



wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 11:38 pm BST

PDB ID : 6RAY
EMDB ID : EMD-4787
Title : D. melanogaster CMG-DNA, State 2A
Authors : Eickhoff, P.; Martino, F.; Costa, A.
Deposited on : 2019-04-08
Resolution : 4.28 Å(reported)

This is a wwPDB EM Validation Summary 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.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

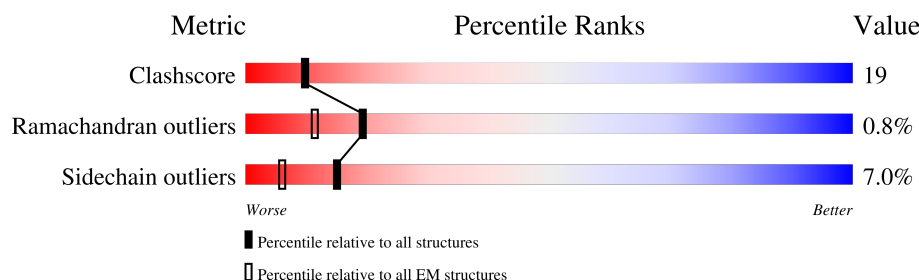
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.28 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	3	819	
2	4	866	
3	7	720	
4	6	817	
5	5	733	
6	A	575	
7	H	202	
8	L	203	

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Mol	Chain	Length	Quality of chain
9	M	212	
10	N	228	
11	2	887	
12	X	13	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	ATP	3	901	-	-	X	-
13	ATP	4	901	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 39071 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 DNA replication licensing factor Mcm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	600	Total	C	N	O	S	0	0
			4685	2927	839	893	26		

- Molecule 2 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	617	Total	C	N	O	S	0	0
			4901	3071	870	938	22		

- Molecule 3 is a protein called DNA replication licensing factor Mcm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	587	Total	C	N	O	S	0	0
			4577	2865	819	873	20		

- Molecule 4 is a protein called DNA replication licensing factor Mcm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	600	Total	C	N	O	S	0	0
			4748	2968	848	908	24		

- Molecule 5 is a protein called DNA replication licensing factor Mcm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	577	Total	C	N	O	S	0	0
			4505	2832	796	850	27		

- Molecule 6 is a protein called CDC45L.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	567	Total	C	N	O	S	0	0
			4555	2885	788	860	22		

- Molecule 7 is a protein called IP07275p.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	189	Total	C	N	O	S	0	0
			1504	961	263	273	7		

- Molecule 8 is a protein called Probable DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	177	Total	C	N	O	S	0	0
			1422	915	239	256	12		

- Molecule 9 is a protein called AT18545p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	167	Total	C	N	O	S	0	0
			1377	875	244	254	4		

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	206	Total	C	N	O	S	0	0
			1627	1007	279	328	13		

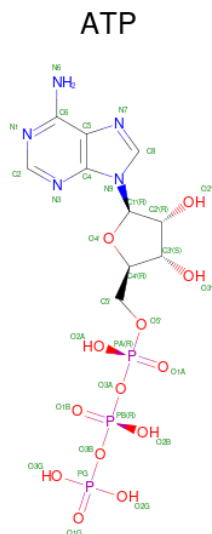
- Molecule 11 is a protein called DNA replication licensing factor Mcm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	600	Total	C	N	O	S	0	0
			4731	2988	827	885	31		

- Molecule 12 is a DNA chain called DNA (5'-D(P*AP*TP*TP*TP*TP*TP*TP*TP*T
P*TP*TP*T)-3').

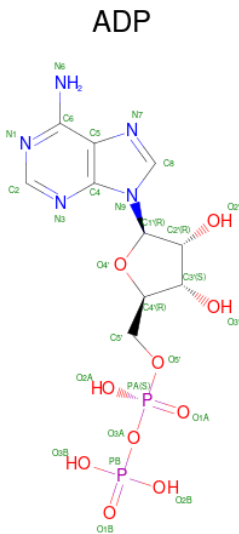
Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	13	Total	C	N	O	P	0	0
			261	130	29	89	13		

- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



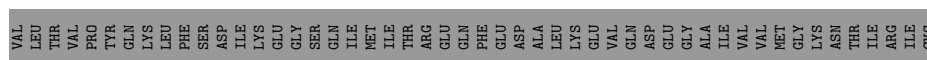
Mol	Chain	Residues	Atoms					AltConf
13	3	1	Total 31	C 10	N 5	O 13	P 3	0
13	4	1	Total 31	C 10	N 5	O 13	P 3	0
13	6	1	Total 31	C 10	N 5	O 13	P 3	0
13	2	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



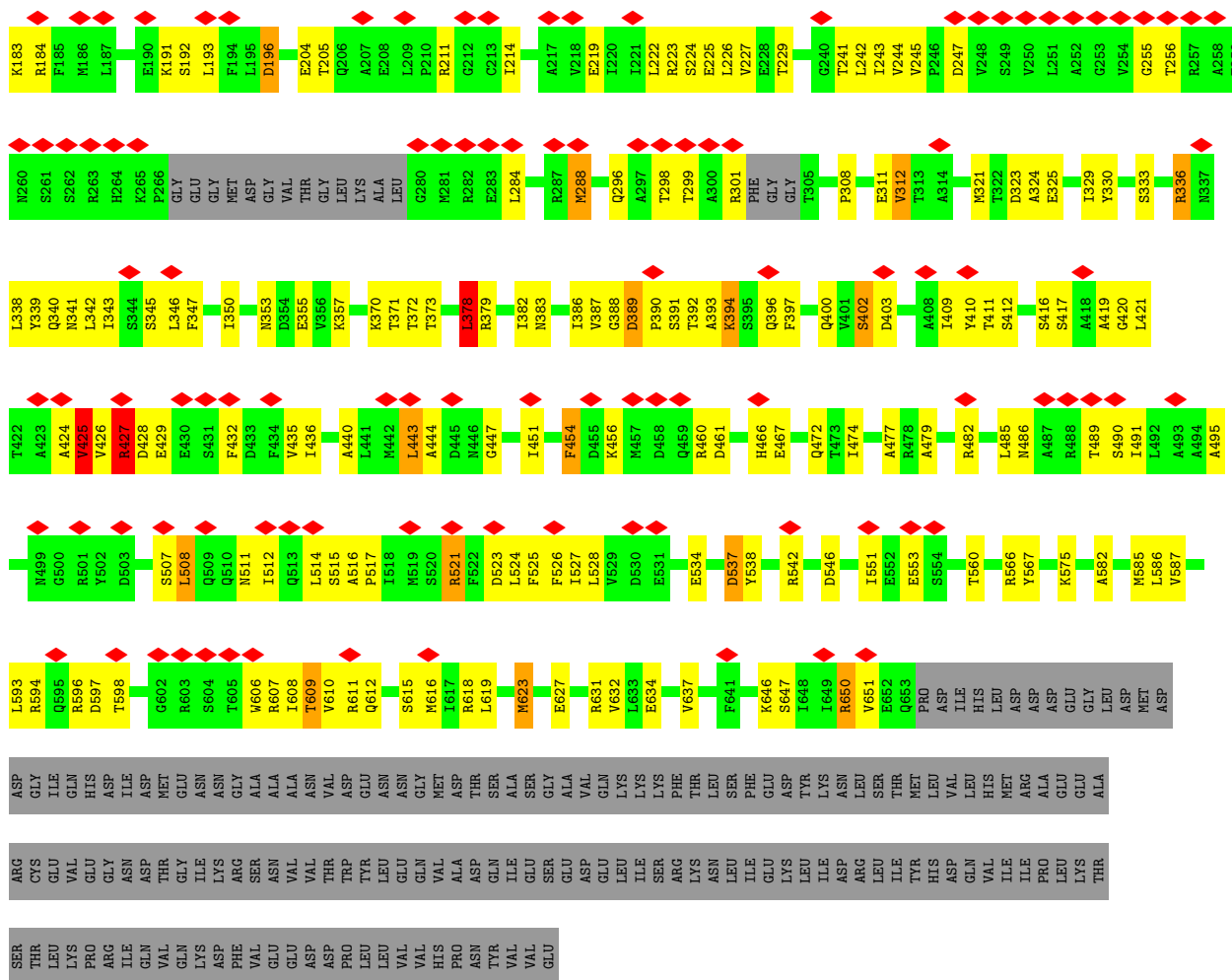
Mol	Chain	Residues	Atoms					AltConf
14	7	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	5	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 2: DNA replication licensing factor MCM4

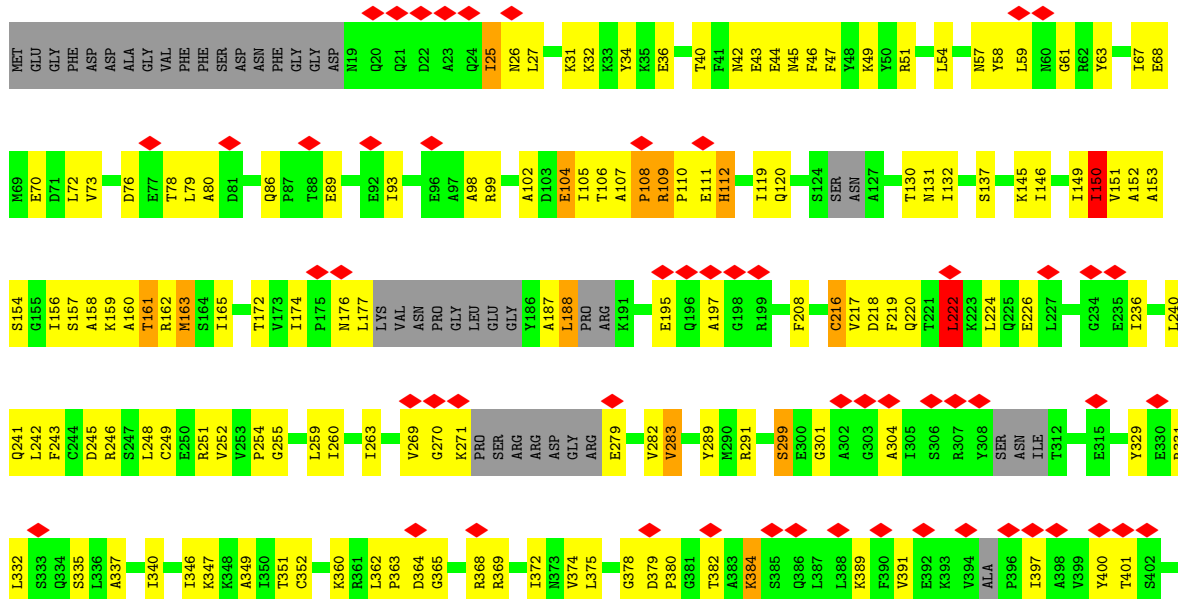


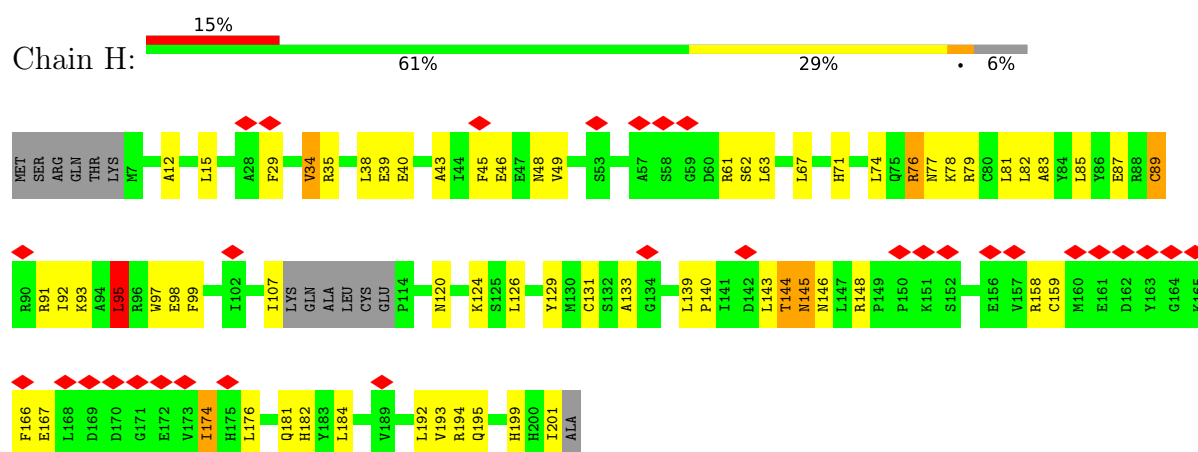
- Molecule 3: DNA replication licensing factor Mcm7



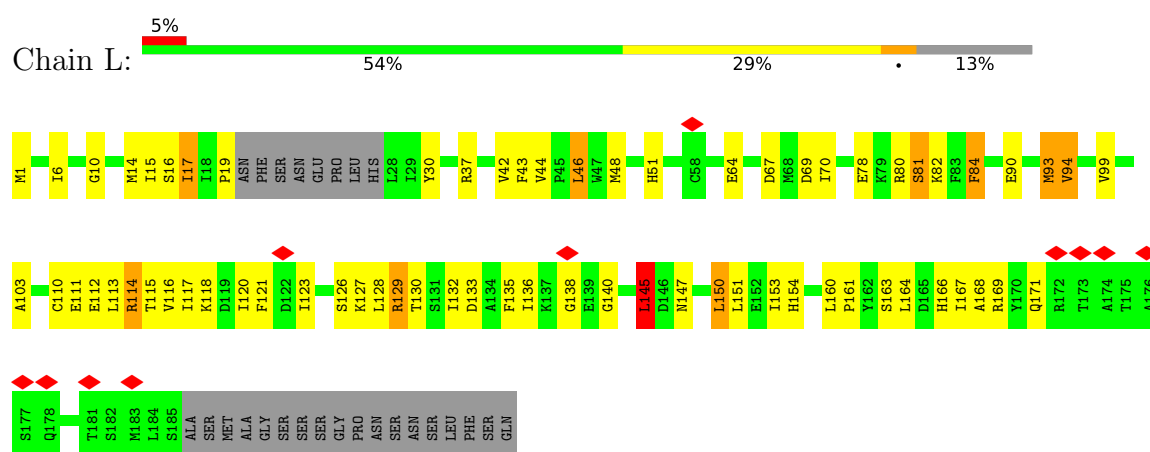


• Molecule 5: DNA replication licensing factor Mcm5

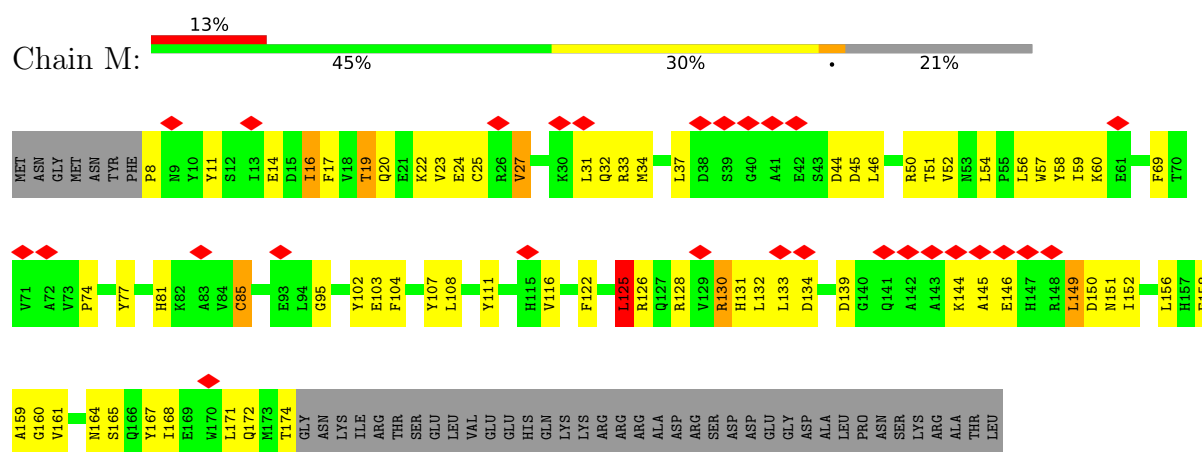




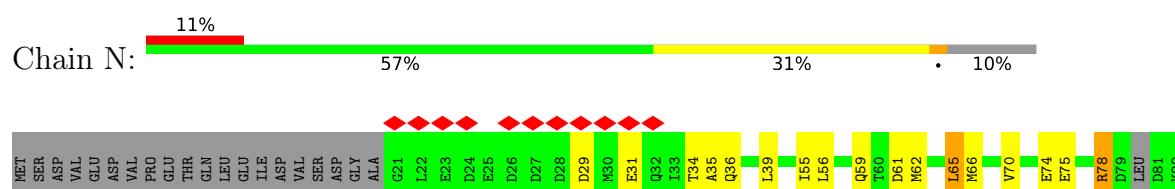
• Molecule 8: Probable DNA replication complex GINS protein PSF2



• Molecule 9: AT18545p

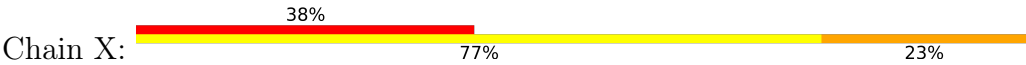


• Molecule 10: DNA replication complex GINS protein SLD5



PRO	PHE	TYR	GLU	SER	ASP	LEU	PHE	ARG	THR	ASN	GLY	PHE	SER	TYR	ASP	PRO	LYS	ARG	ARG	ILE	ILE	LEU	GLN	ILE	VAL	VAL	ASP	GLY	ASN	THR	ALA
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● Molecule 12: DNA (5'-D(P*AP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')



A26	T27	T28	T29	T30	T31	T32	T33	T34	T35	T36	T37	T38
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52214	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	3	0.54	0/4747	0.93	15/6394 (0.2%)
2	4	0.62	3/4986 (0.1%)	1.06	42/6744 (0.6%)
3	7	0.58	5/4636 (0.1%)	0.95	34/6246 (0.5%)
4	6	0.56	2/4819 (0.0%)	0.91	12/6502 (0.2%)
5	5	0.56	0/4571	1.02	20/6151 (0.3%)
6	A	0.52	1/4647 (0.0%)	0.83	7/6283 (0.1%)
7	H	0.57	0/1538	0.91	3/2077 (0.1%)
8	L	0.65	1/1454 (0.1%)	0.86	3/1966 (0.2%)
9	M	0.62	0/1409	0.84	2/1909 (0.1%)
10	N	0.54	0/1647	0.87	5/2226 (0.2%)
11	2	0.57	2/4813 (0.0%)	1.01	25/6499 (0.4%)
12	X	0.96	0/287	1.66	5/441 (1.1%)
All	All	0.57	14/39554 (0.0%)	0.96	173/53438 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	3	0	14
2	4	2	10
3	7	0	7
4	6	0	6
5	5	1	12
6	A	0	6
7	H	0	3
8	L	0	2
9	M	0	2
11	2	1	8
All	All	4	70

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7	254	THR	C-N	14.41	1.67	1.34
2	4	588	VAL	C-N	14.04	1.66	1.34
3	7	267	PRO	C-N	11.66	1.54	1.33
3	7	431	GLY	C-N	-8.39	1.18	1.33
4	6	108	PHE	C-N	8.12	1.52	1.34

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	510	ARG	NE-CZ-NH2	-14.63	112.99	120.30
5	5	425	VAL	CB-CA-C	-14.16	84.50	111.40
3	7	629	ASP	O-C-N	-13.85	100.55	122.70
5	5	270	GLY	C-N-CA	13.64	155.79	121.70
3	7	267	PRO	O-C-N	13.55	146.24	123.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	4	472	ILE	CB
2	4	575	ILE	CB
5	5	464	ILE	CB
11	2	310	ILE	CB

5 of 70 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3	219	ASP	Peptide
1	3	223	VAL	Peptide
1	3	257	LEU	Peptide
1	3	28	ILE	Peptide
1	3	69	GLU	Peptide

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	3	4685	0	4739	173	0
2	4	4901	0	4838	209	0
3	7	4577	0	4548	259	0
4	6	4748	0	4725	178	0
5	5	4505	0	4511	185	0
6	A	4555	0	4468	159	0
7	H	1504	0	1460	46	0
8	L	1422	0	1443	55	0
9	M	1377	0	1346	59	0
10	N	1627	0	1565	49	0
11	2	4731	0	4765	227	0
12	X	261	0	156	24	0
13	2	31	0	12	4	0
13	3	31	0	12	10	0
13	4	31	0	12	13	0
13	6	31	0	11	5	0
14	5	27	0	12	2	0
14	7	27	0	12	8	0
All	All	39071	0	38635	1496	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 19.

The worst 5 of 1496 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)
4:6:466:HIS:CD2	4:6:521:ARG:NH2	2.03	1.25
5:5:425:VAL:CG2	5:5:425:VAL:O	1.78	1.24
2:4:590:HIS:NE2	13:6:901:ATP:O2G	1.75	1.19
4:6:587:VAL:HG11	11:2:658:GLN:HB3	1.32	1.10
2:4:393:VAL:HG13	2:4:423:HIS:O	1.51	1.08

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	3	582/819 (71%)	471 (81%)	108 (19%)	3 (0%)	25	63
2	4	611/866 (71%)	494 (81%)	108 (18%)	9 (2%)	8	39
3	7	561/720 (78%)	468 (83%)	83 (15%)	10 (2%)	7	34
4	6	590/817 (72%)	495 (84%)	93 (16%)	2 (0%)	37	72
5	5	555/733 (76%)	439 (79%)	109 (20%)	7 (1%)	10	42
6	A	565/575 (98%)	475 (84%)	89 (16%)	1 (0%)	44	78
7	H	185/202 (92%)	149 (80%)	35 (19%)	1 (0%)	25	63
8	L	173/203 (85%)	137 (79%)	36 (21%)	0	100	100
9	M	165/212 (78%)	129 (78%)	36 (22%)	0	100	100
10	N	200/228 (88%)	168 (84%)	32 (16%)	0	100	100
11	2	588/887 (66%)	482 (82%)	102 (17%)	4 (1%)	19	56
All	All	4775/6262 (76%)	3907 (82%)	831 (17%)	37 (1%)	19	53

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	7	383	PRO
4	6	425	VAL
11	2	314	CYS
2	4	488	GLY
2	4	538	ARG

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	3	513/699 (73%)	478 (93%)	35 (7%)	13	34
2	4	540/759 (71%)	502 (93%)	38 (7%)	12	33
3	7	492/630 (78%)	440 (89%)	52 (11%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	6	519/718 (72%)	480 (92%)	39 (8%)	11	31
5	5	491/630 (78%)	462 (94%)	29 (6%)	16	39
6	A	491/501 (98%)	465 (95%)	26 (5%)	19	42
7	H	156/176 (89%)	145 (93%)	11 (7%)	12	33
8	L	159/184 (86%)	149 (94%)	10 (6%)	15	37
9	M	148/188 (79%)	139 (94%)	9 (6%)	15	38
10	N	178/205 (87%)	162 (91%)	16 (9%)	8	25
11	2	526/781 (67%)	498 (95%)	28 (5%)	19	42
All	All	4213/5471 (77%)	3920 (93%)	293 (7%)	15	33

5 of 293 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	L	14	MET
11	2	541	LEU
8	L	129	ARG
10	N	154	LYS
3	7	333	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
7	H	48	ASN
10	N	110	GLN
11	2	586	HIS
4	6	584	HIS
4	6	466	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
13	ATP	3	901	-	26,33,33	0.92	1 (3%)	31,52,52	1.96	5 (16%)
13	ATP	4	901	-	26,33,33	1.01	1 (3%)	31,52,52	2.12	9 (29%)
14	ADP	7	801	-	24,29,29	0.96	1 (4%)	29,45,45	1.56	5 (17%)
13	ATP	2	901	-	26,33,33	0.96	1 (3%)	31,52,52	1.86	7 (22%)
14	ADP	5	801	-	24,29,29	1.03	2 (8%)	29,45,45	1.72	5 (17%)
13	ATP	6	901	-	26,33,33	0.90	1 (3%)	31,52,52	1.78	8 (25%)

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
13	ATP	3	901	-	-	5/18/38/38	0/3/3/3
13	ATP	4	901	-	-	5/18/38/38	0/3/3/3
14	ADP	7	801	-	-	0/12/32/32	0/3/3/3
13	ATP	2	901	-	-	5/18/38/38	0/3/3/3
14	ADP	5	801	-	-	0/12/32/32	0/3/3/3
13	ATP	6	901	-	-	5/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	5	801	ADP	C5-C4	2.73	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	901	ATP	C5-C4	2.72	1.48	1.40
14	7	801	ADP	C5-C4	2.59	1.47	1.40
13	2	901	ATP	C5-C4	2.58	1.47	1.40
14	5	801	ADP	O4'-C1'	2.11	1.44	1.41

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	901	ATP	PA-O3A-PB	-5.68	113.35	132.83
13	4	901	ATP	C3'-C2'-C1'	5.30	108.95	100.98
14	5	801	ADP	PA-O3A-PB	-5.28	114.70	132.83
13	3	901	ATP	PB-O3B-PG	-5.18	115.04	132.83
13	2	901	ATP	PA-O3A-PB	-4.96	115.80	132.83

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	3	901	ATP	C5'-O5'-PA-O1A
13	3	901	ATP	C5'-O5'-PA-O2A
13	4	901	ATP	C5'-O5'-PA-O1A
13	4	901	ATP	C5'-O5'-PA-O2A
13	6	901	ATP	C5'-O5'-PA-O2A

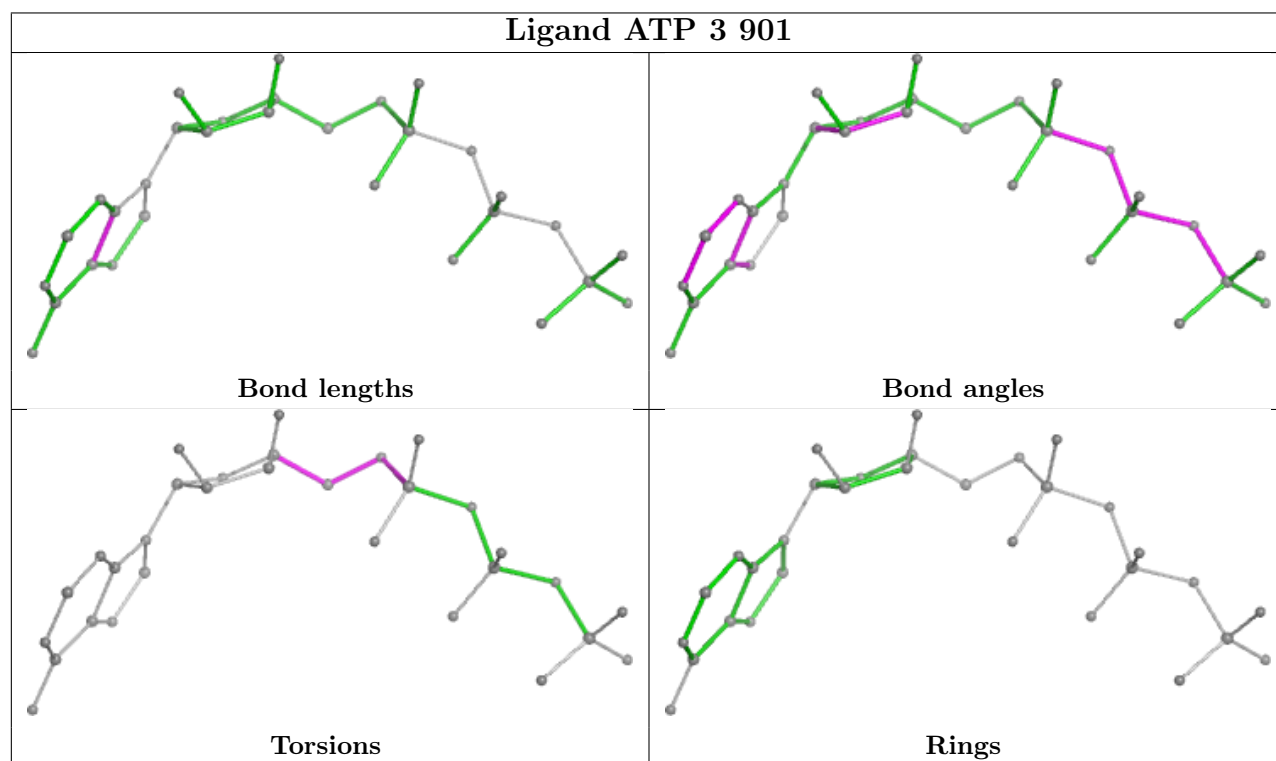
There are no ring outliers.

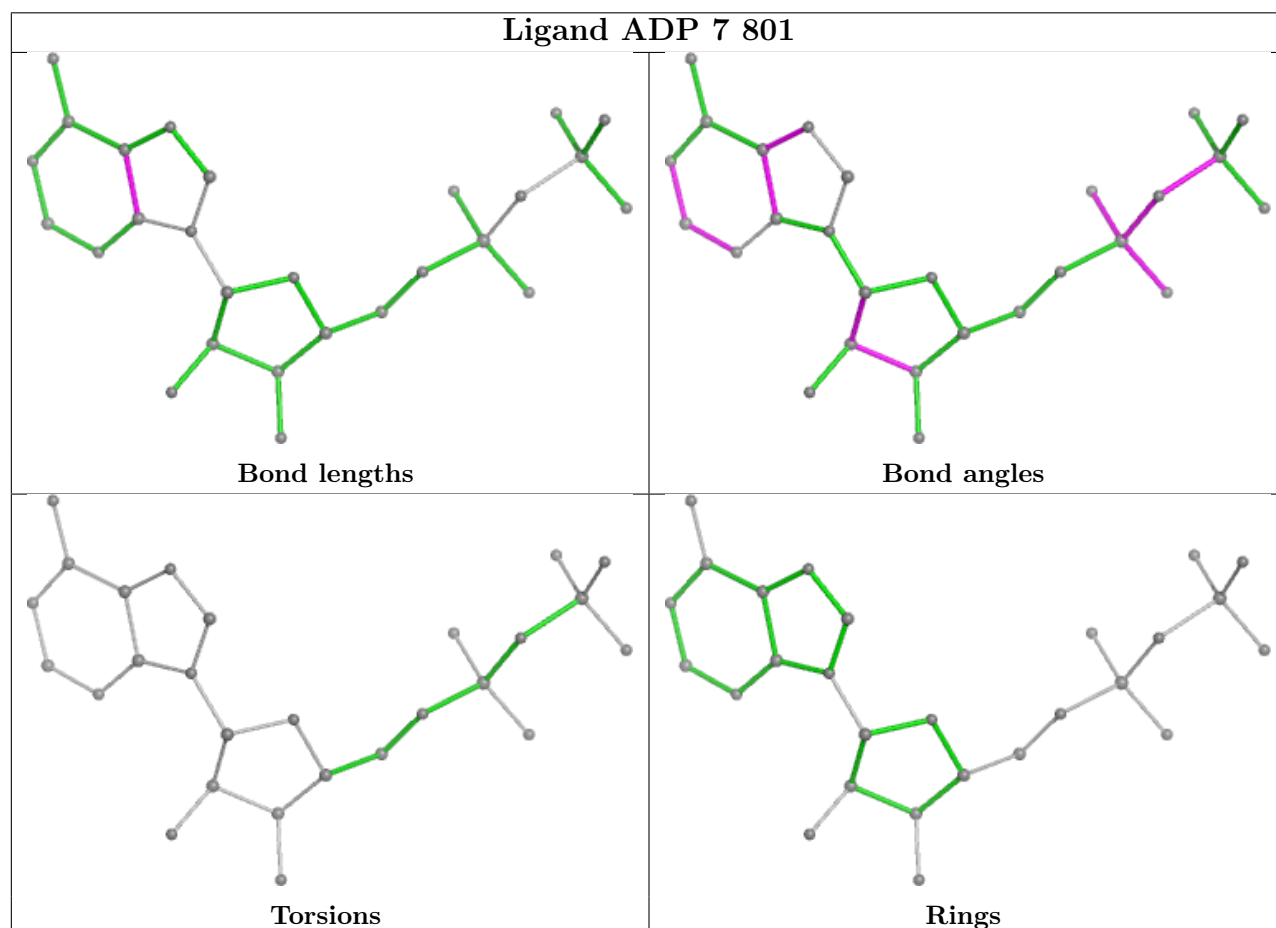
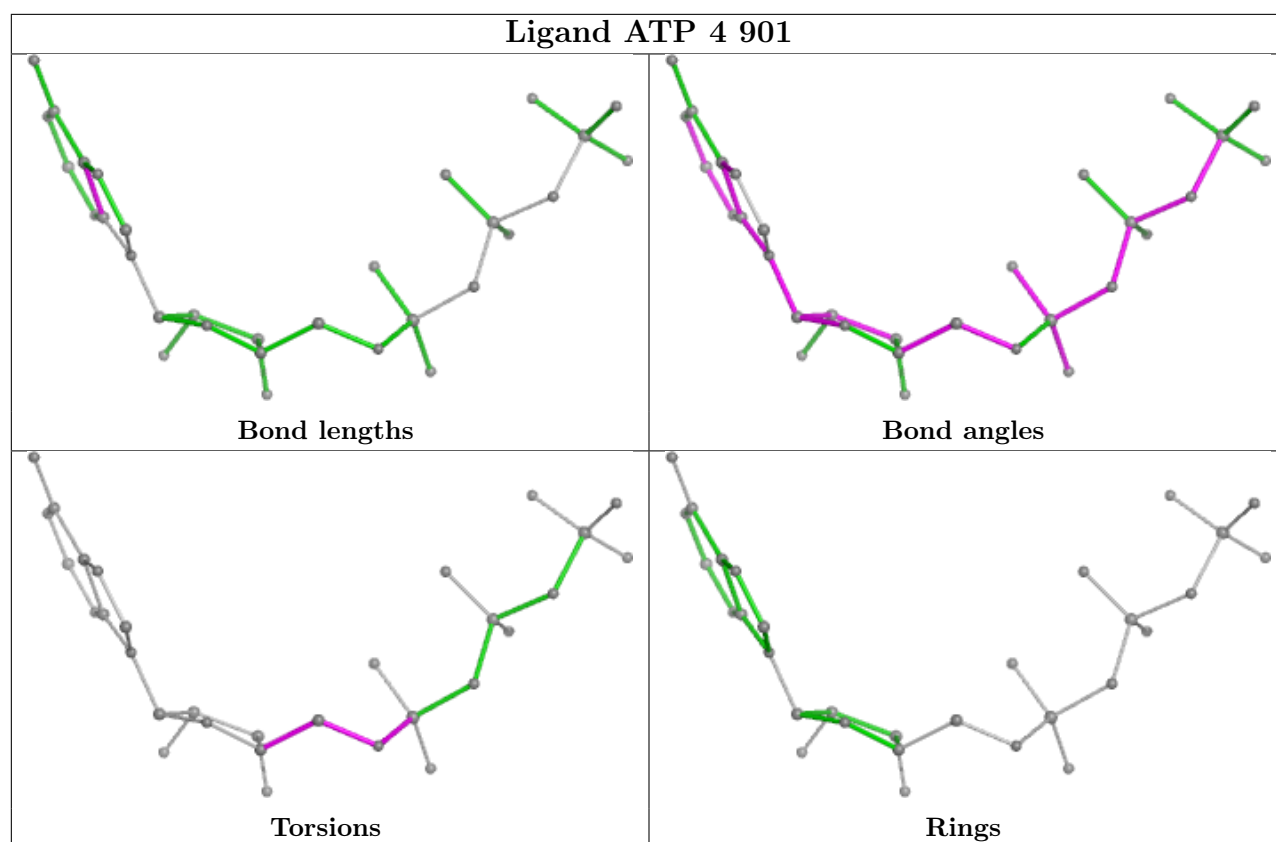
6 monomers are involved in 42 short contacts:

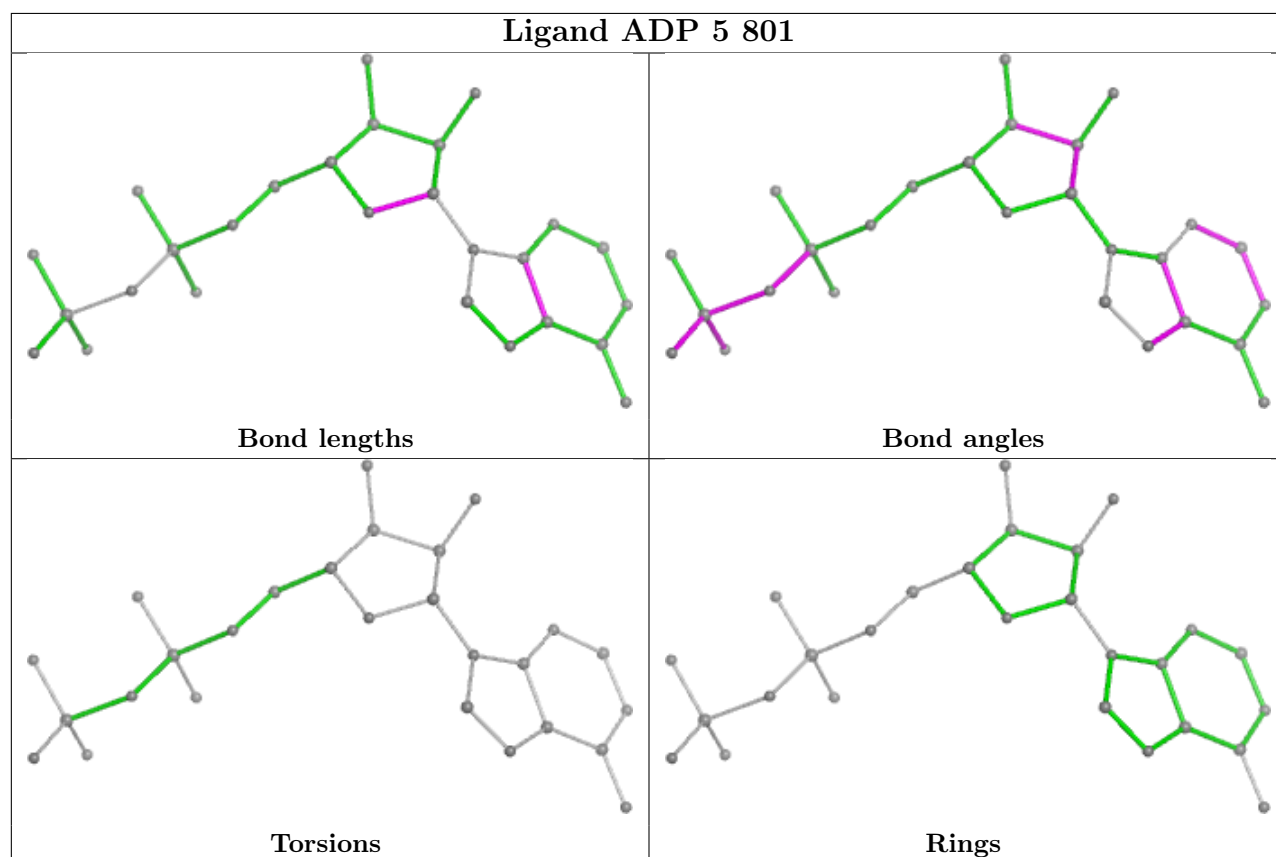
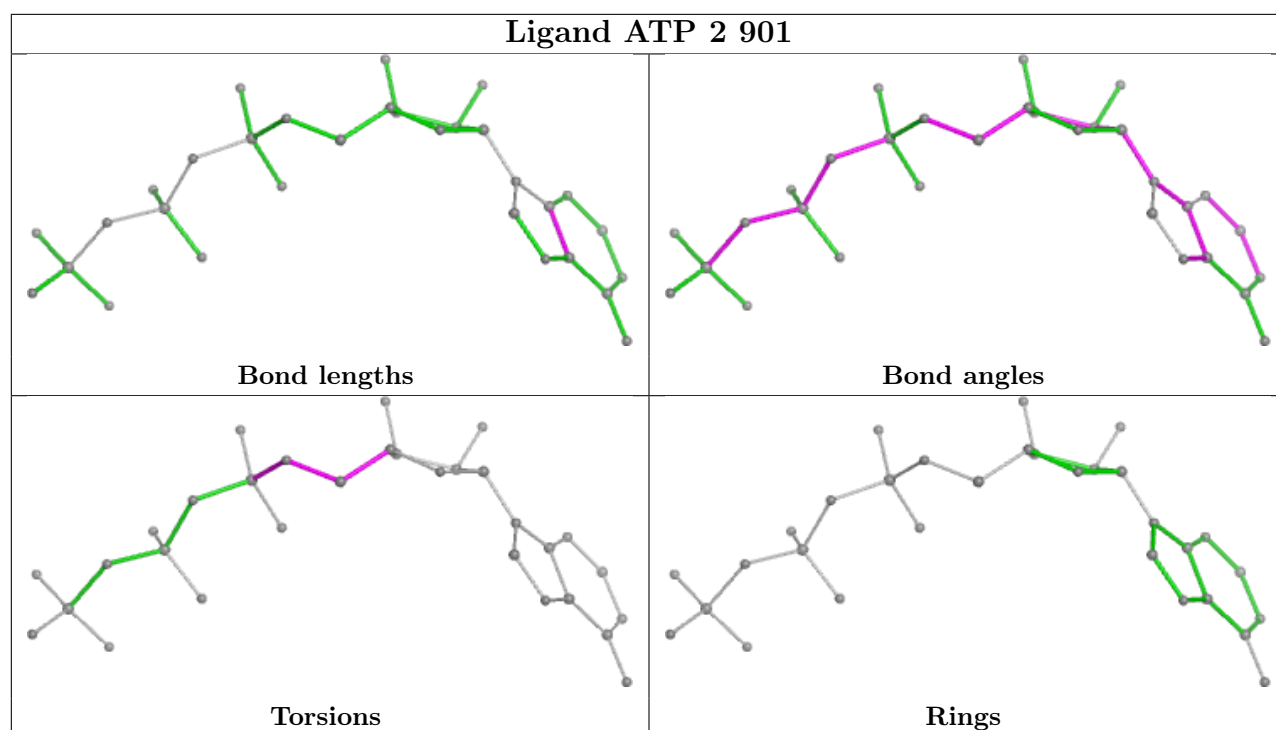
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	3	901	ATP	10	0
13	4	901	ATP	13	0
14	7	801	ADP	8	0
13	2	901	ATP	4	0
14	5	801	ADP	2	0
13	6	901	ATP	5	0

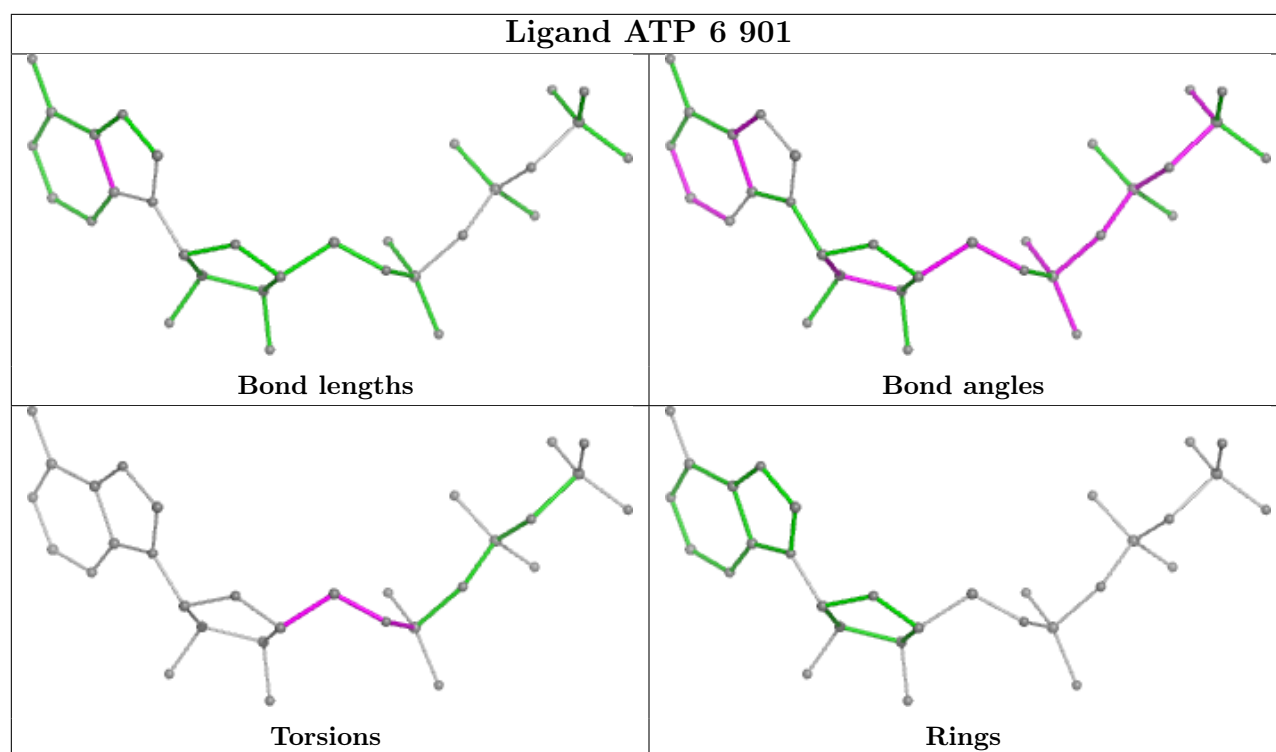
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	4	2
3	7	2
11	2	1
5	5	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	442:ILE	C	443:PHE	N	14.43
1	2	441:LEU	C	442:THR	N	10.58
1	5	405:GLY	C	408:SER	N	6.53
1	7	254:THR	C	255:ILE	N	1.67
1	4	588:VAL	C	589:LEU	N	1.66

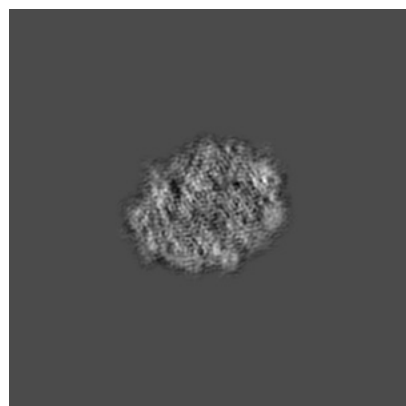
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4787. These allow visual inspection of the internal detail of the map and identification of artifacts.

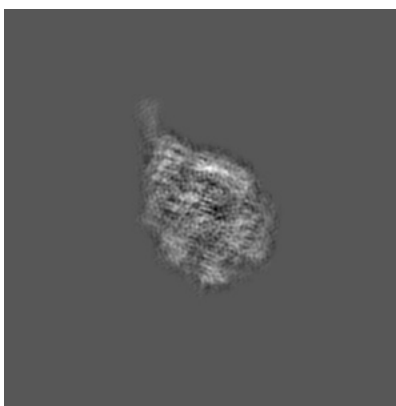
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

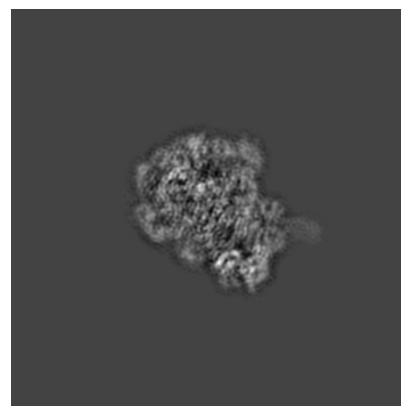
6.1.1 Primary map



X

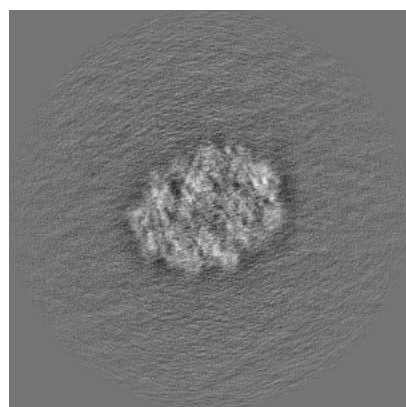


Y

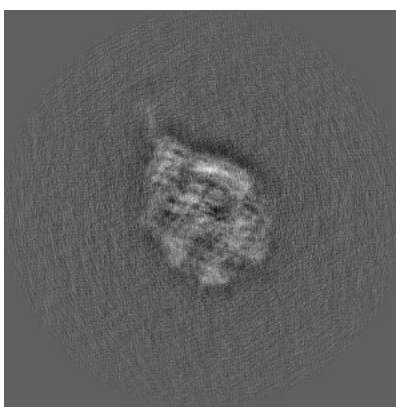


Z

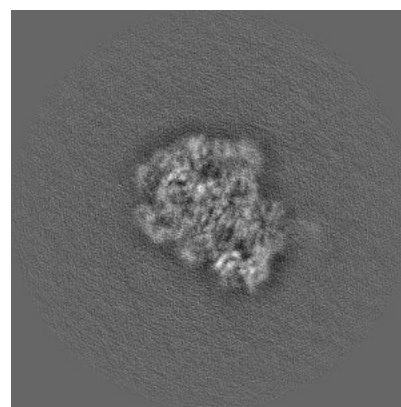
6.1.2 Raw map



X



Y

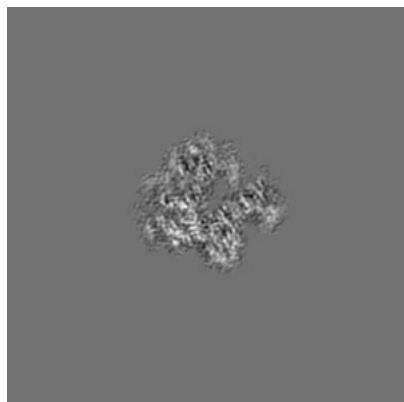


Z

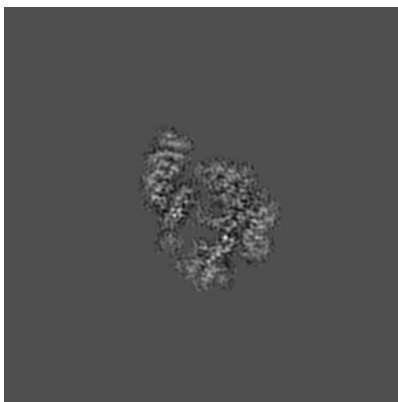
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

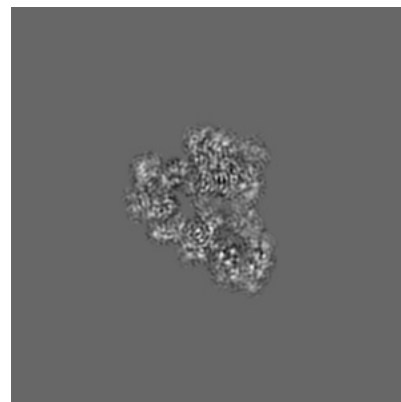
6.2.1 Primary map



X Index: 192

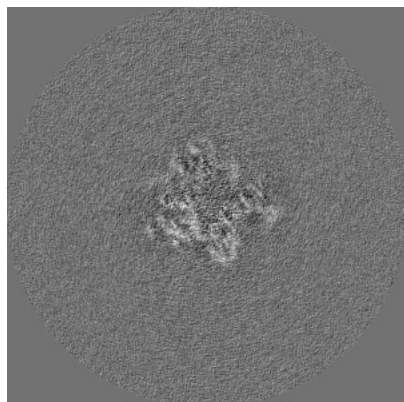


Y Index: 192

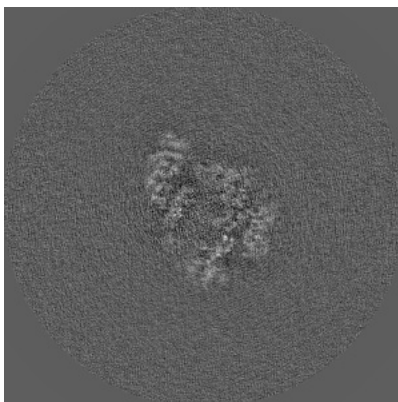


Z Index: 192

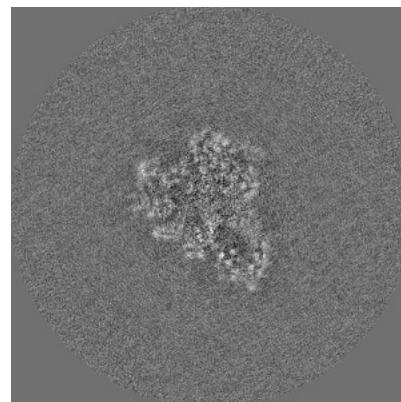
6.2.2 Raw map



X Index: 192



Y Index: 192

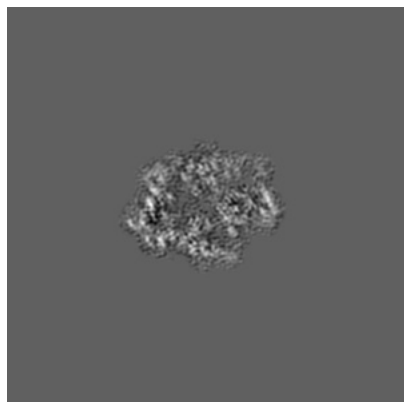


Z Index: 192

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

6.3 Largest variance slices [i](#)

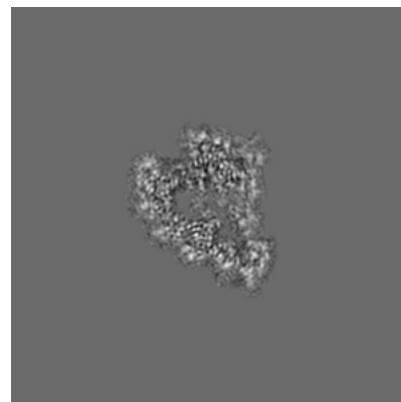
6.3.1 Primary map



X Index: 207

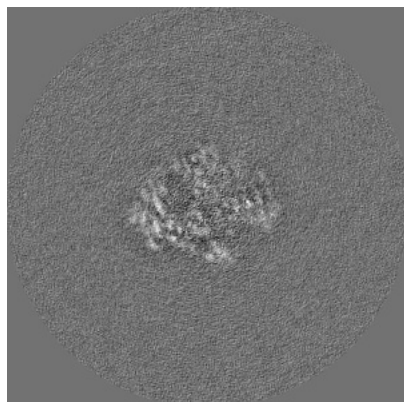


Y Index: 180

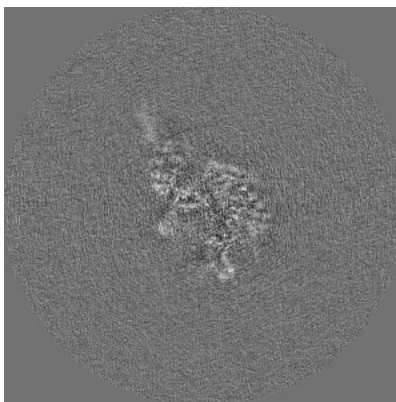


Z Index: 197

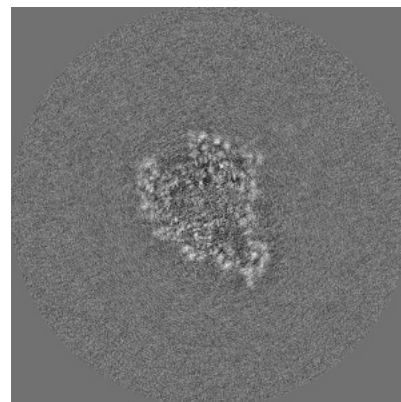
6.3.2 Raw map



X Index: 202



Y Index: 180

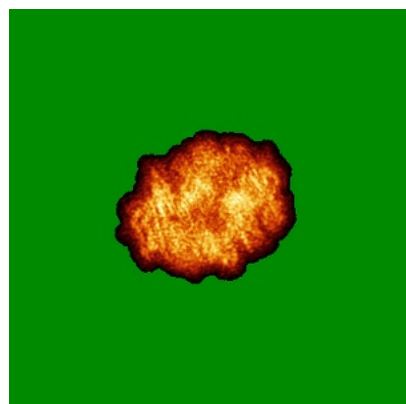


Z Index: 197

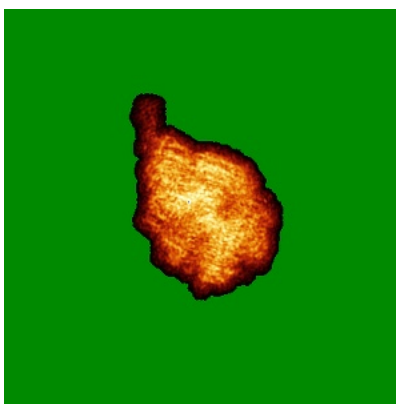
The images above show the largest variance slices of the map in three orthogonal directions.

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

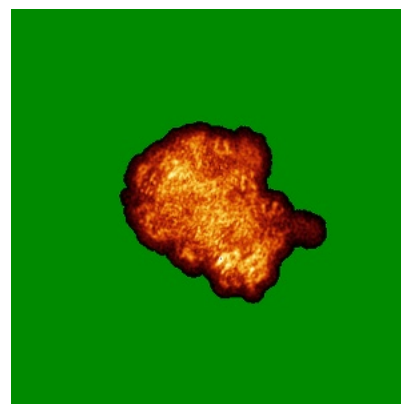
6.4.1 Primary map



X

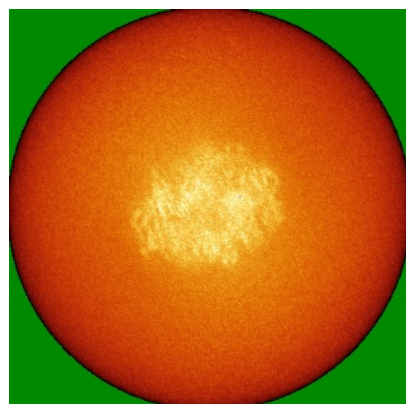


Y

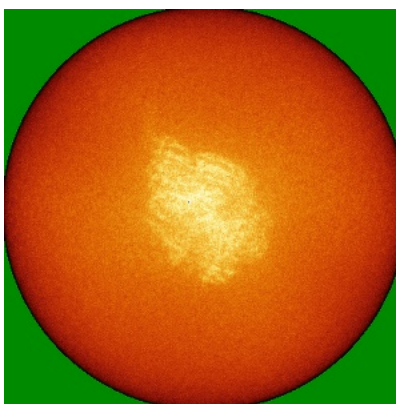


Z

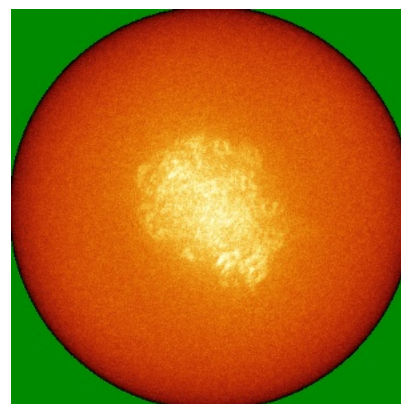
6.4.2 Raw map



X



Y

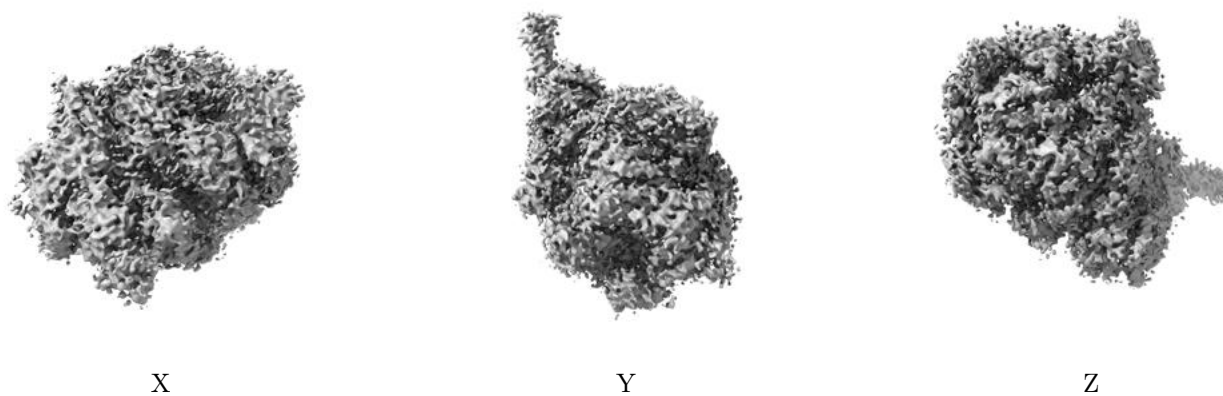


Z

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.

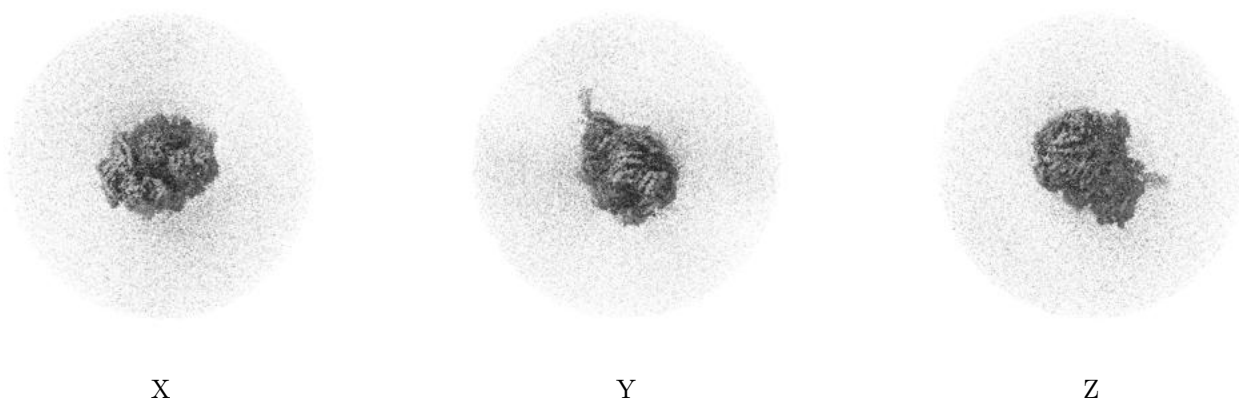
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

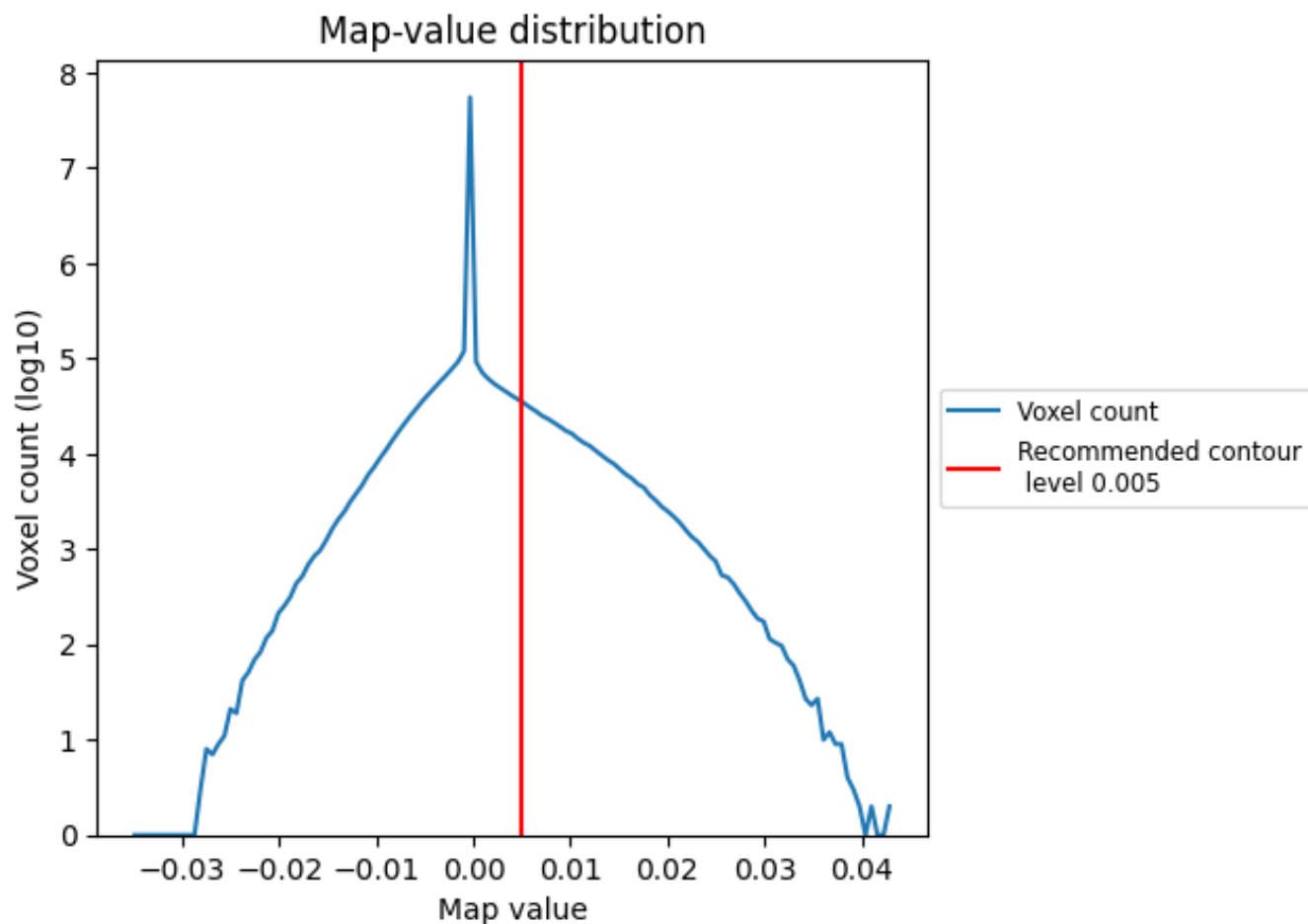
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

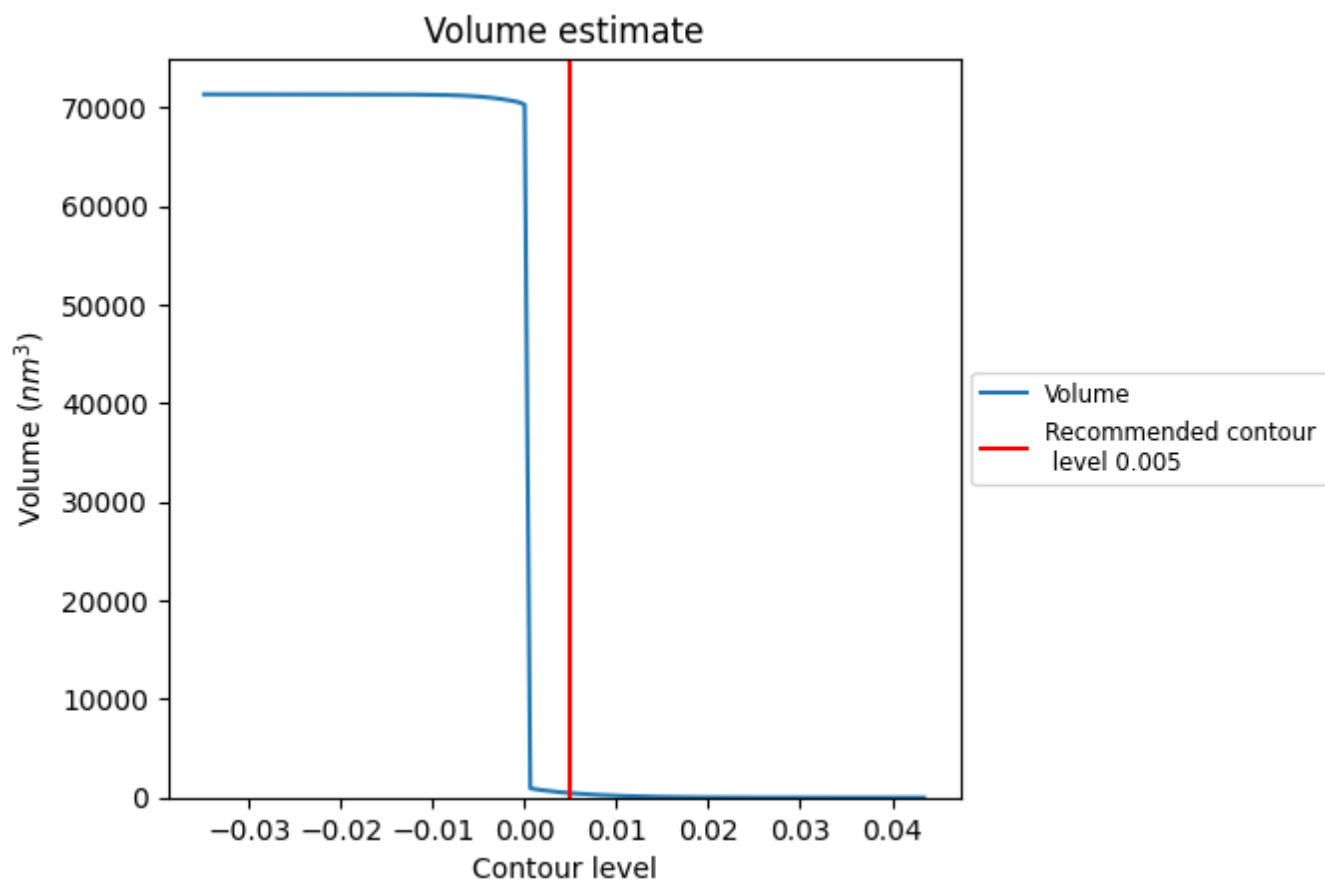
This section contains the results of statistical analysis of the map.

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.

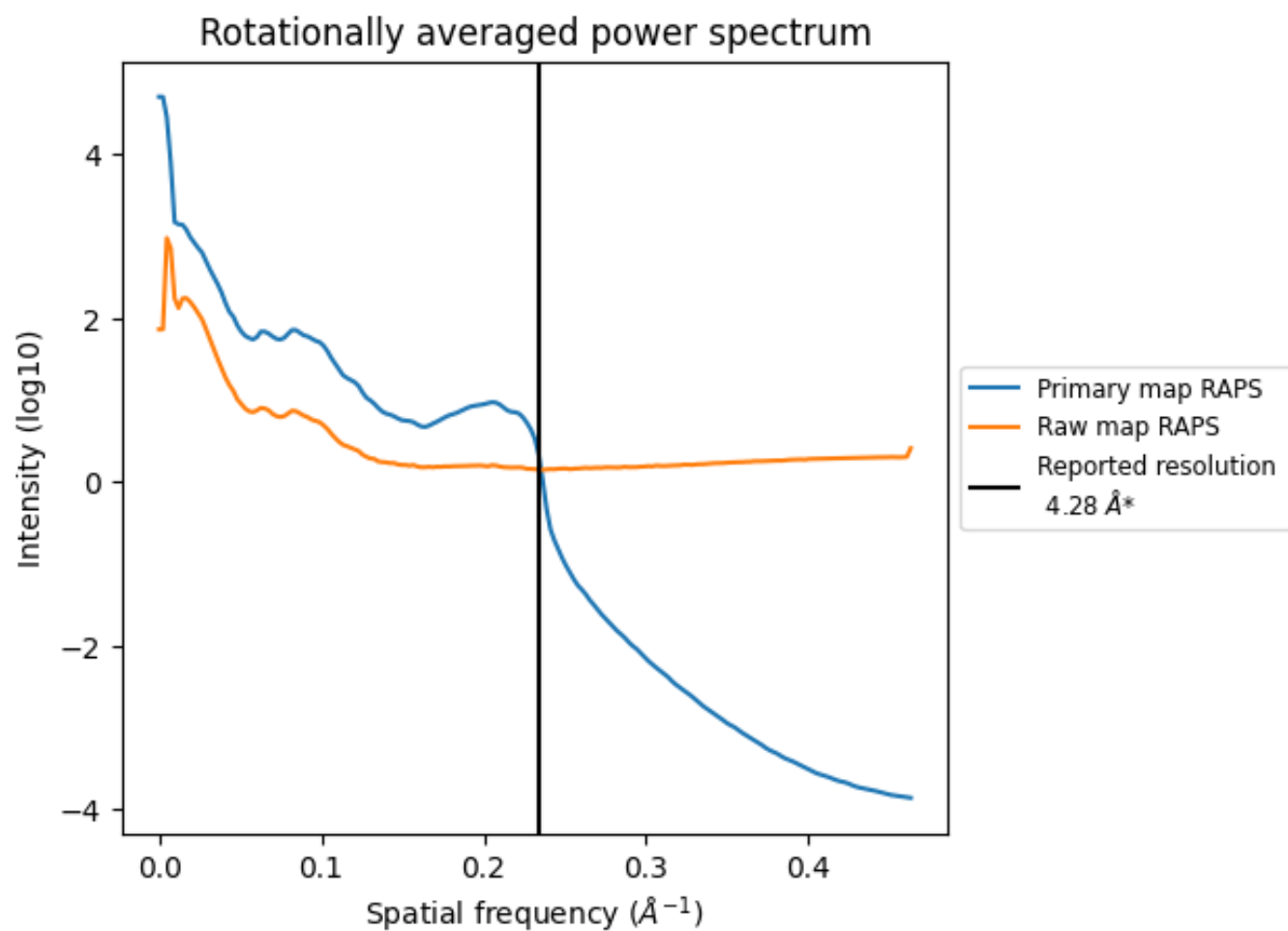
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 452 nm³; this corresponds to an approximate mass of 408 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 ⓘ

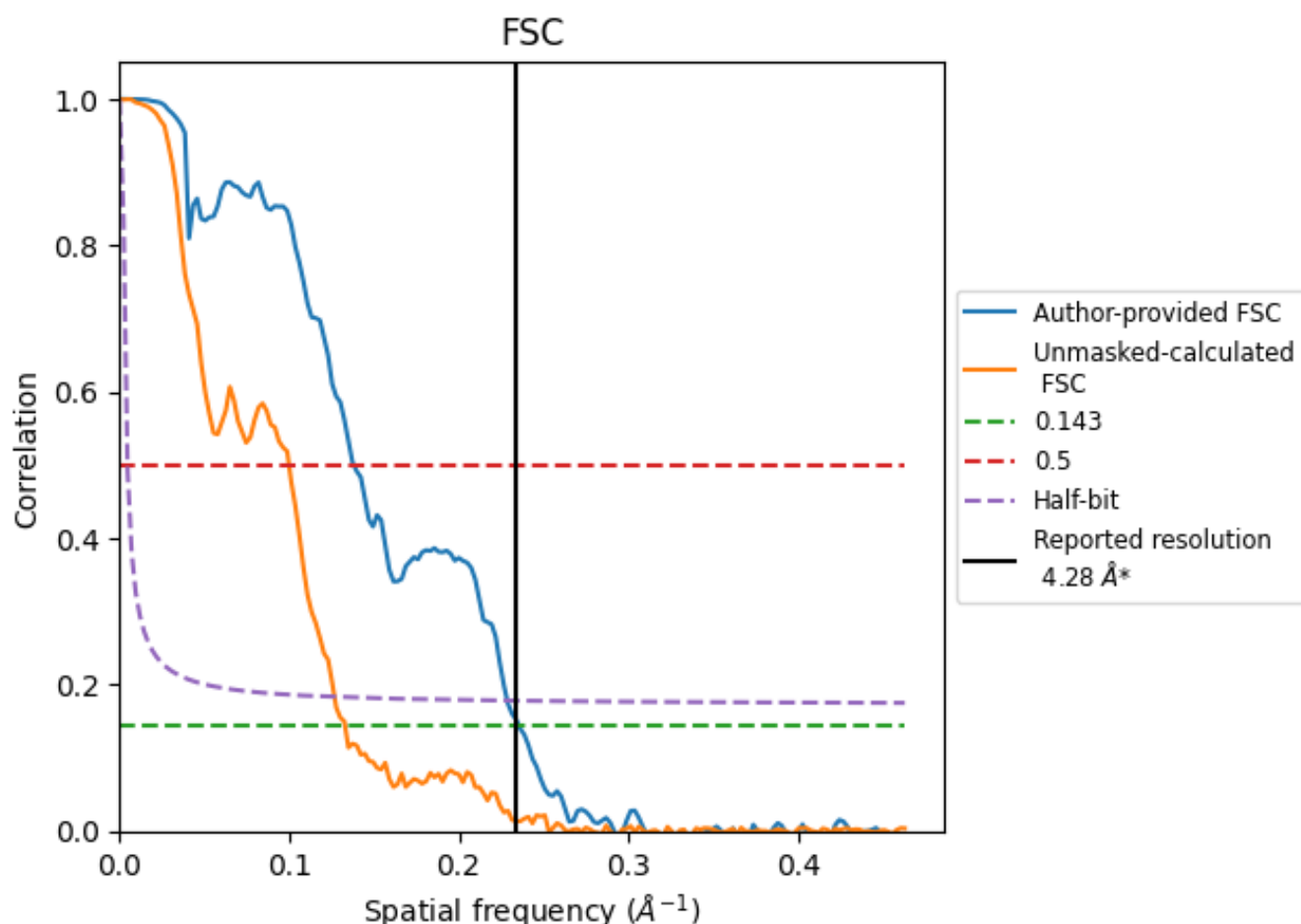


*Reported resolution corresponds to spatial frequency of 0.234 Å⁻¹

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 0.234 Å⁻¹

8.2 Resolution estimates [i](#)

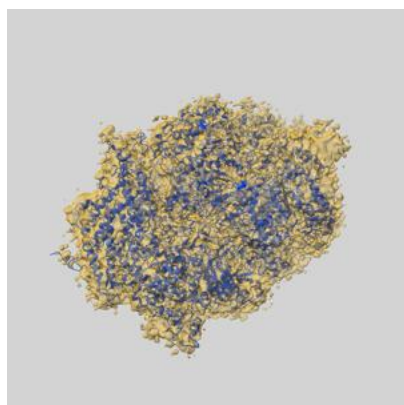
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.28	-	-
Author-provided FSC curve	4.24	7.24	4.37
Unmasked-calculated*	7.52	10.01	7.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.52 differs from the reported value 4.28 by more than 10 %

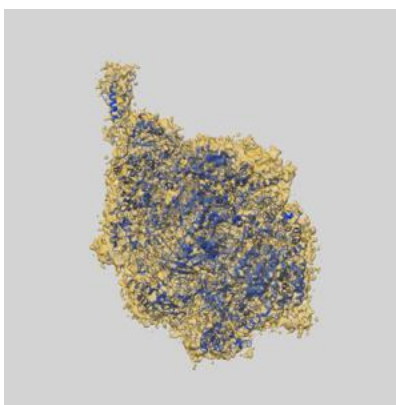
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4787 and PDB model 6RAY. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

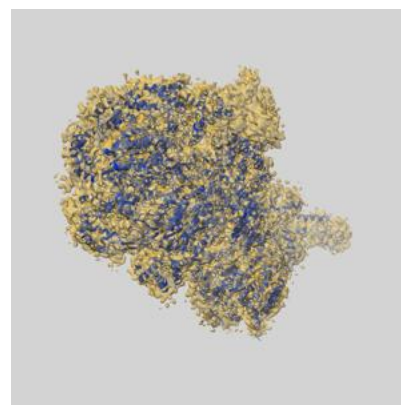
9.1 Map-model overlay [i](#)



X



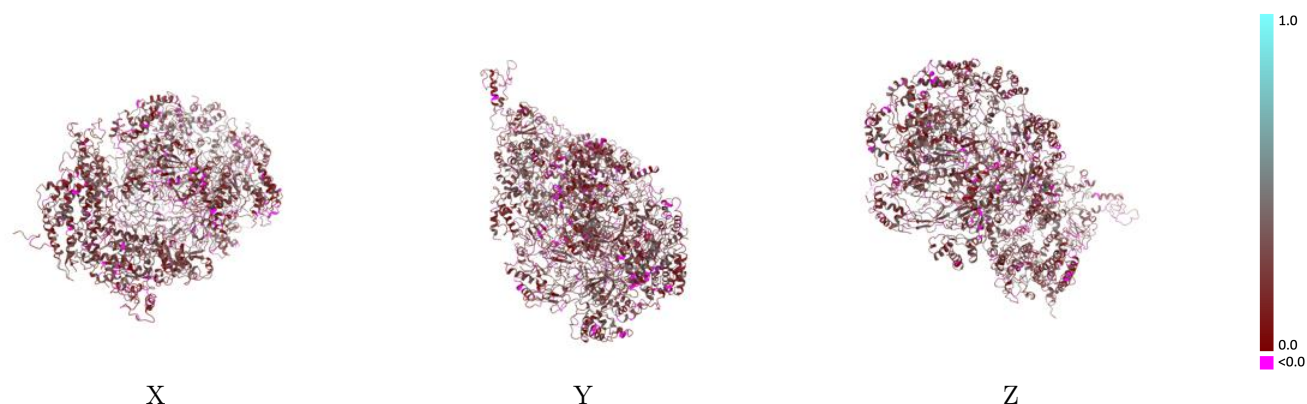
Y



Z

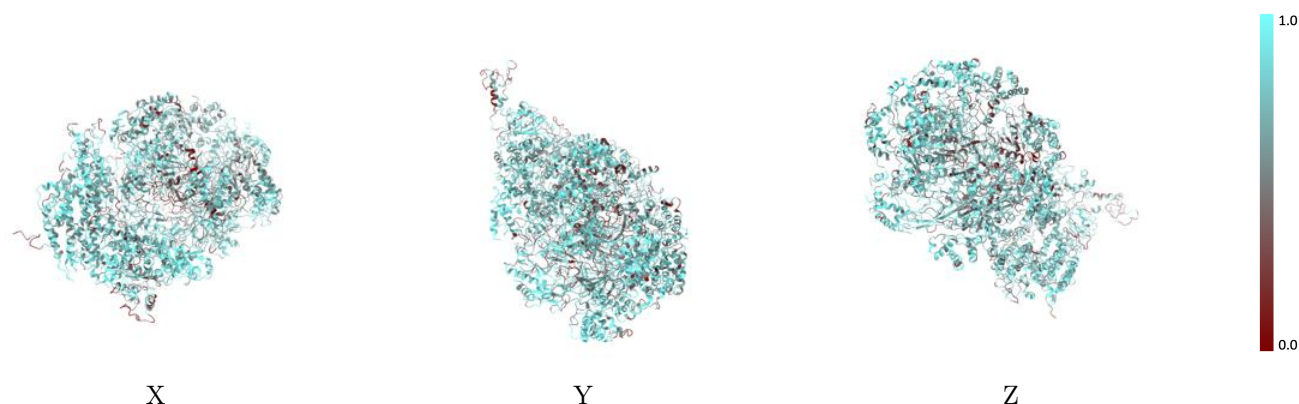
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



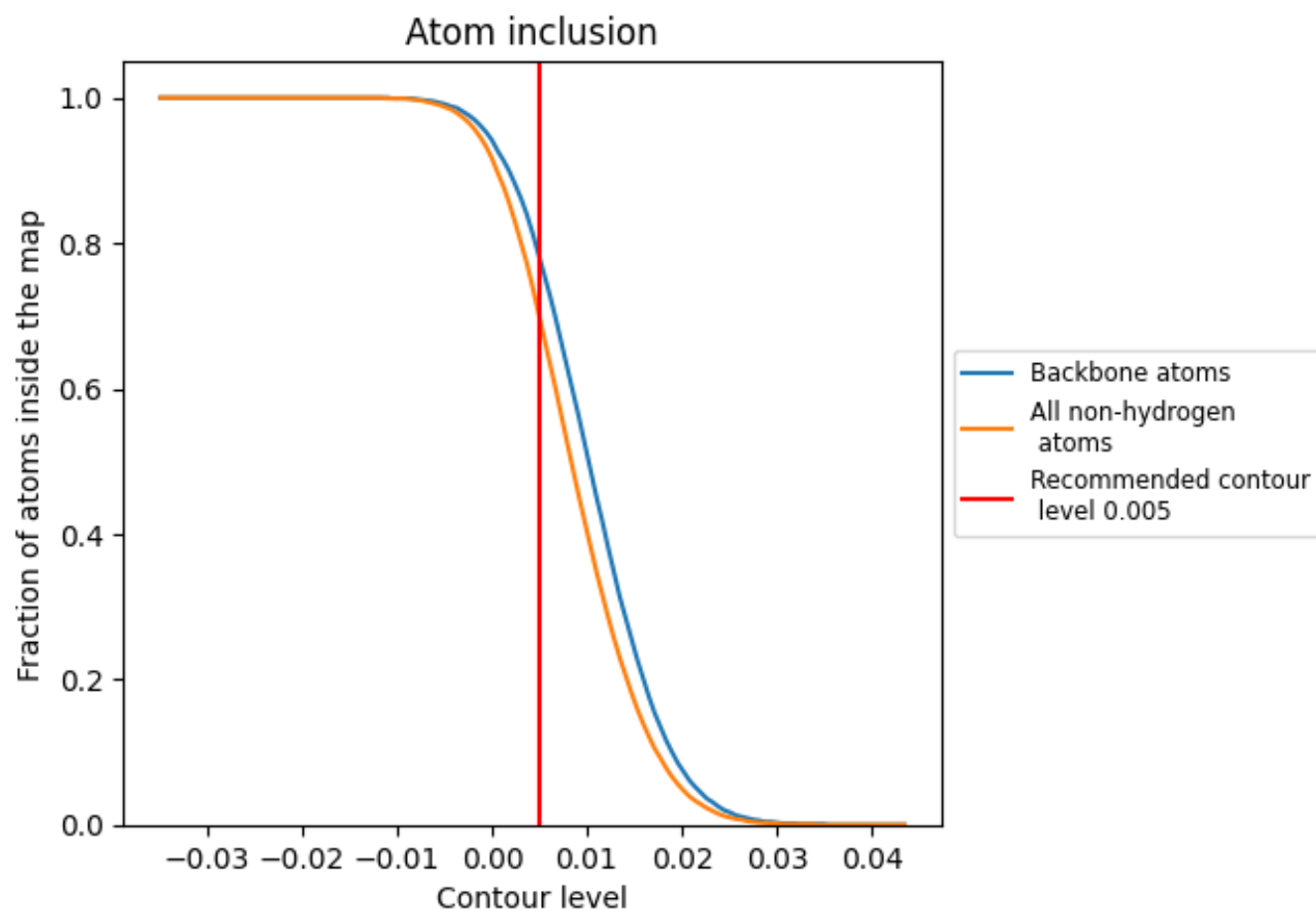
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6990	<div></div> 0.2350
2	<div></div> 0.6740	<div></div> 0.2130
3	<div></div> 0.7080	<div></div> 0.2460
4	<div></div> 0.7180	<div></div> 0.2440
5	<div></div> 0.6610	<div></div> 0.2370
6	<div></div> 0.6710	<div></div> 0.2230
7	<div></div> 0.7080	<div></div> 0.2600
A	<div></div> 0.7190	<div></div> 0.2350
H	<div></div> 0.7230	<div></div> 0.1890
L	<div></div> 0.7860	<div></div> 0.2630
M	<div></div> 0.6690	<div></div> 0.2200
N	<div></div> 0.7530	<div></div> 0.2390
X	<div></div> 0.5330	<div></div> 0.2370

1.0

0.0

<0.0