



Full wwPDB EM Validation Report ⓘ

Sep 15, 2026 – 12:32 PM EDT

PDB ID : 9OJ2 / pdb_00009oj2
EMDB ID : EMD-70529
Title : sx20S complex (NSF-alphaSNAP-syntaxin-1a), non-hydrolyzing, class 1
Authors : White, K.I.; Brunger, A.T.
Deposited on : 2025-05-06
Resolution : 3.75 Å(reported)
Based on initial models : 1N7S, 6MDM

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:

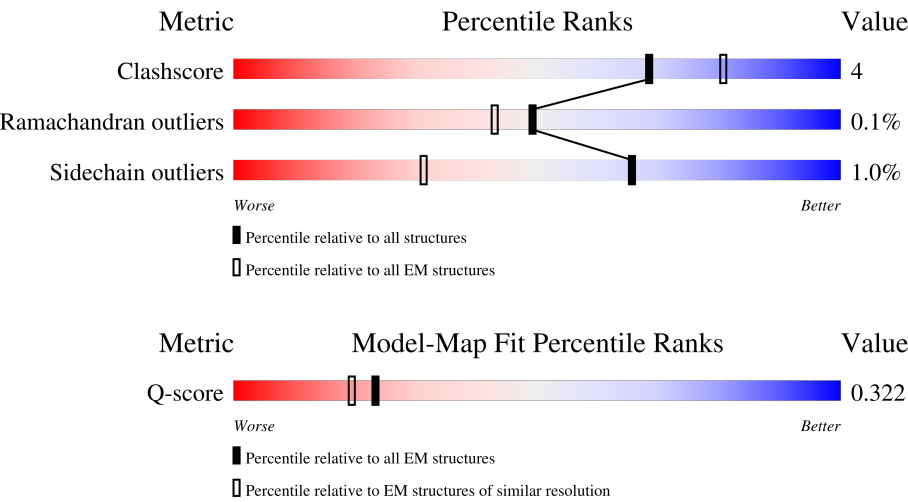
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 3.75 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.



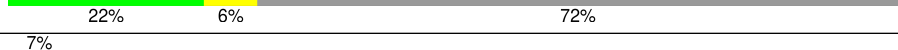
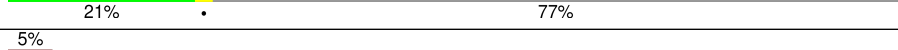
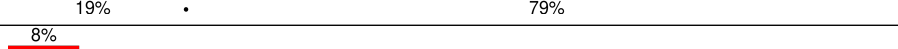
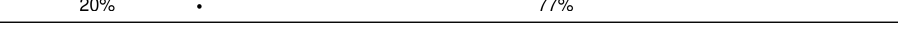
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10301 (3.25 - 4.25)

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

Mol	Chain	Length	Quality of chain
1	A	747	64% 6% 30%
1	B	747	22% 89% 8%
1	C	747	24% 88% 9%
1	D	747	24% 88% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	747	
1	F	747	
2	K	296	
2	L	296	
2	M	296	
2	N	296	
3	G	253	
3	H	253	
3	I	253	
3	J	253	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 81636 atoms, of which 40943 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	523	Total	C	H	N	O	S	3	0
			8298	2579	4221	715	761	22		
1	B	726	Total	C	H	N	O	S	2	0
			11460	3581	5796	984	1068	31		
1	C	726	Total	C	H	N	O	S	4	0
			11483	3587	5810	986	1069	31		
1	D	726	Total	C	H	N	O	S	2	0
			11463	3582	5799	984	1067	31		
1	E	536	Total	C	H	N	O	S	3	0
			8533	2654	4336	736	784	23		
1	F	517	Total	C	H	N	O	S	3	0
			8199	2551	4164	706	757	21		

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 Alpha-soluble NSF attachment protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	K	287	Total	C	H	N	O	S	0	0
			4467	1424	2212	375	438	18		
2	M	287	Total	C	H	N	O	S	0	0
			4467	1424	2212	375	438	18		
2	N	287	Total	C	H	N	O	S	0	0
			4467	1424	2212	375	438	18		
2	L	279	Total	C	H	N	O	S	0	0
			4331	1384	2143	363	423	18		

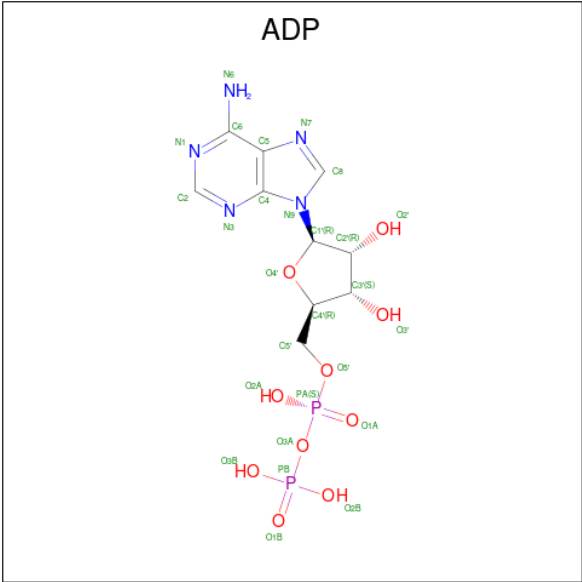
There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Syntaxin-1A.

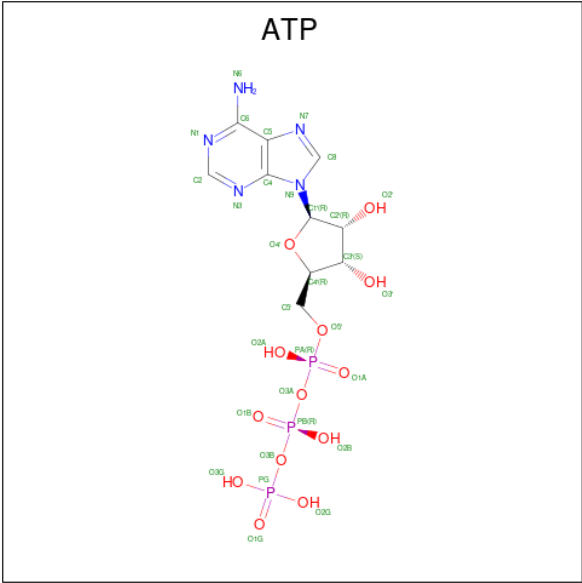
Mol	Chain	Residues	Atoms						AltConf	Trace
3	H	58	Total	C	H	N	O	S	2	0
			959	303	470	82	99	5		
3	G	71	Total	C	H	N	O	S	2	0
			1129	352	558	96	117	6		
3	I	52	Total	C	H	N	O	S	0	0
			829	263	403	71	87	5		
3	J	57	Total	C	H	N	O	S	2	0
			941	294	463	82	97	5		

- Molecule 4 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
4	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

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



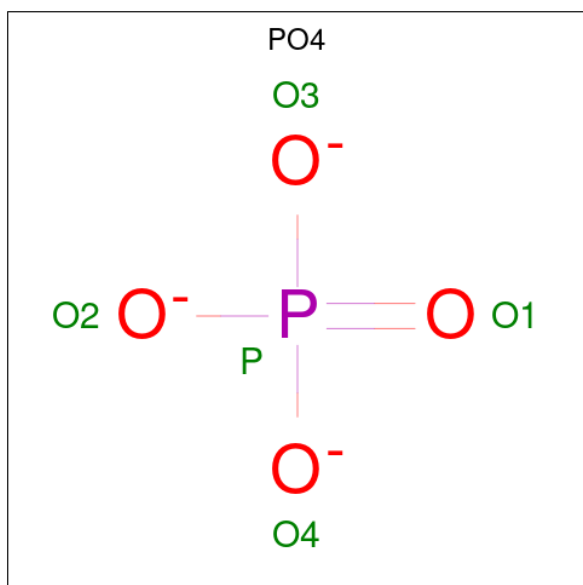
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

Continued on next page...

Continued from previous page...

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

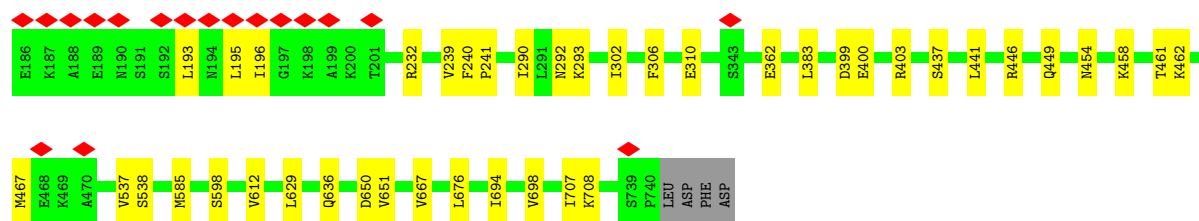
- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



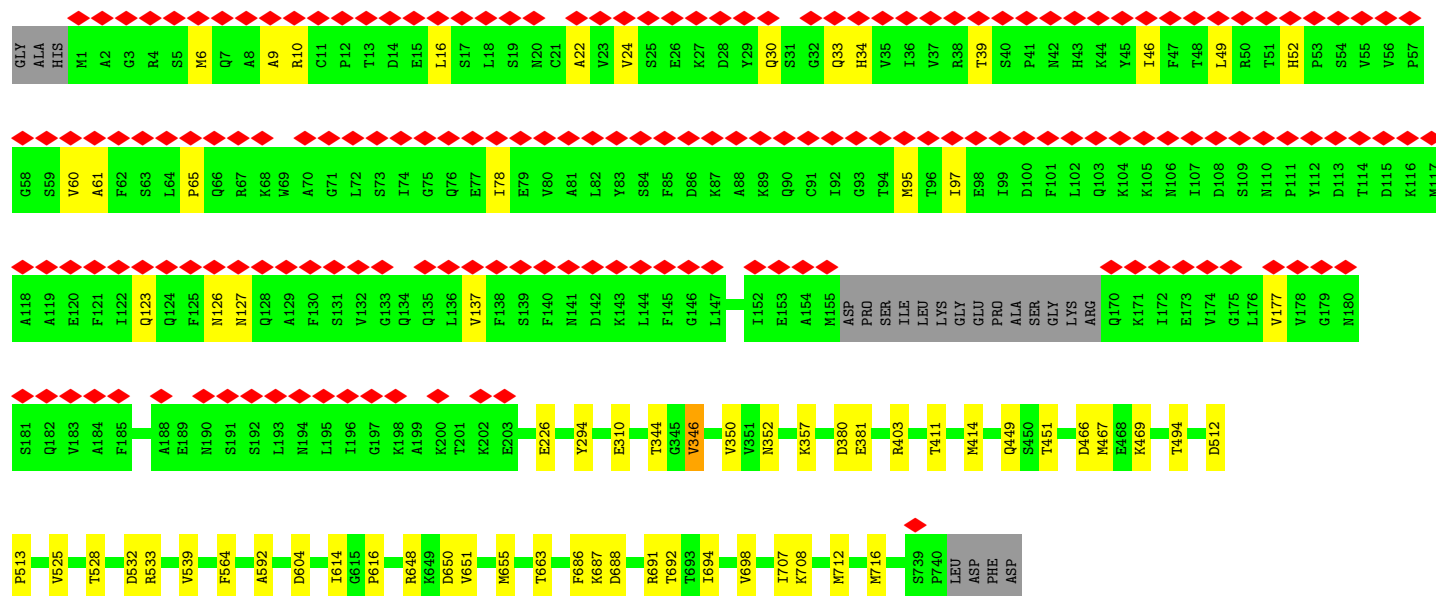
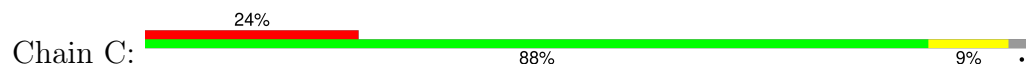
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	O	P	0
			5	4	1	

- Molecule 7 is water.

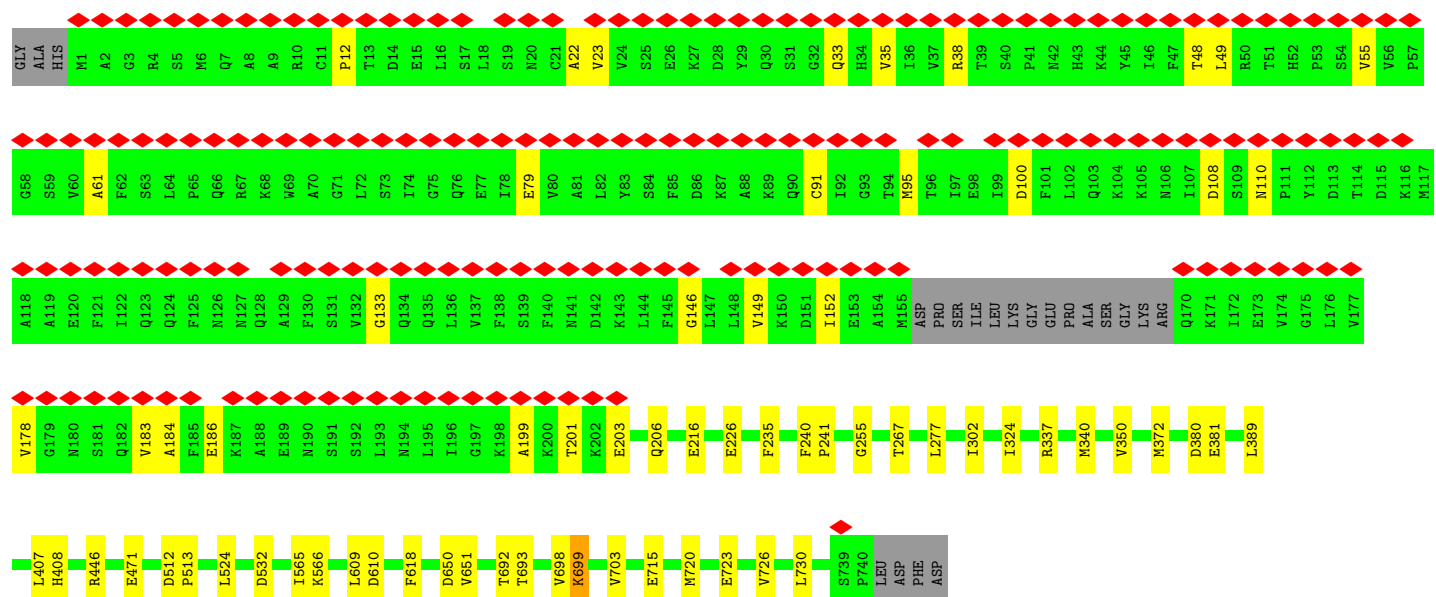
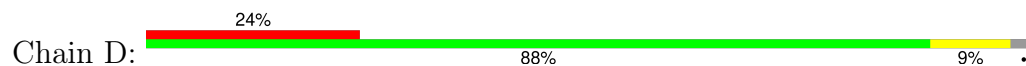
Mol	Chain	Residues	Atoms		AltConf
7	A	11	Total 11	O 11	0
7	B	26	Total 26	O 26	0
7	C	31	Total 31	O 31	0
7	D	20	Total 20	O 20	0
7	E	3	Total 3	O 3	0
7	F	2	Total 2	O 2	0



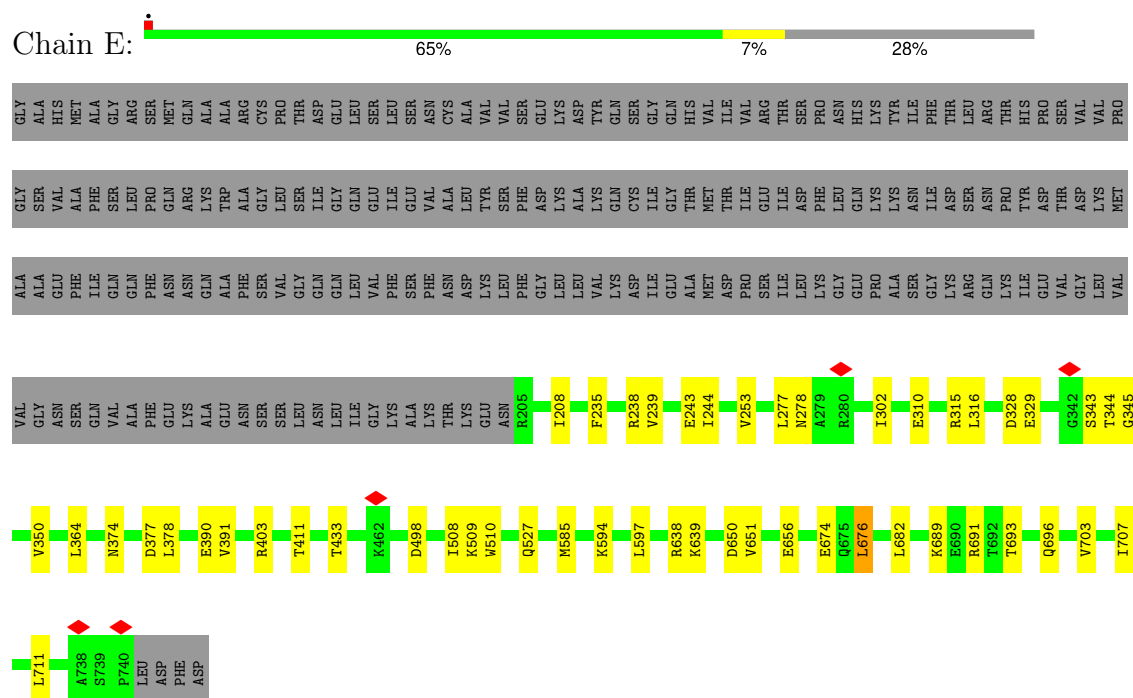
• Molecule 1: Vesicle-fusing ATPase



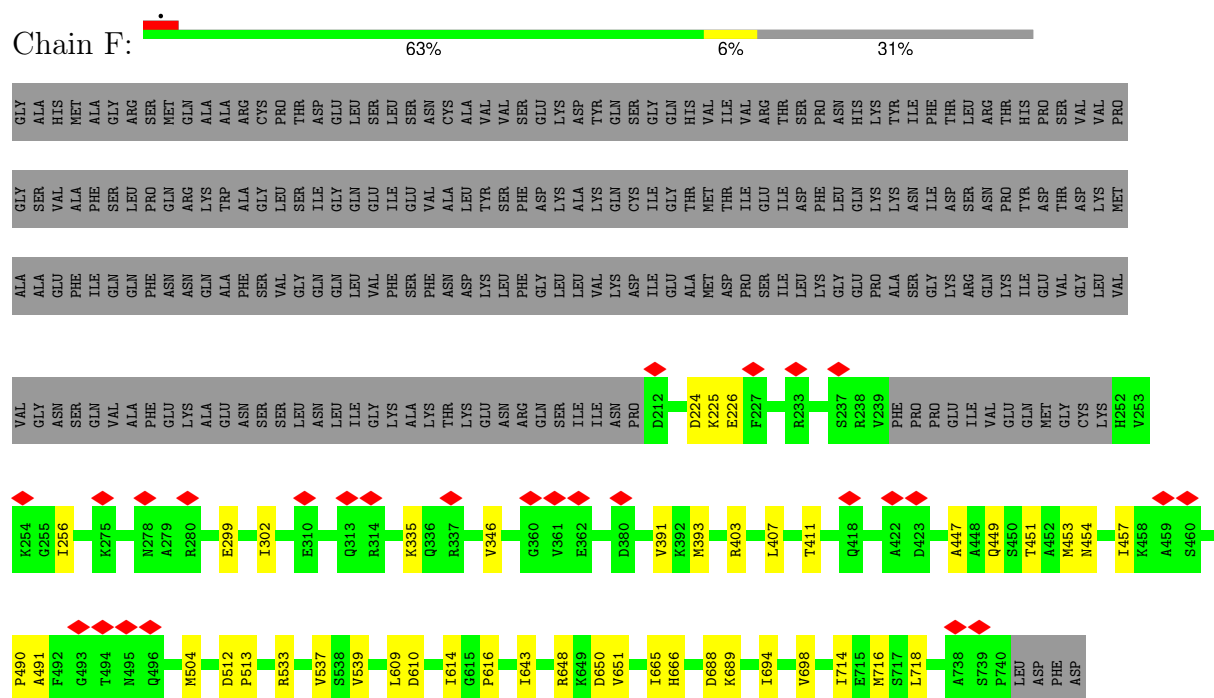
• Molecule 1: Vesicle-fusing ATPase



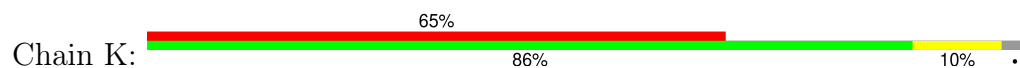
- Molecule 1: Vesicle-fusing ATPase

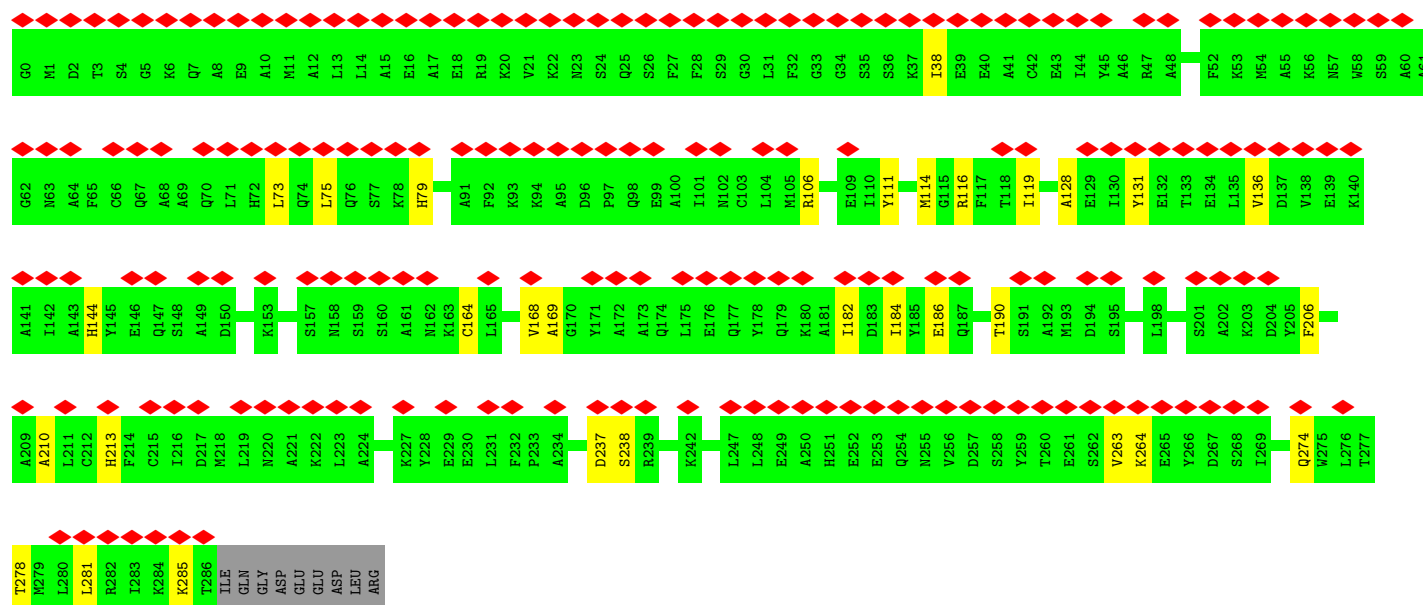


- Molecule 1: Vesicle-fusing ATPase



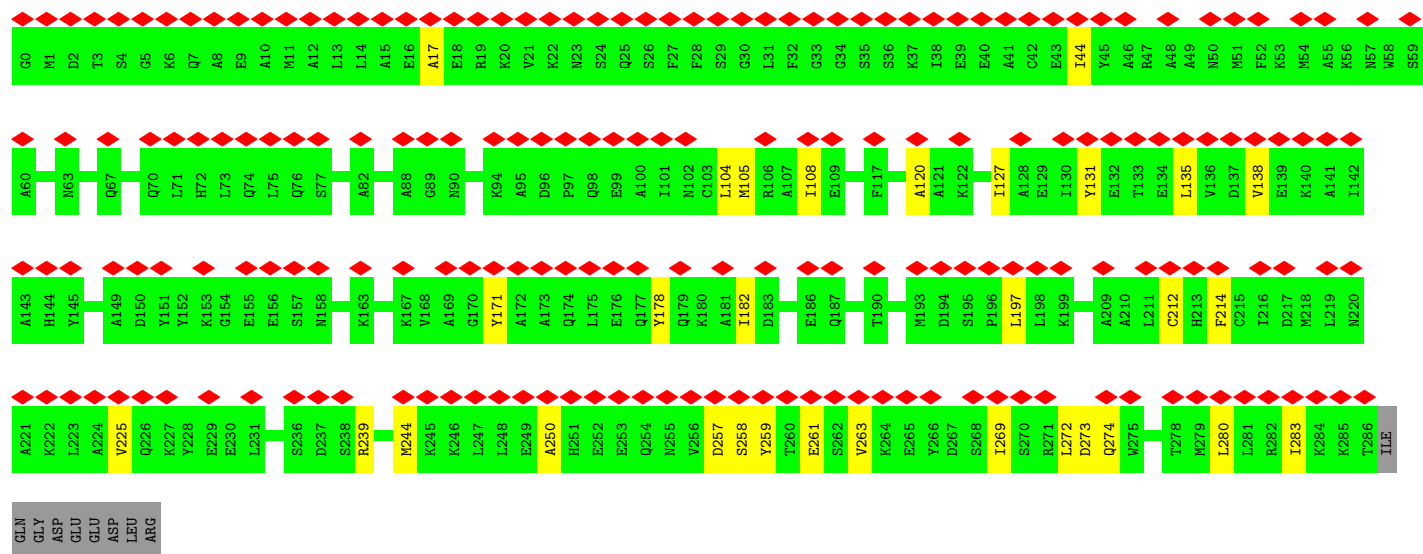
- Molecule 2: Alpha-soluble NSF attachment protein





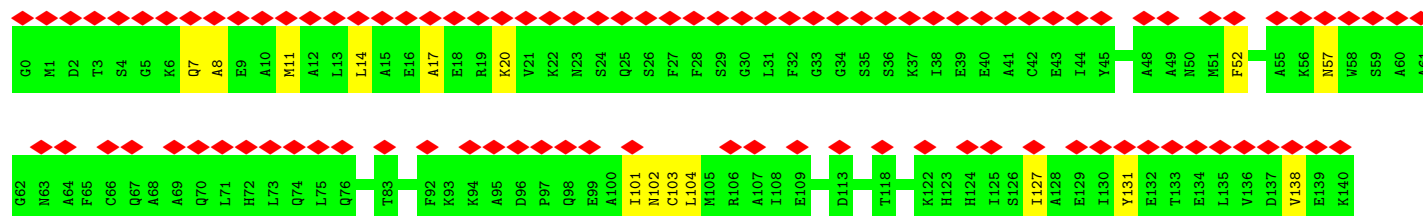
• Molecule 2: Alpha-soluble NSF attachment protein

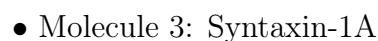
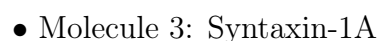
Chain M: 65% 86% 10%



• Molecule 2: Alpha-soluble NSF attachment protein

Chain N: 68% 84% 12%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53244	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 ($e^-/\text{\AA}^2$)	27.608	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.424	Depositor
Minimum map value	-1.223	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	322.224, 322.224, 322.224	wwPDB
Map dimensions	294, 294, 294	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ADP, ATP, PO4

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	0.52	1/4154 (0.0%)	0.78	0/5593
1	B	0.50	1/5756 (0.0%)	0.72	0/7756
1	C	0.43	2/5780 (0.0%)	0.61	0/7788
1	D	0.49	1/5763 (0.0%)	0.69	0/7765
1	E	0.54	0/4267	0.77	0/5749
1	F	0.36	0/4107	0.57	0/5531
2	K	0.07	0/2295	0.22	0/3084
2	L	0.08	0/2227	0.22	0/2992
2	M	0.23	0/2295	0.38	0/3084
2	N	0.21	0/2295	0.43	0/3084
3	G	0.71	0/582	1.03	0/780
3	H	0.08	0/503	0.23	0/675
3	I	0.08	0/431	0.21	0/578
3	J	0.21	0/496	0.39	0/664
All	All	0.42	5/40951 (0.0%)	0.63	0/55123

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	403	ARG	C-N	8.81	1.44	1.33
1	A	232	ARG	C-N	-7.79	1.22	1.33
1	C	352	ASN	C-N	-7.15	1.24	1.33
1	D	446	ARG	C-N	-5.58	1.26	1.33
1	B	446	ARG	C-N	-5.46	1.26	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4077	4221	4204	30	0
1	B	5664	5796	5794	43	0
1	C	5673	5810	5792	41	0
1	D	5664	5799	5789	45	0
1	E	4197	4336	4326	28	0
1	F	4035	4164	4149	31	0
2	K	2255	2212	2212	16	0
2	L	2188	2143	2143	13	0
2	M	2255	2212	2212	18	0
2	N	2255	2212	2212	23	0
3	G	571	558	552	17	0
3	H	489	470	463	7	0
3	I	426	403	403	6	0
3	J	478	463	453	7	0
4	A	27	12	12	0	0
5	A	31	12	12	0	0
5	B	62	24	24	0	0
5	C	62	24	24	0	0
5	D	62	24	24	0	0
5	E	62	24	24	1	0
5	F	62	24	24	0	0
6	A	5	0	0	0	0
7	A	11	0	0	0	0
7	B	26	0	0	0	0
7	C	31	0	0	0	0
7	D	20	0	0	0	0
7	E	3	0	0	0	0
7	F	2	0	0	0	0
All	All	40693	40943	40848	300	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 4.

All (300) 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)
3:G:223:VAL:HG21	3:J:219:MET:HE1	1.49	0.93
1:D:267:THR:HA	1:D:372:MET:HE1	1.52	0.89
1:C:6:MET:HE1	1:C:60:VAL:HG23	1.61	0.82
3:G:223:VAL:HG21	3:J:219:MET:CE	2.09	0.82
1:F:609:LEU:HD12	1:F:609:LEU:O	1.84	0.77
2:L:203:LYS:HD2	2:L:238:SER:OG	1.87	0.74
2:N:102:ASN:OD1	2:N:103:CYS:N	2.22	0.73
1:C:6:MET:CE	1:C:60:VAL:HG23	2.19	0.71
2:L:203:LYS:CD	2:L:238:SER:OG	2.39	0.71
1:C:686:PHE:O	1:C:691:ARG:NH2	2.24	0.70
1:B:24:VAL:HG12	1:B:60:VAL:HG22	1.74	0.70
2:N:7:GLN:OE1	2:N:57:ASN:ND2	2.25	0.68
1:C:380:ASP:OD1	1:C:381:GLU:N	2.26	0.68
1:C:226:GLU:OE1	1:C:226:GLU:N	2.28	0.66
1:B:97:ILE:HD12	1:B:183:VAL:HG11	1.76	0.66
1:E:403:ARG:NH1	1:E:433:THR:O	2.28	0.66
2:M:257:ASP:OD1	2:M:258:SER:N	2.28	0.66
1:B:6:MET:HE3	1:B:60:VAL:HG23	1.77	0.66
1:A:650:ASP:OD1	1:A:651:VAL:N	2.29	0.65
1:F:694:ILE:O	1:F:698:VAL:HG22	1.97	0.65
2:M:225:VAL:HG13	2:M:244:MET:HE3	1.79	0.65
1:C:30:GLN:N	1:C:33:GLN:OE1	2.30	0.65
1:C:123:GLN:O	1:C:126:ASN:ND2	2.30	0.65
1:F:716:MET:HE3	1:F:716:MET:HA	1.77	0.65
3:H:234:GLU:O	3:H:237:VAL:HG12	1.96	0.64
1:D:35:VAL:HG13	1:D:49:LEU:HD11	1.78	0.64
1:D:720:MET:HA	1:D:720:MET:HE2	1.79	0.63
1:D:186:GLU:OE1	1:D:201:THR:HG21	1.99	0.63
2:M:239:ARG:NH1	2:M:269:ILE:HG21	2.13	0.63
1:D:186:GLU:OE1	1:D:201:THR:CG2	2.46	0.63
2:K:263:VAL:HG13	2:K:264:LYS:HD2	1.80	0.62
1:E:377:ASP:OD1	1:E:378:LEU:N	2.31	0.62
3:G:181:ILE:HG23	3:G:181:ILE:O	1.99	0.62
1:F:224:ASP:OD1	1:F:225:LYS:N	2.33	0.62
2:N:101:ILE:HD13	2:N:131:TYR:CZ	2.35	0.62
1:D:302:ILE:HD11	1:D:350:VAL:HG13	1.82	0.62
2:L:211:LEU:HD13	2:L:279:MET:HE1	1.81	0.62
2:N:183:ASP:OD1	2:N:184:ILE:N	2.34	0.61
1:C:414:MET:SD	1:C:449:GLN:NE2	2.71	0.61
2:L:207:PHE:CE2	2:L:211:LEU:HD11	2.36	0.61
2:K:237:ASP:OD1	2:K:238:SER:N	2.34	0.61
3:H:230:ILE:HG22	3:I:229:MET:HE3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ILE:CD1	1:B:302:ILE:HD11	2.31	0.61
1:D:267:THR:CA	1:D:372:MET:HE1	2.29	0.60
1:E:208:ILE:HD13	1:E:238:ARG:HB3	1.83	0.60
2:N:222:LYS:HA	2:N:248:LEU:HD21	1.84	0.60
1:C:650:ASP:OD1	1:C:651:VAL:N	2.35	0.59
1:A:433:THR:HG22	1:A:436:PHE:CE2	2.36	0.59
1:A:663:THR:HG22	1:A:664:THR:H	1.68	0.59
1:F:346:VAL:HG12	1:F:346:VAL:O	2.03	0.59
2:M:178:TYR:O	2:M:182:ILE:HD12	2.03	0.59
1:B:290:ILE:HD12	1:B:302:ILE:HD11	1.84	0.58
1:D:302:ILE:CD1	1:D:350:VAL:HG13	2.34	0.58
1:B:650:ASP:OD1	1:B:651:VAL:N	2.36	0.58
1:D:108:ASP:OD2	1:D:110:ASN:OD1	2.21	0.58
2:K:116:ARG:HG3	2:K:119:ILE:HG22	1.86	0.57
1:D:235:PHE:CE1	1:D:277:LEU:HD21	2.40	0.57
1:C:564:PHE:CE2	1:C:592:ALA:HB2	2.40	0.57
1:C:95:MET:HE2	1:C:97:ILE:HD11	1.86	0.56
1:D:277:LEU:HD12	1:D:324:ILE:HD11	1.87	0.56
2:N:263:VAL:HG11	2:N:280:LEU:HD21	1.88	0.56
1:C:24:VAL:HG12	1:C:60:VAL:HG22	1.88	0.56
2:N:179:GLN:HA	2:N:182:ILE:HG22	1.87	0.56
1:E:391:VAL:HG13	1:E:391:VAL:O	2.05	0.55
1:C:310:GLU:OE2	1:C:357:LYS:NZ	2.39	0.55
1:B:39:THR:HG22	1:B:78:ILE:HG22	1.87	0.55
1:B:38:ARG:HD2	1:B:44:LYS:HE3	1.88	0.55
1:D:650:ASP:OD1	1:D:651:VAL:N	2.39	0.55
1:B:292:ASN:OD1	1:B:293:LYS:N	2.38	0.55
1:B:636[A]:GLN:OE1	1:B:636[A]:GLN:N	2.38	0.55
1:E:328:ASP:OD1	1:E:329:GLU:N	2.40	0.55
1:B:403:ARG:HG2	1:B:441:LEU:HD11	1.88	0.55
1:F:539:VAL:HG13	1:F:643:ILE:HG23	1.87	0.55
1:C:411:THR:HG22	1:C:411:THR:O	2.06	0.54
2:M:273:ASP:OD1	2:M:274:GLN:N	2.41	0.54
1:C:688:ASP:O	1:C:692:THR:HG23	2.07	0.54
1:F:504:MET:HA	1:F:504:MET:HE3	1.89	0.54
1:A:712:MET:HA	1:A:712:MET:HE2	1.89	0.54
1:F:650:ASP:OD1	1:F:651:VAL:N	2.41	0.53
1:E:508:ILE:HD11	1:E:682:LEU:HD12	1.91	0.53
1:D:216:GLU:N	1:D:216:GLU:OE1	2.42	0.53
1:D:35:VAL:CG1	1:D:49:LEU:HD11	2.39	0.53
1:E:310:GLU:HA	1:E:364:LEU:HD11	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:694:ILE:O	1:C:698:VAL:HG12	2.09	0.53
1:E:676:LEU:HD12	1:E:703:VAL:HG11	1.90	0.53
1:F:449:GLN:C	1:F:453:MET:HE3	2.34	0.53
1:B:676:LEU:HD23	1:B:698:VAL:HG21	1.90	0.52
1:E:508:ILE:HG23	1:E:508:ILE:O	2.08	0.52
3:G:216:PHE:CE1	3:G:219:MET:HE2	2.44	0.52
1:B:38:ARG:HG3	1:B:44:LYS:NZ	2.24	0.52
1:C:614:ILE:O	1:C:616:PRO:HA	2.10	0.52
2:L:215:CYS:SG	2:L:283:ILE:HD11	2.49	0.52
1:A:295:VAL:HG12	3:G:181:ILE:HG13	1.90	0.52
2:M:105:MET:SD	2:M:127:ILE:HD13	2.50	0.52
3:G:182:ILE:CG2	3:G:183:MET:HE2	2.40	0.52
2:L:267:ASP:OD1	2:L:268:SER:N	2.43	0.52
3:H:219:MET:HE1	2:N:197:LEU:CD2	2.40	0.51
1:E:508:ILE:HG22	5:E:802:ATP:N7	2.25	0.51
1:D:12:PRO:HD2	1:D:23:VAL:HG11	1.91	0.51
1:D:22:ALA:N	1:D:48:THR:O	2.44	0.51
1:B:97:ILE:HD12	1:B:183:VAL:CG1	2.39	0.51
1:F:614:ILE:O	1:F:616:PRO:HA	2.10	0.51
3:G:234:GLU:OE1	3:J:229:MET:HE1	2.10	0.51
1:F:454:ASN:HA	1:F:457:ILE:HD12	1.92	0.51
1:B:667:VAL:HG23	1:B:667:VAL:O	2.10	0.51
2:K:274:GLN:O	2:K:278:THR:HG23	2.11	0.51
2:M:104:LEU:HB3	2:M:127:ILE:HD11	1.92	0.51
2:N:244:MET:O	2:N:248:LEU:HD13	2.11	0.51
1:A:503:ILE:O	1:A:503:ILE:HG13	2.11	0.50
1:C:687:LYS:HE2	1:C:687:LYS:HA	1.93	0.50
1:B:22:ALA:O	1:B:50:ARG:N	2.45	0.50
1:B:585:MET:HE3	1:B:629:LEU:HD12	1.94	0.50
1:D:723:GLU:OE1	1:D:723:GLU:N	2.42	0.50
2:N:138:VAL:HG21	2:N:175:LEU:HD21	1.93	0.50
1:B:22:ALA:N	1:B:48:THR:O	2.44	0.50
1:D:255:GLY:HA3	1:D:389:LEU:HD23	1.93	0.50
2:L:11:MET:HA	2:L:11:MET:HE3	1.94	0.50
1:D:23:VAL:HB	1:D:61:ALA:HB3	1.94	0.49
1:B:100:ASP:O	1:B:146:GLY:N	2.43	0.49
1:C:39:THR:HG22	1:C:78:ILE:HG22	1.93	0.49
1:E:508:ILE:O	1:E:509:LYS:C	2.55	0.49
1:E:510:TRP:CD1	1:E:707:ILE:CD1	2.96	0.49
1:C:294:TYR:CD1	3:G:187:ILE:CG2	2.96	0.49
1:F:411:THR:HG22	1:F:411:THR:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:GLU:N	1:D:471:GLU:OE1	2.46	0.49
1:D:380:ASP:OD1	1:D:381:GLU:N	2.46	0.49
1:E:411:THR:HG22	1:E:411:THR:O	2.13	0.49
1:E:343:SER:O	1:E:344:THR:OG1	2.26	0.49
1:A:663:THR:HG22	1:A:664:THR:N	2.27	0.49
3:J:243:TYR:O	3:J:247:ALA:N	2.46	0.49
1:B:461:THR:O	1:B:461:THR:HG22	2.12	0.48
1:C:127:ASN:N	1:C:177:VAL:O	2.45	0.48
1:C:539:VAL:HG23	1:C:663:THR:HG23	1.95	0.48
1:A:294:TYR:O	1:A:295:VAL:C	2.53	0.48
2:K:164:CYS:O	2:K:168:VAL:HG23	2.13	0.48
1:E:650:ASP:OD1	1:E:651:VAL:N	2.47	0.48
2:N:14:LEU:HD11	2:N:52:PHE:CE2	2.49	0.48
1:B:10:ARG:O	1:B:61:ALA:HB1	2.14	0.48
1:B:537:VAL:HG12	1:B:538:SER:N	2.28	0.48
1:A:505:ASN:OD1	1:F:533:ARG:HD2	2.14	0.47
2:M:108:ILE:HG23	2:M:120:ALA:HB1	1.96	0.47
2:M:250:ALA:CB	2:M:259:TYR:HB2	2.44	0.47
2:M:263:VAL:HG21	2:M:280:LEU:HD13	1.97	0.47
1:A:585:MET:HE1	1:A:626:LEU:HG	1.97	0.47
1:C:651:VAL:HG12	1:C:655:MET:HE3	1.95	0.47
1:B:38:ARG:HH21	1:B:41:PRO:HA	1.80	0.47
1:C:564:PHE:HE2	1:C:592:ALA:HB2	1.77	0.47
1:D:186:GLU:OE1	1:D:201:THR:HG23	2.15	0.47
3:G:230:ILE:O	3:G:233:ILE:HG22	2.14	0.47
2:M:17:ALA:HA	2:M:44:ILE:HD12	1.97	0.47
2:M:197:LEU:HD11	3:G:220:ALA:HB1	1.96	0.47
1:D:532:ASP:OD1	1:D:532:ASP:N	2.47	0.47
1:C:10:ARG:O	1:C:61:ALA:HB1	2.15	0.47
3:G:182:ILE:HG21	3:G:183:MET:HE2	1.97	0.47
1:F:449:GLN:O	1:F:453:MET:HE3	2.16	0.46
1:B:537:VAL:HG12	1:B:538:SER:H	1.79	0.46
1:F:256:ILE:HG23	1:F:393:MET:HE1	1.98	0.46
3:H:219:MET:HE2	3:H:219:MET:HA	1.96	0.46
2:N:169:ALA:HB2	2:N:184:ILE:HG21	1.96	0.46
2:N:210:ALA:HB1	2:N:244:MET:HE3	1.98	0.46
3:G:223:VAL:CG2	3:J:219:MET:HE1	2.34	0.46
1:F:610:ASP:OD1	1:F:610:ASP:N	2.47	0.46
1:A:418:GLN:C	1:A:419:LEU:HD12	2.41	0.46
1:D:610:ASP:O	1:D:618:PHE:HA	2.16	0.46
3:G:243:TYR:HB3	3:I:248:VAL:HG21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:216:ILE:HG23	2:L:217:ASP:N	2.30	0.46
1:C:466:ASP:O	1:C:467:MET:C	2.58	0.46
2:K:281:LEU:O	2:K:285:LYS:N	2.49	0.46
1:F:391:VAL:HG12	1:F:393:MET:SD	2.56	0.45
2:N:17:ALA:O	2:N:20:LYS:HG2	2.17	0.45
1:A:346:VAL:HG21	3:G:181:ILE:CG2	2.46	0.45
1:A:676:LEU:O	1:A:680:LEU:HD23	2.17	0.45
1:B:193:LEU:HD21	1:B:195:LEU:HD21	1.96	0.45
1:D:240:PHE:CG	1:D:241:PRO:HD2	2.51	0.45
2:M:182:ILE:HD12	2:M:182:ILE:H	1.82	0.45
1:B:6:MET:SD	1:B:7:GLN:N	2.89	0.45
1:C:712:MET:HG3	1:C:716:MET:HE3	1.98	0.45
1:D:512:ASP:N	1:D:513:PRO:CD	2.79	0.45
3:H:201:GLU:HG3	3:J:202:ILE:HG21	1.99	0.45
2:N:8:ALA:HA	2:N:11:MET:HE2	1.98	0.45
1:F:688:ASP:OD1	1:F:689:LYS:N	2.50	0.45
1:F:714:ILE:O	1:F:718:LEU:HD23	2.17	0.45
1:A:330:ILE:HG22	1:A:373:THR:HB	1.99	0.45
1:D:133:GLY:N	1:D:149:VAL:O	2.46	0.45
3:G:215:MET:HB3	3:I:216:PHE:CZ	2.51	0.45
1:B:36:ILE:HD11	1:B:44:LYS:HB3	1.99	0.45
1:B:362:GLU:OE2	1:B:362:GLU:HA	2.16	0.45
1:C:65:PRO:CG	1:C:137:VAL:HG13	2.47	0.45
2:N:57:ASN:OD1	2:N:57:ASN:O	2.35	0.45
1:B:232:ARG:NH1	1:C:451:THR:OG1	2.51	0.44
1:C:707:ILE:HG23	1:C:708:LYS:N	2.33	0.44
1:D:184:ALA:HA	1:D:199:ALA:HB1	1.99	0.44
1:E:315:ARG:HE	1:E:316:LEU:HG	1.82	0.44
1:F:512:ASP:N	1:F:513:PRO:CD	2.80	0.44
2:K:111:TYR:CD2	2:K:119:ILE:HG21	2.52	0.44
1:C:350:VAL:HG12	1:C:350:VAL:O	2.16	0.44
1:D:149:VAL:HG11	1:D:152:ILE:HD11	2.00	0.44
2:K:38:ILE:HG21	2:K:75:LEU:HD11	1.99	0.44
1:C:532:ASP:OD1	1:C:533:ARG:N	2.51	0.44
1:C:22:ALA:HB3	1:C:49:LEU:HD23	1.98	0.44
1:E:302:ILE:HD11	1:E:350:VAL:HG13	1.99	0.44
2:K:186:GLU:O	2:K:190:THR:HG22	2.18	0.44
2:N:165:LEU:HB3	2:N:184:ILE:HD11	2.00	0.44
1:B:38:ARG:HG3	1:B:44:LYS:HZ2	1.82	0.44
1:E:656:GLU:OE2	1:F:648:ARG:NH2	2.50	0.44
1:D:100:ASP:O	1:D:146:GLY:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:VAL:HG23	1:B:180:ASN:OD1	2.18	0.43
1:D:255:GLY:CA	1:D:389:LEU:HD23	2.48	0.43
1:E:278:ASN:OD1	1:E:278:ASN:O	2.36	0.43
1:F:403:ARG:O	1:F:407:LEU:HD13	2.18	0.43
2:N:247:LEU:HD11	2:N:251:HIS:CE1	2.53	0.43
1:C:525:VAL:O	1:C:528:THR:HG22	2.18	0.43
1:D:23:VAL:HG12	1:D:55:VAL:CG2	2.48	0.43
1:E:253:VAL:HG13	1:E:390:GLU:OE1	2.18	0.43
3:G:181:ILE:O	3:G:181:ILE:CG2	2.65	0.43
1:D:726:VAL:O	1:D:730:LEU:HD23	2.18	0.43
1:F:447:ALA:O	1:F:451:THR:HG23	2.19	0.43
1:A:694:ILE:O	1:A:698:VAL:HG22	2.19	0.43
1:B:6:MET:CE	1:B:60:VAL:HG23	2.45	0.43
1:B:6:MET:HE1	1:B:60:VAL:N	2.34	0.43
1:B:306:PHE:O	1:B:310:GLU:HG3	2.18	0.43
1:E:594:LYS:O	1:E:638:ARG:NH1	2.51	0.43
1:E:597:LEU:HD13	1:E:639:LYS:HB2	2.01	0.43
3:H:230:ILE:HG22	3:I:229:MET:CE	2.47	0.43
1:A:351:VAL:HG12	1:A:355:LEU:HD12	2.01	0.43
1:B:612:VAL:HG13	1:B:612:VAL:O	2.18	0.43
2:M:131:TYR:CD1	2:M:135:LEU:HD12	2.54	0.43
1:F:346:VAL:O	1:F:346:VAL:CG1	2.66	0.42
1:F:609:LEU:O	1:F:610:ASP:C	2.61	0.42
2:K:169:ALA:HB2	2:K:184:ILE:HG21	2.00	0.42
2:L:184:ILE:O	2:L:188:VAL:HG12	2.19	0.42
2:L:272:LEU:HD23	2:L:272:LEU:H	1.84	0.42
1:E:243:GLU:OE1	1:E:243:GLU:N	2.46	0.42
1:D:38:ARG:N	1:D:79:GLU:O	2.51	0.42
1:D:609:LEU:HD12	1:D:609:LEU:O	2.19	0.42
3:I:215:MET:HE1	2:L:197:LEU:O	2.19	0.42
1:A:241:PRO:HG3	1:B:467:MET:HE2	2.00	0.42
1:A:295:VAL:HG22	1:B:293:LYS:HA	2.02	0.42
1:D:698:VAL:O	1:D:699:LYS:C	2.63	0.42
1:A:505:ASN:OD1	1:F:533:ARG:CD	2.67	0.42
1:B:240:PHE:CD2	1:B:241:PRO:HD2	2.55	0.42
1:F:490:PRO:O	1:F:491:ALA:HB3	2.20	0.42
2:K:73:LEU:HD22	2:K:106:ARG:NH2	2.35	0.42
2:K:128:ALA:HB2	2:K:144:HIS:HB3	2.01	0.42
1:A:232:ARG:HG2	1:B:454:ASN:CG	2.45	0.42
1:A:512:ASP:N	1:A:513:PRO:CD	2.83	0.42
1:B:707:ILE:HG23	1:B:708:LYS:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ALA:N	1:C:60:VAL:O	2.52	0.42
2:M:182:ILE:HD11	2:M:212:CYS:HB3	2.01	0.42
2:N:142:ILE:HG23	2:N:168:VAL:HG23	2.01	0.42
2:K:182:ILE:HD12	2:K:213:HIS:HB2	2.01	0.41
2:L:214:PHE:CD1	2:L:244:MET:HE1	2.55	0.41
1:E:344:THR:HG22	1:E:345:GLY:N	2.35	0.41
1:B:399:ASP:O	1:B:400:GLU:C	2.63	0.41
1:C:10:ARG:C	1:C:61:ALA:HB1	2.46	0.41
1:A:295:VAL:HG12	3:G:181:ILE:CG1	2.50	0.41
1:E:208:ILE:HG22	1:E:277:LEU:HG	2.02	0.41
1:D:33:GLN:HB2	1:D:49:LEU:HD12	2.01	0.41
1:D:95:MET:SD	1:D:183:VAL:HG22	2.60	0.41
1:A:231:PHE:O	1:A:232:ARG:C	2.64	0.41
1:C:34:HIS:CE1	1:C:46:ILE:HG23	2.55	0.41
1:C:687:LYS:HG3	1:C:688:ASP:H	1.86	0.41
2:N:231:LEU:O	2:N:231:LEU:HD23	2.21	0.41
2:N:274:GLN:O	2:N:277:THR:OG1	2.34	0.41
2:L:133:THR:HG23	2:L:134:GLU:N	2.36	0.41
1:A:452:ALA:CB	1:A:476:THR:HG22	2.51	0.41
1:B:239:VAL:HG22	1:B:239:VAL:O	2.21	0.41
1:E:235:PHE:O	1:E:239:VAL:HG23	2.20	0.41
2:K:131:TYR:O	2:K:136:VAL:N	2.54	0.41
1:A:579:THR:O	1:A:583:GLN:HG2	2.21	0.41
1:B:383:LEU:HG	1:B:383:LEU:O	2.20	0.41
1:C:16:LEU:HD11	1:C:52:HIS:CD2	2.55	0.41
1:F:299:GLU:HA	1:F:302:ILE:HG22	2.02	0.41
2:M:272:LEU:HD23	2:M:272:LEU:H	1.84	0.41
3:J:230:ILE:HA	3:J:233:ILE:HG22	2.03	0.41
2:N:259:TYR:O	2:N:263:VAL:HG12	2.21	0.41
1:C:648:ARG:HE	1:C:651:VAL:HG21	1.85	0.41
1:D:715:GLU:OE1	1:D:715:GLU:HA	2.21	0.41
1:F:226:GLU:OE1	1:F:226:GLU:N	2.54	0.41
3:H:219:MET:HE2	3:H:219:MET:CA	2.50	0.41
1:A:505:ASN:OD1	1:F:533:ARG:HG2	2.20	0.40
1:A:517:VAL:HG11	1:A:552:LEU:HD23	2.02	0.40
1:D:226:GLU:OE1	1:D:226:GLU:N	2.54	0.40
2:K:79:HIS:CE1	2:K:114:MET:HE1	2.56	0.40
2:K:206:PHE:O	2:K:210:ALA:N	2.47	0.40
2:M:138:VAL:HG13	2:M:171:TYR:CD1	2.56	0.40
2:N:104:LEU:HB3	2:N:127:ILE:HD11	2.03	0.40
1:C:512:ASP:N	1:C:513:PRO:CD	2.84	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:VAL:HG13	1:D:49:LEU:CD1	2.47	0.40
1:D:91:CYS:SG	1:D:178:VAL:HG11	2.62	0.40
1:E:244:ILE:HD12	1:E:244:ILE:H	1.87	0.40
1:F:665:ILE:HG22	1:F:666:HIS:N	2.36	0.40
1:A:573:MET:HE2	1:A:581:LYS:HG2	2.03	0.40
1:D:337:ARG:HH22	1:E:374:ASN:HD22	1.68	0.40
1:D:565:ILE:HG22	1:D:566:LYS:N	2.36	0.40
2:M:214:PHE:HD1	2:M:283:ILE:HD12	1.86	0.40
1:A:417:HIS:HB3	1:A:419:LEU:HD13	2.04	0.40
1:A:525:VAL:HA	1:A:528:THR:HG22	2.03	0.40
3:I:213:HIS:O	3:I:216:PHE:HB3	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/747 (70%)	500 (96%)	20 (4%)	2 (0%)	30	61
1	B	724/747 (97%)	702 (97%)	22 (3%)	0	100	100
1	C	726/747 (97%)	690 (95%)	35 (5%)	1 (0%)	48	79
1	D	724/747 (97%)	690 (95%)	34 (5%)	0	100	100
1	E	537/747 (72%)	513 (96%)	23 (4%)	1 (0%)	43	72
1	F	516/747 (69%)	491 (95%)	25 (5%)	0	100	100
2	K	285/296 (96%)	281 (99%)	4 (1%)	0	100	100
2	L	275/296 (93%)	271 (98%)	4 (2%)	0	100	100
2	M	285/296 (96%)	281 (99%)	4 (1%)	0	100	100
2	N	285/296 (96%)	278 (98%)	7 (2%)	0	100	100
3	G	70/253 (28%)	64 (91%)	6 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	58/253 (23%)	58 (100%)	0	0	100	100
3	I	50/253 (20%)	50 (100%)	0	0	100	100
3	J	57/253 (22%)	57 (100%)	0	0	100	100
All	All	5114/6678 (77%)	4926 (96%)	184 (4%)	4 (0%)	49	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	GLU
1	C	346	VAL
1	A	215	PHE
1	E	498	ASP

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	448/638 (70%)	442 (99%)	6 (1%)	61	71
1	B	623/638 (98%)	616 (99%)	7 (1%)	65	72
1	C	626/638 (98%)	621 (99%)	5 (1%)	73	75
1	D	624/638 (98%)	615 (99%)	9 (1%)	59	70
1	E	461/638 (72%)	452 (98%)	9 (2%)	48	64
1	F	442/638 (69%)	440 (100%)	2 (0%)	81	81
2	K	235/243 (97%)	235 (100%)	0	100	100
2	L	227/243 (93%)	227 (100%)	0	100	100
2	M	235/243 (97%)	234 (100%)	1 (0%)	84	82
2	N	235/243 (97%)	235 (100%)	0	100	100
3	G	65/233 (28%)	62 (95%)	3 (5%)	24	47
3	H	56/233 (24%)	56 (100%)	0	100	100
3	I	48/233 (21%)	48 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	55/233 (24%)	55 (100%)	0	100	100
All	All	4380/5732 (76%)	4338 (99%)	42 (1%)	65	73

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	PHE
1	A	232	ARG
1	A	299	GLU
1	A	344	THR
1	A	542	GLU
1	A	645	THR
1	B	196	ILE
1	B	437	SER
1	B	449	GLN
1	B	458	LYS
1	B	462	LYS
1	B	598	SER
1	B	694	ILE
1	C	344	THR
1	C	346	VAL
1	C	469	LYS
1	C	494	THR
1	C	604	ASP
1	D	203	GLU
1	D	206	GLN
1	D	340	MET
1	D	408	HIS
1	D	524	LEU
1	D	692	THR
1	D	693	THR
1	D	699	LYS
1	D	703	VAL
1	E	527	GLN
1	E	585	MET
1	E	674	GLU
1	E	676	LEU
1	E	689	LYS
1	E	691	ARG
1	E	693	THR
1	E	696	GLN
1	E	711	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	335	LYS
1	F	537	VAL
2	M	261	GLU
3	G	198	ARG
3	G	205	LEU
3	G	218	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	474	GLN
1	A	561	ASN
1	A	624	GLN
1	B	7	GLN
1	B	20	ASN
1	B	43	HIS
1	B	128	GLN
1	B	495	ASN
1	B	505	ASN
1	B	685	ASN
1	C	103	GLN
1	C	106	ASN
1	C	170	GLN
1	C	417	HIS
1	C	486	ASN
1	C	496	GLN
1	C	530	ASN
1	D	474	GLN
1	E	374	ASN
1	E	405	GLN
1	E	505	ASN
1	E	685	ASN
1	E	697	GLN
1	F	286	ASN
1	F	336	GLN
1	F	353	GLN
1	F	374	ASN
1	F	685	ASN
2	K	23	ASN
2	M	102	ASN
3	H	239	HIS
3	J	213	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	90	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 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	$\# Z > 2$
5	ATP	C	801	-	32,33,33	0.67	1 (3%)	48,52,52	0.56	0
5	ATP	C	802	-	32,33,33	0.57	0	48,52,52	0.58	0
5	ATP	E	801	-	32,33,33	0.54	0	48,52,52	0.63	0
5	ATP	F	802	-	32,33,33	0.58	0	48,52,52	0.61	0
5	ATP	D	801	-	32,33,33	0.57	0	48,52,52	0.60	0
5	ATP	F	801	-	32,33,33	0.54	0	48,52,52	0.62	0
5	ATP	B	802	-	32,33,33	0.56	0	48,52,52	0.59	0
5	ATP	B	801	-	32,33,33	0.63	0	48,52,52	0.55	0
6	PO4	A	803	-	4,4,4	0.70	0	6,6,6	0.49	0
5	ATP	A	802	-	32,33,33	0.57	0	48,52,52	0.64	0
5	ATP	E	802	-	32,33,33	0.54	0	48,52,52	0.63	0
4	ADP	A	801	-	28,29,29	0.51	0	43,45,45	0.47	0
5	ATP	D	802	-	32,33,33	0.58	0	48,52,52	0.57	0

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
5	ATP	C	801	-	-	3/22/38/38	0/3/3/3
5	ATP	C	802	-	-	2/22/38/38	0/3/3/3
5	ATP	E	801	-	-	7/22/38/38	0/3/3/3
5	ATP	F	802	-	-	5/22/38/38	0/3/3/3
5	ATP	D	801	-	-	0/22/38/38	0/3/3/3
5	ATP	F	801	-	-	3/22/38/38	0/3/3/3
5	ATP	B	802	-	-	2/22/38/38	0/3/3/3
5	ATP	B	801	-	-	2/22/38/38	0/3/3/3
5	ATP	A	802	-	-	5/22/38/38	0/3/3/3
5	ATP	E	802	-	-	4/22/38/38	0/3/3/3
4	ADP	A	801	-	-	4/16/32/32	0/3/3/3
5	ATP	D	802	-	-	1/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	801	ATP	PG-O2G	-2.05	1.47	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	ADP	C5'-O5'-PA-O3A
5	A	802	ATP	C5'-O5'-PA-O1A
5	B	802	ATP	PB-O3B-PG-O3G
5	C	801	ATP	PB-O3B-PG-O2G
5	C	801	ATP	C5'-O5'-PA-O1A
5	E	801	ATP	PB-O3B-PG-O3G
5	E	801	ATP	C5'-O5'-PA-O3A
5	A	802	ATP	C3'-C4'-C5'-O5'
5	E	802	ATP	C3'-C4'-C5'-O5'
5	A	802	ATP	O4'-C4'-C5'-O5'
5	E	801	ATP	O4'-C4'-C5'-O5'
5	E	801	ATP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	E	802	ATP	O4'-C4'-C5'-O5'
5	D	802	ATP	O4'-C4'-C5'-O5'
5	F	801	ATP	C2'-C1'-N9-C4
5	E	801	ATP	PB-O3B-PG-O2G
4	A	801	ADP	PB-O3A-PA-O2A
5	F	802	ATP	PA-O3A-PB-O1B
5	F	801	ATP	C2'-C1'-N9-C8
4	A	801	ADP	C5'-O5'-PA-O1A
5	C	801	ATP	C5'-O5'-PA-O3A
5	C	802	ATP	C5'-O5'-PA-O2A
5	E	801	ATP	C5'-O5'-PA-O1A
5	B	802	ATP	PB-O3B-PG-O1G
5	A	802	ATP	PA-O3A-PB-O2B
5	B	801	ATP	PA-O3A-PB-O2B
5	F	802	ATP	PA-O3A-PB-O2B
5	F	802	ATP	O4'-C4'-C5'-O5'
5	E	801	ATP	PB-O3B-PG-O1G
5	F	802	ATP	PB-O3B-PG-O3G
5	F	802	ATP	O4'-C1'-N9-C8
5	B	801	ATP	PA-O3A-PB-O1B
5	E	802	ATP	O4'-C1'-N9-C8
5	A	802	ATP	O4'-C1'-N9-C8
4	A	801	ADP	PB-O3A-PA-O1A
5	C	802	ATP	PA-O3A-PB-O1B
5	E	802	ATP	PG-O3B-PB-O2B
5	F	801	ATP	PA-O3A-PB-O2B

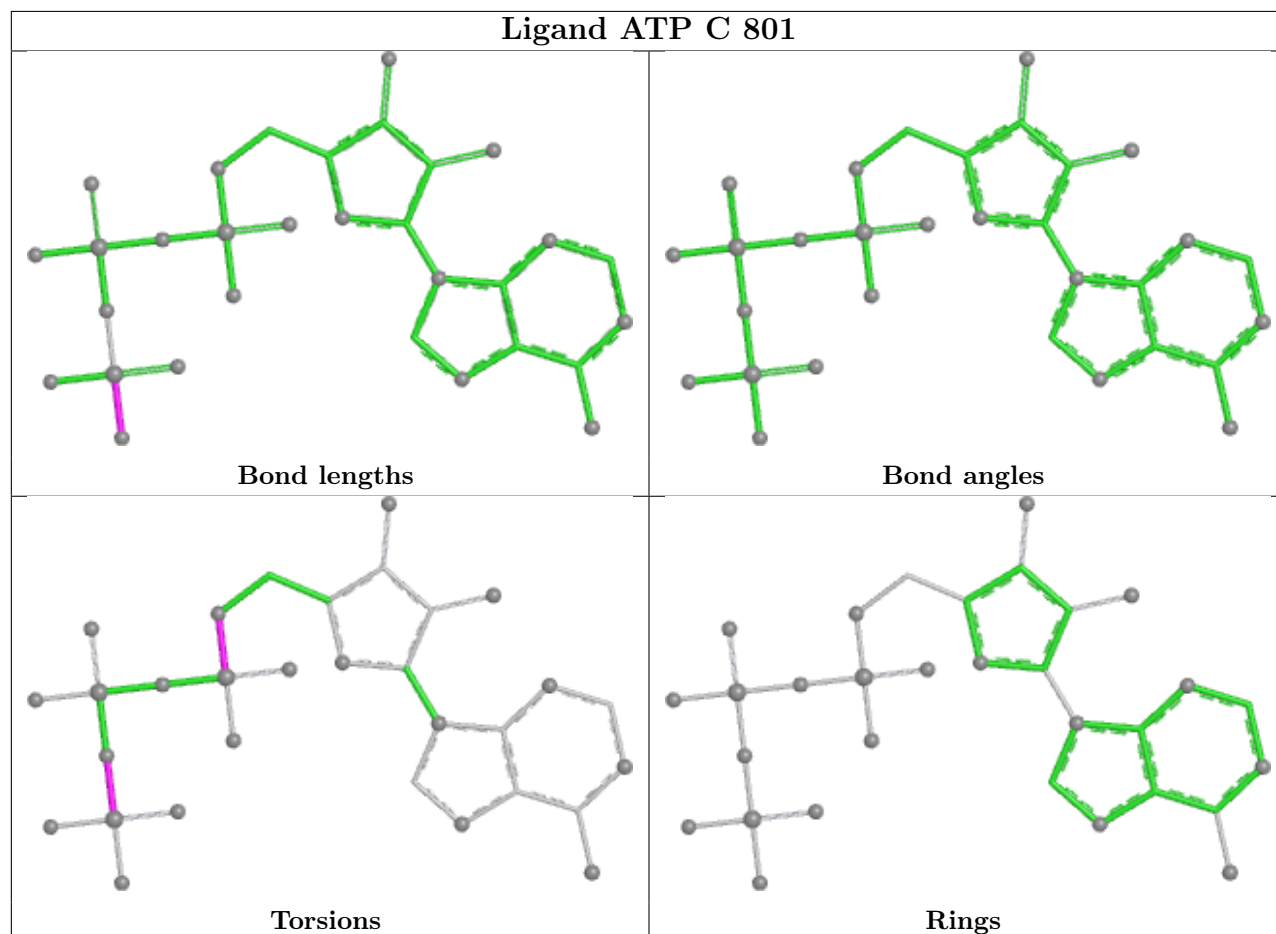
There are no ring outliers.

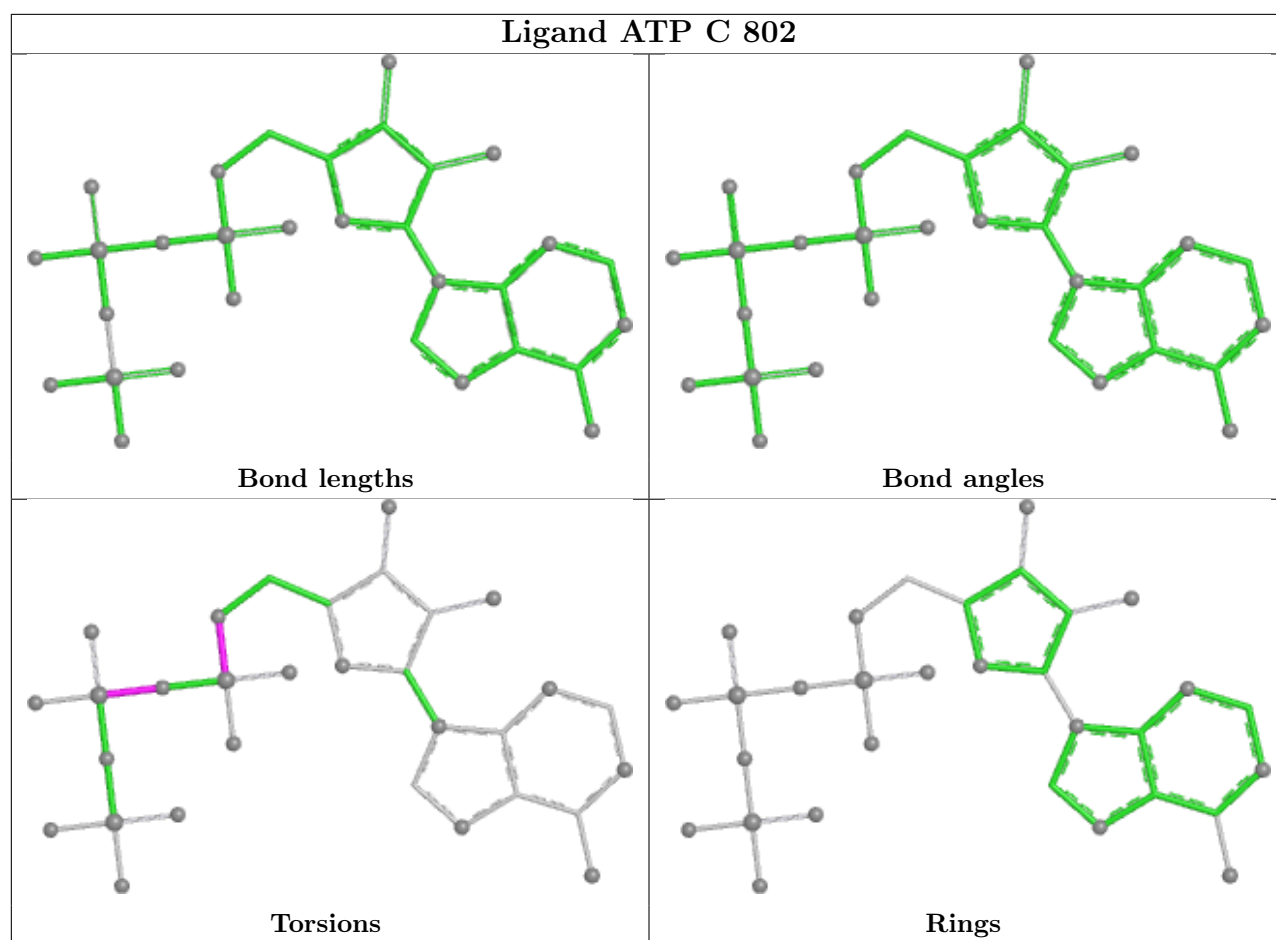
1 monomer is involved in 1 short contact:

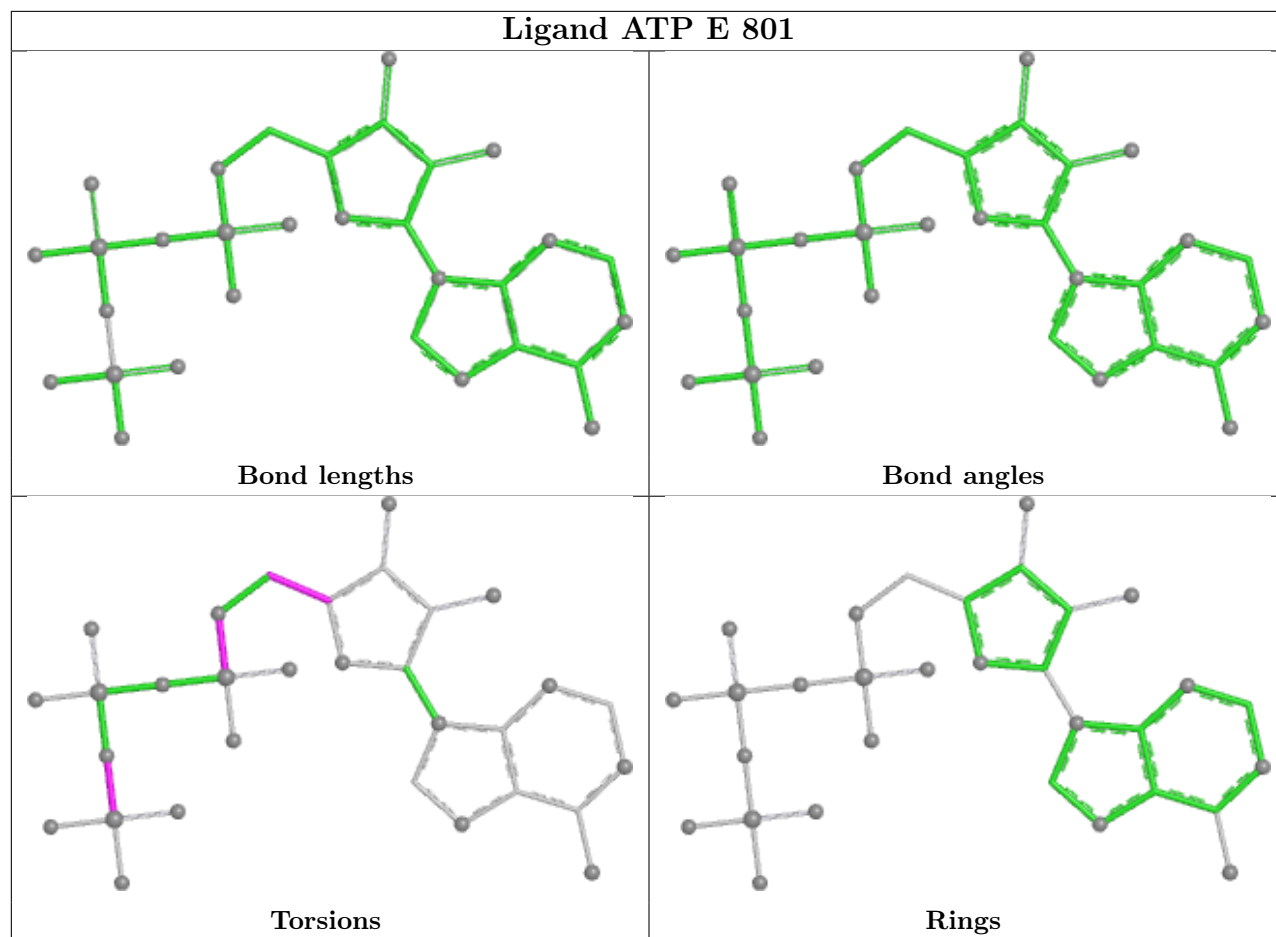
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	802	ATP	1	0

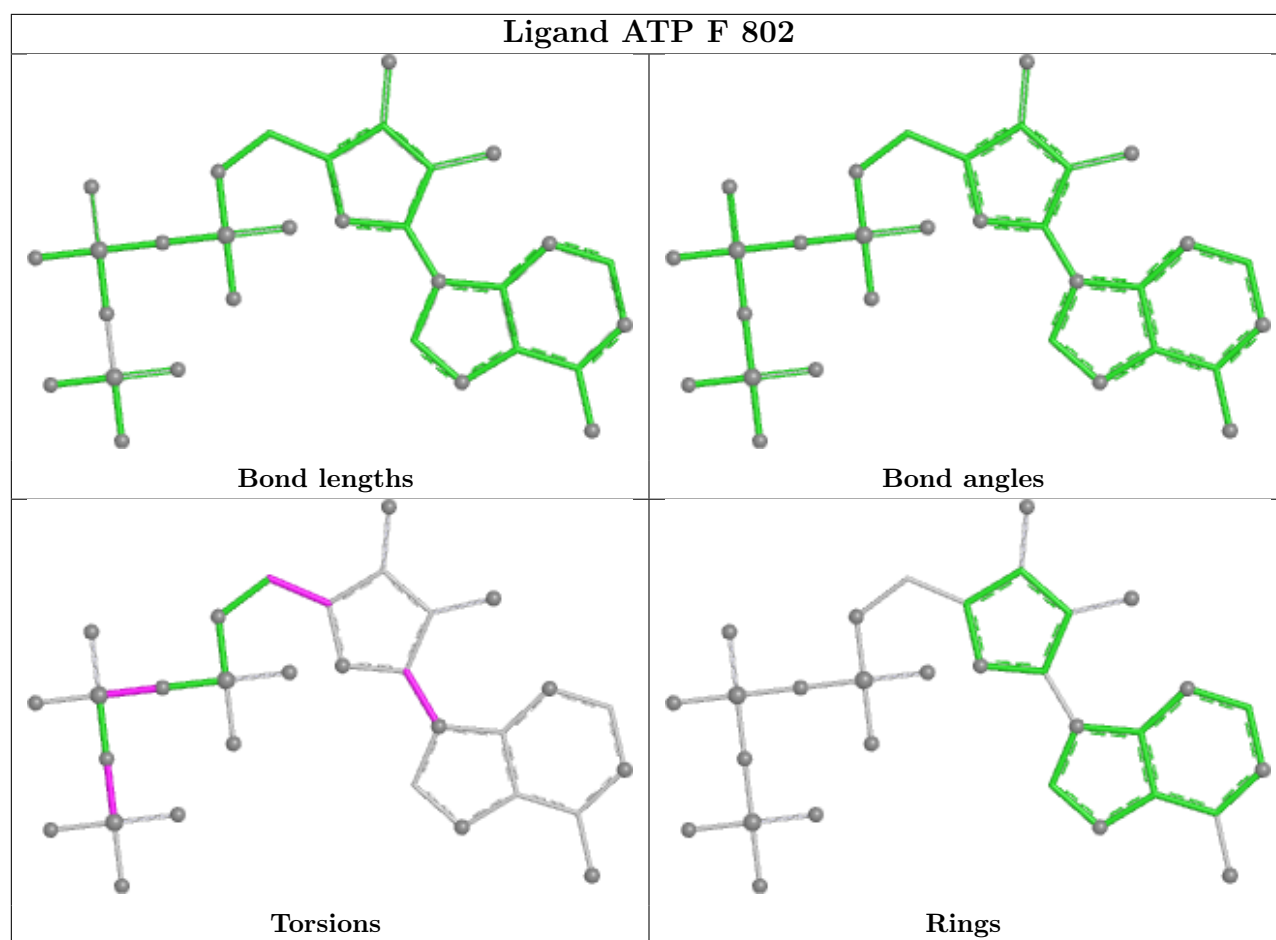
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

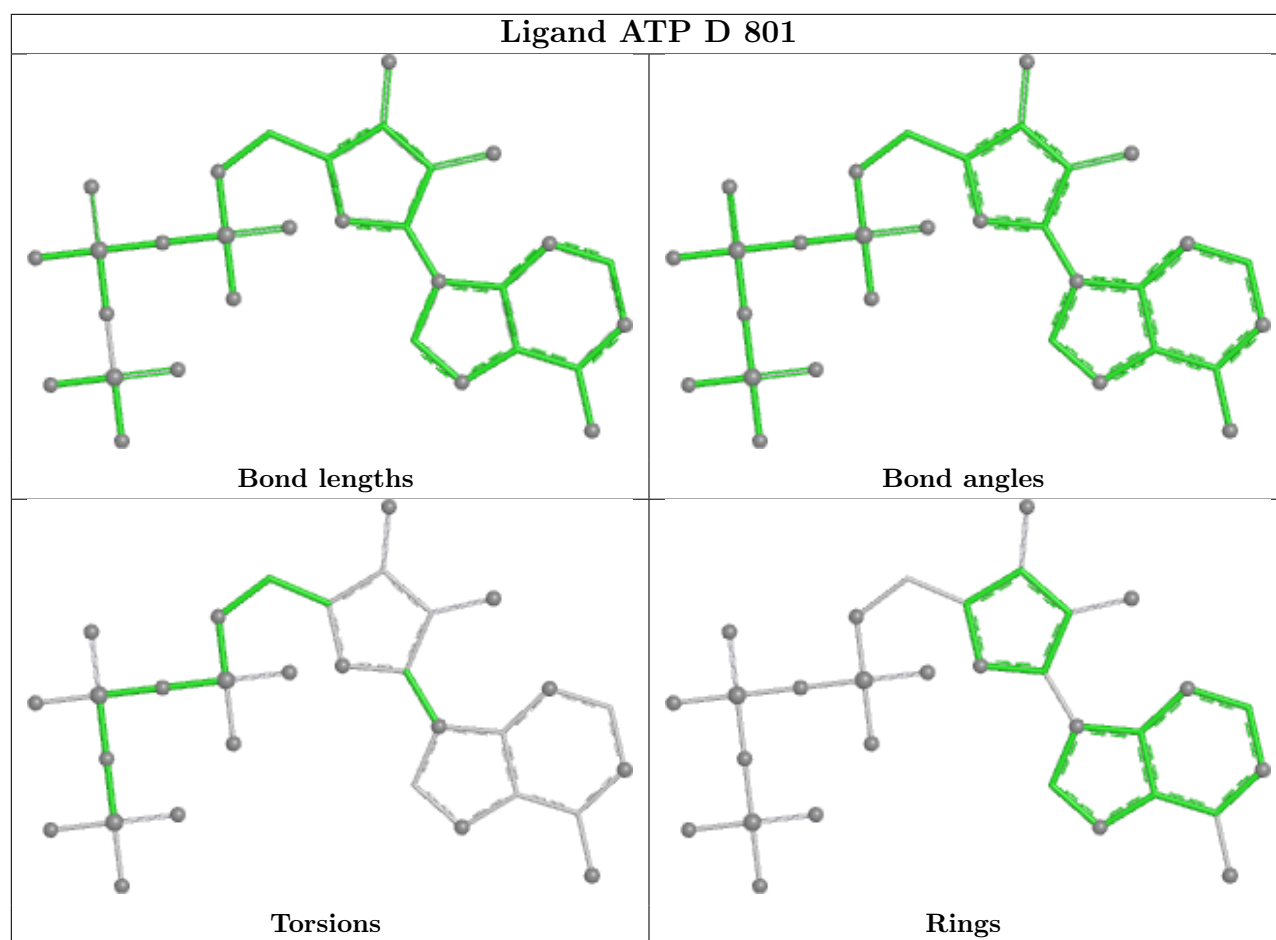
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

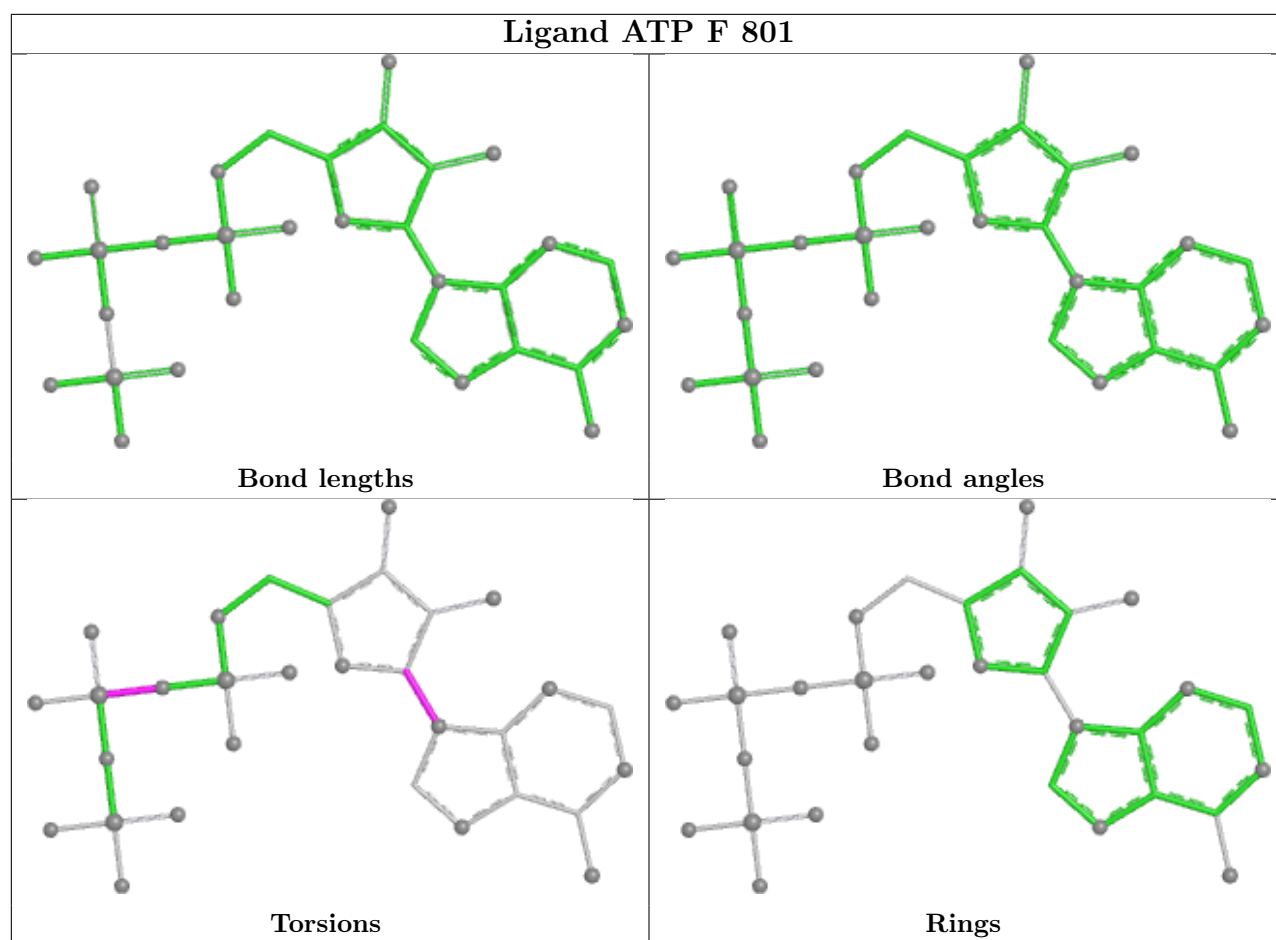


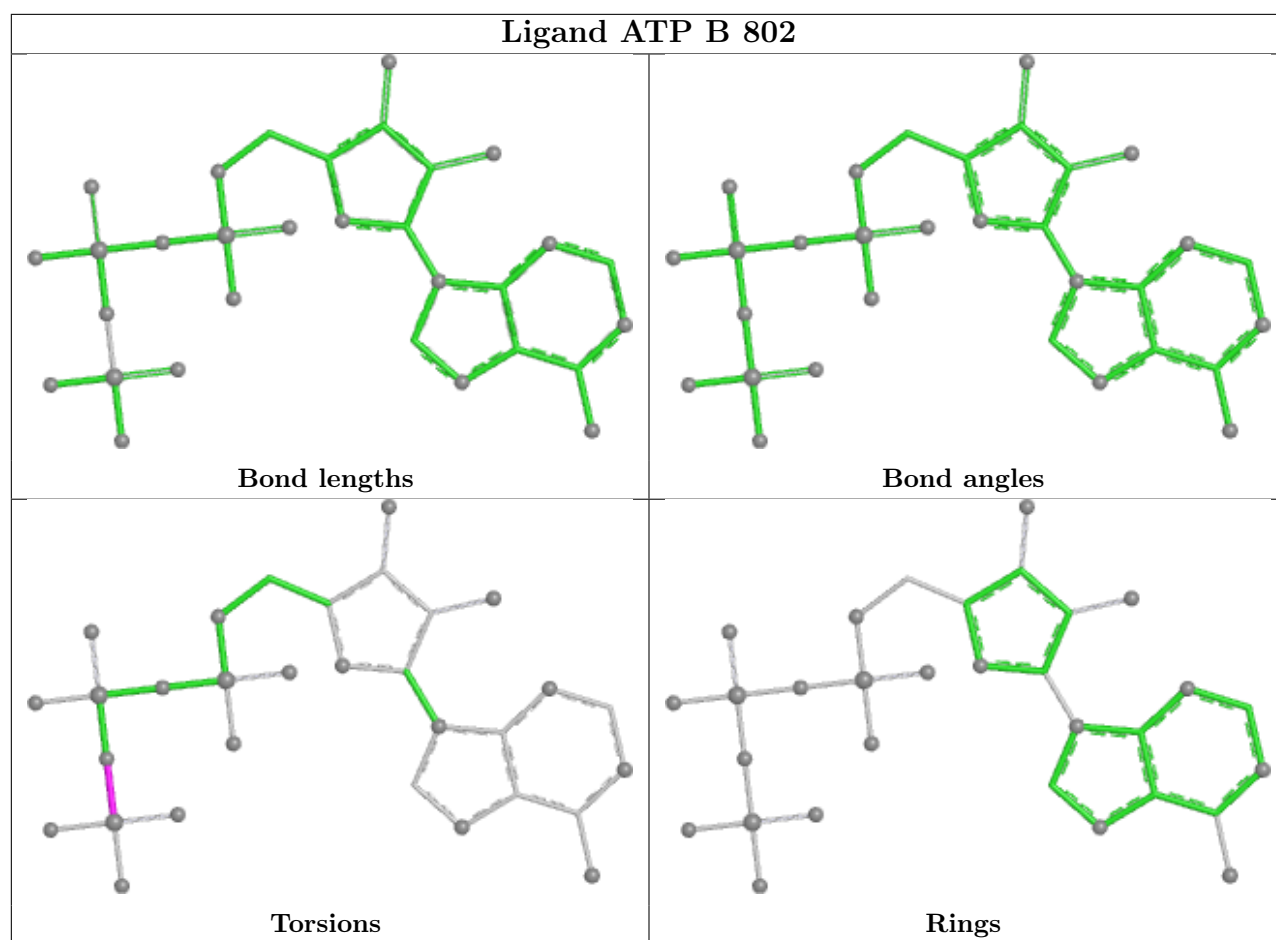


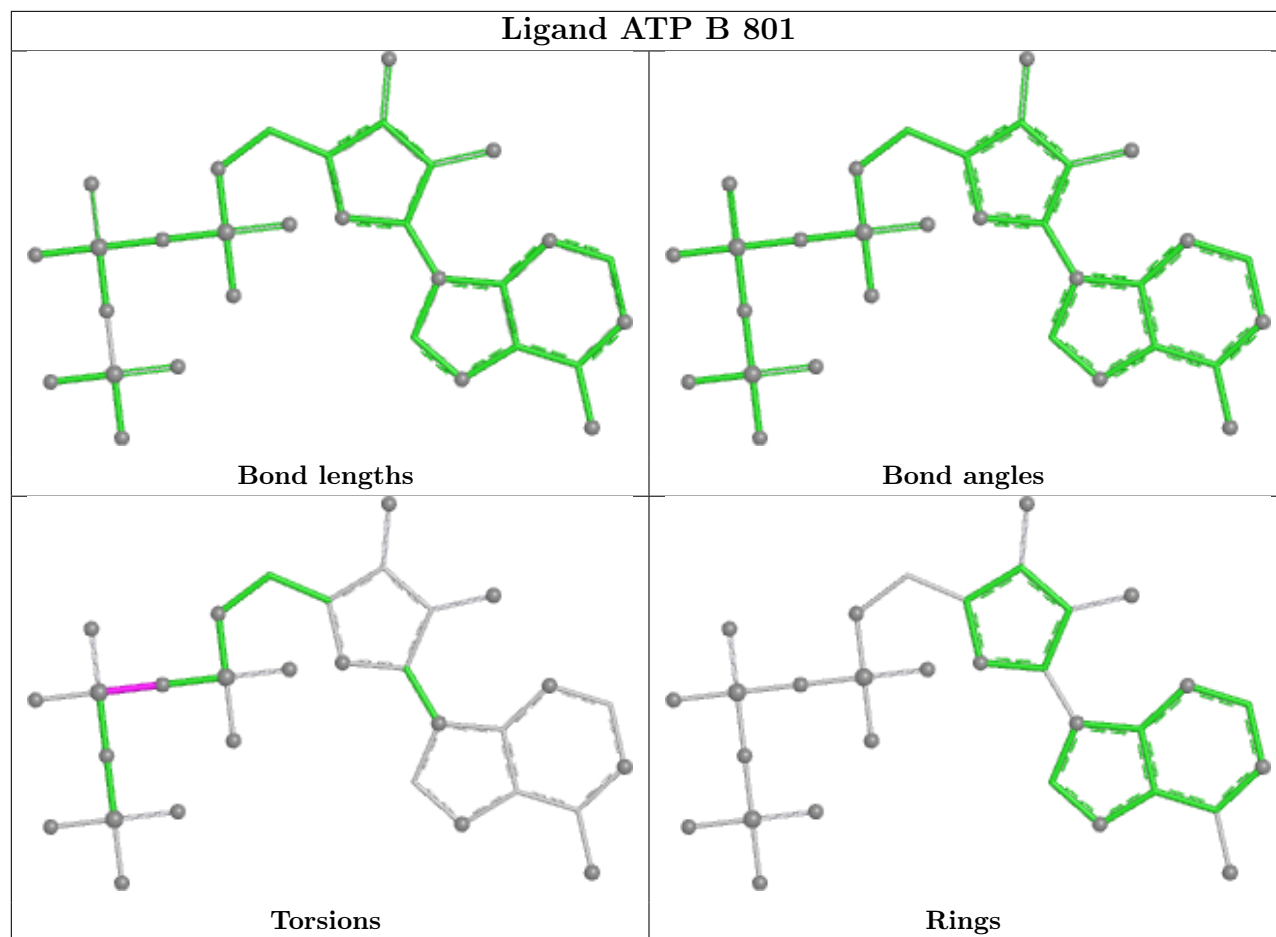


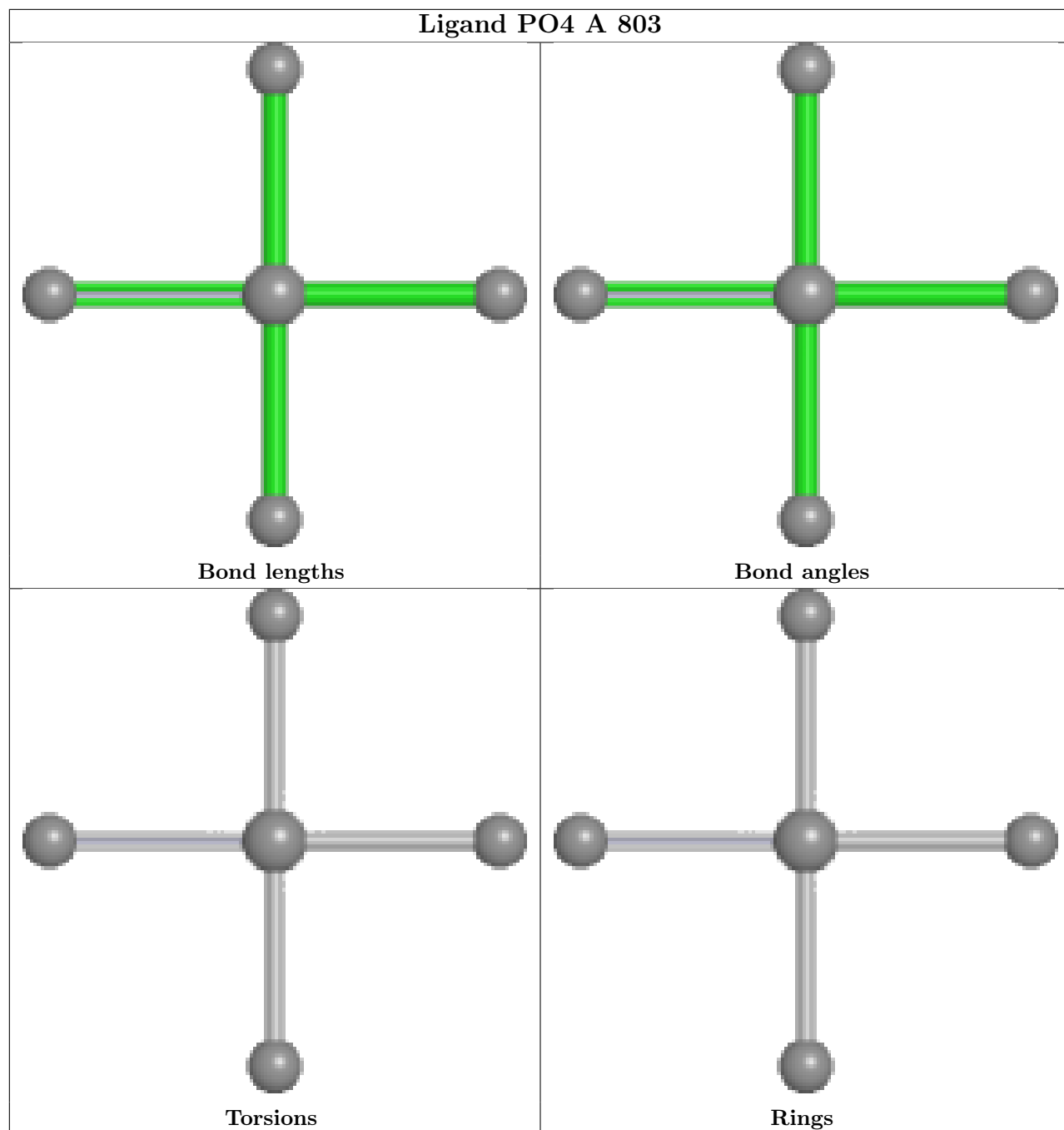


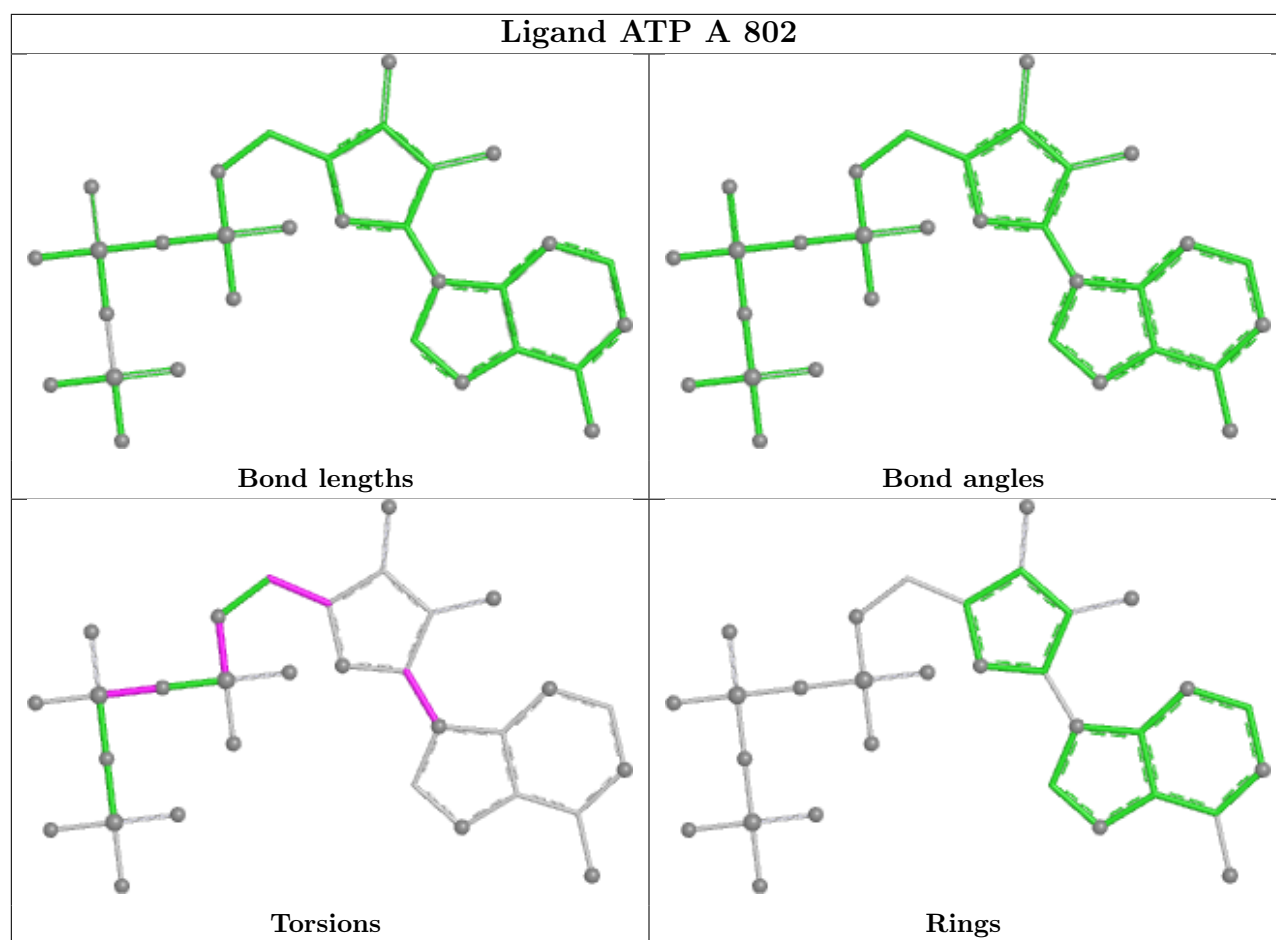




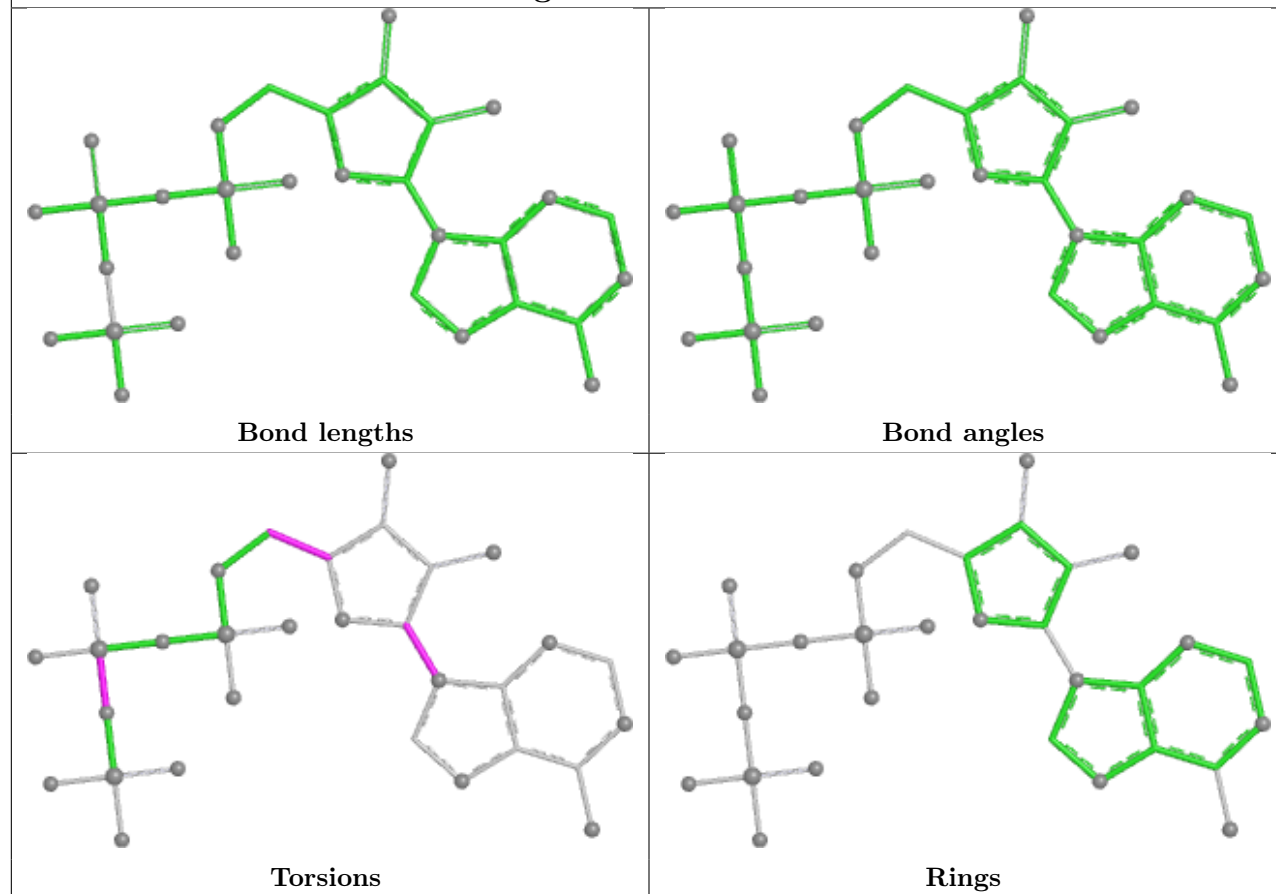




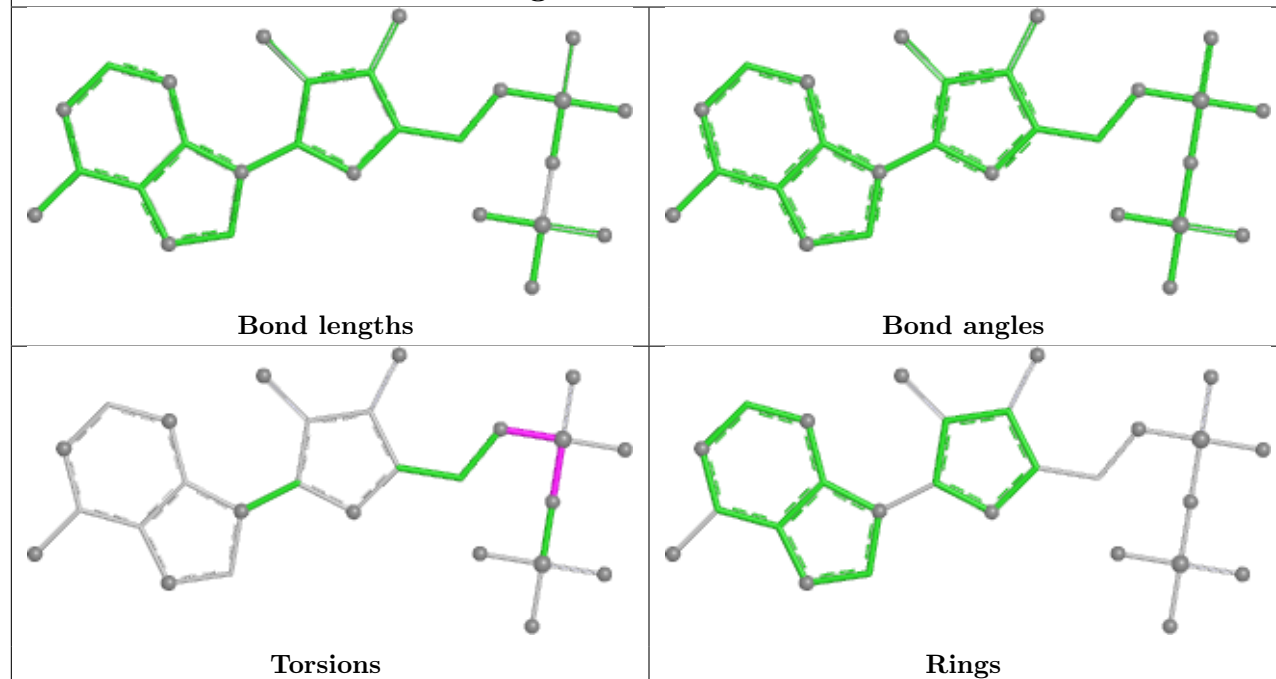


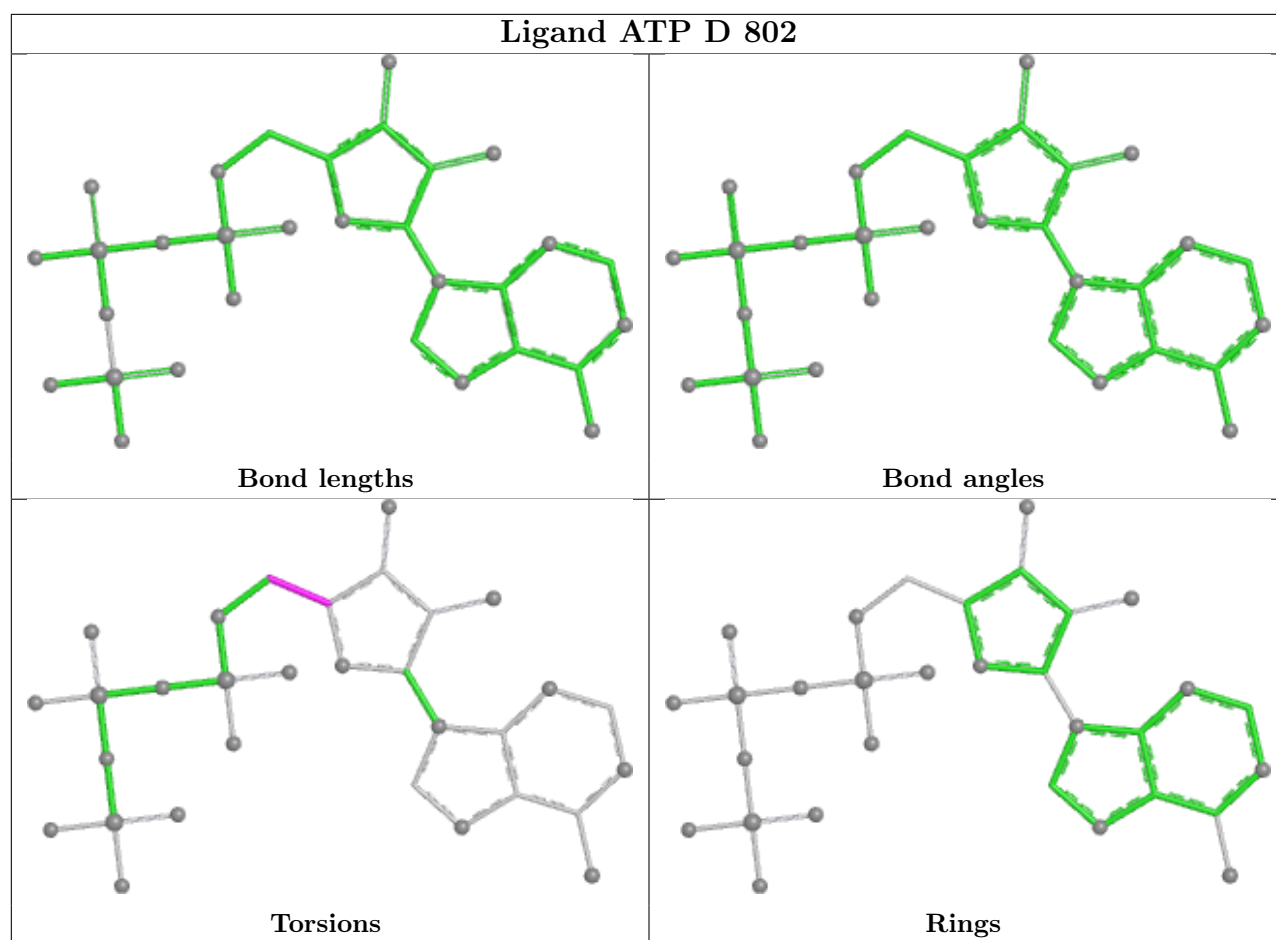


Ligand ATP E 802



Ligand ADP A 801





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.

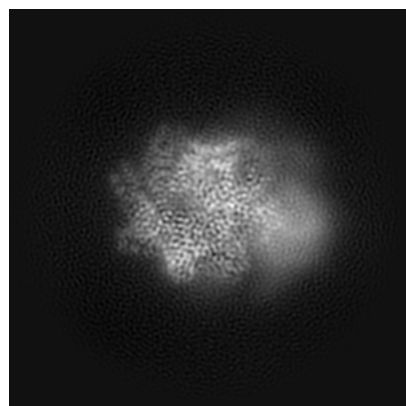
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70529. These allow visual inspection of the internal detail of the map and identification of artifacts.

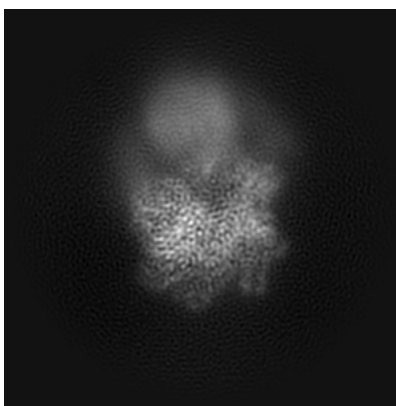
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

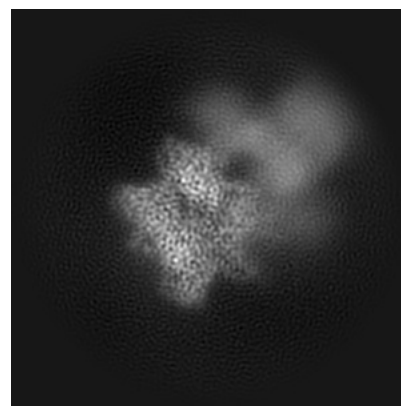
6.1.1 Primary map



X

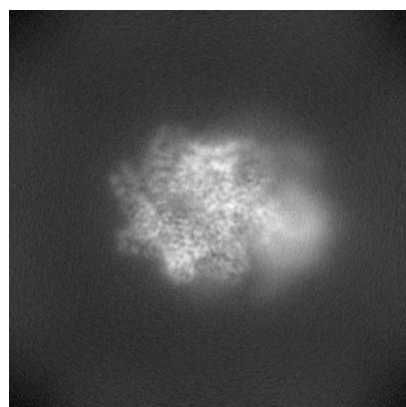


Y

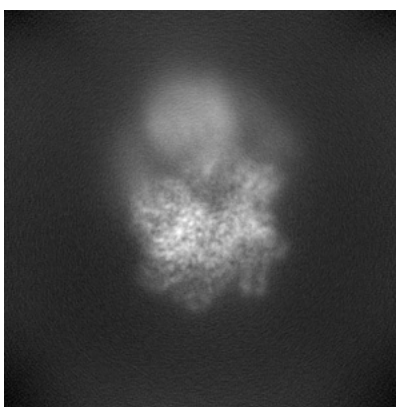


Z

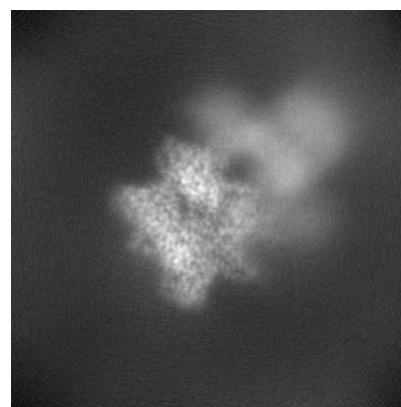
6.1.2 Raw map



X



Y

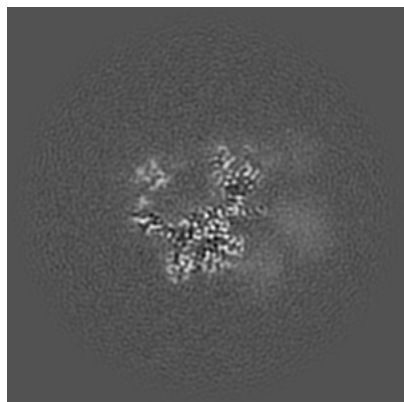


Z

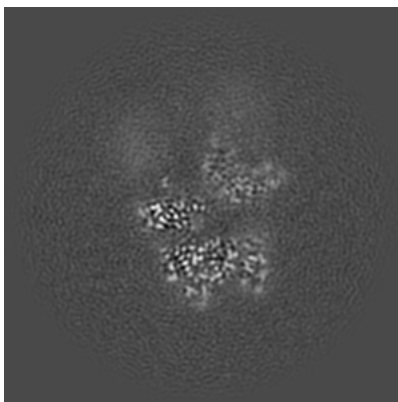
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

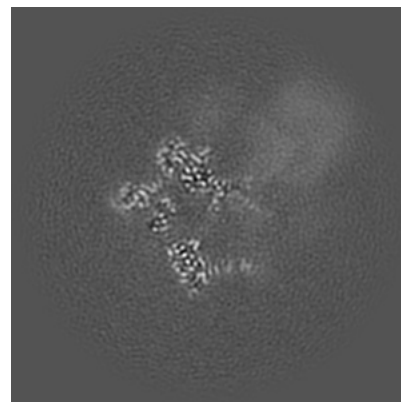
6.2.1 Primary map



X Index: 147

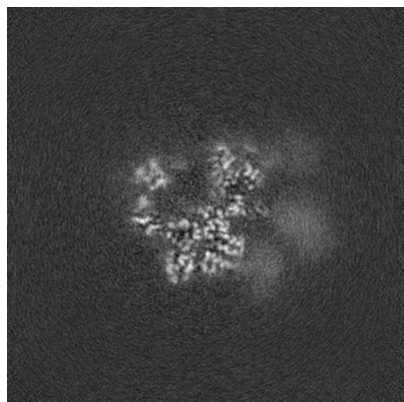


Y Index: 147

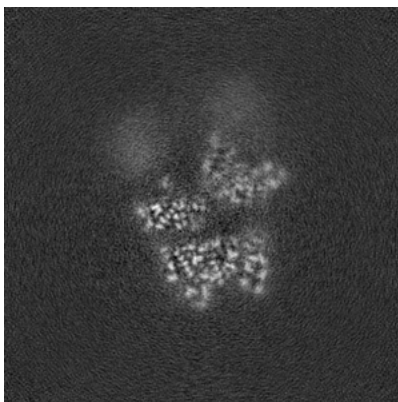


Z Index: 147

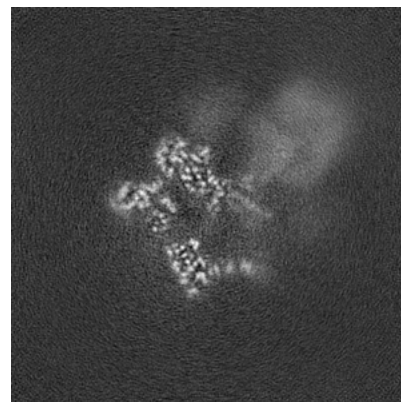
6.2.2 Raw map



X Index: 147



Y Index: 147

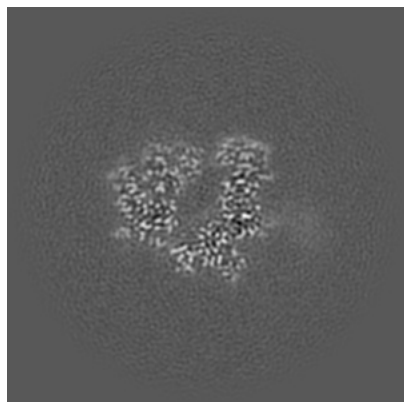


Z Index: 147

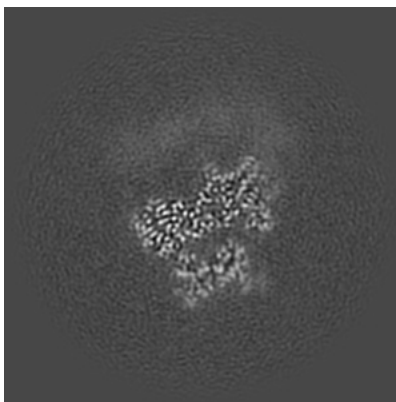
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

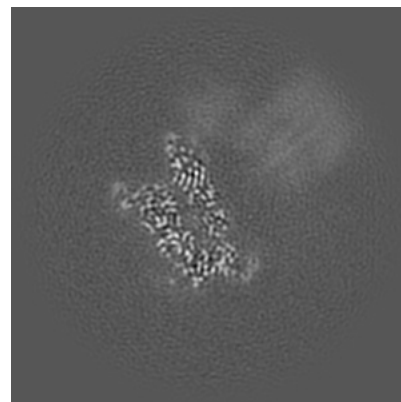
6.3.1 Primary map



X Index: 133

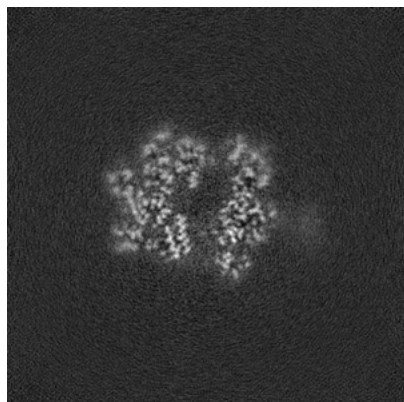


Y Index: 160

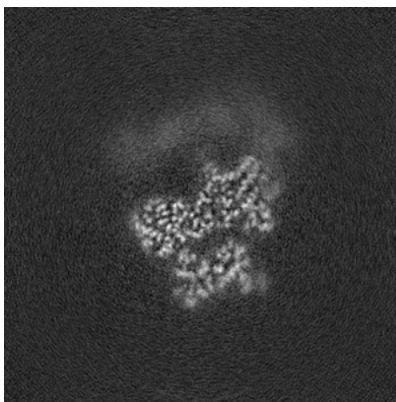


Z Index: 135

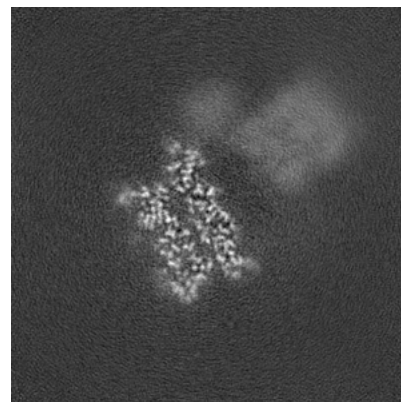
6.3.2 Raw map



X Index: 128



Y Index: 160

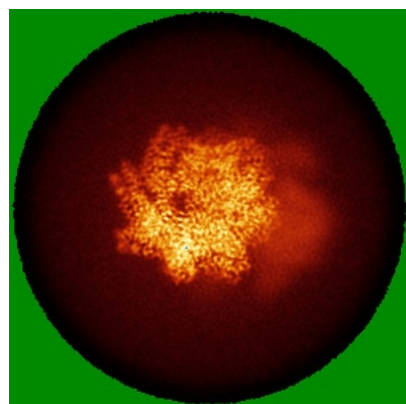


Z Index: 130

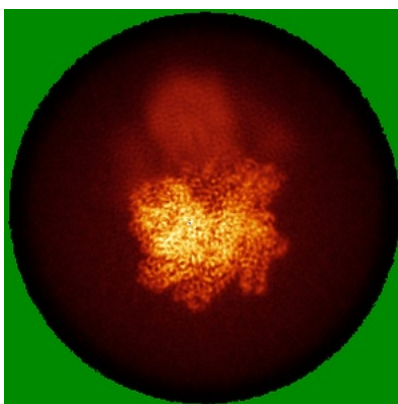
The images above show the largest variance slices of the map in three orthogonal directions.

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

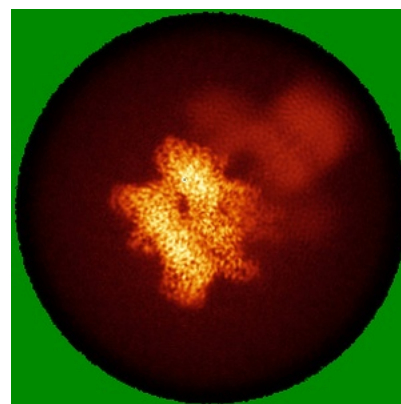
6.4.1 Primary map



X

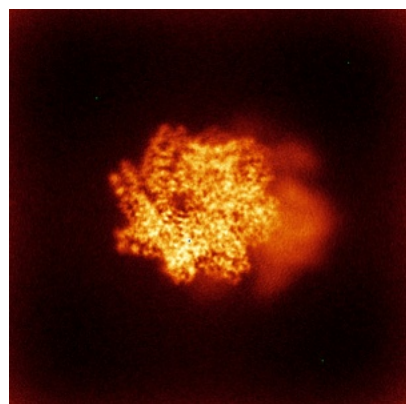


Y

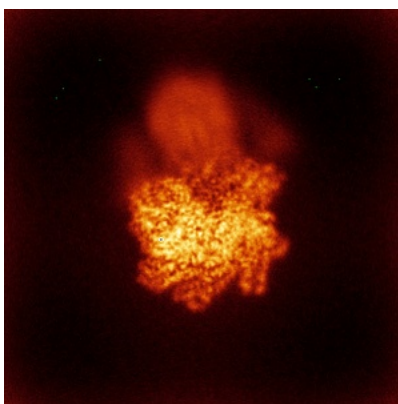


Z

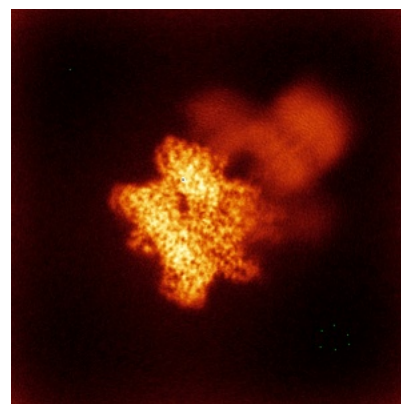
6.4.2 Raw map



X



Y

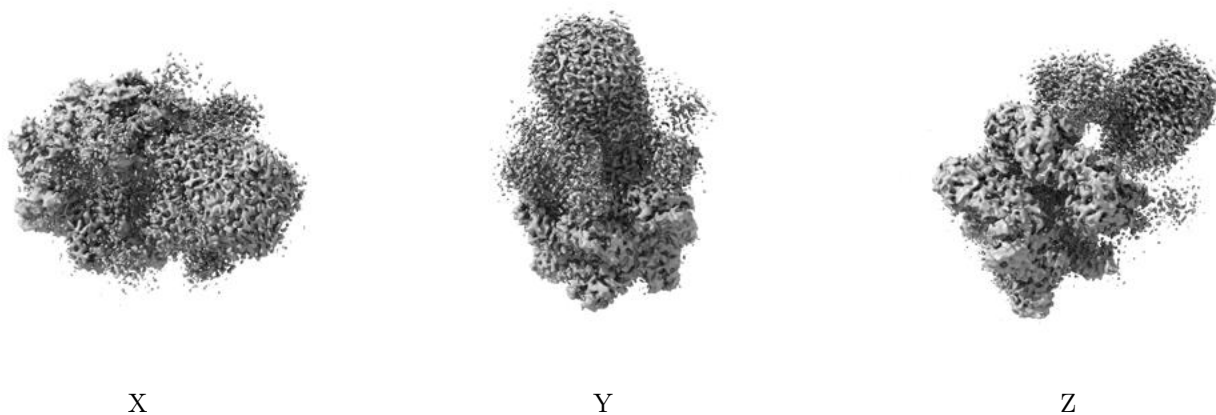


Z

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.

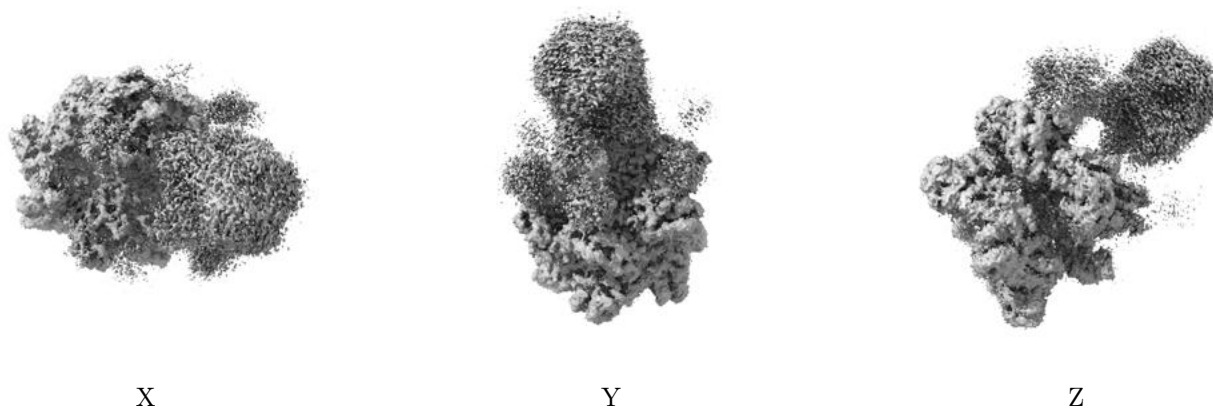
6.5 Orthogonal surface views [i](#)

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.

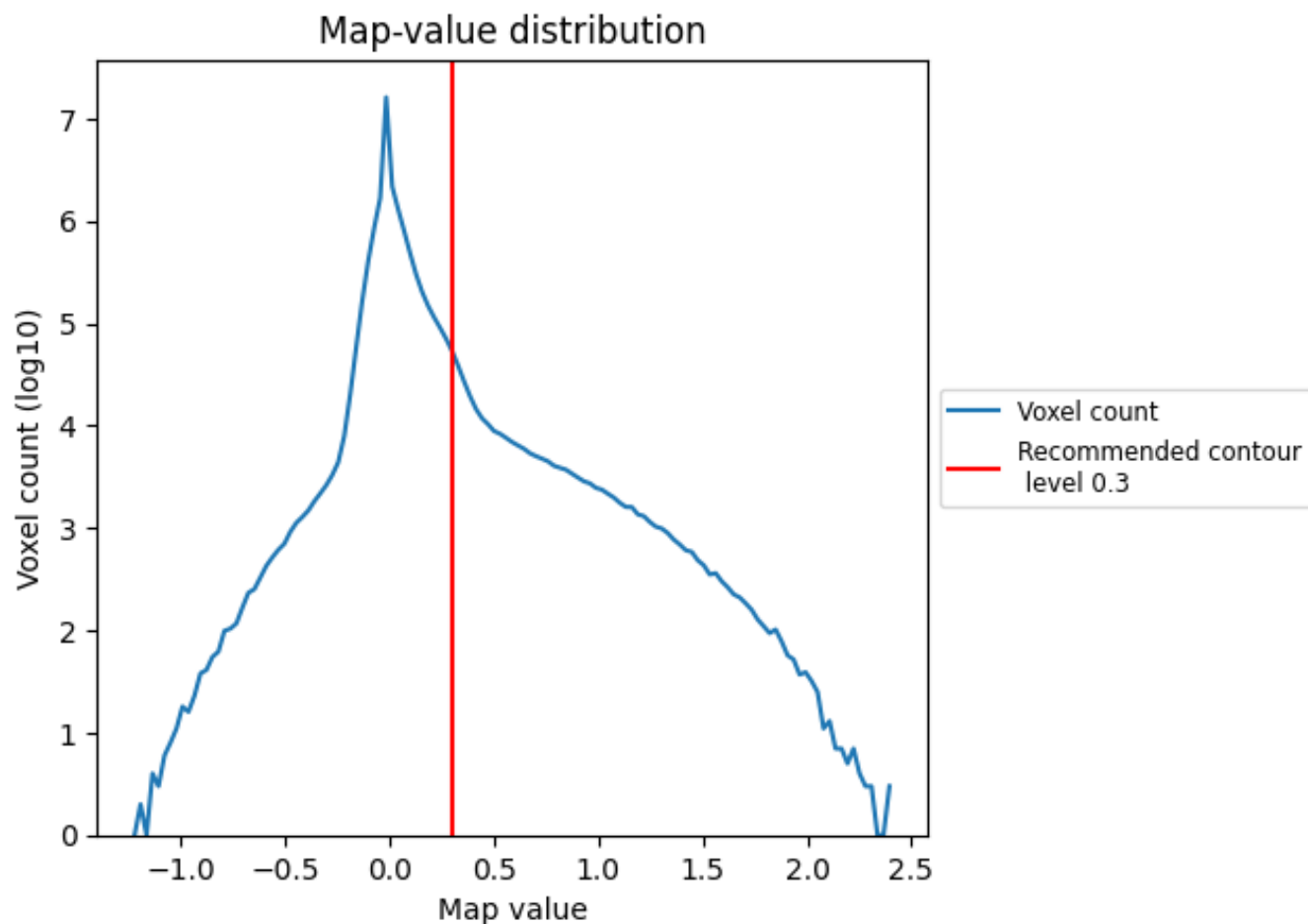
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

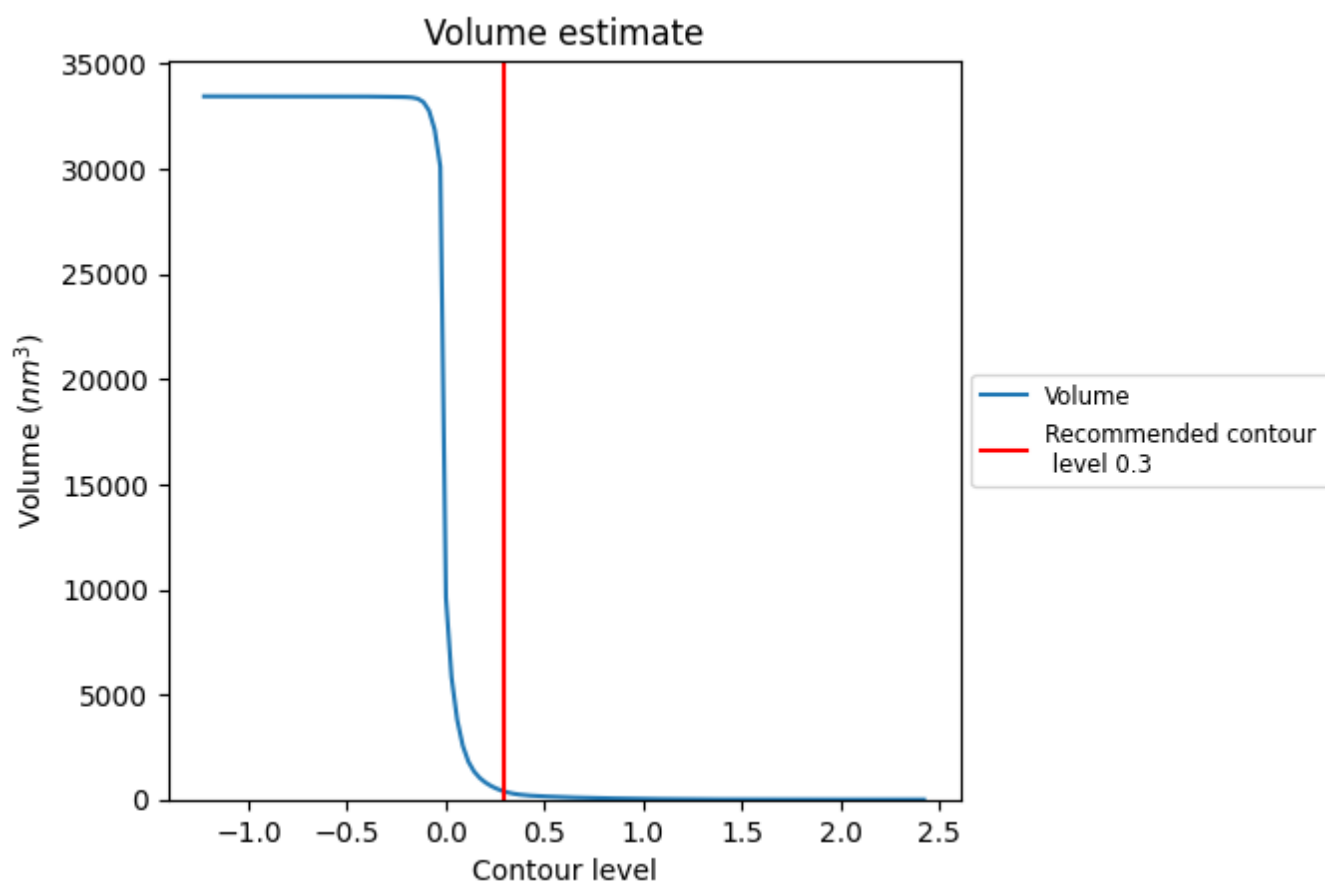
This section contains the results of statistical analysis of the map.

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.

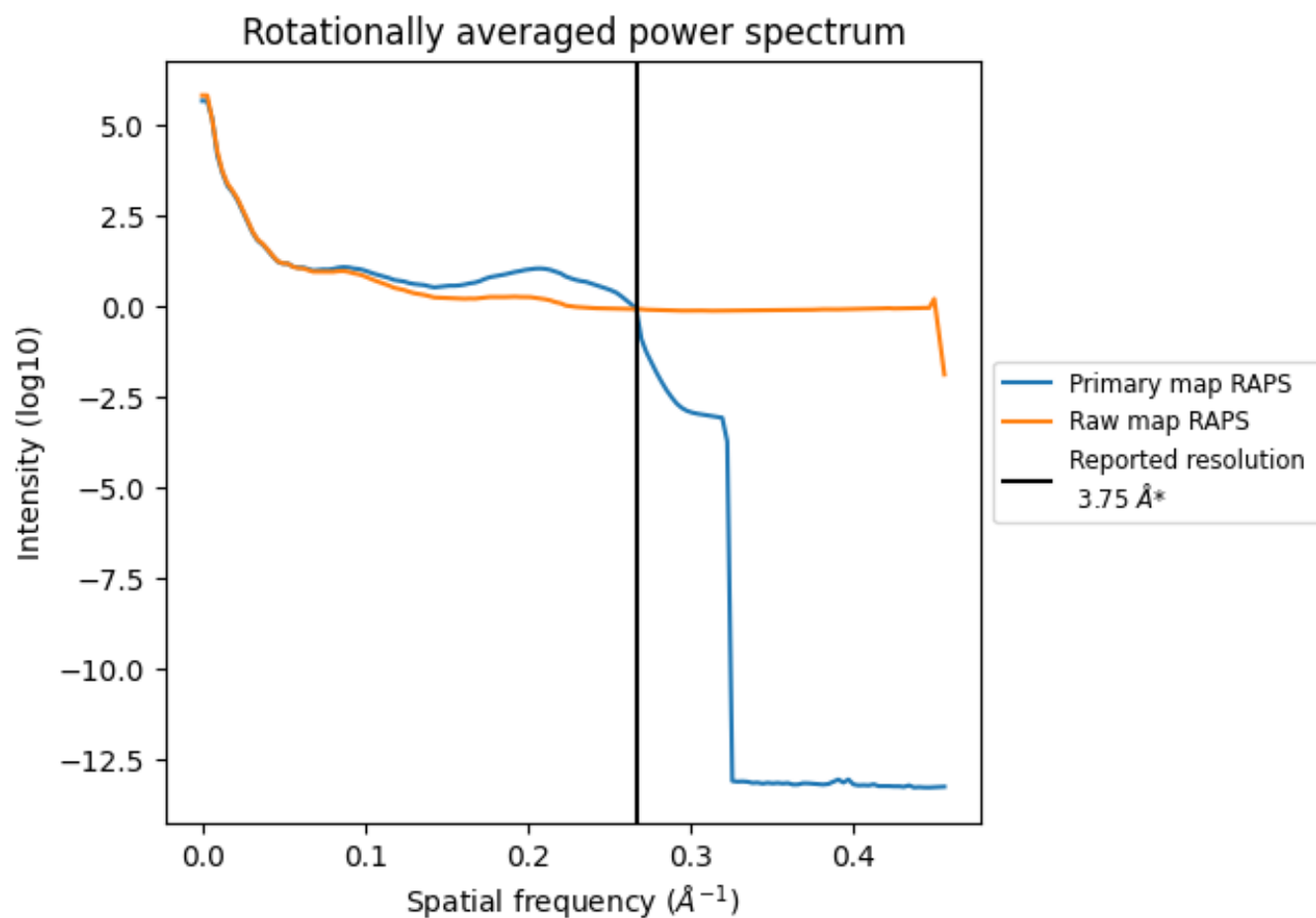
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 381 nm³; this corresponds to an approximate mass of 344 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 ⓘ

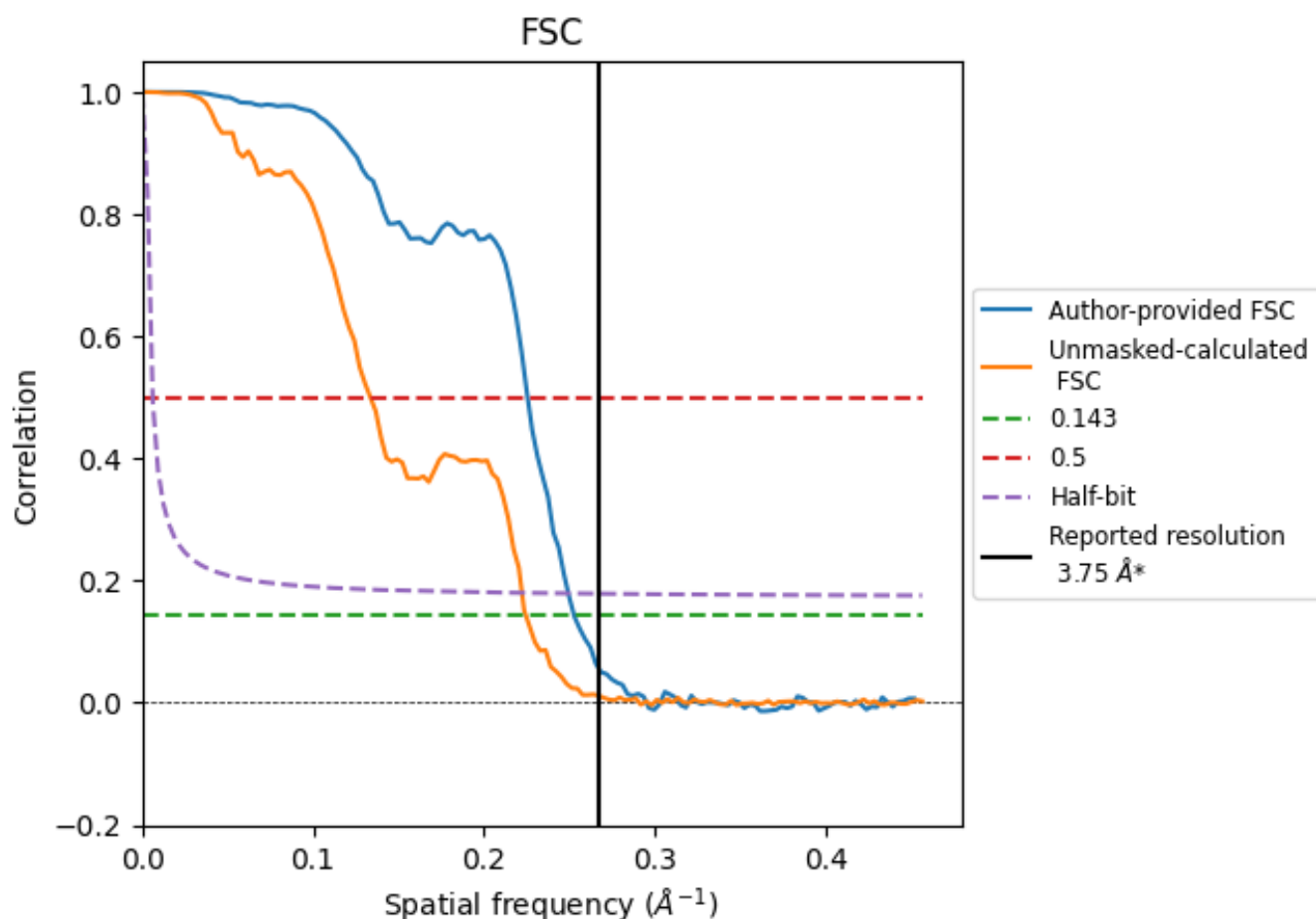


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

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 0.267 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

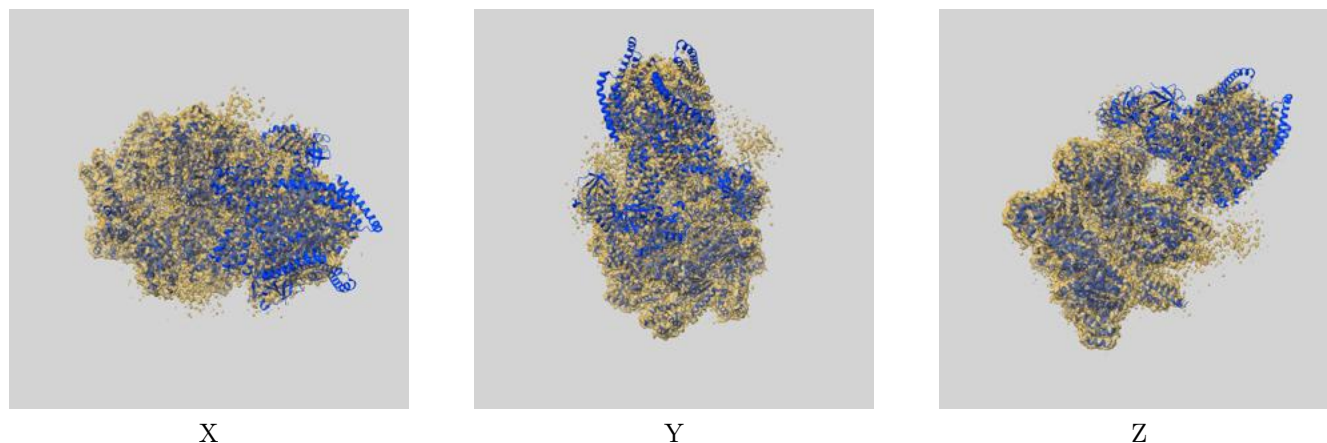
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.96	4.44	4.01
Unmasked-calculated*	4.46	7.49	4.50

*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 4.46 differs from the reported value 3.75 by more than 10 %

9 Map-model fit [i](#)

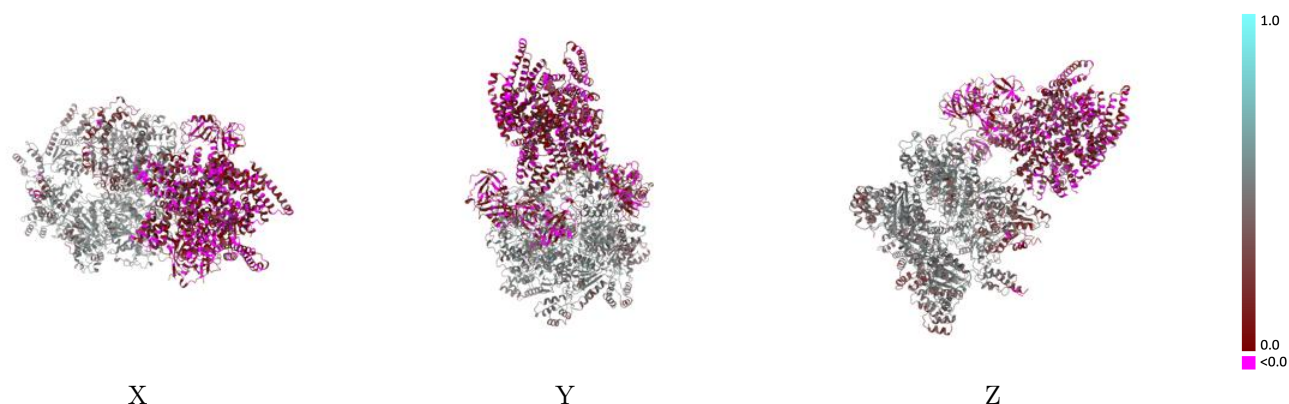
This section contains information regarding the fit between EMDB map EMD-70529 and PDB model 9OJ2. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



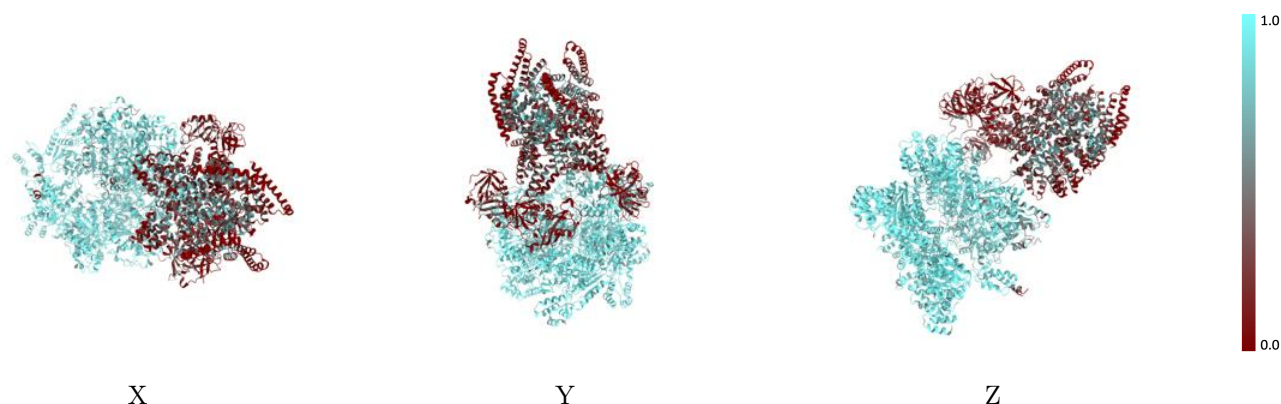
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



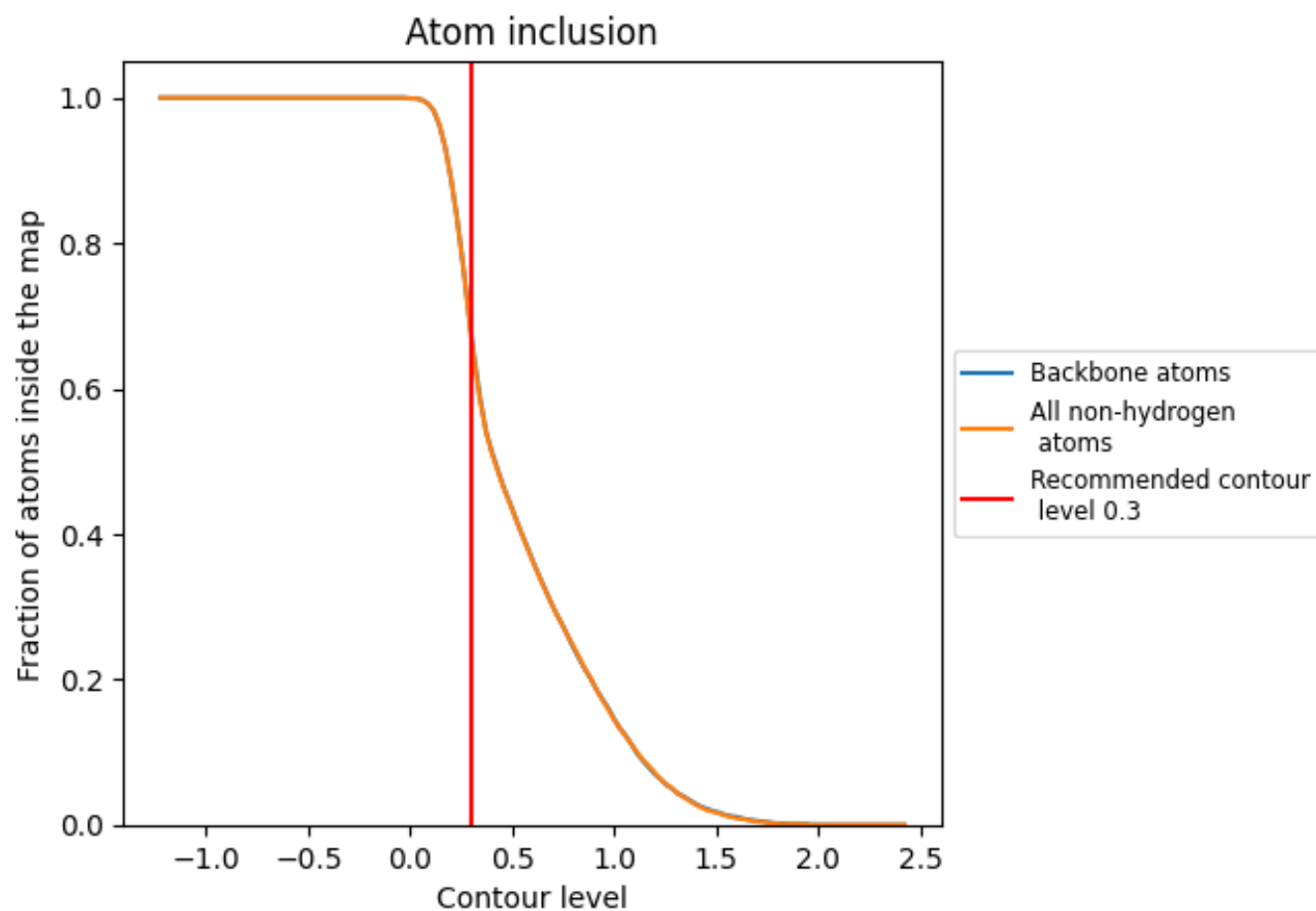
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 67% of all backbone atoms, 67% 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	 0.6700	 0.3220
A	 0.9220	 0.4640
B	 0.7450	 0.3940
C	 0.7300	 0.3900
D	 0.7240	 0.3710
E	 0.9180	 0.4470
F	 0.8250	 0.3740
G	 0.6460	 0.2140
H	 0.5290	 0.1310
I	 0.6220	 0.1480
J	 0.5360	 0.0860
K	 0.3020	 0.1190
L	 0.2650	 0.0890
M	 0.2980	 0.0780
N	 0.2850	 0.0760

