



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:57 PM UTC

PDB ID : 9NLU / pdb_00009nlu
EMDB ID : EMD-49522
Title : Y20S (Sec18-Sec17-Sec9-Sso1-Snc1) EDTA - Class 5
Authors : Khan, Y.A.; Brunger, A.T.
Deposited on : 2025-03-03
Resolution : 4.29 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

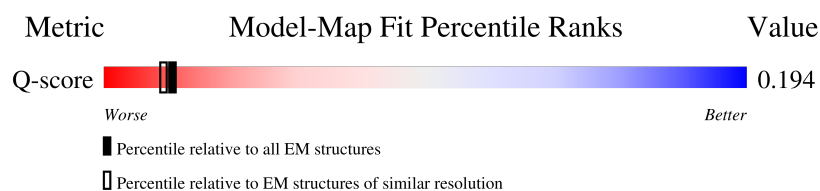
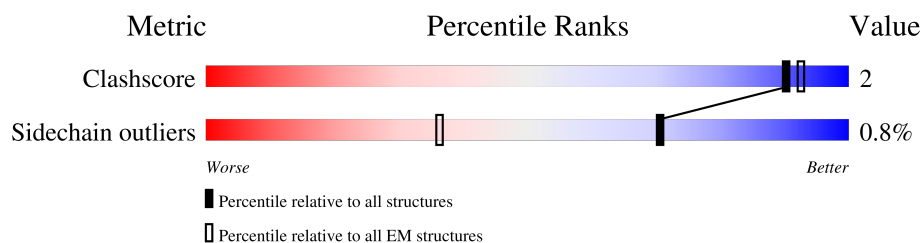
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

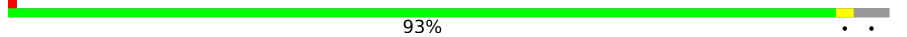
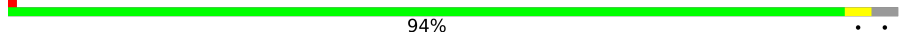
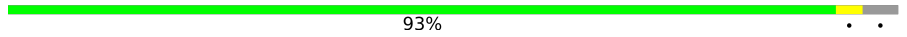
The reported resolution of this entry is 4.29 Å.

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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4494 (3.79 - 4.79)

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	761	
1	B	761	
1	C	761	
1	D	761	
1	E	761	

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Mol	Chain	Length	Quality of chain
1	F	761	63%36%
2	G	293	95%. .
2	H	293	93%. 6%
2	I	293	38%97%. .
3	J	97	57%5%38%
4	K	269	25%7%. 67%
5	L	222	48%9%. 42%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 39736 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Vesicular-fusion protein SEC18.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	513	Total	C	N	O	S	0	0
			3994	2522	690	764	18		
1	B	731	Total	C	N	O	S	1	0
			5726	3610	998	1095	23		
1	C	735	Total	C	N	O	S	0	0
			5736	3621	999	1093	23		
1	D	730	Total	C	N	O	S	0	0
			5699	3595	992	1089	23		
1	E	714	Total	C	N	O	S	0	0
			5575	3525	964	1063	23		
1	F	489	Total	C	N	O	S	0	0
			3809	2401	658	732	18		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P18759
A	-1	ALA	-	expression tag	UNP P18759
A	0	HIS	-	expression tag	UNP P18759
B	-2	GLY	-	expression tag	UNP P18759
B	-1	ALA	-	expression tag	UNP P18759
B	0	HIS	-	expression tag	UNP P18759
C	-2	GLY	-	expression tag	UNP P18759
C	-1	ALA	-	expression tag	UNP P18759
C	0	HIS	-	expression tag	UNP P18759
D	-2	GLY	-	expression tag	UNP P18759
D	-1	ALA	-	expression tag	UNP P18759
D	0	HIS	-	expression tag	UNP P18759
E	-2	GLY	-	expression tag	UNP P18759
E	-1	ALA	-	expression tag	UNP P18759
E	0	HIS	-	expression tag	UNP P18759
F	-2	GLY	-	expression tag	UNP P18759
F	-1	ALA	-	expression tag	UNP P18759
F	0	HIS	-	expression tag	UNP P18759

- Molecule 2 is a protein called Alpha-soluble NSF attachment protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	287	Total	C	N	O	S	0	0
			2264	1419	380	454	11		
2	H	275	Total	C	N	O	S	0	0
			2158	1355	354	439	10		
2	I	286	Total	C	N	O	S	0	0
			2261	1420	378	453	10		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	GLY	-	expression tag	UNP P32602
H	0	GLY	-	expression tag	UNP P32602
I	0	GLY	-	expression tag	UNP P32602

- Molecule 3 is a protein called Synaptobrevin homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	60	Total	C	N	O	S	0	0
			468	282	92	92	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-3	GLY	-	expression tag	UNP P31109
J	-2	ALA	-	expression tag	UNP P31109
J	-1	SER	-	expression tag	UNP P31109
J	0	HIS	-	expression tag	UNP P31109

- Molecule 4 is a protein called Protein SSO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	89	Total	C	N	O	S	0	0
			698	426	126	144	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	GLY	-	expression tag	UNP P32867
K	-2	ALA	-	expression tag	UNP P32867
K	-1	SER	-	expression tag	UNP P32867
K	0	HIS	-	expression tag	UNP P32867

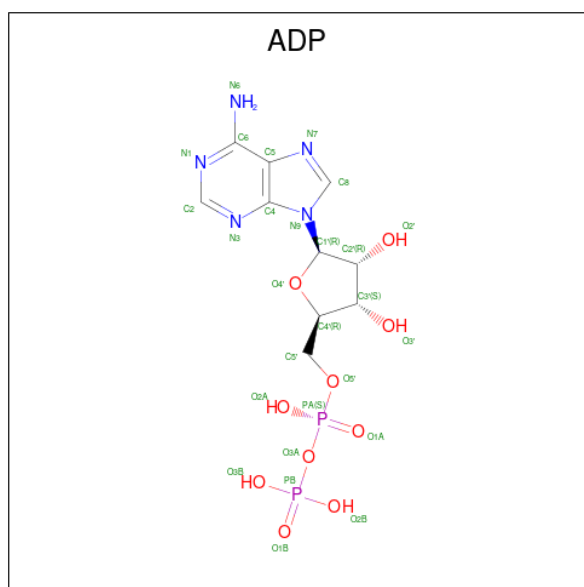
- Molecule 5 is a protein called Protein transport protein SEC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	129	Total	C	N	O	S	0	0
			1015	614	186	208	7		

There are 4 discrepancies between the modelled and reference sequences:

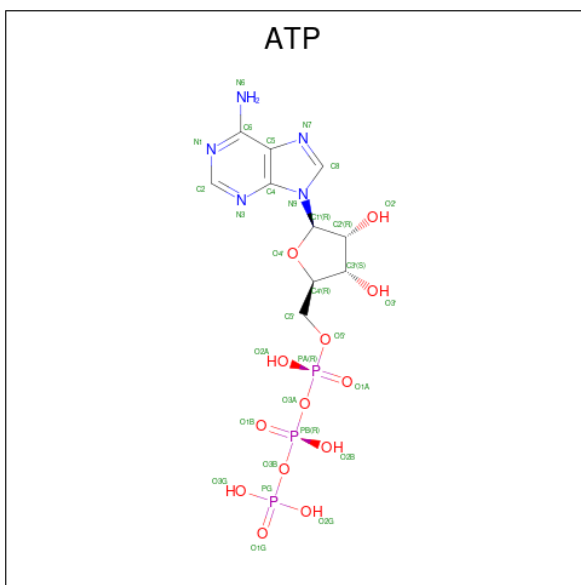
Chain	Residue	Modelled	Actual	Comment	Reference
L	429	GLY	-	expression tag	UNP P40357
L	430	ALA	-	expression tag	UNP P40357
L	431	SER	-	expression tag	UNP P40357
L	432	HIS	-	expression tag	UNP P40357

- Molecule 6 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
6	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

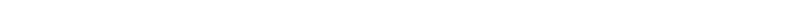
- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



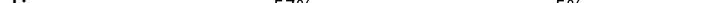
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total 31	C 10	N 5	O 13	P 3	0
7	B	1	Total 31	C 10	N 5	O 13	P 3	0
7	B	1	Total 31	C 10	N 5	O 13	P 3	0
7	C	1	Total 31	C 10	N 5	O 13	P 3	0
7	C	1	Total 31	C 10	N 5	O 13	P 3	0
7	D	1	Total 31	C 10	N 5	O 13	P 3	0
7	D	1	Total 31	C 10	N 5	O 13	P 3	0
7	E	1	Total 31	C 10	N 5	O 13	P 3	0
7	F	1	Total 31	C 10	N 5	O 13	P 3	0

- Chain H: 93% 6%

GLY M1 S18 S19 G20 G21 F21 F22 M22 K23 K24 L24 Y47 A48 L49 LEU LEU ARG ARG LYS E52 D74 E75 R110 GLY GLN PHE ARG R115 L156 L157 SER MET GLY ASN ARG ARG LEU LEU GLN TRP L292

- Chain I:  38% 97%

[illegible]

- Chain J: 

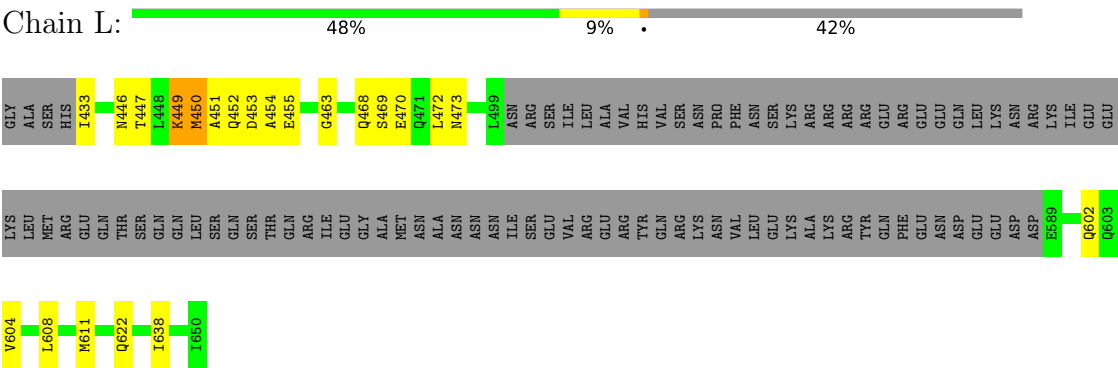
GLY	ALA	SER	HIS	MET	SER	SER	PRO	PRO	THR	PRO	PHE	ASP	PRO	PRO	TYR	ALA	LEU	SER	HIS	ASP	GLU	GLU	GLU	ARG	PRO	ASN	VAL	GLN	SER	SER	LYS	S27	L32	V40	M43	R44	R56	R76	W86	TYR	LYS	ASP	LEU	LYS	MET
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- Chain K: 25% 7% 67%

[illegible]

L177	L178	N151	E156	T188	A189	L190	V193	L201	A208	F214	E218	E219	E223	E226	E236	L240	A256	R257	LYS	ALA	ARG	LYS	ASN	LYS	ILE	ARG
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● Molecule 5: Protein transport protein SEC9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33084	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	-0.010	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00205	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

5.1 Standard geometry

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	0.24	0/4049	0.42	0/5459
1	B	0.25	0/5818	0.41	0/7854
1	C	0.26	0/5826	0.44	0/7861
1	D	0.27	0/5788	0.45	0/7813
1	E	0.24	0/5663	0.45	0/7642
1	F	0.23	0/3858	0.41	0/5198
2	G	0.37	0/2300	0.56	0/3086
2	H	0.27	0/2189	0.49	0/2936
2	I	0.24	0/2297	0.47	0/3082
3	J	0.28	0/470	0.58	0/628
4	K	0.52	0/701	0.89	1/941 (0.1%)
5	L	0.48	0/1016	0.75	0/1355
All	All	0.28	0/39975	0.47	1/53855 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	218	GLU	CB-CA-C	-5.48	102.27	110.88

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	3994	0	4090	8	0
1	B	5726	0	5786	10	0
1	C	5736	0	5820	14	0
1	D	5699	0	5773	14	0
1	E	5575	0	5646	31	0
1	F	3809	0	3903	11	0
2	G	2264	0	2191	23	0
2	H	2158	0	2087	4	0
2	I	2261	0	2195	3	0
3	J	468	0	470	6	0
4	K	698	0	692	29	0
5	L	1015	0	1034	25	0
6	A	27	0	12	0	0
6	E	27	0	12	0	0
7	A	31	0	12	0	0
7	B	62	0	24	0	0
7	C	62	0	24	0	0
7	D	62	0	24	0	0
7	E	31	0	12	0	0
7	F	31	0	12	0	0
All	All	39736	0	39819	131	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 2.

All (131) 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)
5:L:447:THR:HA	5:L:450:MET:HE2	1.57	0.85
5:L:469:SER:HB2	5:L:622:GLN:NE2	2.02	0.73
1:F:461:GLU:O	1:F:465:LEU:HD12	1.88	0.73
1:A:698:ASN:O	1:A:702:ILE:HG23	1.93	0.69
2:G:196:TRP:CZ2	5:L:450:MET:HE3	2.28	0.67
2:H:74:ASP:HB2	4:K:240:LEU:HD11	1.76	0.66
2:G:114:ARG:HD3	4:K:226:GLU:HB3	1.78	0.66
1:B:161:GLU:OE1	1:C:93:LEU:HB2	2.00	0.62
1:E:691:MET:HE2	1:E:733:THR:HG21	1.83	0.61
1:E:346:ILE:HD12	1:E:346:ILE:O	2.01	0.60
1:E:691:MET:CE	1:E:733:THR:HG21	2.32	0.60
1:D:145:ARG:HH22	1:E:96:ASP:N	2.00	0.59
1:E:316:VAL:CG1	4:K:178:LEU:HD13	2.34	0.57
1:E:718:GLU:OE1	1:E:747:VAL:HG21	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:PHE:CZ	1:F:474:ILE:HG23	2.39	0.57
1:D:715:VAL:HG12	1:D:747:VAL:HG13	1.87	0.56
1:E:229:VAL:HG23	1:E:230:ILE:HD12	1.86	0.56
1:C:524:VAL:HG12	1:C:524:VAL:O	2.05	0.56
2:G:114:ARG:CD	4:K:226:GLU:HB3	2.36	0.56
2:G:156:LEU:HD11	4:K:223:GLU:HG3	1.87	0.56
1:E:316:VAL:HG12	4:K:178:LEU:HD13	1.87	0.55
1:A:236:PHE:CZ	1:A:249:THR:HG22	2.41	0.55
1:E:603:ILE:HG23	1:E:646:MET:HE2	1.88	0.54
1:E:240:GLY:O	1:E:430:ILE:HD13	2.07	0.54
2:G:196:TRP:CH2	5:L:450:MET:HE3	2.43	0.54
1:A:702:ILE:HG22	1:A:712:ARG:NH2	2.23	0.54
1:F:323:ILE:HG13	1:F:371:VAL:HG23	1.89	0.54
2:G:236:ARG:NH2	4:K:201:LEU:HD13	2.23	0.54
1:F:715:VAL:HG12	1:F:747:VAL:HG13	1.89	0.53
1:A:562:ILE:CG2	1:A:666:THR:HG22	2.38	0.53
1:E:619:ASN:HB2	1:E:661:LEU:HD12	1.91	0.53
5:L:468:GLN:O	5:L:472:LEU:HG	2.09	0.53
5:L:447:THR:CA	5:L:450:MET:HE2	2.32	0.52
5:L:453:ASP:C	5:L:455:GLU:N	2.67	0.52
2:H:74:ASP:HB3	4:K:236:GLU:CG	2.41	0.51
5:L:454:ALA:HB3	5:L:608:LEU:CD1	2.41	0.50
1:D:145:ARG:HH22	1:E:95:GLN:C	2.20	0.50
2:I:74:ASP:OD2	5:L:638:ILE:HD11	2.11	0.50
1:B:161:GLU:CD	1:C:93:LEU:HD12	2.37	0.50
1:D:367:VAL:O	1:D:371:VAL:HG23	2.12	0.50
2:G:114:ARG:HD3	4:K:226:GLU:CB	2.41	0.50
2:I:114:ARG:HH11	3:J:56:ARG:NH2	2.10	0.50
3:J:40:VAL:CG1	3:J:44:ARG:HE	2.25	0.50
4:K:188:THR:O	5:L:433:ILE:HD13	2.11	0.50
1:E:275:LYS:NZ	1:E:382:VAL:HG21	2.28	0.49
1:D:232:PRO:O	1:E:485:THR:HG23	2.11	0.49
2:G:114:ARG:NE	4:K:226:GLU:HB3	2.28	0.49
1:E:316:VAL:HB	4:K:178:LEU:HD13	1.94	0.49
2:G:196:TRP:CZ2	4:K:208:ALA:HA	2.48	0.49
5:L:455:GLU:HG2	5:L:611:MET:HE1	1.95	0.49
1:A:315:TYR:HD1	4:K:170:GLN:HB3	1.77	0.49
1:C:205:ASN:OD1	1:C:223:ARG:NH1	2.45	0.49
5:L:453:ASP:O	5:L:455:GLU:N	2.46	0.48
1:B:426:GLN:O	1:B:430:ILE:HG23	2.13	0.48
1:C:223:ARG:HB3	1:C:223:ARG:CZ	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:457:PHE:CE2	1:F:465:LEU:HD11	2.48	0.48
1:D:715:VAL:CG1	1:D:747:VAL:HG22	2.44	0.48
2:G:49:LEU:HD21	2:I:109:HIS:HA	1.96	0.48
1:A:379:MET:HE3	1:A:390:VAL:HG11	1.96	0.47
5:L:446:ASN:C	5:L:450:MET:HE2	2.40	0.47
2:H:156:LEU:HD21	5:L:463:GLY:HA2	1.96	0.47
2:G:196:TRP:CH2	4:K:208:ALA:HB2	2.50	0.47
1:E:630:VAL:O	1:E:630:VAL:HG12	2.15	0.47
5:L:469:SER:HB2	5:L:622:GLN:HE21	1.79	0.47
1:E:323:ILE:HD12	1:E:371:VAL:HG23	1.97	0.46
1:B:230:ILE:HG22	1:B:231:ARG:N	2.31	0.46
5:L:453:ASP:C	5:L:455:GLU:H	2.23	0.46
1:E:692:THR:HG22	1:E:727:ASN:OD1	2.16	0.46
1:E:702:ILE:HG22	1:E:712:ARG:NE	2.31	0.46
2:G:196:TRP:CZ2	5:L:450:MET:SD	3.09	0.46
1:F:688:VAL:HG23	1:F:688:VAL:O	2.16	0.46
2:G:148:TYR:CE1	2:G:156:LEU:HD13	2.51	0.46
5:L:450:MET:O	5:L:453:ASP:HB2	2.16	0.46
2:G:236:ARG:NH2	4:K:201:LEU:HD22	2.31	0.45
4:K:178:LEU:HD21	4:K:181:ASN:HA	1.98	0.45
2:H:75:GLU:HG3	4:K:240:LEU:HD12	1.97	0.45
1:C:172:ARG:HH22	1:C:231:ARG:HD2	1.81	0.45
2:G:155:ALA:HB1	4:K:219:GLU:HG2	1.99	0.45
1:C:728:VAL:HG13	1:C:729:GLY:N	2.31	0.45
1:C:188:VAL:CG2	1:D:485:THR:HG21	2.47	0.45
1:D:382:VAL:HG12	1:D:382:VAL:O	2.17	0.44
1:F:543:ALA:HA	1:F:546:VAL:HG12	2.00	0.44
1:A:315:TYR:CD1	4:K:170:GLN:HB3	2.52	0.44
1:B:730:ILE:H	1:B:730:ILE:HD12	1.83	0.44
1:C:570:LYS:HG2	1:C:688:VAL:HG21	1.99	0.44
1:E:728:VAL:HG13	1:E:729:GLY:N	2.33	0.44
3:J:32:LEU:HD13	5:L:602:GLN:HA	2.00	0.43
1:D:145:ARG:NH2	1:E:96:ASP:CG	2.75	0.43
1:C:223:ARG:NH1	1:C:223:ARG:HB3	2.33	0.43
2:G:196:TRP:CE2	4:K:208:ALA:HA	2.54	0.43
1:D:715:VAL:HG12	1:D:747:VAL:HG22	2.01	0.43
2:G:231:ASN:N	5:L:449:LYS:HZ3	2.17	0.43
3:J:43:MET:HE2	4:K:214:PHE:CG	2.54	0.43
4:K:173:PHE:HB3	4:K:174:SER:H	1.71	0.43
5:L:449:LYS:HE3	5:L:449:LYS:HB2	1.86	0.43
1:A:261:PHE:HB2	1:A:266:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:711:GLY:O	1:F:715:VAL:HG13	2.18	0.43
5:L:451:ALA:C	5:L:604:VAL:HG11	2.44	0.43
1:E:275:LYS:HZ3	1:E:382:VAL:HG21	1.83	0.42
1:E:316:VAL:CB	4:K:178:LEU:HD13	2.49	0.42
1:B:223:ARG:N	1:B:224:PRO:HD3	2.34	0.42
1:E:346:ILE:HD12	1:E:346:ILE:C	2.43	0.42
2:G:155:ALA:HB1	4:K:219:GLU:CB	2.49	0.42
4:K:188:THR:O	4:K:189:ALA:HB3	2.20	0.42
1:B:161:GLU:OE1	1:C:93:LEU:HD12	2.19	0.42
1:B:296:THR:O	1:B:296:THR:HG22	2.19	0.42
1:D:266:ILE:HD11	1:D:271:ILE:HD11	2.01	0.42
1:E:365:THR:HG23	4:K:177:LEU:HD13	2.02	0.42
1:E:702:ILE:HG22	1:E:712:ARG:HE	1.85	0.42
1:D:128:LYS:O	1:D:130:VAL:HG23	2.20	0.42
1:D:728:VAL:HG23	1:D:729:GLY:N	2.35	0.42
1:D:114:LEU:HD22	1:D:174:VAL:HG13	2.03	0.41
3:J:40:VAL:HG12	3:J:44:ARG:HE	1.85	0.41
1:C:347:ILE:HG22	1:C:391:ILE:CG2	2.50	0.41
1:F:457:PHE:CD2	1:F:465:LEU:HD11	2.56	0.41
1:E:114:LEU:HD22	1:E:174:VAL:HG13	2.03	0.41
1:E:261:PHE:CE2	1:F:474:ILE:HD12	2.56	0.41
1:B:711:GLY:O	1:B:715:VAL:HG12	2.21	0.41
1:C:711:GLY:O	1:C:715:VAL:HG13	2.20	0.41
1:F:630:VAL:O	1:F:630:VAL:HG12	2.20	0.41
2:G:196:TRP:CH2	5:L:450:MET:CE	3.03	0.40
3:J:40:VAL:O	3:J:44:ARG:HG3	2.21	0.40
2:G:155:ALA:CB	4:K:219:GLU:HA	2.52	0.40
2:G:231:ASN:O	2:G:235:SER:HB3	2.21	0.40
5:L:449:LYS:HA	5:L:452:GLN:OE1	2.22	0.40
1:E:277:LEU:HD12	1:E:412:VAL:HG23	2.04	0.40
2:G:196:TRP:CZ2	5:L:450:MET:CE	3.01	0.40
1:B:684:ASN:HD22	1:B:685:GLU:H	1.68	0.40
1:C:230:ILE:O	1:C:231:ARG:HB2	2.21	0.40
1:E:378:LYS:O	1:E:382:VAL:HG12	2.21	0.40
2:G:196:TRP:CZ3	4:K:208:ALA:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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	370/656 (56%)	369 (100%)	1 (0%)	86	84
1	B	637/656 (97%)	627 (98%)	10 (2%)	55	69
1	C	637/656 (97%)	632 (99%)	5 (1%)	73	77
1	D	633/656 (96%)	629 (99%)	4 (1%)	78	80
1	E	618/656 (94%)	613 (99%)	5 (1%)	73	77
1	F	427/656 (65%)	427 (100%)	0	100	100
2	G	240/245 (98%)	240 (100%)	0	100	100
2	H	230/245 (94%)	230 (100%)	0	100	100
2	I	240/245 (98%)	240 (100%)	0	100	100
3	J	48/82 (58%)	48 (100%)	0	100	100
4	K	75/234 (32%)	68 (91%)	7 (9%)	8	27
5	L	115/201 (57%)	111 (96%)	4 (4%)	32	54
All	All	4270/5188 (82%)	4234 (99%)	36 (1%)	70	77

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	438	ASN
1	B	122	SER
1	B	123	PHE
1	B	124	ARG
1	B	160	MET
1	B	221	SER
1	B	222	LEU

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Mol	Chain	Res	Type
1	B	223	ARG
1	B	225	ARG
1	B	684	ASN
1	B	707	LEU
1	C	122	SER
1	C	123	PHE
1	C	124	ARG
1	C	160	MET
1	C	217	LYS
1	D	122	SER
1	D	123	PHE
1	D	124	ARG
1	D	160	MET
1	E	122	SER
1	E	123	PHE
1	E	124	ARG
1	E	160	MET
1	E	239	LEU
4	K	172	ILE
4	K	173	PHE
4	K	175	GLN
4	K	185	GLU
4	K	188	THR
4	K	190	LEU
4	K	193	VAL
5	L	449	LYS
5	L	450	MET
5	L	470	GLU
5	L	473	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	698	ASN
1	A	699	ASN
1	B	136	GLN
1	B	357	GLN
1	B	373	ASN
1	B	456	ASN
1	C	136	GLN
1	C	395	ASN
1	C	727	ASN

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Mol	Chain	Res	Type
1	D	142	GLN
1	D	273	HIS
1	D	395	ASN
1	D	725	ASN
1	E	373	ASN
1	E	374	GLN
1	E	536	ASN
1	E	641	ASN
1	E	725	ASN
1	F	456	ASN
1	F	727	ASN
2	G	109	HIS
2	G	118	ASN
2	I	118	ASN
4	K	175	GLN
4	K	215	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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
7	ATP	B	802	-	32,33,33	0.90	2 (6%)	48,52,52	0.56	0
7	ATP	B	801	-	32,33,33	1.00	2 (6%)	48,52,52	0.63	1 (2%)
7	ATP	F	801	-	32,33,33	0.87	2 (6%)	48,52,52	0.63	0
7	ATP	D	802	-	32,33,33	0.64	1 (3%)	48,52,52	0.52	0
7	ATP	C	802	-	32,33,33	0.74	2 (6%)	48,52,52	0.58	0
7	ATP	A	802	-	32,33,33	0.81	2 (6%)	48,52,52	0.59	0
7	ATP	E	802	-	32,33,33	0.97	2 (6%)	48,52,52	0.51	0
7	ATP	D	801	-	32,33,33	0.87	2 (6%)	48,52,52	0.63	0
6	ADP	E	801	-	28,29,29	1.34	5 (17%)	43,45,45	1.87	9 (20%)
7	ATP	C	801	-	32,33,33	0.81	2 (6%)	48,52,52	0.56	0
6	ADP	A	801	-	28,29,29	1.33	4 (14%)	43,45,45	1.93	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ATP	B	802	-	-	4/22/38/38	0/3/3/3
7	ATP	B	801	-	-	3/22/38/38	0/3/3/3
7	ATP	F	801	-	-	7/22/38/38	0/3/3/3
7	ATP	D	802	-	-	10/22/38/38	0/3/3/3
7	ATP	C	802	-	-	1/22/38/38	0/3/3/3
7	ATP	A	802	-	-	5/22/38/38	0/3/3/3
7	ATP	E	802	-	-	2/22/38/38	0/3/3/3
7	ATP	D	801	-	-	8/22/38/38	0/3/3/3
6	ADP	E	801	-	-	4/16/32/32	0/3/3/3
7	ATP	C	801	-	-	2/22/38/38	0/3/3/3
6	ADP	A	801	-	-	5/16/32/32	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	ADP	C5-C4	4.36	1.46	1.39
6	E	801	ADP	C5-C4	4.28	1.46	1.39
7	E	802	ATP	PB-O3B	-3.82	1.55	1.59
7	B	801	ATP	PB-O3B	-3.79	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	802	ATP	PA-O3A	-3.64	1.55	1.59
7	F	801	ATP	PB-O3B	-3.62	1.55	1.59
7	A	802	ATP	PB-O3B	-3.58	1.55	1.59
7	B	801	ATP	PA-O3A	-3.58	1.55	1.59
7	D	801	ATP	PB-O3B	-3.47	1.55	1.59
7	E	802	ATP	PA-O3A	-3.44	1.55	1.59
7	C	802	ATP	PB-O3B	-3.15	1.56	1.59
7	C	801	ATP	PB-O3B	-3.11	1.56	1.59
7	D	802	ATP	PB-O3B	-3.10	1.56	1.59
7	B	802	ATP	PB-O3B	-2.90	1.56	1.59
7	F	801	ATP	PA-O3A	-2.76	1.56	1.59
7	D	801	ATP	PA-O3A	-2.69	1.56	1.59
6	E	801	ADP	C5-C6	2.48	1.47	1.41
6	A	801	ADP	C5-N7	-2.47	1.34	1.39
7	C	801	ATP	PA-O3A	-2.42	1.56	1.59
6	E	801	ADP	C8-N7	2.41	1.36	1.31
6	E	801	ADP	C5-N7	-2.39	1.34	1.39
6	A	801	ADP	C5-C6	2.33	1.47	1.41
7	A	802	ATP	PA-O3A	-2.15	1.57	1.59
7	C	802	ATP	PA-O3A	-2.13	1.57	1.59
6	A	801	ADP	C4-N9	-2.05	1.33	1.37
6	E	801	ADP	C4-N9	-2.04	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	ADP	C5-C4-N3	-5.83	118.69	126.72
6	E	801	ADP	C5-C4-N3	-5.80	118.73	126.72
6	A	801	ADP	N3-C4-N9	5.21	136.02	127.17
6	E	801	ADP	N3-C4-N9	4.69	135.15	127.17
6	E	801	ADP	C2-N3-C4	3.99	121.58	111.83
6	A	801	ADP	C2-N3-C4	3.77	121.04	111.83
6	E	801	ADP	N3-C2-N1	-3.74	122.92	128.58
6	A	801	ADP	N3-C2-N1	-3.62	123.11	128.58
6	A	801	ADP	C4-N9-C8	3.54	109.45	105.74
6	E	801	ADP	C4-C5-N7	-3.27	106.84	110.58
6	E	801	ADP	C4-N9-C8	3.15	109.05	105.74
6	A	801	ADP	C4-C5-N7	-2.80	107.38	110.58
6	E	801	ADP	C5-N7-C8	2.62	107.56	103.45
6	E	801	ADP	N9-C8-N7	-2.47	110.43	113.94
6	A	801	ADP	C5-N7-C8	2.45	107.30	103.45
6	A	801	ADP	N9-C8-N7	-2.36	110.59	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	801	ADP	C6-C5-N7	2.20	136.33	132.09
7	B	801	ATP	O3A-PB-O1B	2.02	116.78	110.70

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	801	ADP	C3'-C4'-C5'-O5'
6	E	801	ADP	O4'-C1'-N9-C8
6	E	801	ADP	O4'-C1'-N9-C4
7	A	802	ATP	C5'-O5'-PA-O2A
7	A	802	ATP	C5'-O5'-PA-O3A
7	A	802	ATP	O4'-C4'-C5'-O5'
7	B	801	ATP	C5'-O5'-PA-O1A
7	B	801	ATP	C5'-O5'-PA-O3A
7	D	801	ATP	C5'-O5'-PA-O3A
7	D	801	ATP	O4'-C1'-N9-C8
7	D	801	ATP	O4'-C1'-N9-C4
7	D	802	ATP	C5'-O5'-PA-O2A
7	F	801	ATP	C5'-O5'-PA-O1A
7	F	801	ATP	C5'-O5'-PA-O2A
7	F	801	ATP	C5'-O5'-PA-O3A
6	A	801	ADP	C3'-C4'-C5'-O5'
6	E	801	ADP	O4'-C4'-C5'-O5'
7	A	802	ATP	C3'-C4'-C5'-O5'
7	F	801	ATP	O4'-C4'-C5'-O5'
7	D	802	ATP	O4'-C4'-C5'-O5'
6	A	801	ADP	O4'-C4'-C5'-O5'
7	D	802	ATP	C3'-C4'-C5'-O5'
7	F	801	ATP	C3'-C4'-C5'-O5'
6	A	801	ADP	PA-O3A-PB-O1B
7	E	802	ATP	PA-O3A-PB-O1B
7	D	802	ATP	PA-O3A-PB-O3B
6	A	801	ADP	PA-O3A-PB-O3B
7	B	802	ATP	PA-O3A-PB-O2B
7	D	801	ATP	PG-O3B-PB-O1B
7	B	802	ATP	C3'-C4'-C5'-O5'
6	A	801	ADP	C5'-O5'-PA-O1A
7	B	801	ATP	C5'-O5'-PA-O2A
7	D	801	ATP	C5'-O5'-PA-O1A
7	D	802	ATP	C5'-O5'-PA-O1A
7	D	802	ATP	C5'-O5'-PA-O3A

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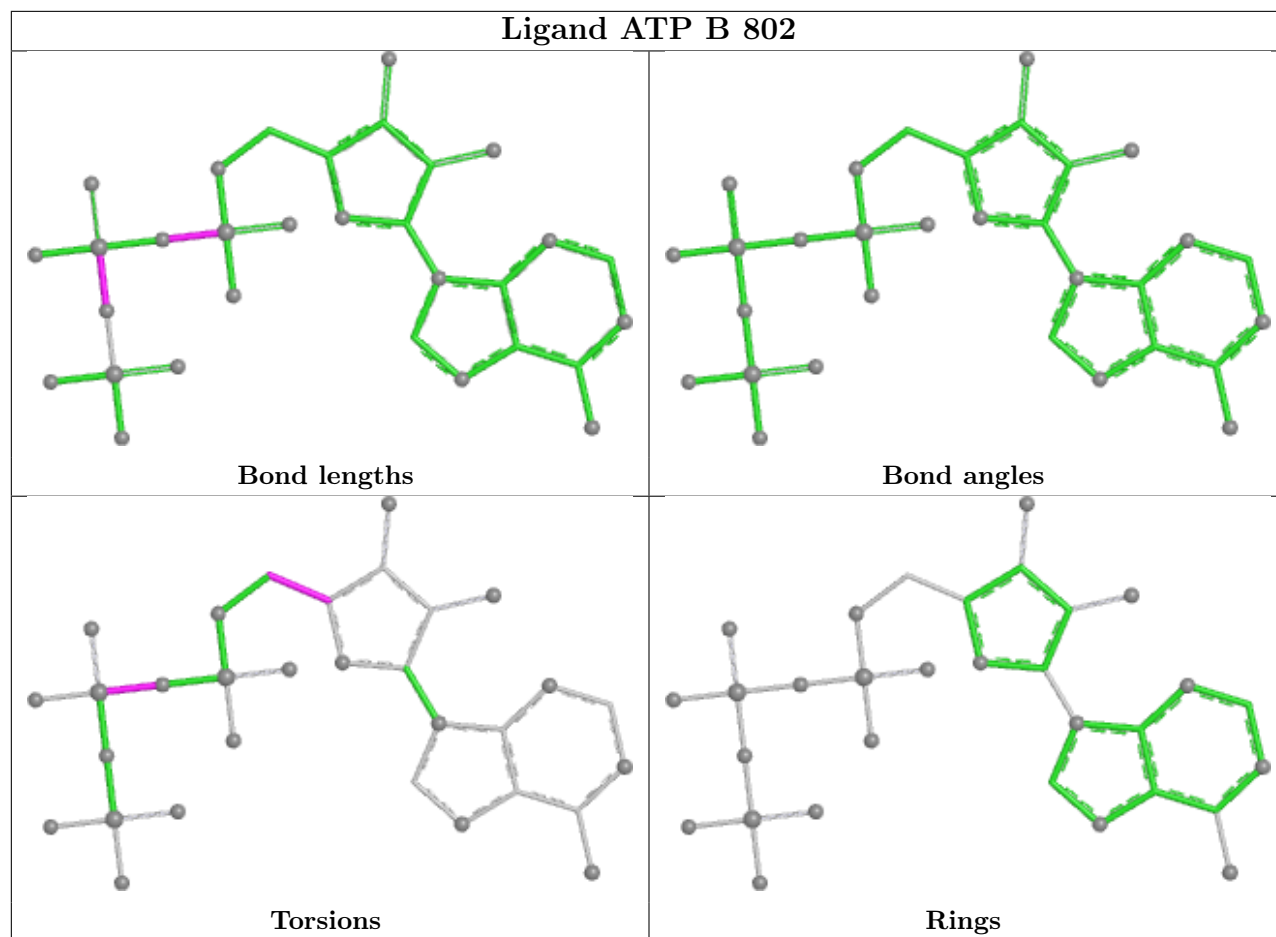
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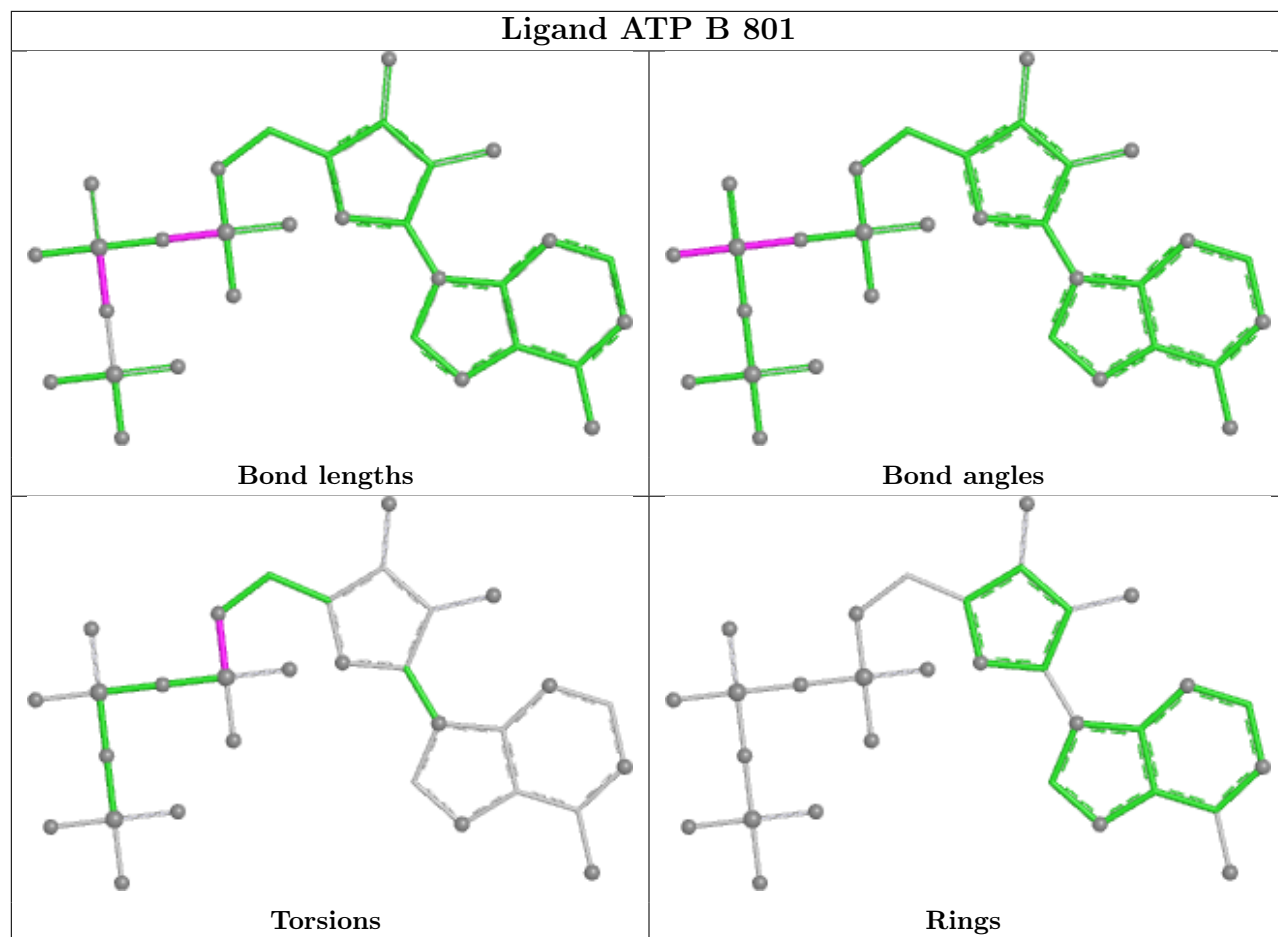
Mol	Chain	Res	Type	Atoms
7	D	801	ATP	C4'-C5'-O5'-PA
7	E	802	ATP	PA-O3A-PB-O2B
7	D	802	ATP	C4'-C5'-O5'-PA
7	F	801	ATP	PA-O3A-PB-O1B
7	B	802	ATP	O4'-C4'-C5'-O5'
7	D	801	ATP	O4'-C4'-C5'-O5'
7	A	802	ATP	PB-O3B-PG-O2G
7	C	802	ATP	C3'-C4'-C5'-O5'
7	B	802	ATP	PA-O3A-PB-O1B
7	C	801	ATP	PB-O3A-PA-O2A
7	D	802	ATP	PA-O3A-PB-O1B
7	F	801	ATP	PA-O3A-PB-O2B
7	C	801	ATP	PG-O3B-PB-O1B
7	D	801	ATP	PG-O3B-PB-O2B
7	D	802	ATP	PA-O3A-PB-O2B
7	D	802	ATP	PB-O3A-PA-O2A

There are no ring outliers.

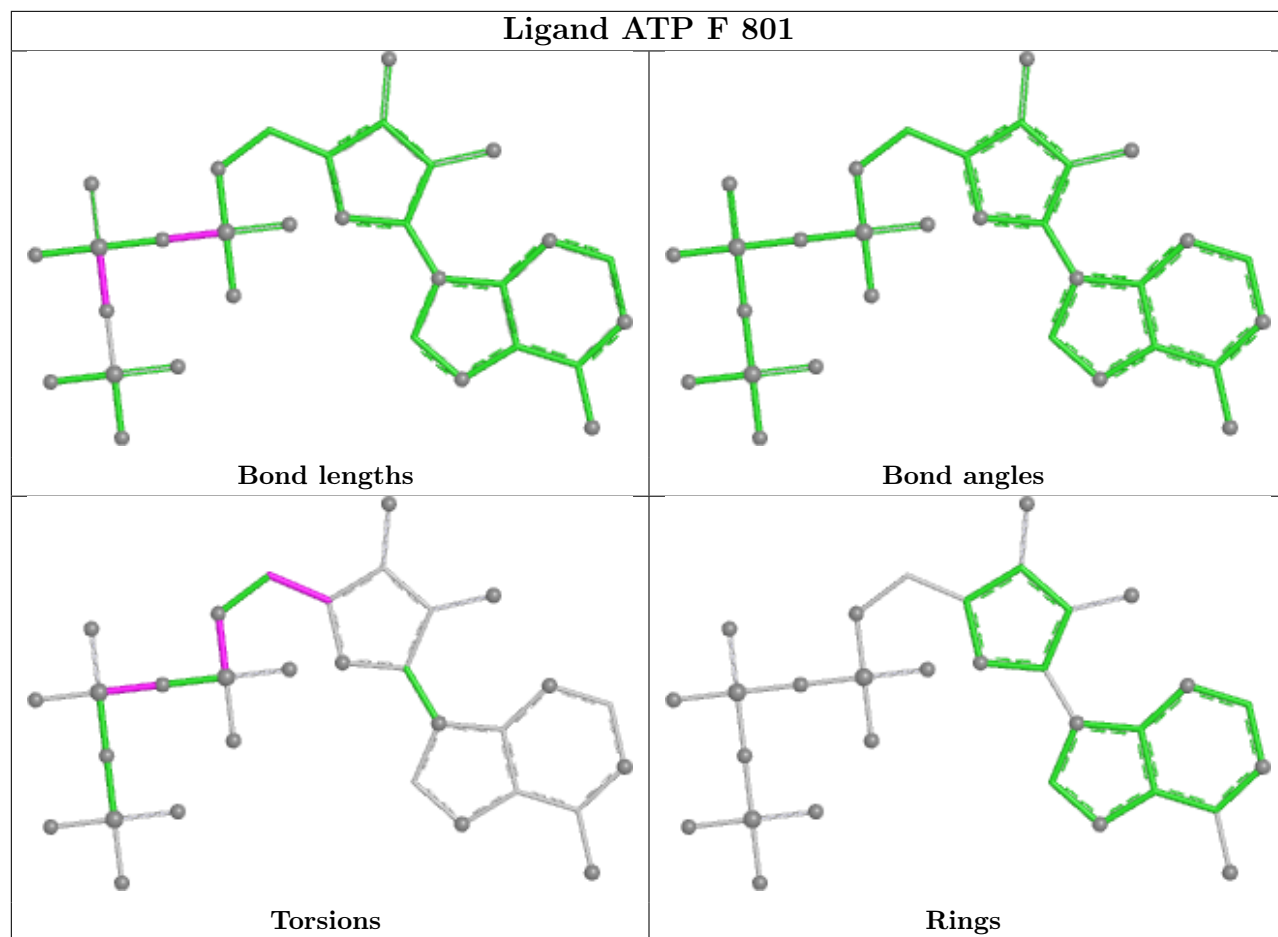
No monomer is involved in short contacts.

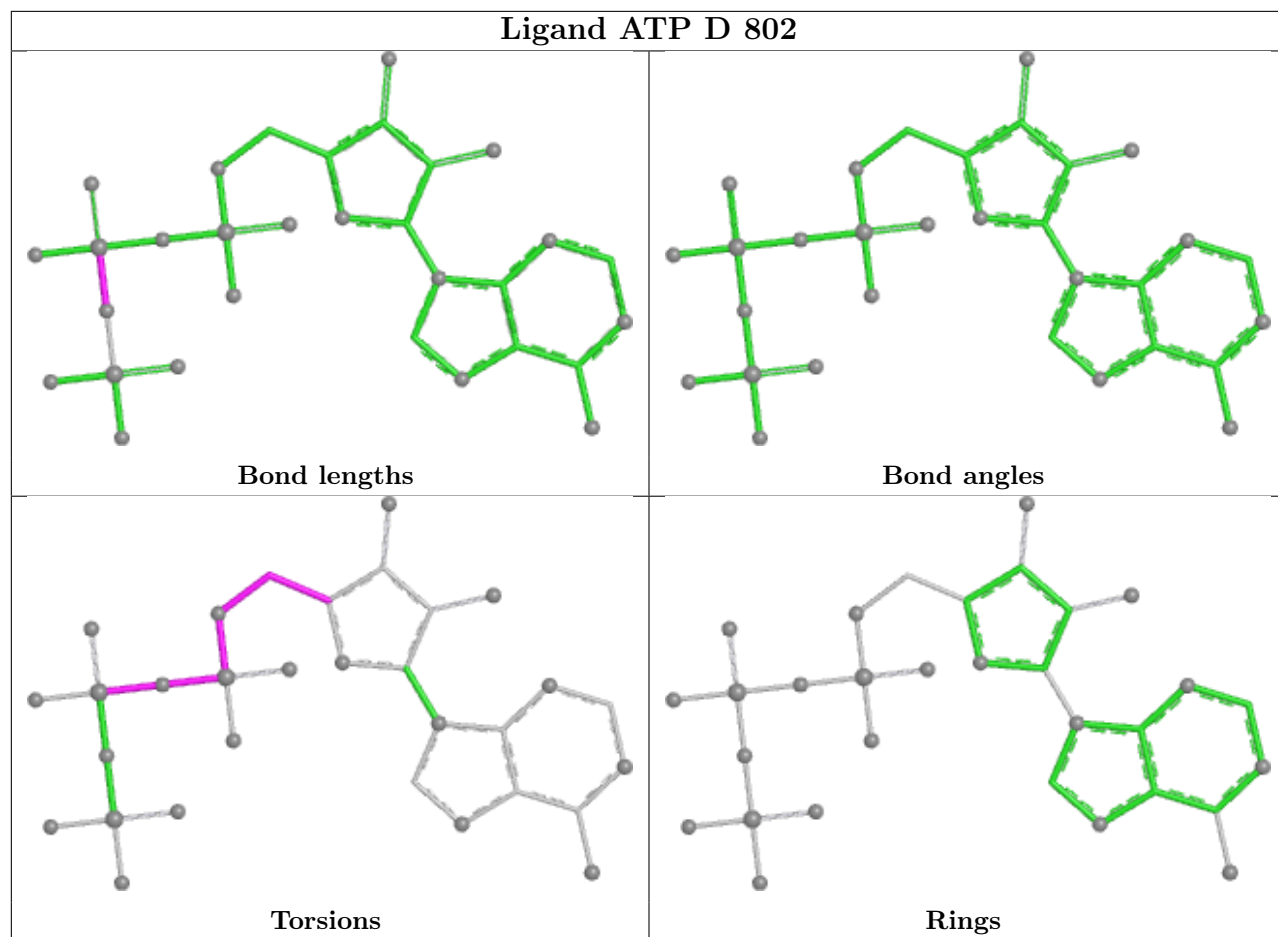
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

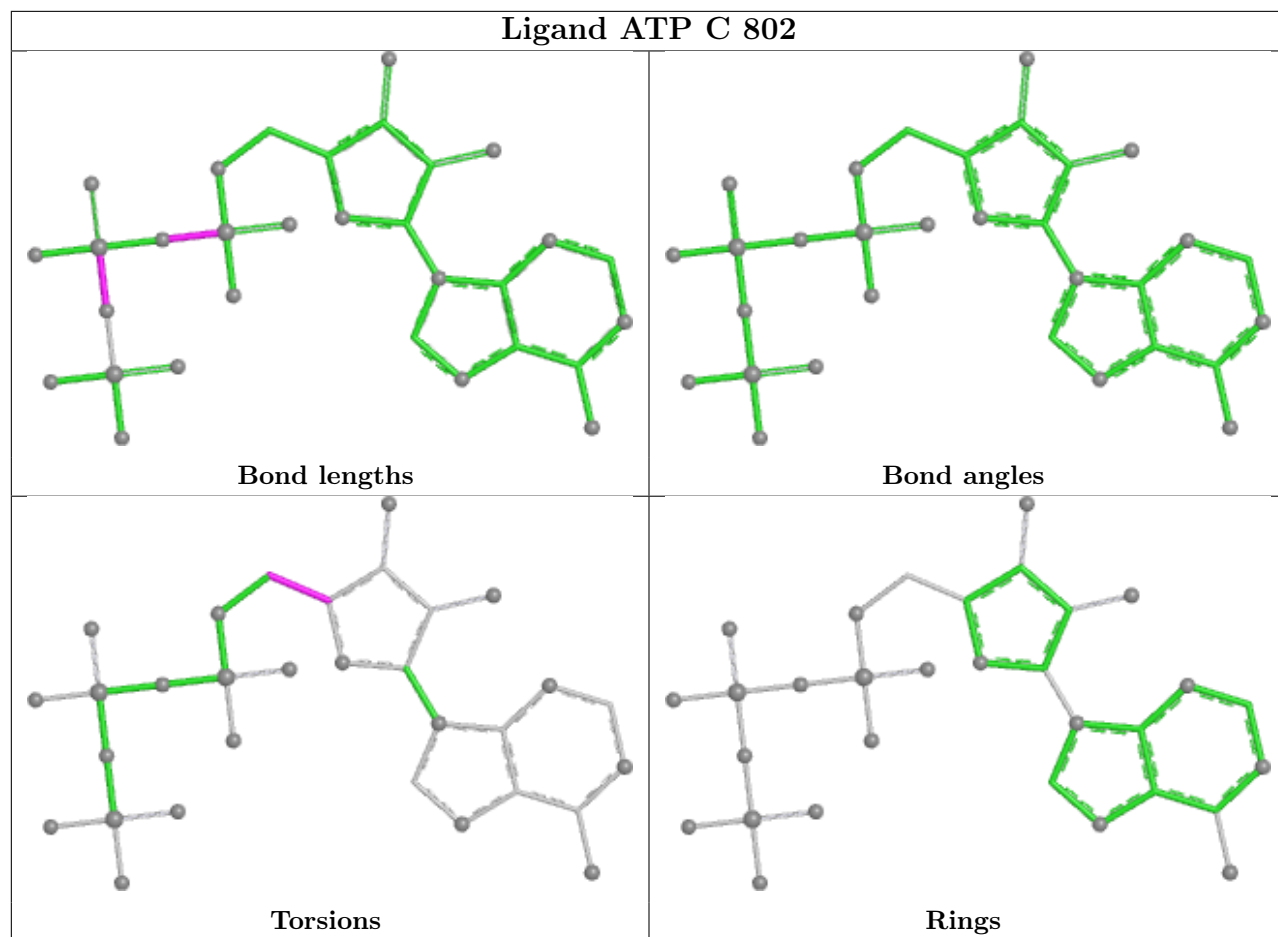


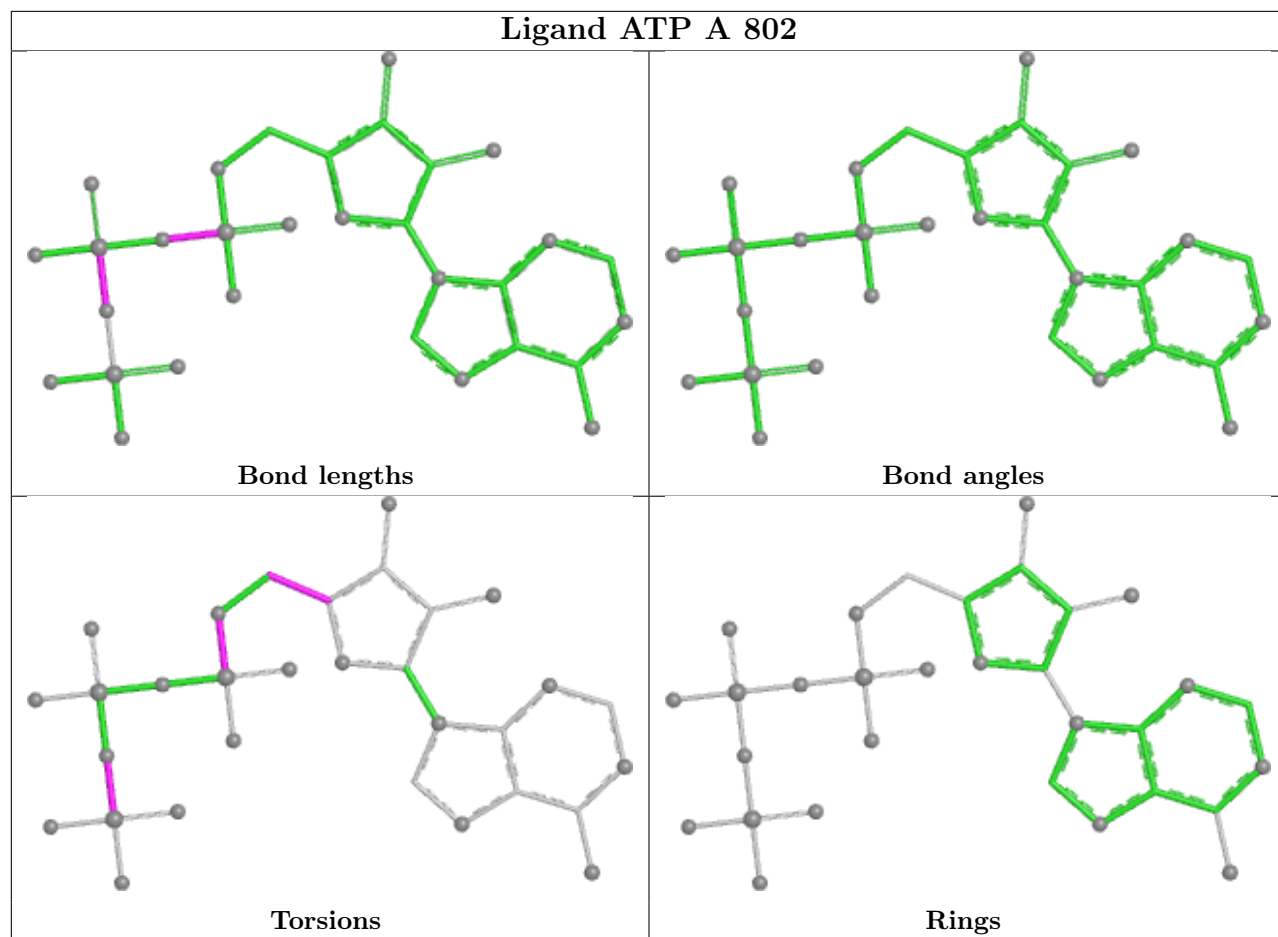


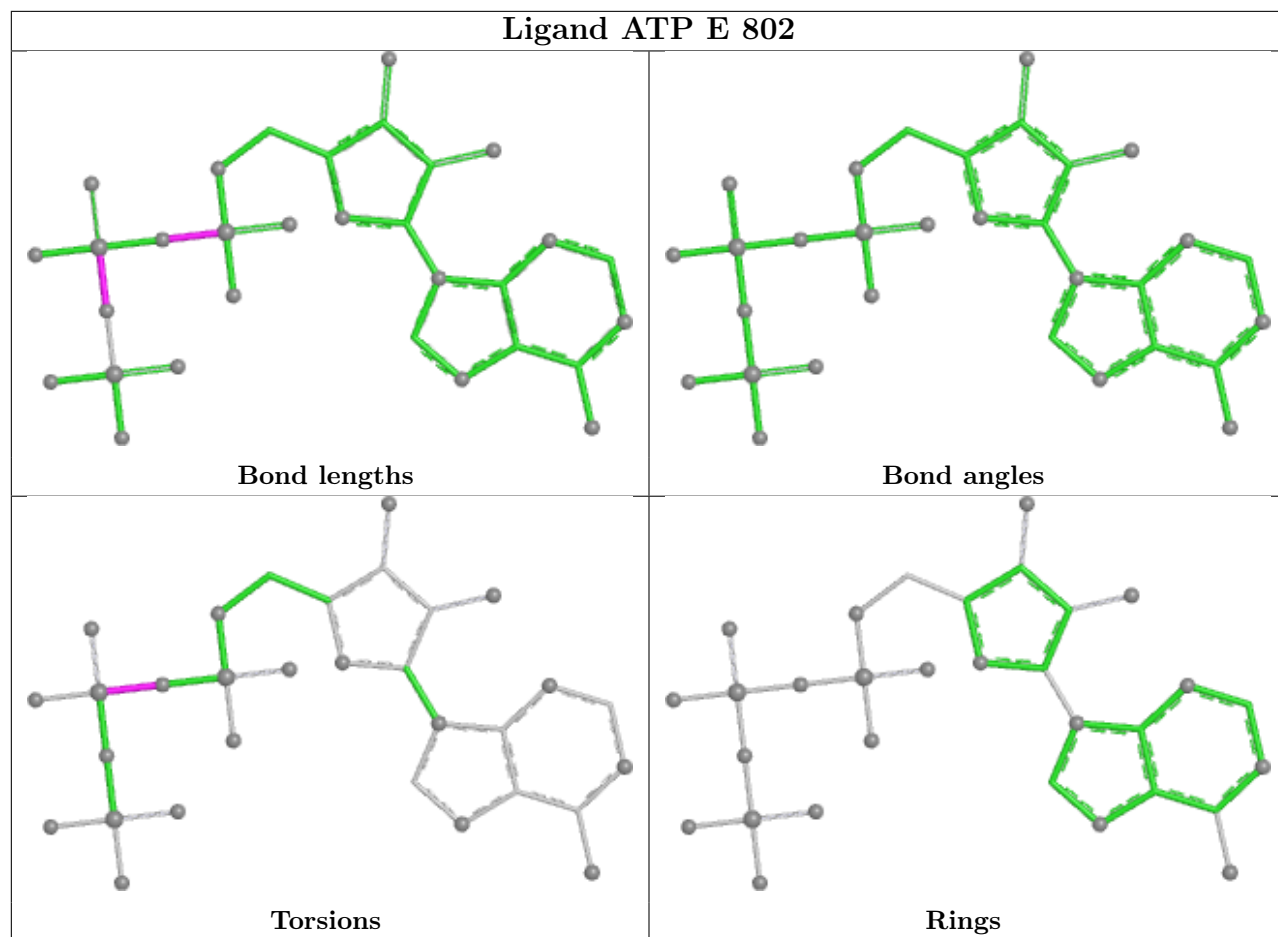
Ligand ATP F 801



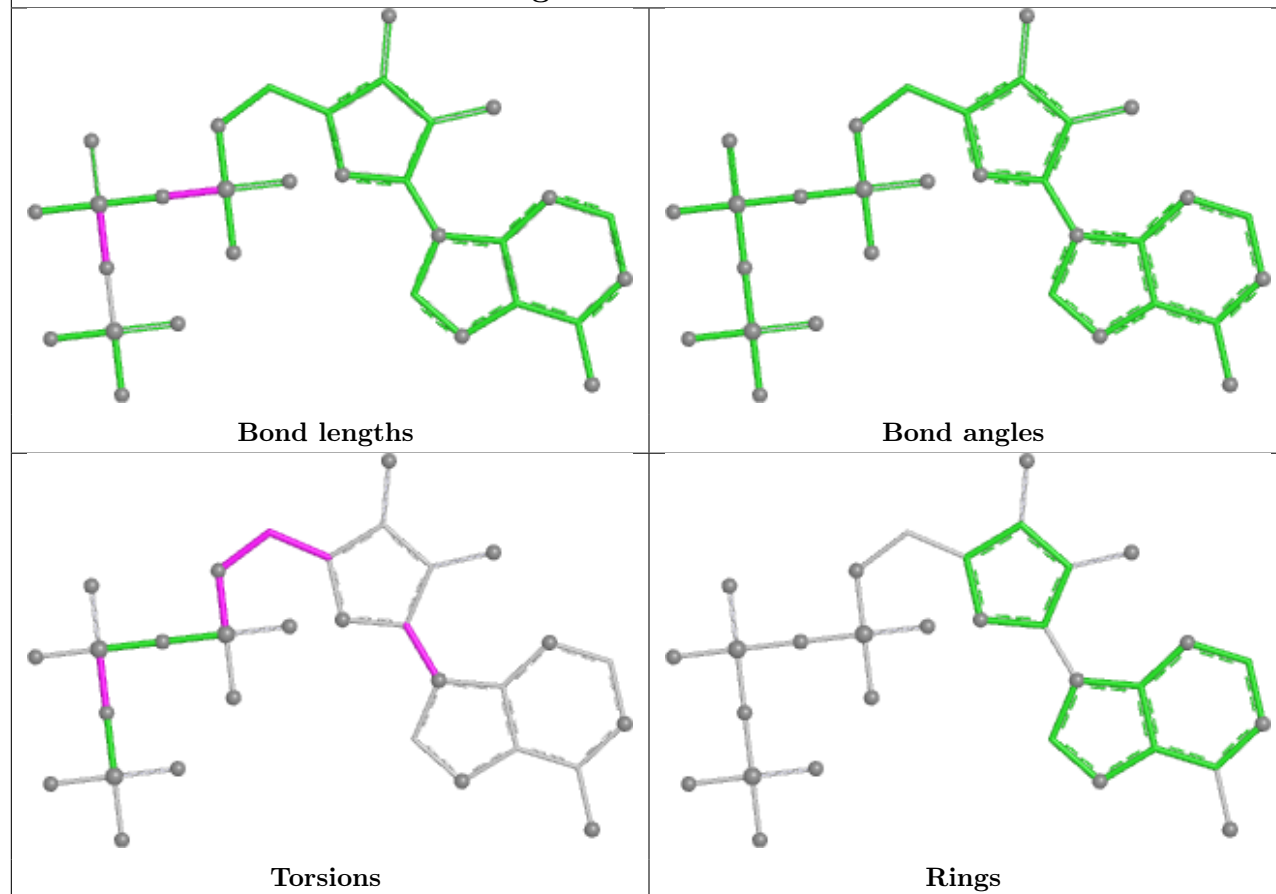




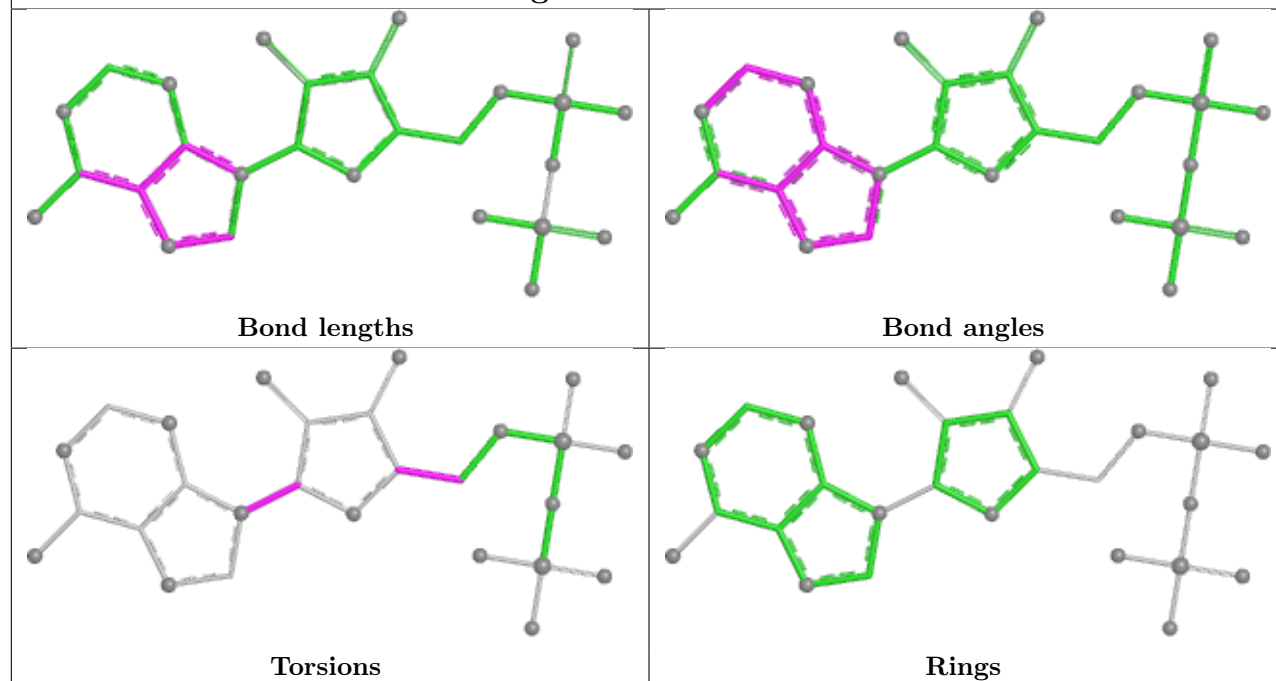




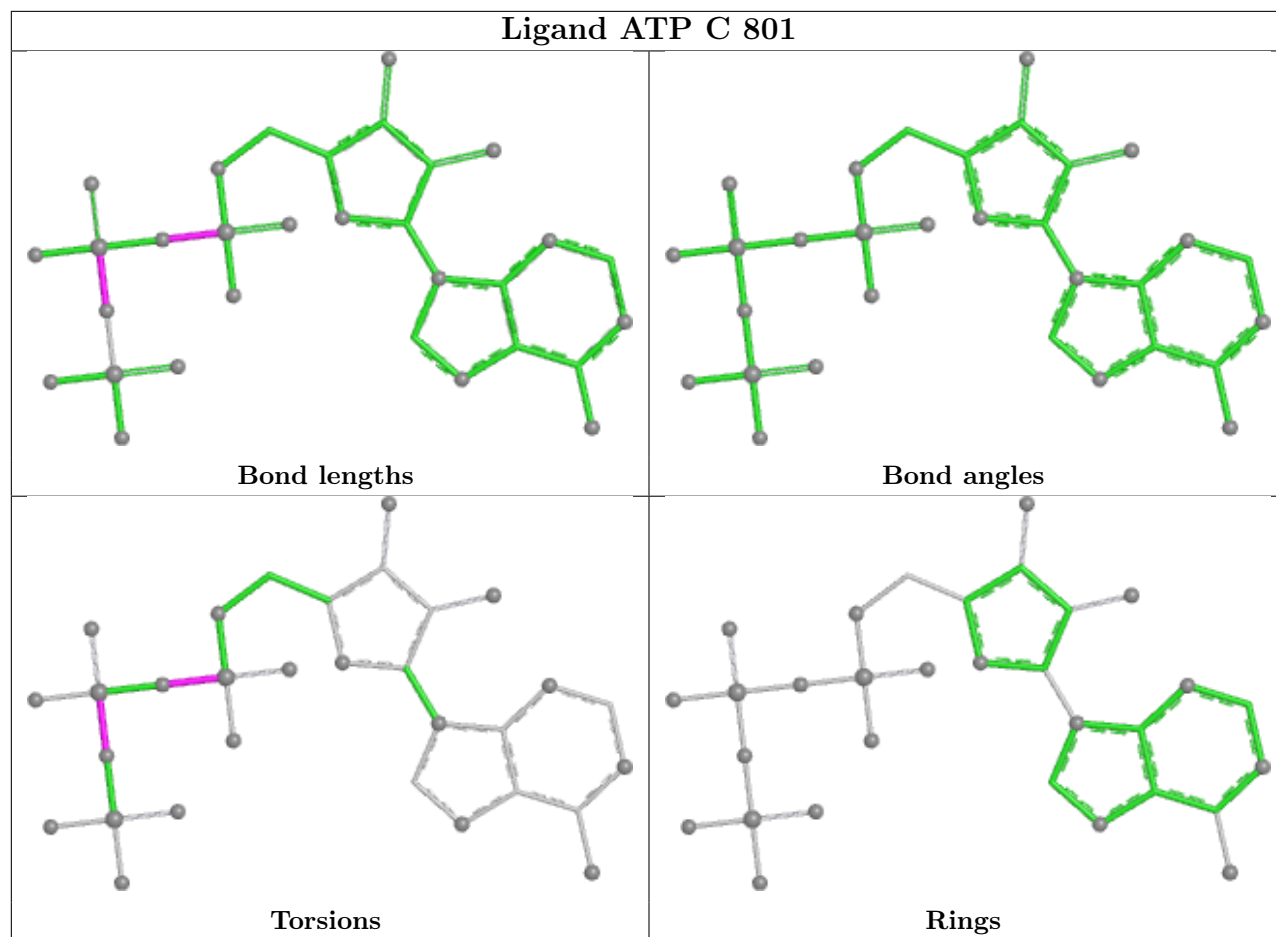
Ligand ATP D 801



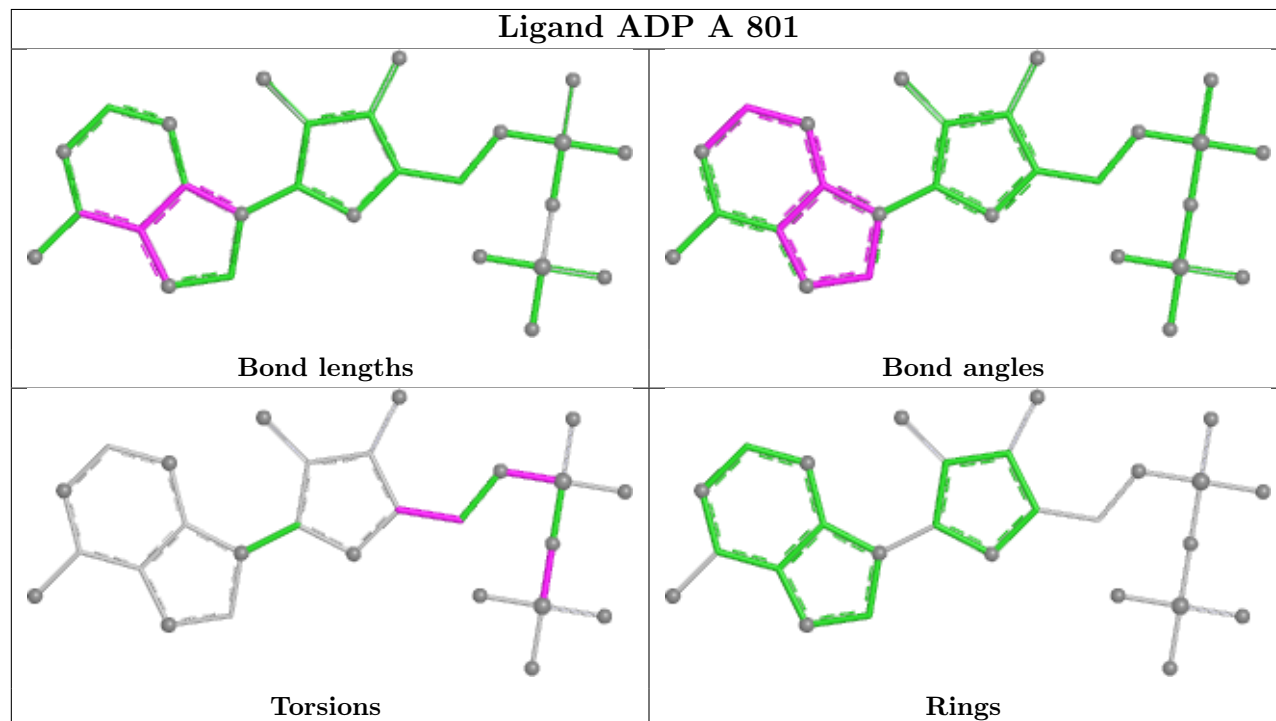
Ligand ADP E 801



Ligand ATP C 801



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.

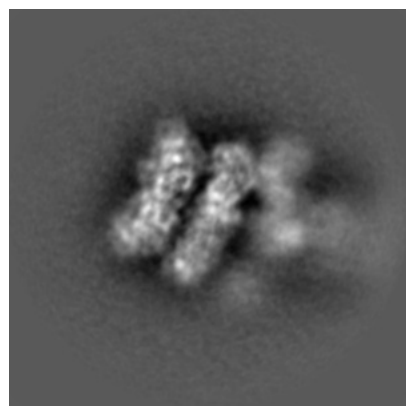
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49522. These allow visual inspection of the internal detail of the map and identification of artifacts.

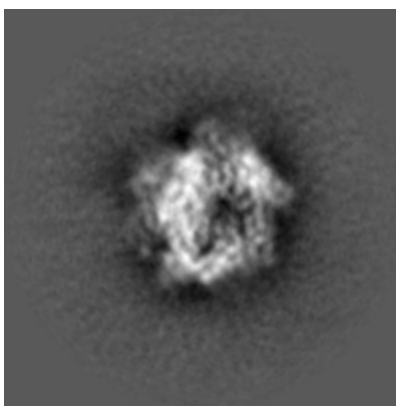
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

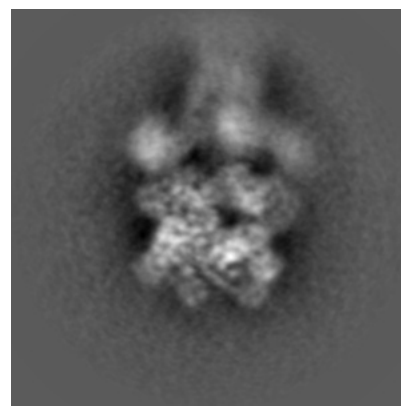
6.1.1 Primary map



X

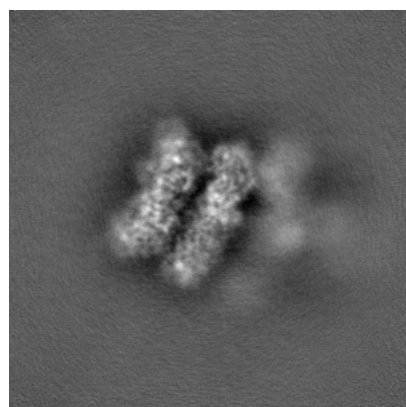


Y

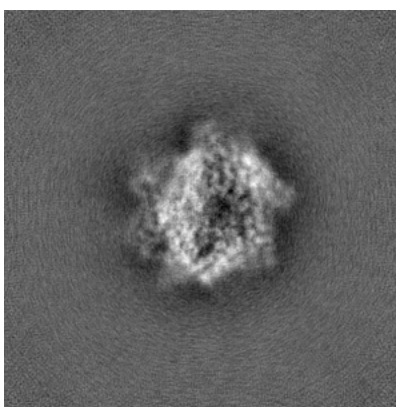


Z

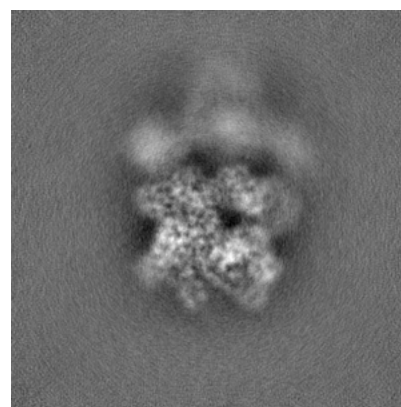
6.1.2 Raw map



X



Y

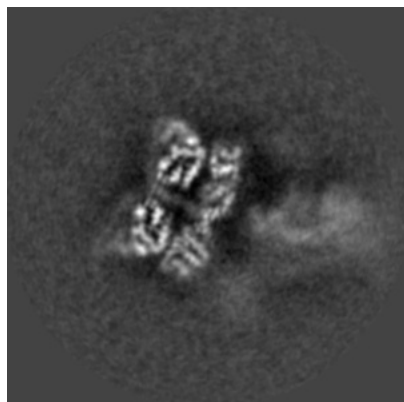


Z

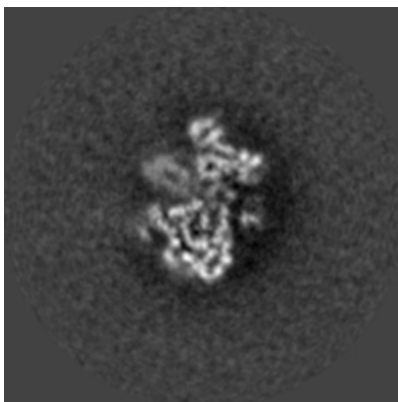
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

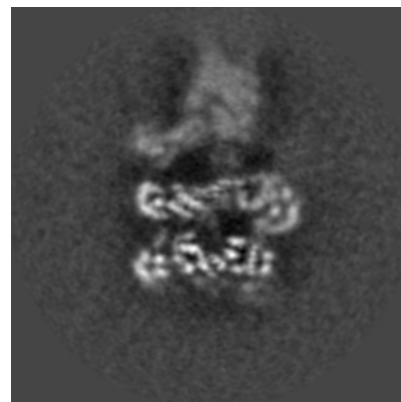
6.2.1 Primary map



X Index: 147

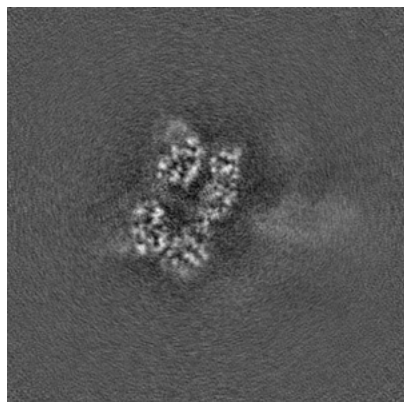


Y Index: 147

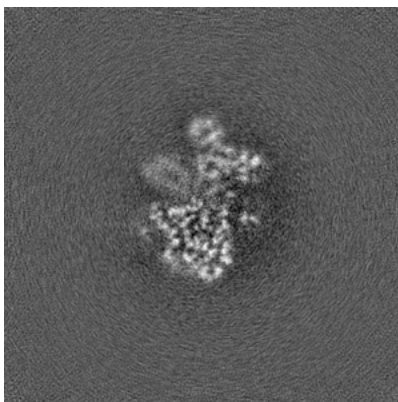


Z Index: 147

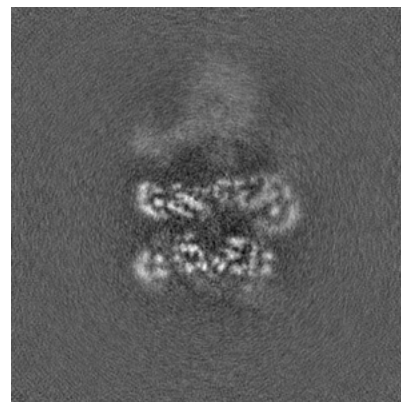
6.2.2 Raw map



X Index: 147



Y Index: 147

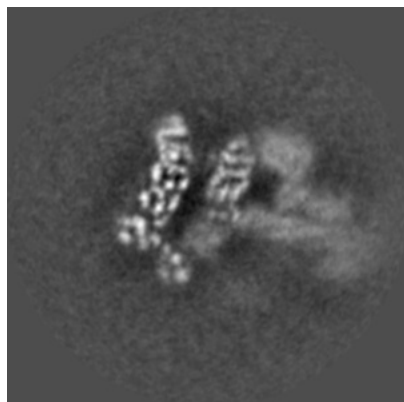


Z Index: 147

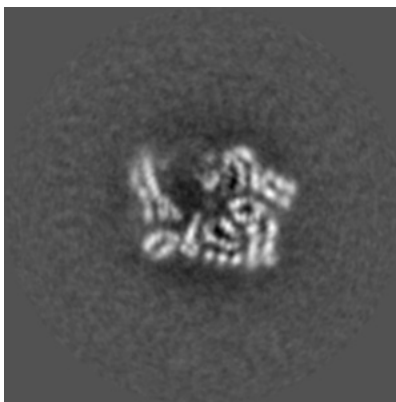
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

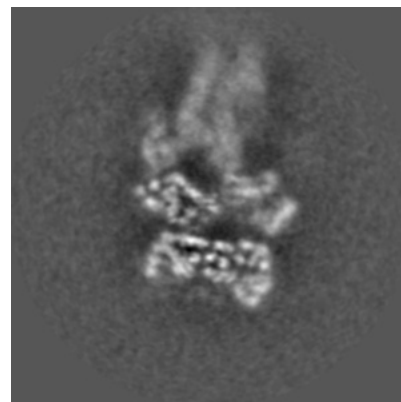
6.3.1 Primary map



X Index: 163

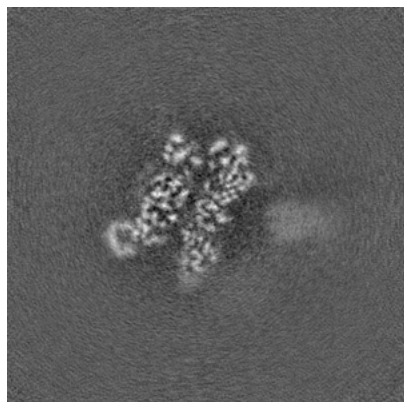


Y Index: 124

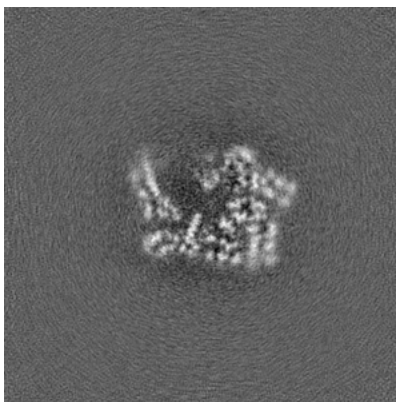


Z Index: 139

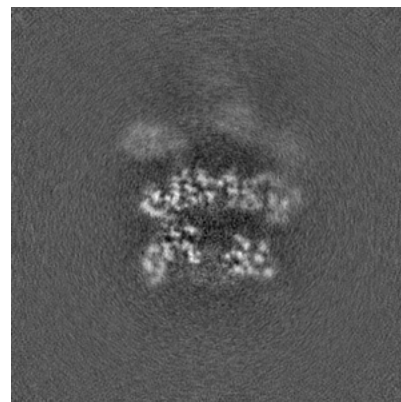
6.3.2 Raw map



X Index: 132



Y Index: 123

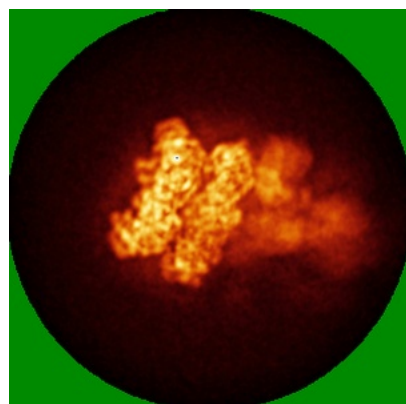


Z Index: 156

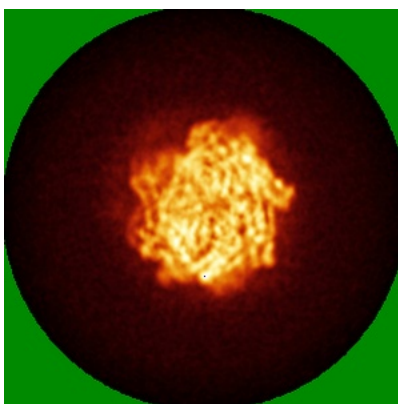
The images above show the largest variance slices of the map in three orthogonal directions.

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

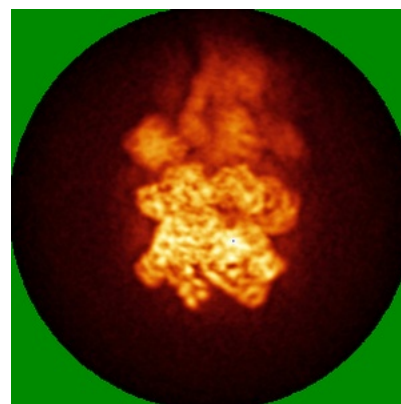
6.4.1 Primary map



X

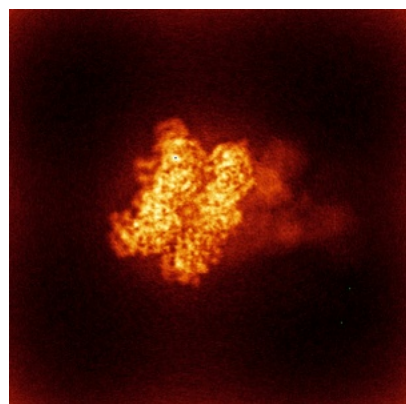


Y

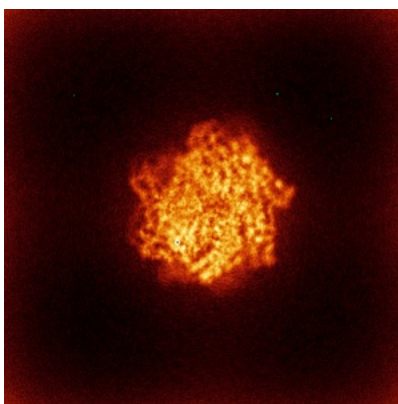


Z

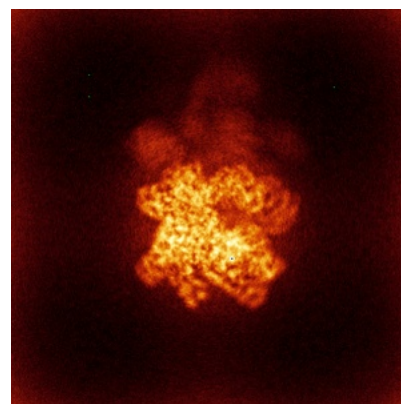
6.4.2 Raw map



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.

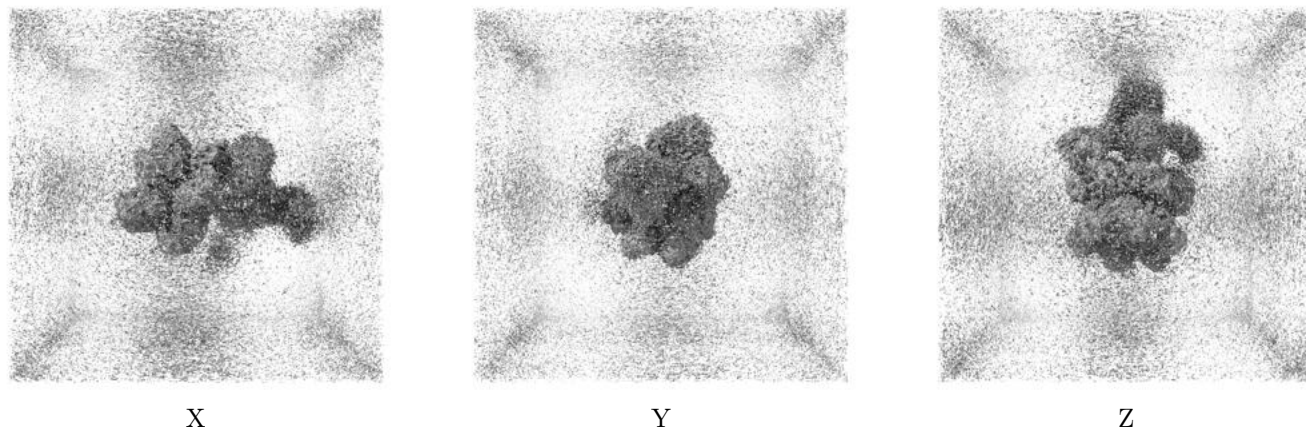
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00205. 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.

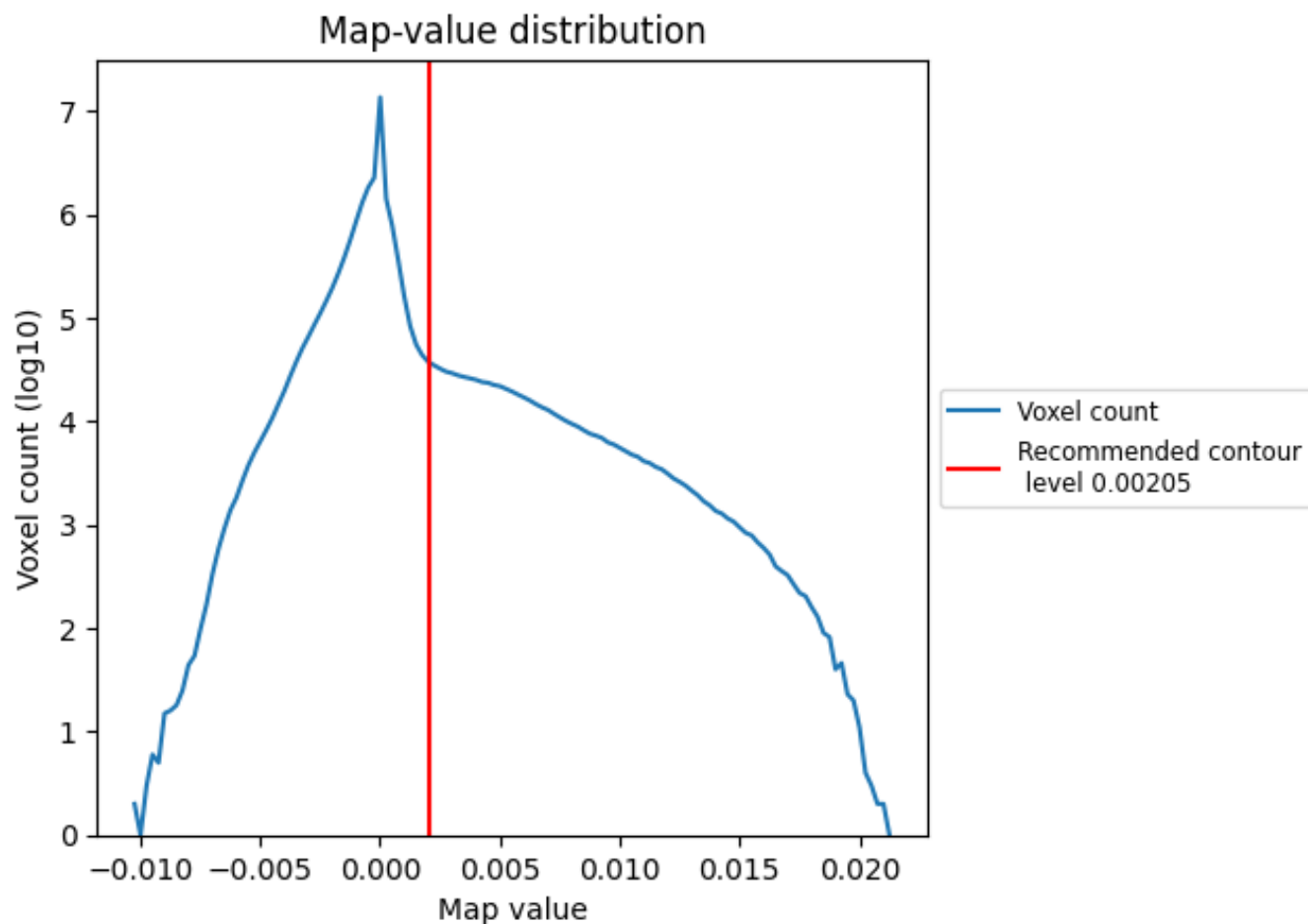
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

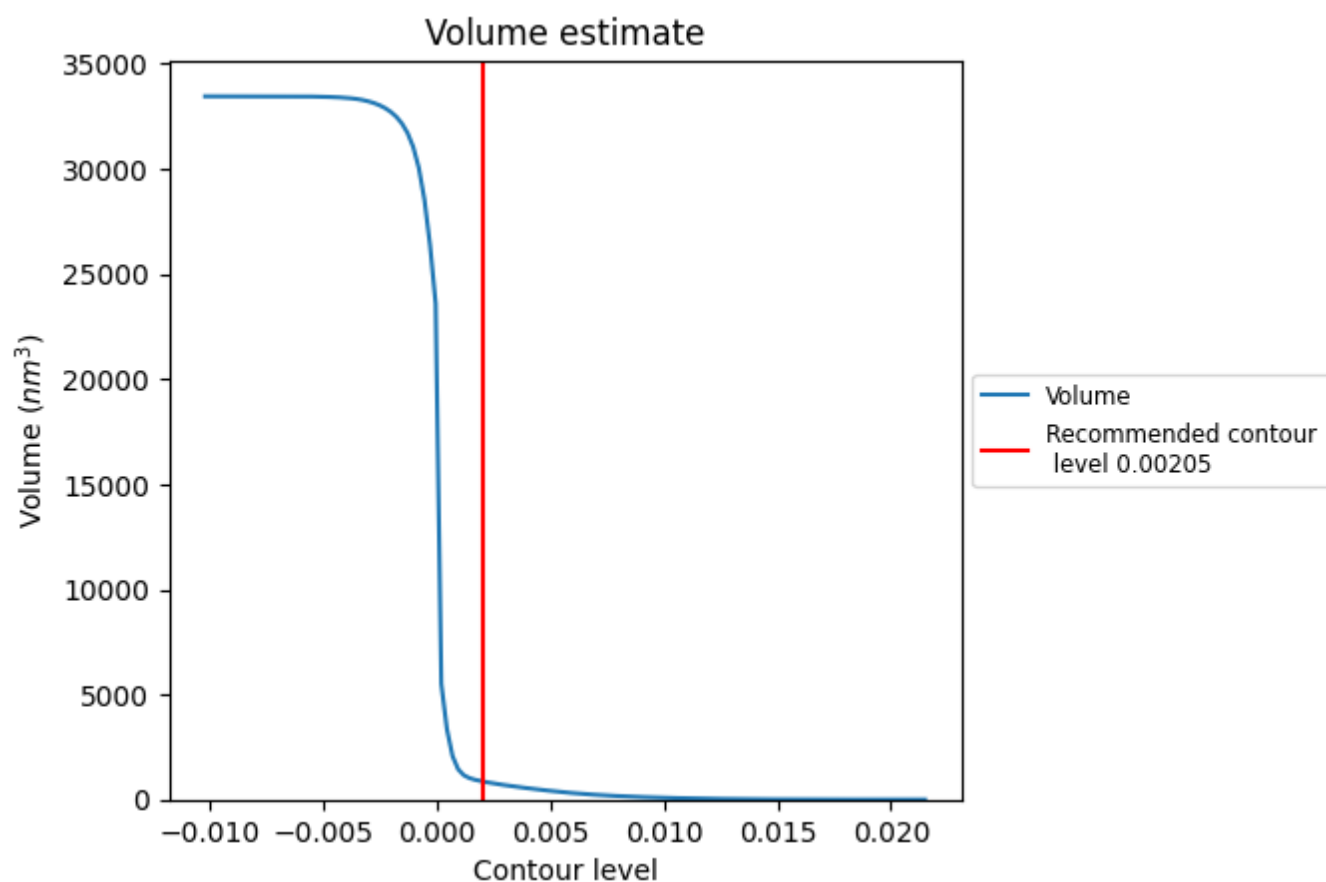
This section contains the results of statistical analysis of the map.

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.

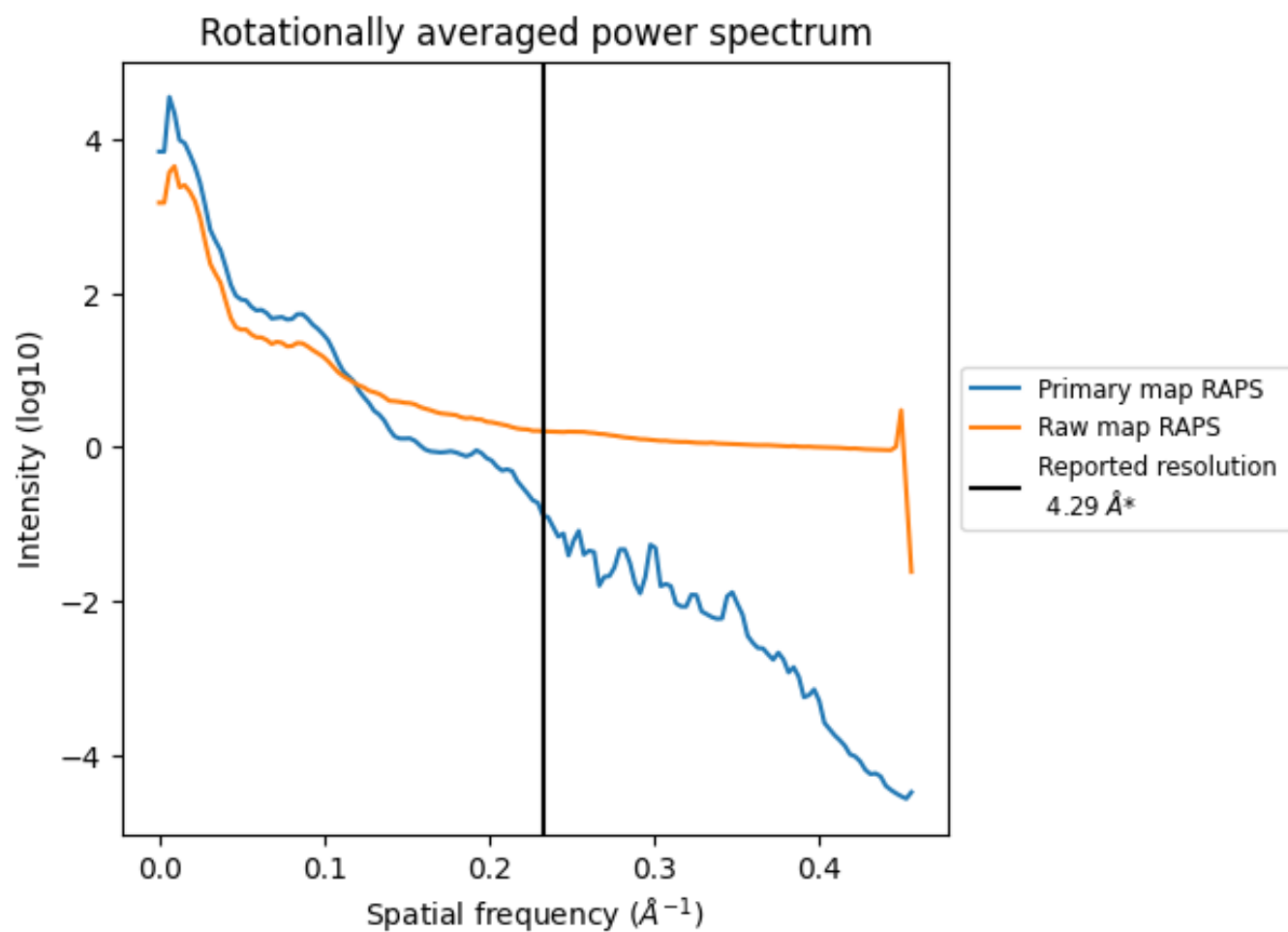
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 851 nm³; this corresponds to an approximate mass of 769 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 ⓘ

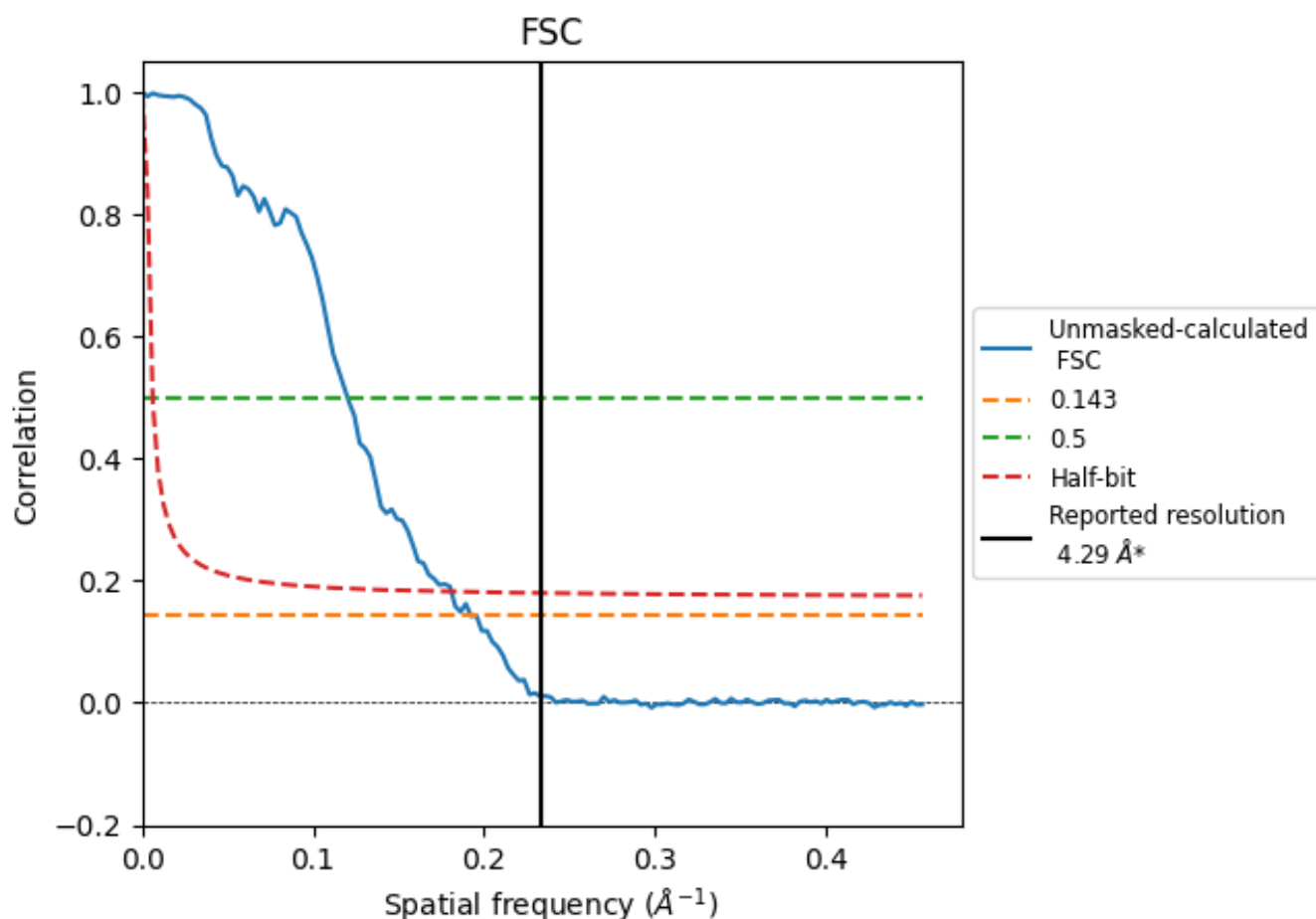


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

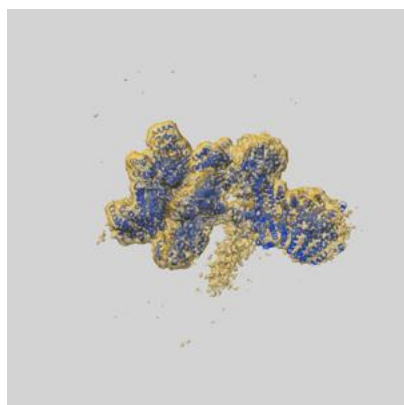
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.29	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.20	8.33	5.53

*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 5.20 differs from the reported value 4.29 by more than 10 %

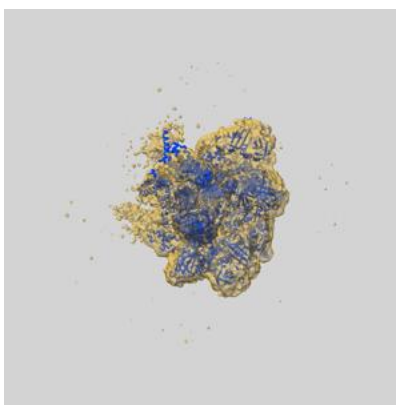
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49522 and PDB model 9NLU. Per-residue inclusion information can be found in section [3](#) on page [8](#).

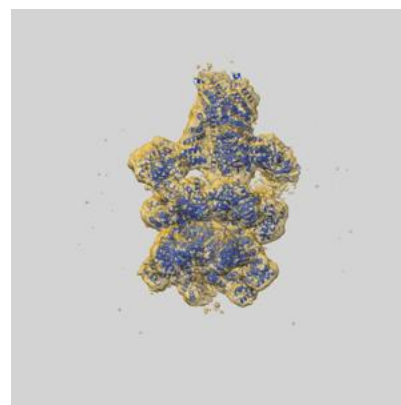
9.1 Map-model overlay [i](#)



X



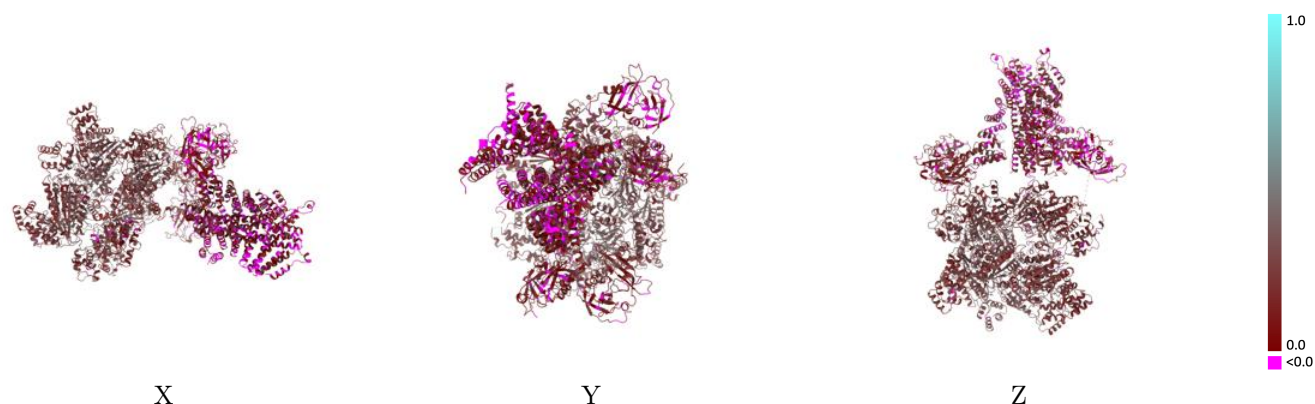
Y



Z

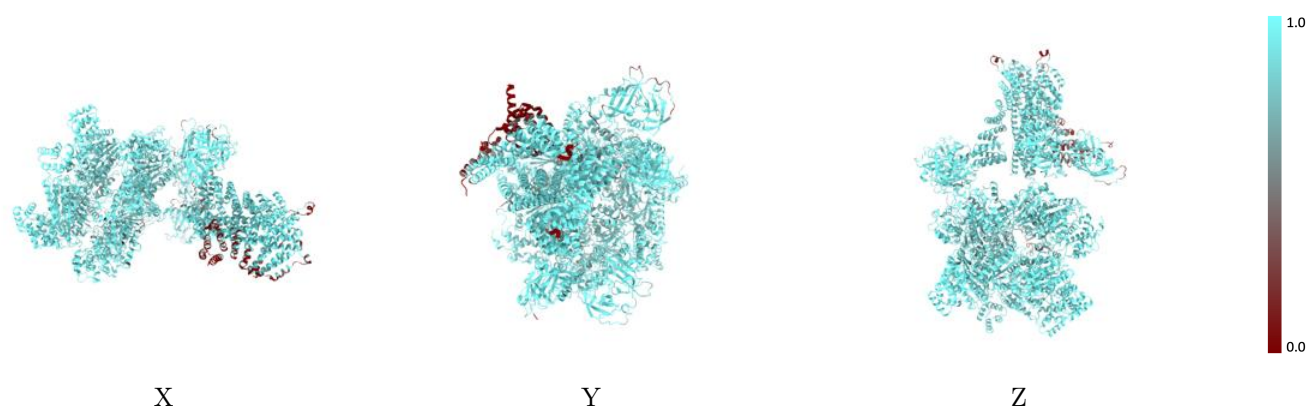
The images above show the 3D surface view of the map at the recommended contour level 0.00205 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



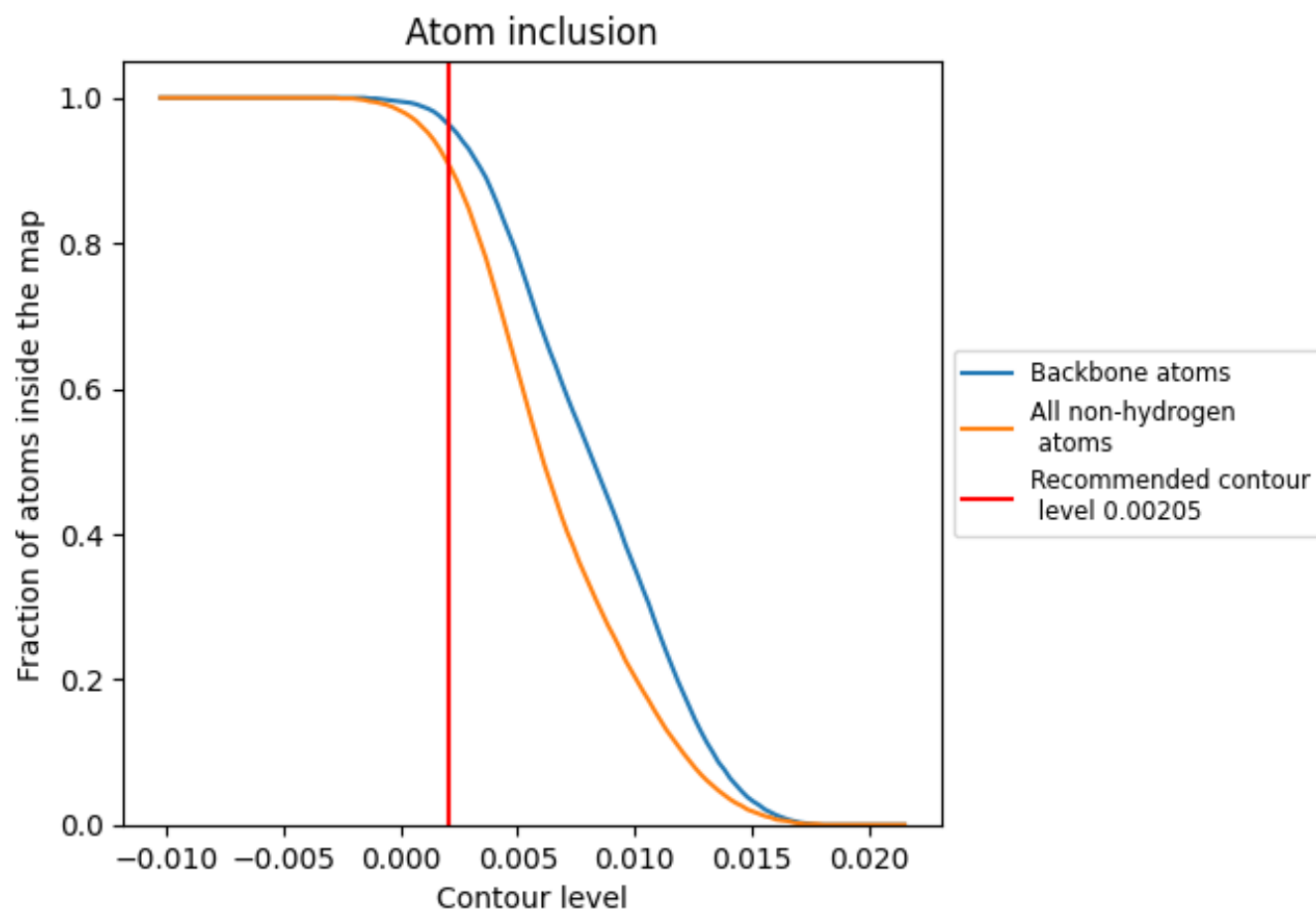
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00205).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.00205) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9080	0.1940
A	0.9350	0.2680
B	0.9310	0.2280
C	0.9300	0.2360
D	0.9330	0.2240
E	0.9160	0.1940
F	0.9030	0.2130
G	0.9210	0.1050
H	0.9440	0.0880
I	0.5780	0.0430
J	0.9380	0.0890
K	0.9490	0.1010
L	0.9710	0.0820

1.0

0.0

<0.0