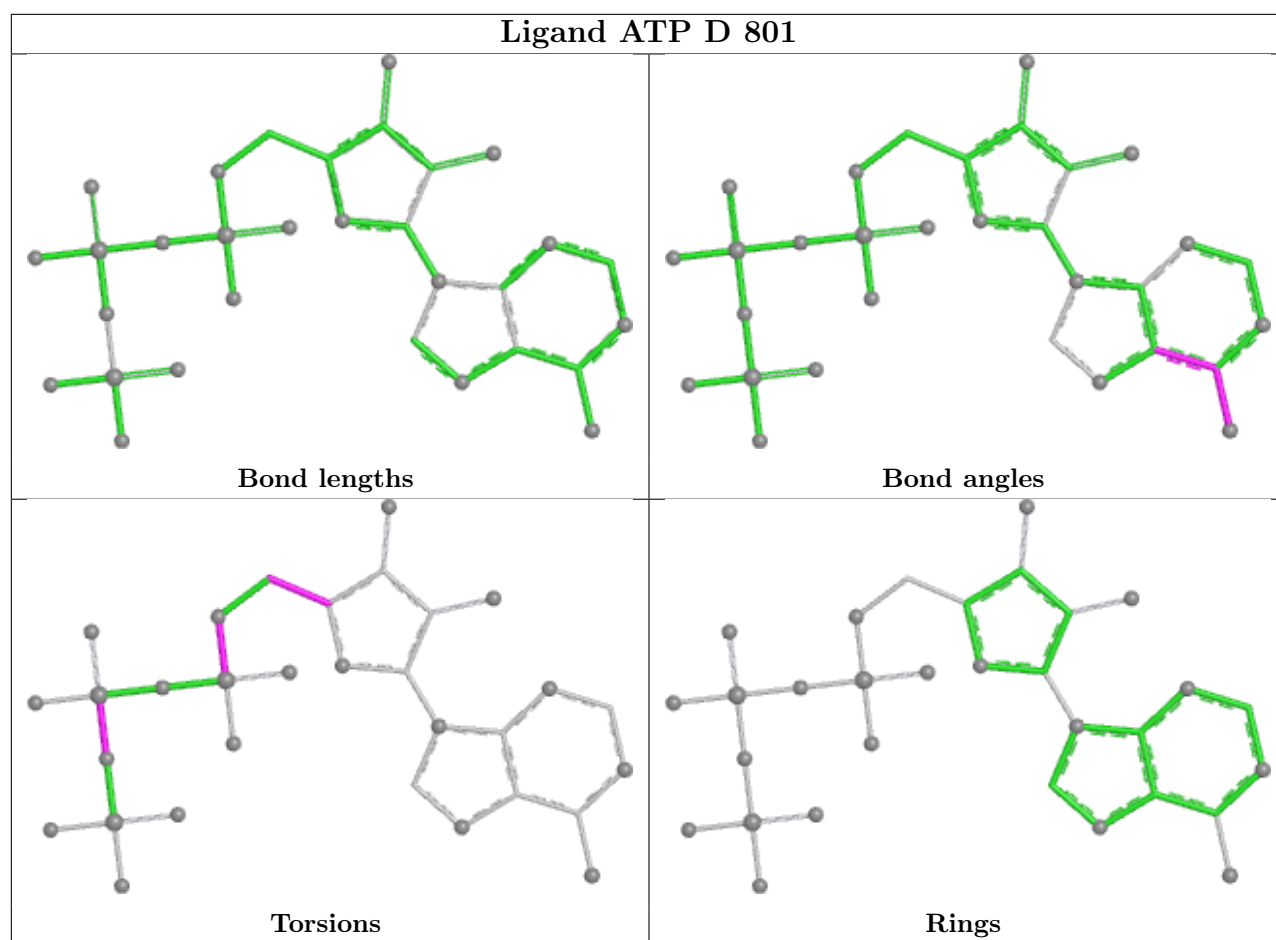












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

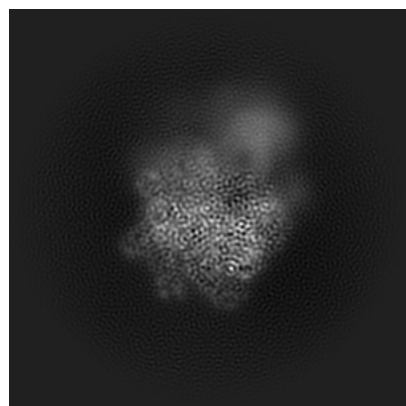
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71475. These allow visual inspection of the internal detail of the map and identification of artifacts.

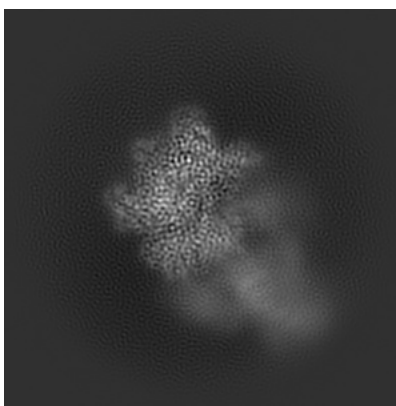
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

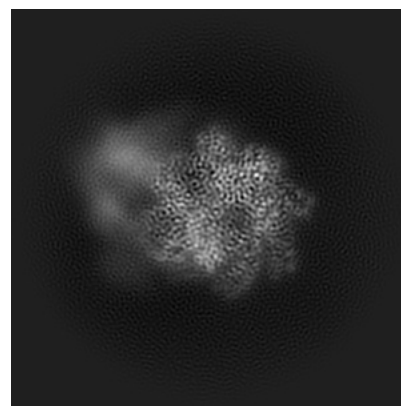
#### 6.1.1 Primary map



X

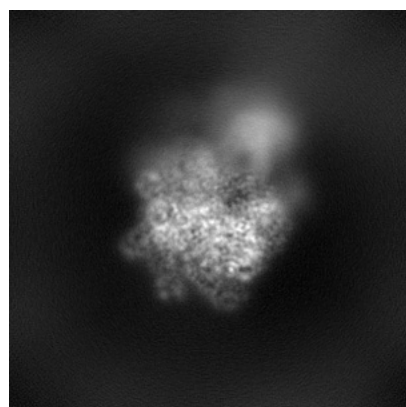


Y

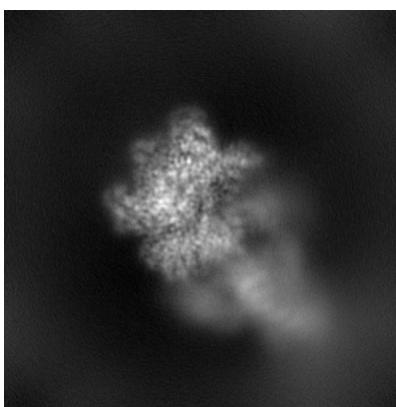


Z

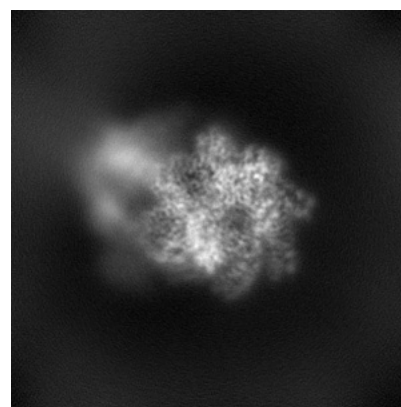
#### 6.1.2 Raw map



X



Y

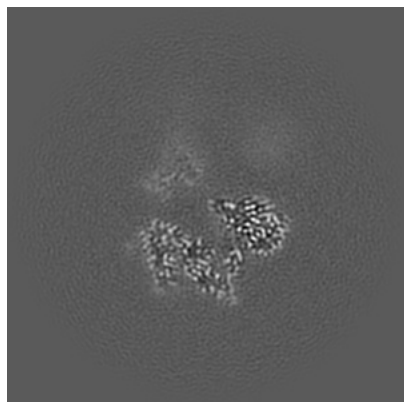


Z

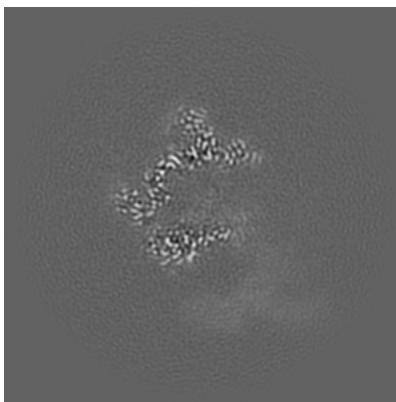
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

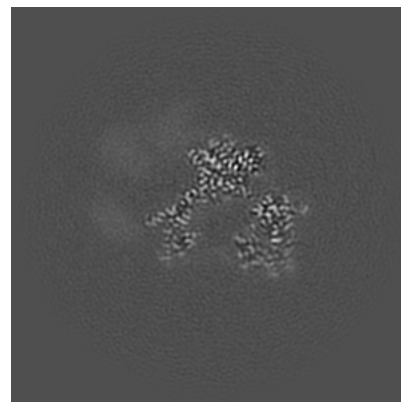
### 6.2.1 Primary map



X Index: 147

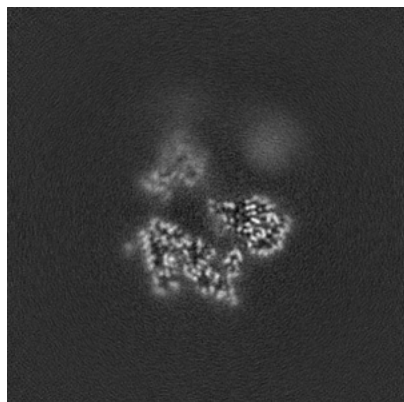


Y Index: 147

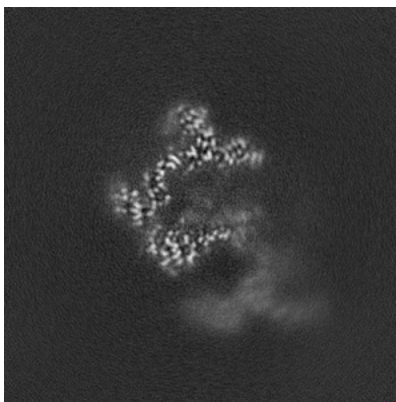


Z Index: 147

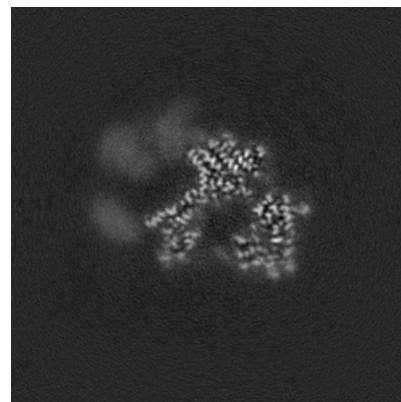
### 6.2.2 Raw map



X Index: 147



Y Index: 147

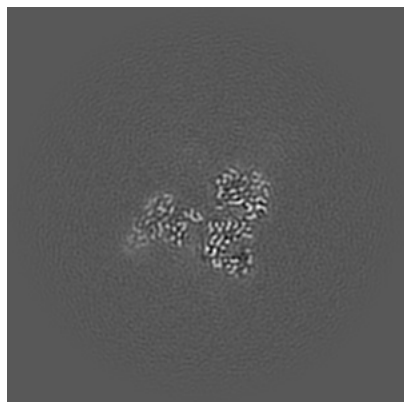


Z Index: 147

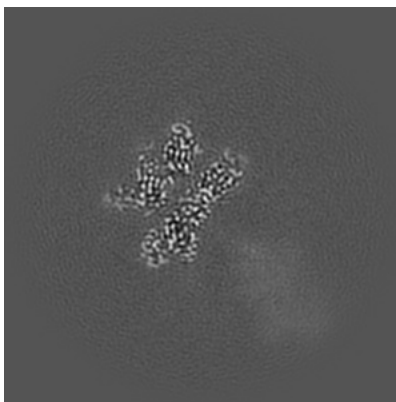
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

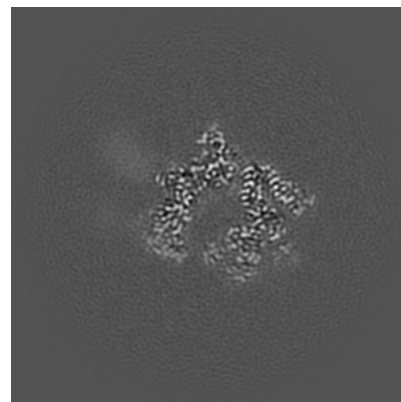
### 6.3.1 Primary map



X Index: 172

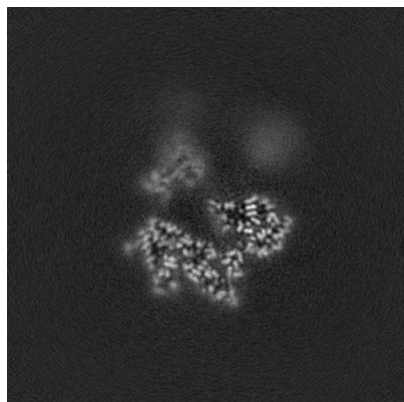


Y Index: 164

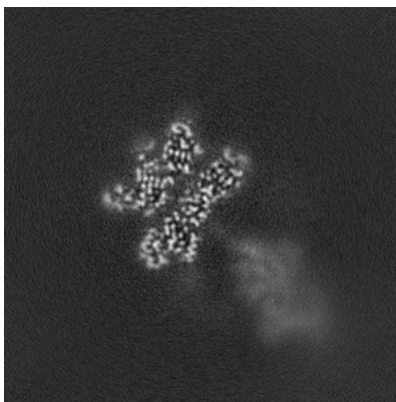


Z Index: 134

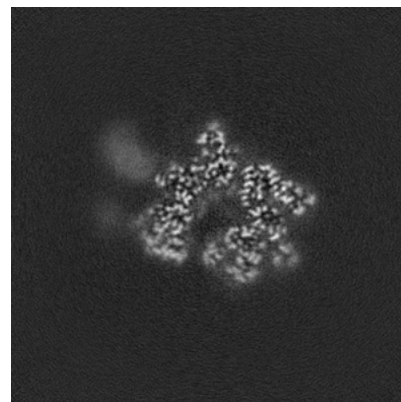
### 6.3.2 Raw map



X Index: 148



Y Index: 164



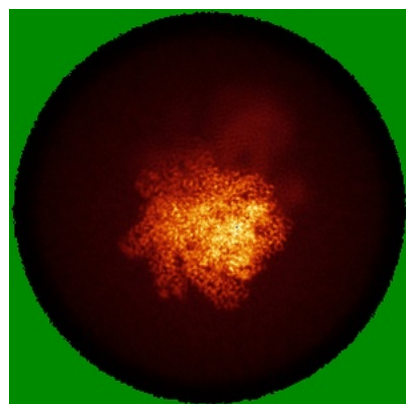
Z Index: 134

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

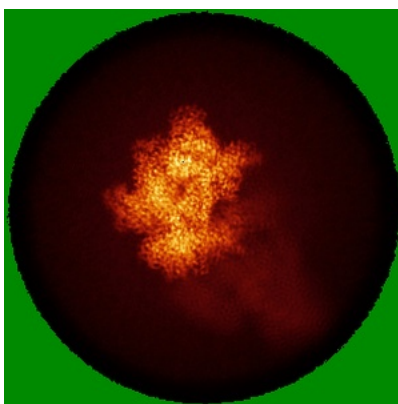


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

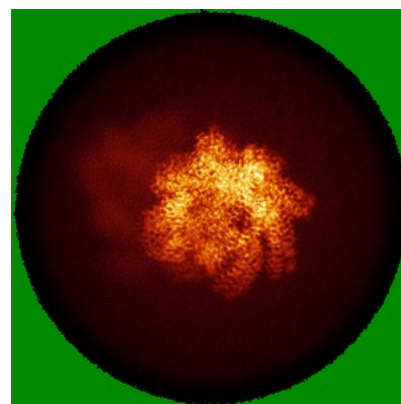
### 6.4.1 Primary map



X

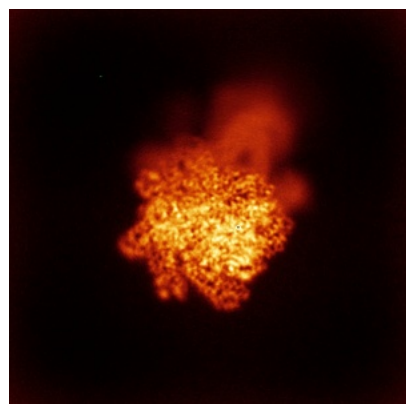


Y

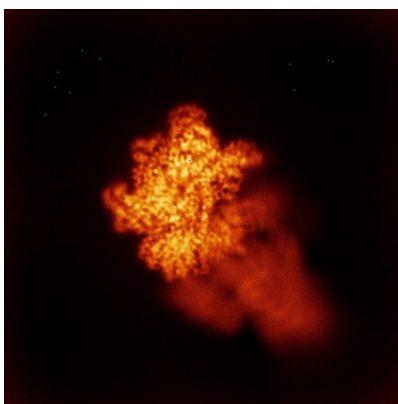


Z

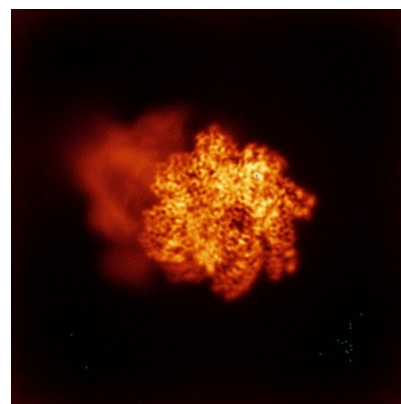
### 6.4.2 Raw map



X



Y



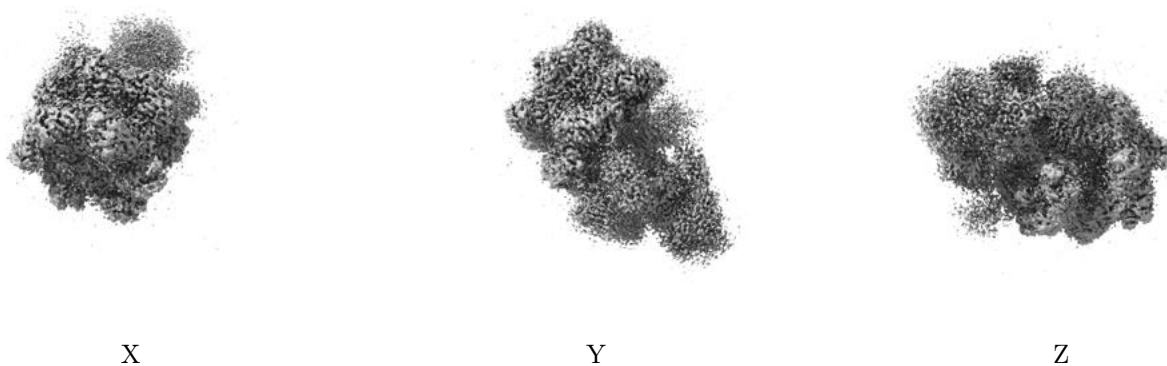
Z

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.



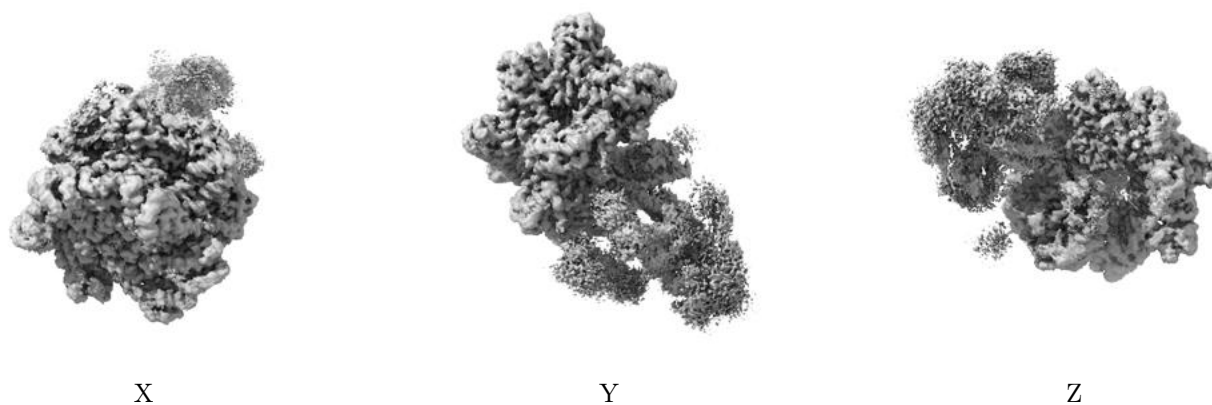
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

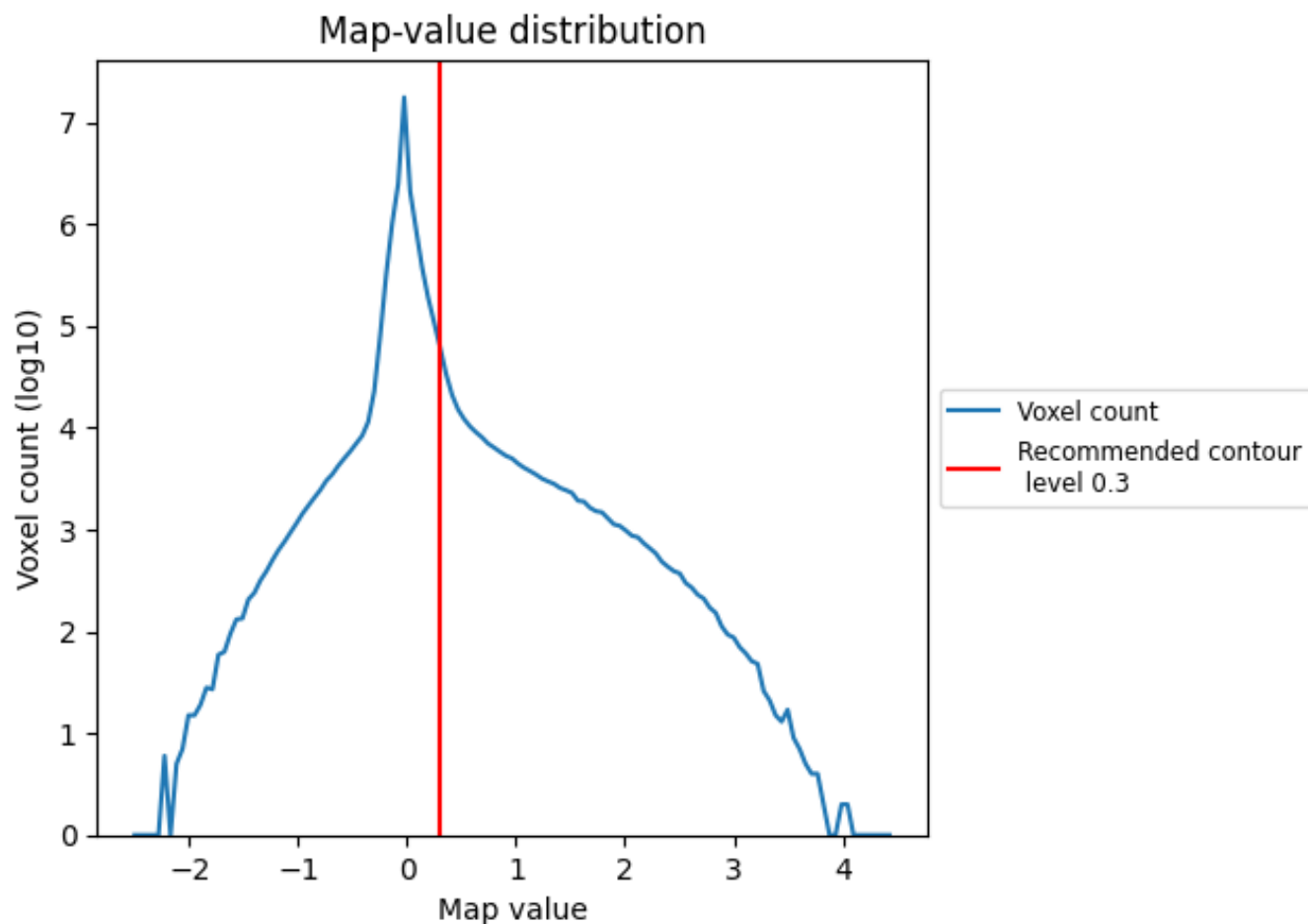
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

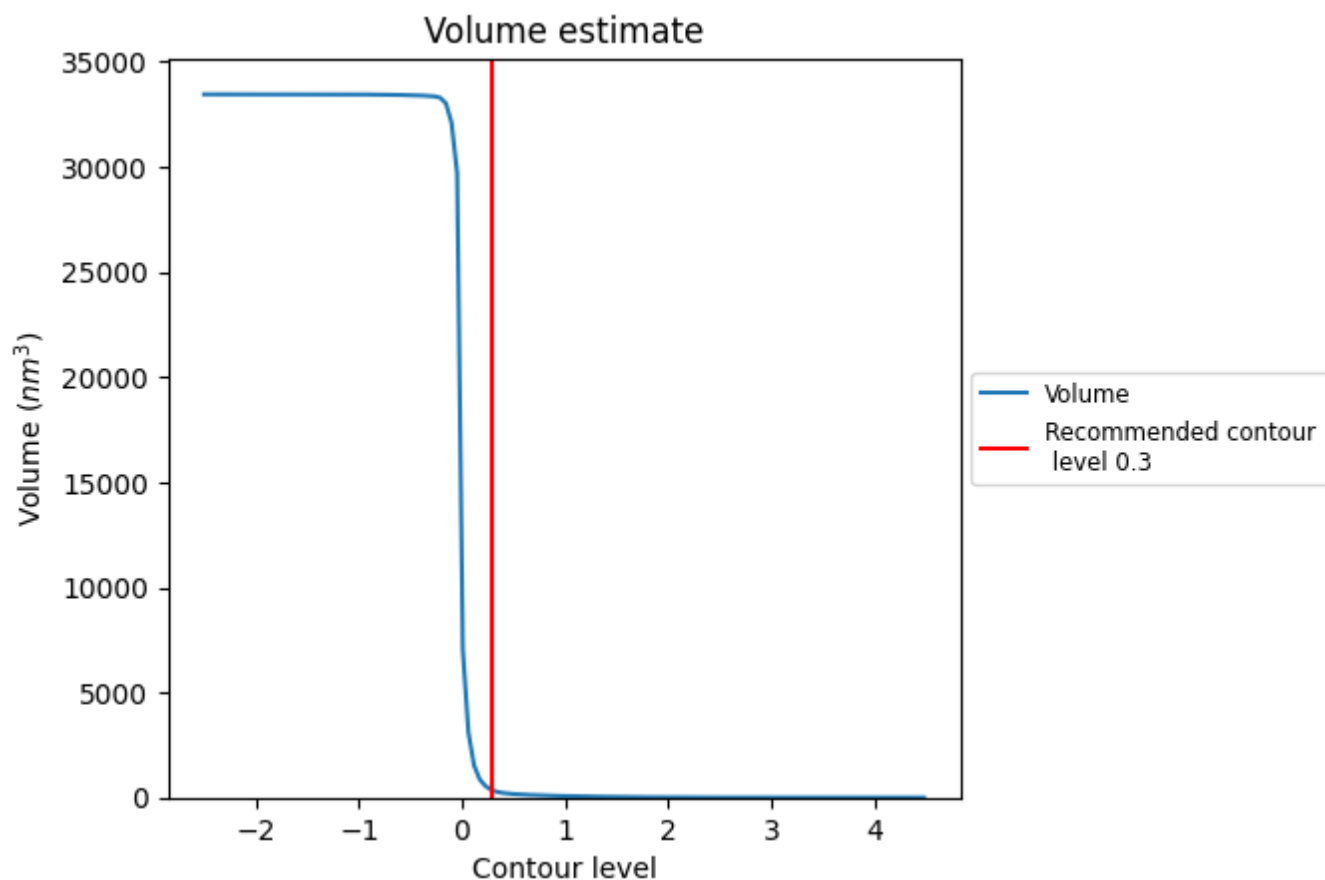
This section contains the results of statistical analysis of the map.

### 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.

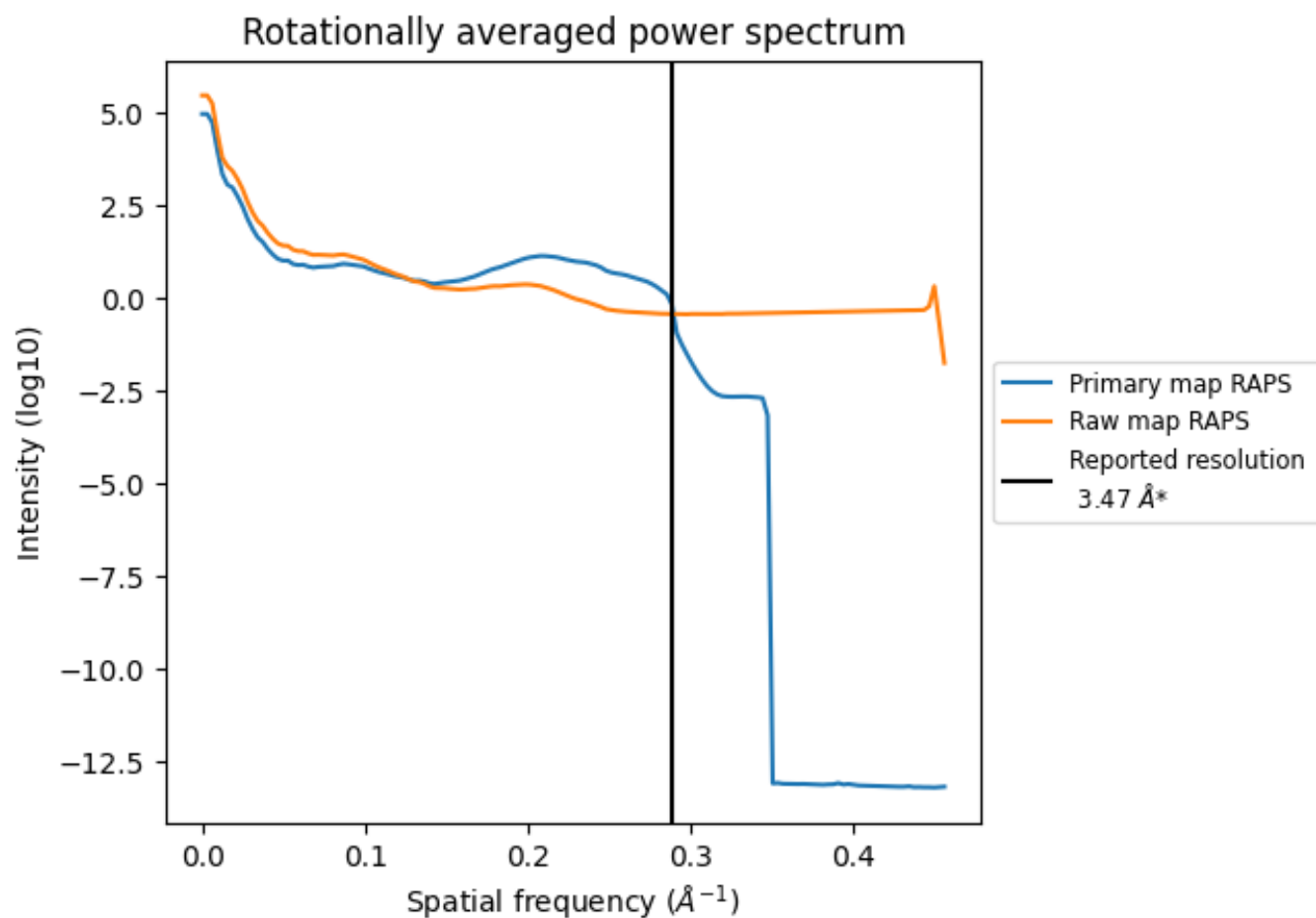
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 345 nm<sup>3</sup>; this corresponds to an approximate mass of 312 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 ⓘ

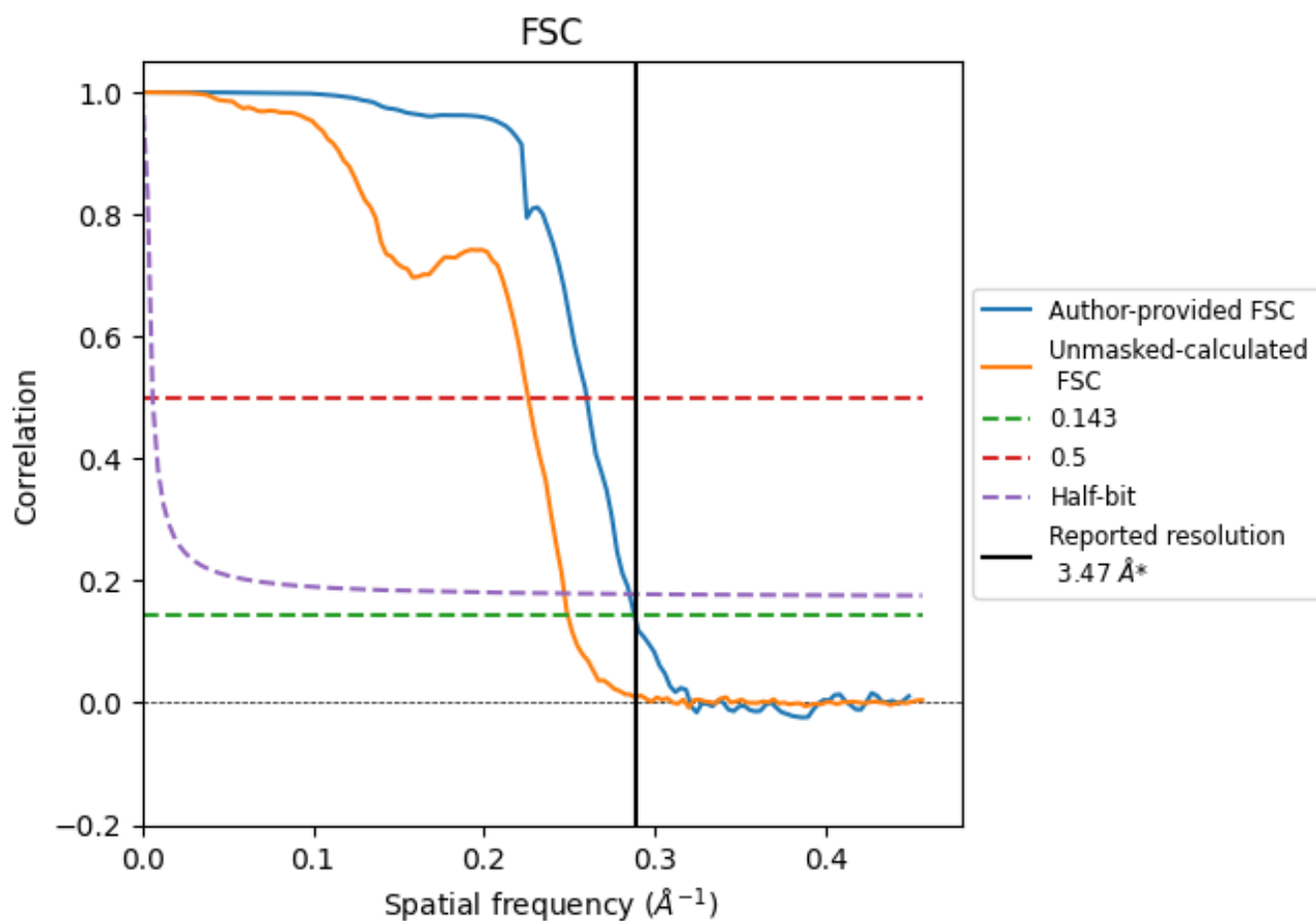


\*Reported resolution corresponds to spatial frequency of 0.288 Å<sup>-1</sup>

## 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 0.288  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

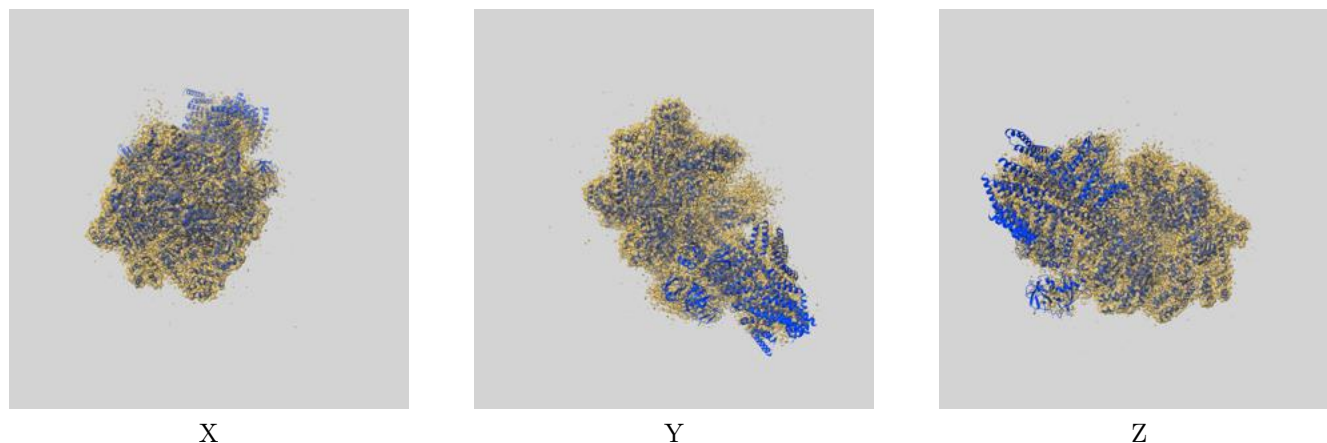
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	3.47	3.85	3.51
Unmasked-calculated*	4.02	4.43	4.05

\*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 4.02 differs from the reported value 3.47 by more than 10 %

## 9 Map-model fit [i](#)

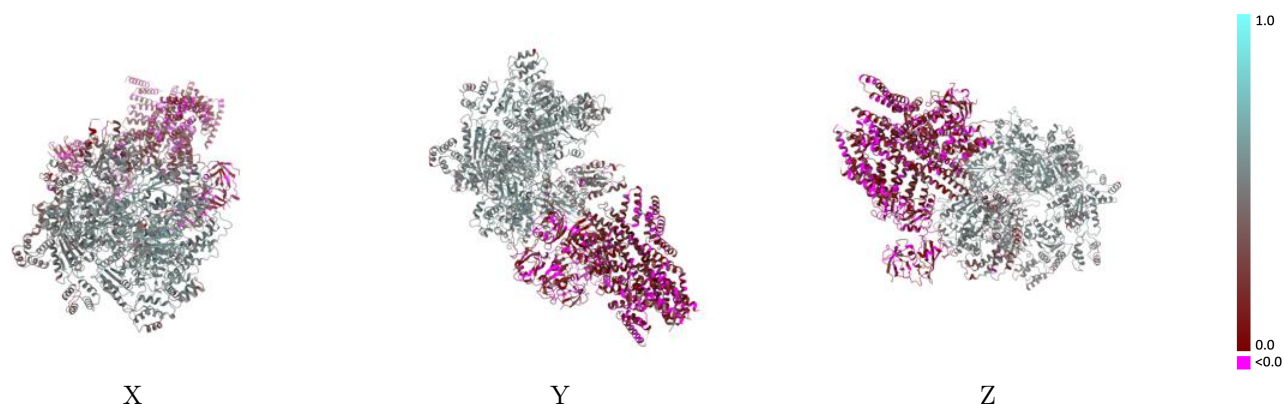
This section contains information regarding the fit between EMDB map EMD-71475 and PDB model 9PBA. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)



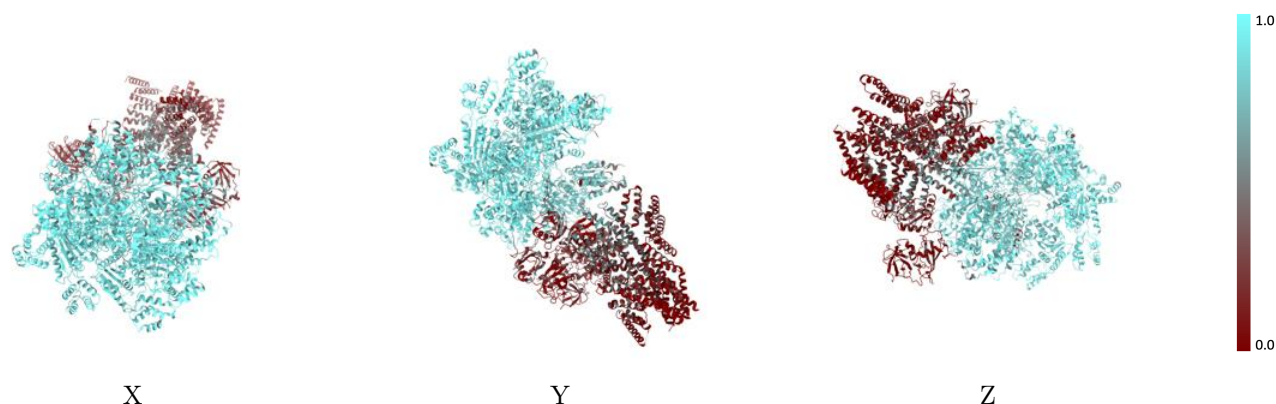
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

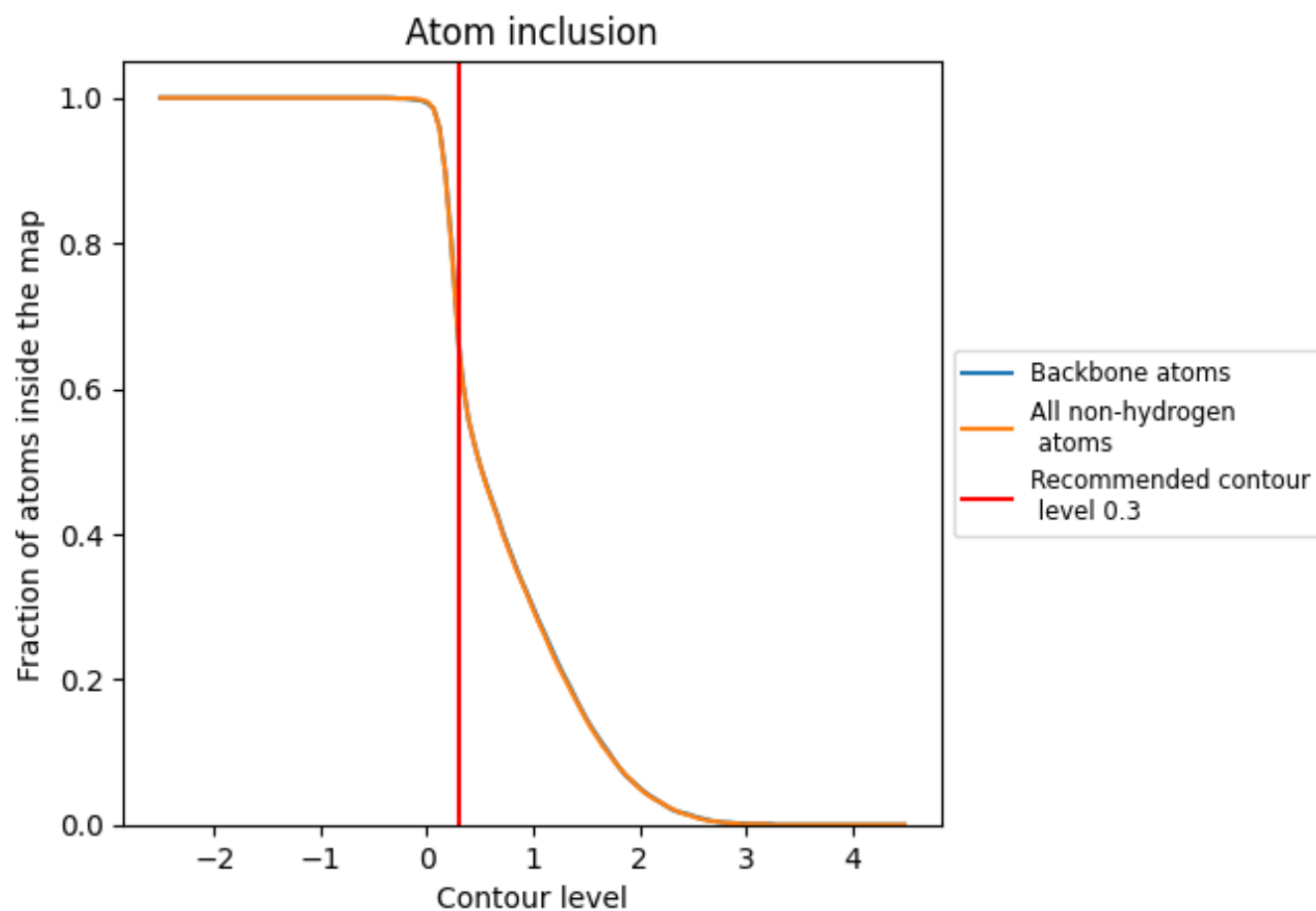
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.3).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6560	<div></div> 0.3610
A	<div></div> 0.9340	<div></div> 0.5190
B	<div></div> 0.7480	<div></div> 0.4240
C	<div></div> 0.7480	<div></div> 0.4260
D	<div></div> 0.7460	<div></div> 0.4110
E	<div></div> 0.7080	<div></div> 0.3900
F	<div></div> 0.8430	<div></div> 0.4270
G	<div></div> 0.2370	<div></div> 0.1160
H	<div></div> 0.3630	<div></div> 0.1450
I	<div></div> 0.3880	<div></div> 0.1900
J	<div></div> 0.1310	<div></div> 0.1020
K	<div></div> 0.2440	<div></div> 0.1050
L	<div></div> 0.2220	<div></div> 0.1280

