



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 04:31 AM UTC

PDB ID : 9E2Y / pdb_00009e2y
EMDB ID : EMD-47472
Title : Cryo-EM structure of yeast CMG helicase stalled at G4-containing DNA template, state 3
Authors : Allwein, B.; Batra, S.; Remus, D.; Hite, R.
Deposited on : 2024-10-23
Resolution : 3.20 Å(reported)
Based on initial model : .

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:

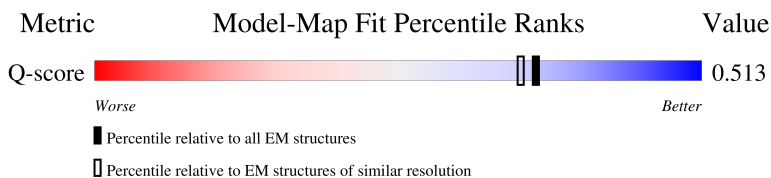
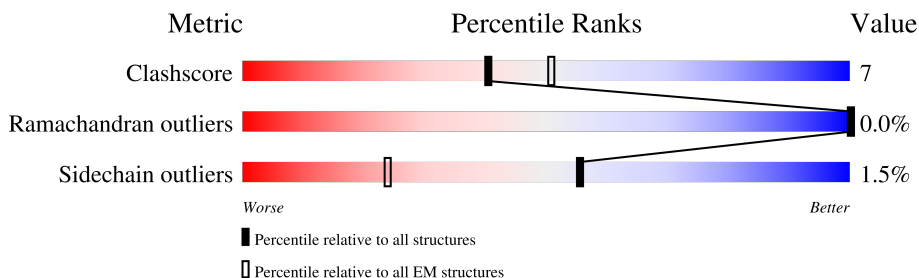
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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.



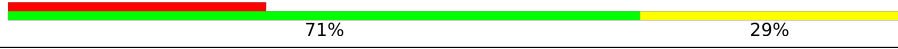
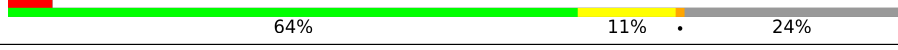
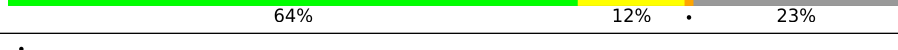
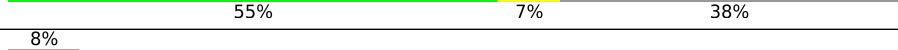
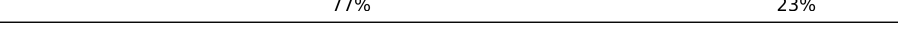
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	208	 84% 10% 6%
2	B	213	 72% 16% 11%
3	C	217	 71% 10% 20%
4	D	294	 63% 13% 24%

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Mol	Chain	Length	Quality of chain
5	E	650	
6	F	35	
7	G	7	
8	2	868	
9	3	971	
10	4	933	
11	5	775	
12	6	1017	
13	7	845	
14	X	43	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 83461 atoms, of which 41584 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 complex GINS protein PSF1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	196	Total	C	H	N	O	S	0	0
			3202	1005	1602	276	310	9		

- Molecule 2 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	189	Total	C	H	N	O	S	0	0
			3193	1014	1616	276	282	5		

- Molecule 3 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	174	Total	C	H	N	O	S	0	0
			2813	912	1413	225	257	6		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	expression tag	UNP Q12146
C	-21	GLY	-	expression tag	UNP Q12146
C	-20	SER	-	expression tag	UNP Q12146
C	-19	SER	-	expression tag	UNP Q12146
C	-18	HIS	-	expression tag	UNP Q12146
C	-17	HIS	-	expression tag	UNP Q12146
C	-16	HIS	-	expression tag	UNP Q12146
C	-15	HIS	-	expression tag	UNP Q12146
C	-14	HIS	-	expression tag	UNP Q12146
C	-13	HIS	-	expression tag	UNP Q12146
C	-12	SER	-	expression tag	UNP Q12146
C	-11	SER	-	expression tag	UNP Q12146
C	-10	GLY	-	expression tag	UNP Q12146
C	-9	LEU	-	expression tag	UNP Q12146
C	-8	VAL	-	expression tag	UNP Q12146

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	PRO	-	expression tag	UNP Q12146
C	-6	ARG	-	expression tag	UNP Q12146
C	-5	GLY	-	expression tag	UNP Q12146
C	-4	SER	-	expression tag	UNP Q12146
C	-3	HIS	-	expression tag	UNP Q12146
C	-2	MET	-	expression tag	UNP Q12146
C	-1	ALA	-	expression tag	UNP Q12146
C	0	SER	-	expression tag	UNP Q12146

- Molecule 4 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	222	Total	C	H	N	O	S	0	0
			3672	1170	1843	300	347	12		

- Molecule 5 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	566	Total	C	H	N	O	S	0	0
			9124	2922	4555	770	863	14		

- Molecule 6 is a DNA chain called Leading strand DNA template.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	35	Total	C	H	N	O	P	0	0
			1047	347	314	133	218	35		

- Molecule 7 is a DNA chain called Lagging strand DNA template.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	7	Total	C	H	N	O	P	0	0
			178	69	32	30	40	7		

- Molecule 8 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	2	664	Total	C	H	N	O	S	0	0
			10572	3305	5305	944	999	19		

- Molecule 9 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	3	618	Total	C	H	N	O	S	0	0
			9718	3044	4893	860	908	13		

- Molecule 10 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	4	612	Total	C	H	N	O	S	0	0
			9785	3067	4921	838	931	28		

- Molecule 11 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	5	595	Total	C	H	N	O	S	0	0
			9407	2951	4730	799	904	23		

- Molecule 12 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	6	634	Total	C	H	N	O	S	0	0
			10036	3159	5031	873	948	25		

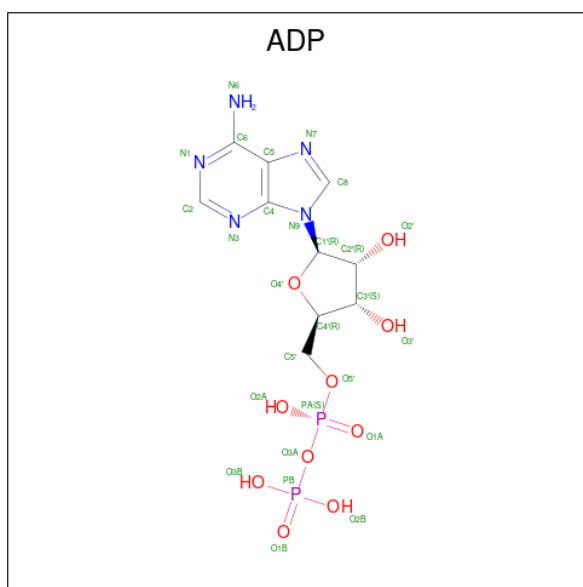
- Molecule 13 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	7	615	Total	C	H	N	O	S	0	0
			9784	3075	4919	847	917	26		

- Molecule 14 is a protein called Topoisomerase 1-associated factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	43	Total	C	H	N	O	0	0
			665	201	338	61	65		

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
15	2	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
16	2	1	Total	Mg	0
			1	1	
16	3	1	Total	Mg	0
			1	1	
16	4	1	Total	Mg	0
			1	1	
16	5	1	Total	Mg	0
			1	1	
16	6	1	Total	Mg	0
			1	1	
16	7	1	Total	Mg	0
			1	1	

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

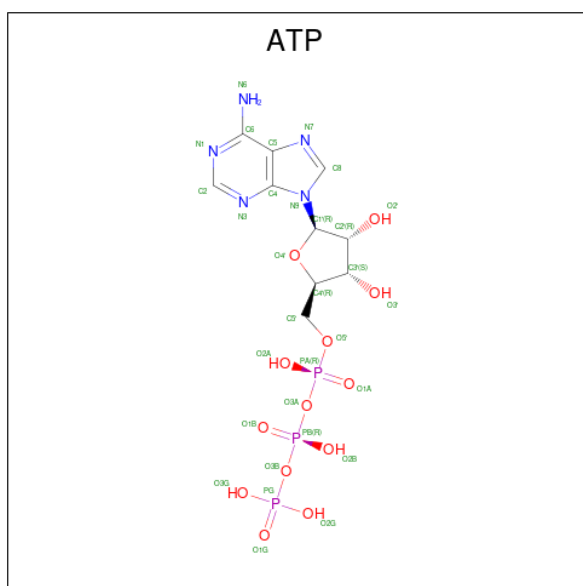
Mol	Chain	Residues	Atoms		AltConf
17	2	1	Total	Zn	0
			1	1	
17	4	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
17	5	1	Total	Zn	0
			1	1	
17	6	1	Total	Zn	0
			1	1	
17	7	1	Total	Zn	0
			1	1	

- Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

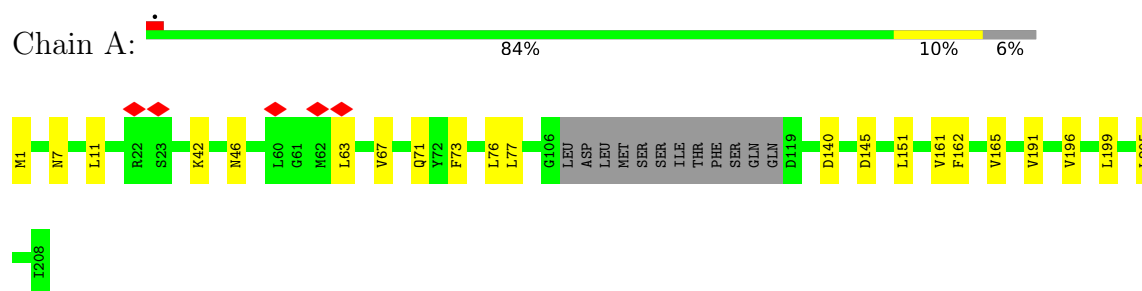


Mol	Chain	Residues	Atoms						AltConf
18	4	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
18	5	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
18	5	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
18	6	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
18	7	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

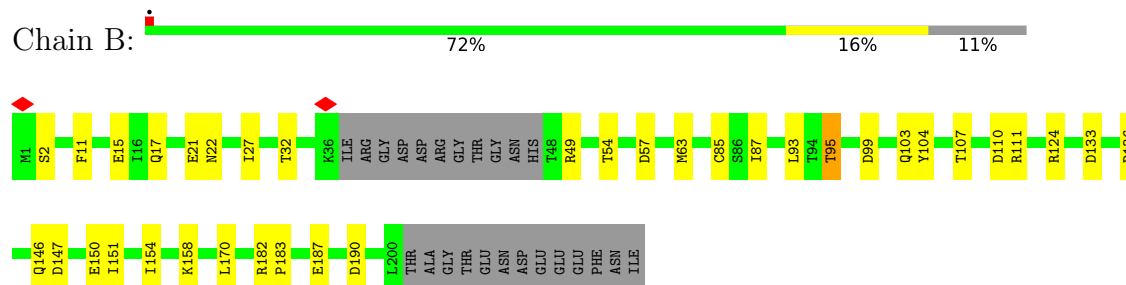
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

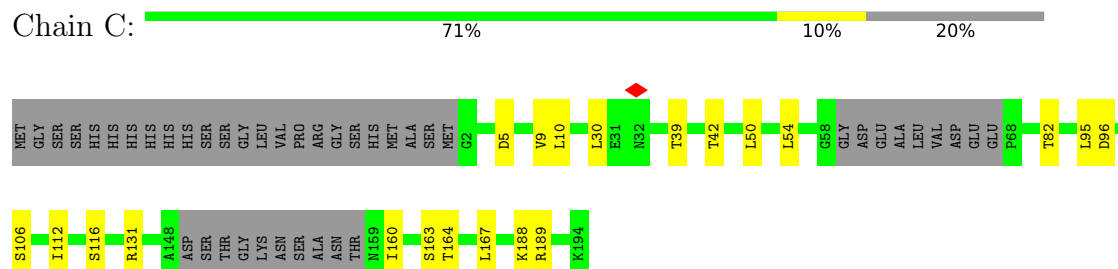
- Molecule 1: DNA replication complex GINS protein PSF1



- Molecule 2: DNA replication complex GINS protein PSF2

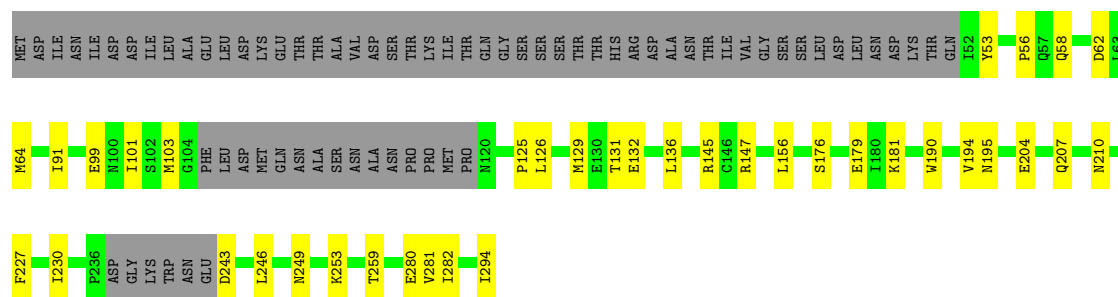


- Molecule 3: DNA replication complex GINS protein PSF3

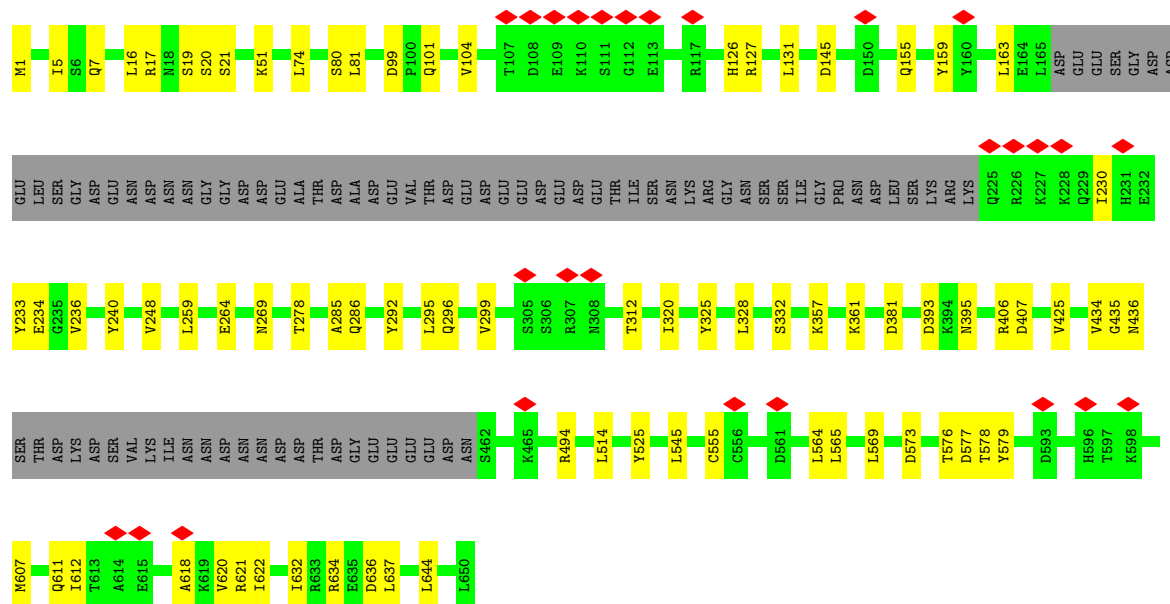


- Molecule 4: DNA replication complex GINS protein SLD5

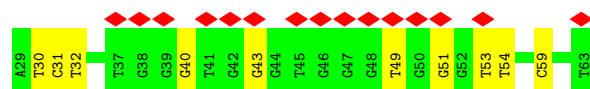




• Molecule 5: Cell division control protein 45



• Molecule 6: Leading strand DNA template



• Molecule 7: Lagging strand DNA template



• Molecule 8: DNA replication licensing factor MCM2



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81996	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 ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	15.407	Depositor
Minimum map value	-9.647	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.320	Depositor
Recommended contour level	0.841	Depositor
Map size ($\text{\AA}$)	370.04797, 370.04797, 370.04797	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8259999, 0.8259999, 0.8259999	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: ZN, MG, ADP, ATP

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	0.18	0/1620	0.33	0/2179
2	B	0.19	0/1609	0.36	0/2177
3	C	0.19	0/1433	0.36	0/1937
4	D	0.19	0/1863	0.36	0/2517
5	E	0.29	2/4656 (0.0%)	0.43	1/6306 (0.0%)
6	F	0.22	0/822	0.47	0/1272
7	G	0.20	0/164	0.36	0/251
8	2	0.89	28/5356 (0.5%)	0.68	23/7233 (0.3%)
9	3	0.17	0/4909	0.34	0/6657
10	4	0.23	0/4936	0.50	4/6671 (0.1%)
11	5	0.41	0/4743	0.70	1/6410 (0.0%)
12	6	0.15	0/5086	0.31	2/6861 (0.0%)
13	7	0.15	0/4943	0.30	0/6682
14	X	0.12	0/329	0.34	0/440
All	All	0.39	30/42469 (0.1%)	0.47	31/57593 (0.1%)

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
2	B	0	2
5	E	0	3
8	2	0	7
9	3	0	3
10	4	0	3
11	5	0	7
12	6	0	2
13	7	0	1
All	All	0	28

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	474	PHE	C-O	-24.57	1.02	1.24
8	2	475	SER	C-O	-15.35	1.04	1.23
8	2	493	ILE	C-O	-14.69	1.06	1.24
8	2	494	ILE	C-O	-14.64	1.04	1.24
8	2	475	SER	CA-CB	-14.26	1.29	1.54

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	4	834	LYS	CA-C-N	-12.93	100.65	120.31
10	4	834	LYS	C-N-CA	-12.93	100.65	120.31
8	2	484	PHE	N-CA-C	-10.40	99.69	112.38
8	2	482	ARG	N-CA-C	-9.17	102.10	113.38
8	2	495	ASP	CB-CA-C	-9.01	93.93	109.07

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	124	ARG	Sidechain
2	B	49	ARG	Sidechain
5	E	17	ARG	Sidechain
5	E	494	ARG	Sidechain
5	E	621	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1600	1602	1602	17	0
2	B	1577	1616	1625	27	0
3	C	1400	1413	1413	11	0
4	D	1829	1843	1844	28	0
5	E	4569	4555	4562	46	0
6	F	733	314	398	12	0
7	G	146	32	79	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	2	5267	5305	5309	59	0
9	3	4825	4893	4897	69	0
10	4	4864	4921	4937	103	0
11	5	4677	4730	4751	72	0
12	6	5005	5031	5032	54	0
13	7	4865	4919	4919	136	0
14	X	327	338	340	17	0
15	2	27	12	12	0	0
16	2	1	0	0	0	0
16	3	1	0	0	0	0
16	4	1	0	0	0	0
16	5	1	0	0	0	0
16	6	1	0	0	0	0
16	7	1	0	0	0	0
17	2	1	0	0	0	0
17	4	1	0	0	0	0
17	5	1	0	0	0	0
17	6	1	0	0	0	0
17	7	1	0	0	0	0
18	4	31	12	12	0	0
18	5	62	24	24	5	0
18	6	31	12	12	2	0
18	7	31	12	12	1	0
All	All	41877	41584	41780	580	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 7.

The worst 5 of 580 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)
11:5:278:CYS:SG	11:5:282:LEU:HB2	1.51	1.48
11:5:278:CYS:SG	11:5:282:LEU:CB	2.04	1.46
10:4:458:LYS:HE2	12:6:431:GLU:O	1.16	1.33
13:7:459:MET:SD	13:7:584:ILE:HD12	1.67	1.32
13:7:538:HIS:CD2	13:7:593:ARG:NH1	2.01	1.28

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	192/208 (92%)	187 (97%)	5 (3%)	0	100	100
2	B	185/213 (87%)	179 (97%)	6 (3%)	0	100	100
3	C	168/217 (77%)	166 (99%)	2 (1%)	0	100	100
4	D	216/294 (74%)	206 (95%)	10 (5%)	0	100	100
5	E	560/650 (86%)	546 (98%)	14 (2%)	0	100	100
8	2	660/868 (76%)	641 (97%)	19 (3%)	0	100	100
9	3	608/971 (63%)	594 (98%)	14 (2%)	0	100	100
10	4	604/933 (65%)	591 (98%)	12 (2%)	1 (0%)	43	73
11	5	583/775 (75%)	555 (95%)	28 (5%)	0	100	100
12	6	622/1017 (61%)	599 (96%)	23 (4%)	0	100	100
13	7	605/845 (72%)	590 (98%)	15 (2%)	0	100	100
14	X	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
All	All	5044/7034 (72%)	4894 (97%)	149 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	4	834	LYS

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	180/193 (93%)	179 (99%)	1 (1%)	78	84
2	B	178/198 (90%)	173 (97%)	5 (3%)	38	68
3	C	156/192 (81%)	152 (97%)	4 (3%)	40	69
4	D	214/279 (77%)	210 (98%)	4 (2%)	50	73
5	E	505/586 (86%)	500 (99%)	5 (1%)	68	80
8	2	582/770 (76%)	573 (98%)	9 (2%)	57	76
9	3	533/835 (64%)	525 (98%)	8 (2%)	57	76
10	4	551/848 (65%)	544 (99%)	7 (1%)	61	78
11	5	535/688 (78%)	524 (98%)	11 (2%)	47	71
12	6	551/886 (62%)	544 (99%)	7 (1%)	61	78
13	7	542/753 (72%)	536 (99%)	6 (1%)	65	79
14	X	37/37 (100%)	36 (97%)	1 (3%)	39	68
All	All	4564/6265 (73%)	4496 (98%)	68 (2%)	55	76

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	6	640	GLU
12	6	767	LYS
13	7	553	ILE
8	2	645	SER
8	2	406	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
10	4	543	GLN
12	6	583	GLN
11	5	64	ASN
11	5	570	ASN
13	7	68	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	ATP	7	1001	16	32,33,33	0.31	0	48,52,52	0.71	0
15	ADP	2	1001	16	28,29,29	1.36	4 (14%)	43,45,45	1.90	10 (23%)
18	ATP	5	802	16	32,33,33	0.41	0	48,52,52	0.73	0
18	ATP	4	1001	16	32,33,33	0.29	0	48,52,52	0.69	0
18	ATP	5	801	16	32,33,33	0.37	0	48,52,52	0.75	0
18	ATP	6	1101	16	32,33,33	0.34	0	48,52,52	0.73	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
18	ATP	7	1001	16	-	6/22/38/38	0/3/3/3
15	ADP	2	1001	16	-	1/16/32/32	0/3/3/3
18	ATP	5	802	16	-	9/22/38/38	0/3/3/3
18	ATP	4	1001	16	-	7/22/38/38	0/3/3/3
18	ATP	5	801	16	-	5/22/38/38	0/3/3/3
18	ATP	6	1101	16	-	0/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	1001	ADP	C5-C4	4.47	1.47	1.39
15	2	1001	ADP	C5-C6	2.59	1.48	1.41
15	2	1001	ADP	C5-N7	-2.35	1.34	1.39
15	2	1001	ADP	C8-N7	2.31	1.36	1.31

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	1001	ADP	C5-C4-N3	-5.82	118.70	126.72
15	2	1001	ADP	N3-C4-N9	4.70	135.15	127.17
15	2	1001	ADP	C2-N3-C4	3.87	121.28	111.83
15	2	1001	ADP	N3-C2-N1	-3.75	122.90	128.58
15	2	1001	ADP	C4-C5-N7	-3.40	106.69	110.58

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	4	1001	ATP	PB-O3B-PG-O2G
18	4	1001	ATP	C5'-O5'-PA-O2A
18	4	1001	ATP	C5'-O5'-PA-O3A
18	5	801	ATP	C5'-O5'-PA-O1A
18	5	801	ATP	C5'-O5'-PA-O3A

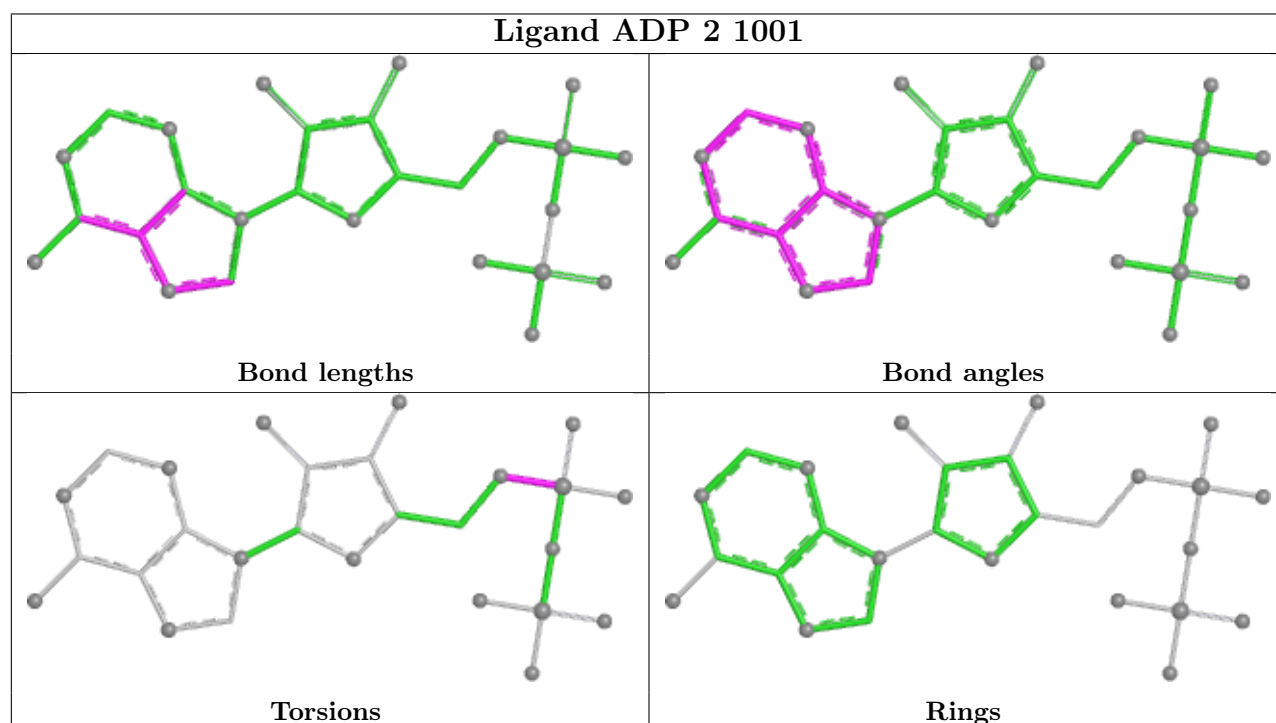
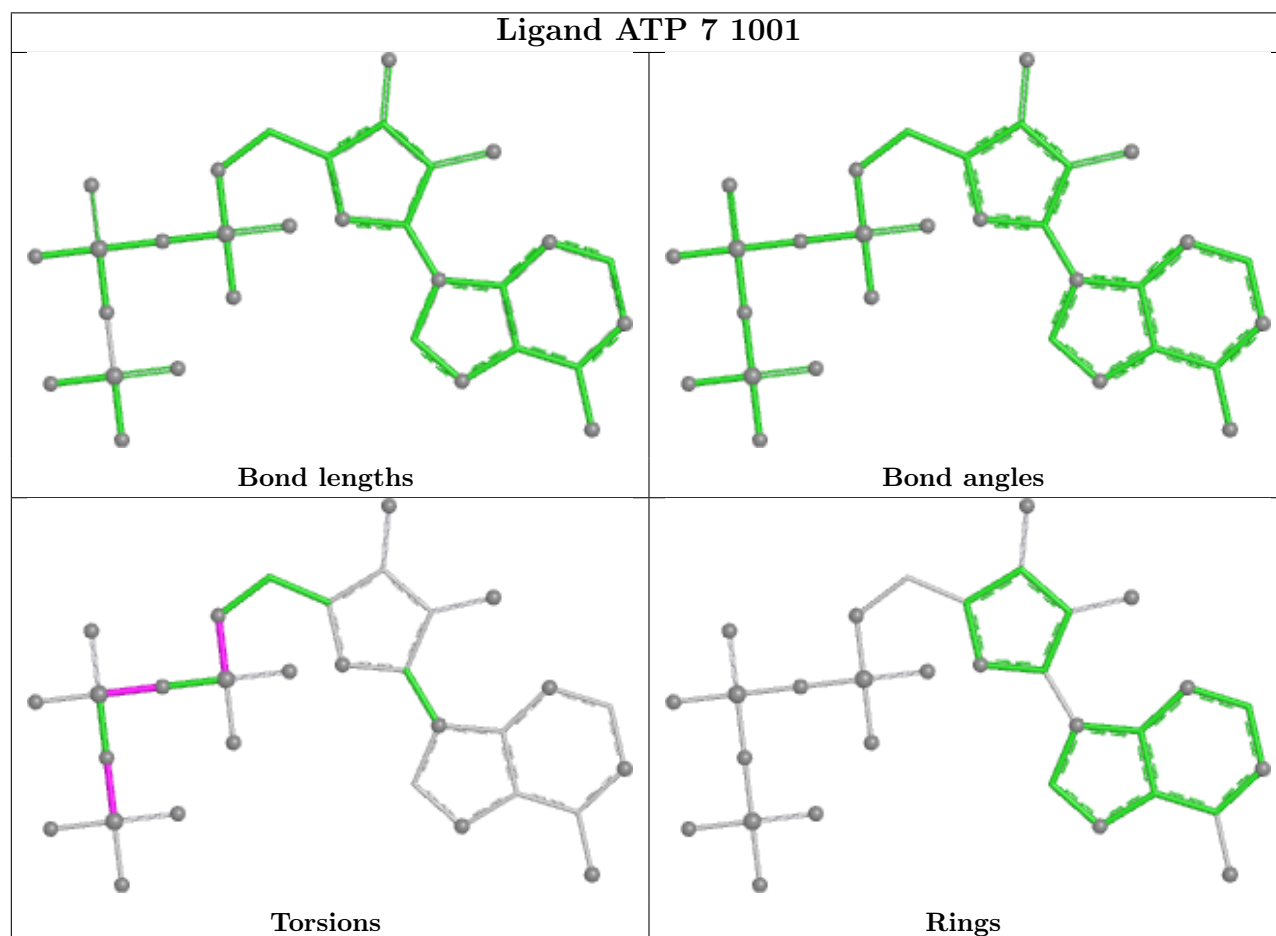
There are no ring outliers.

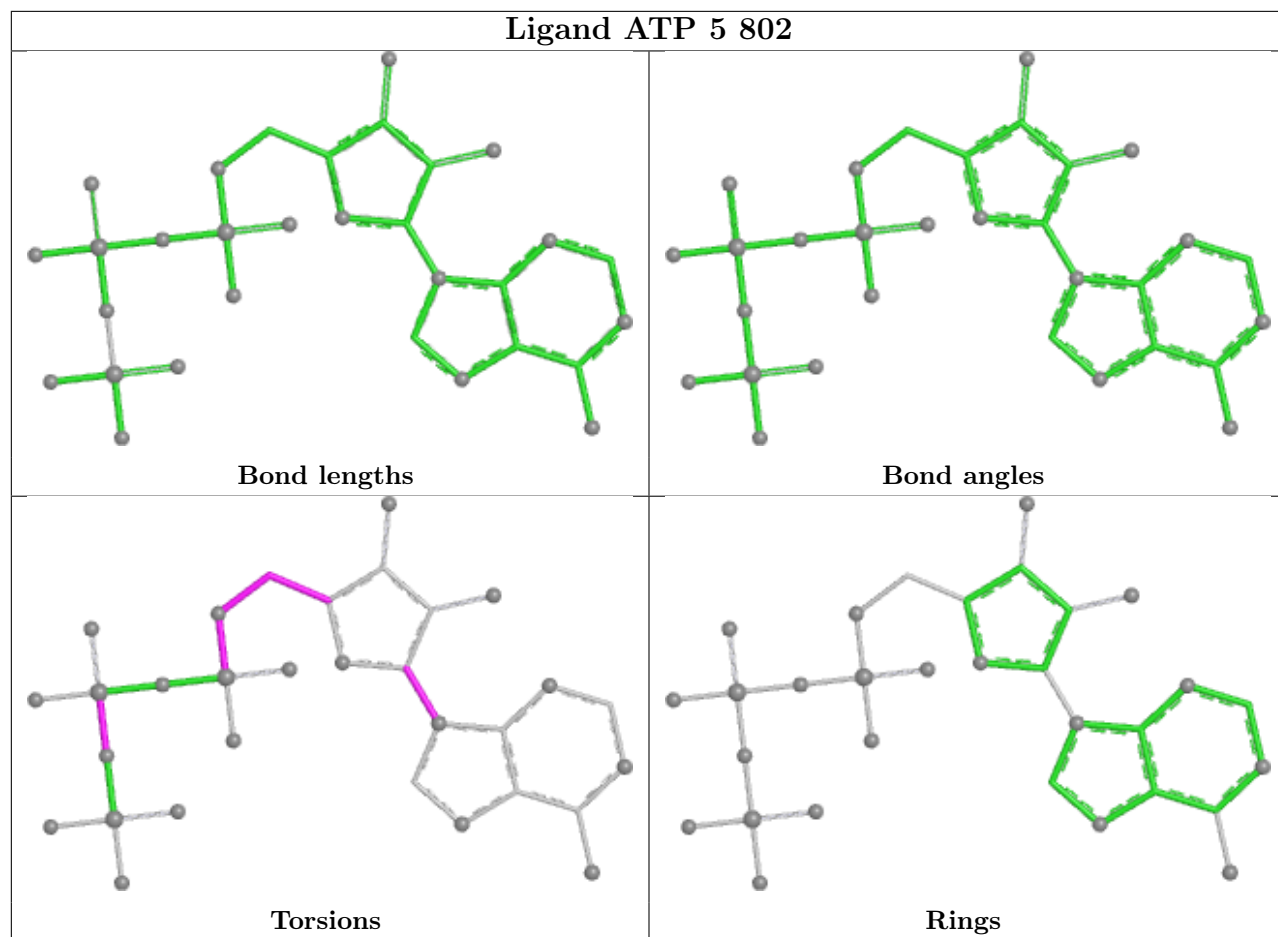
4 monomers are involved in 8 short contacts:

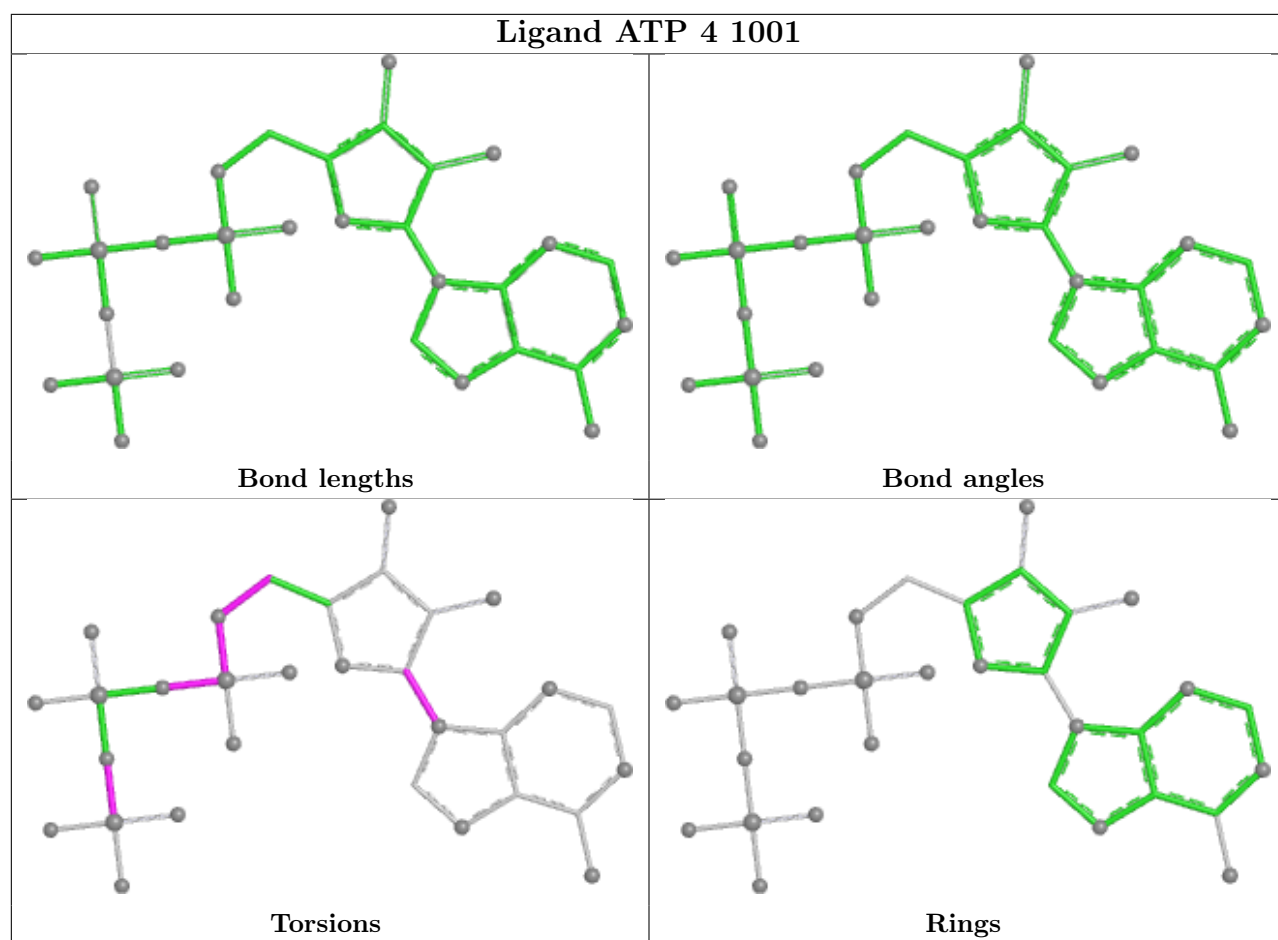
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	7	1001	ATP	1	0
18	5	802	ATP	3	0
18	5	801	ATP	2	0
18	6	1101	ATP	2	0

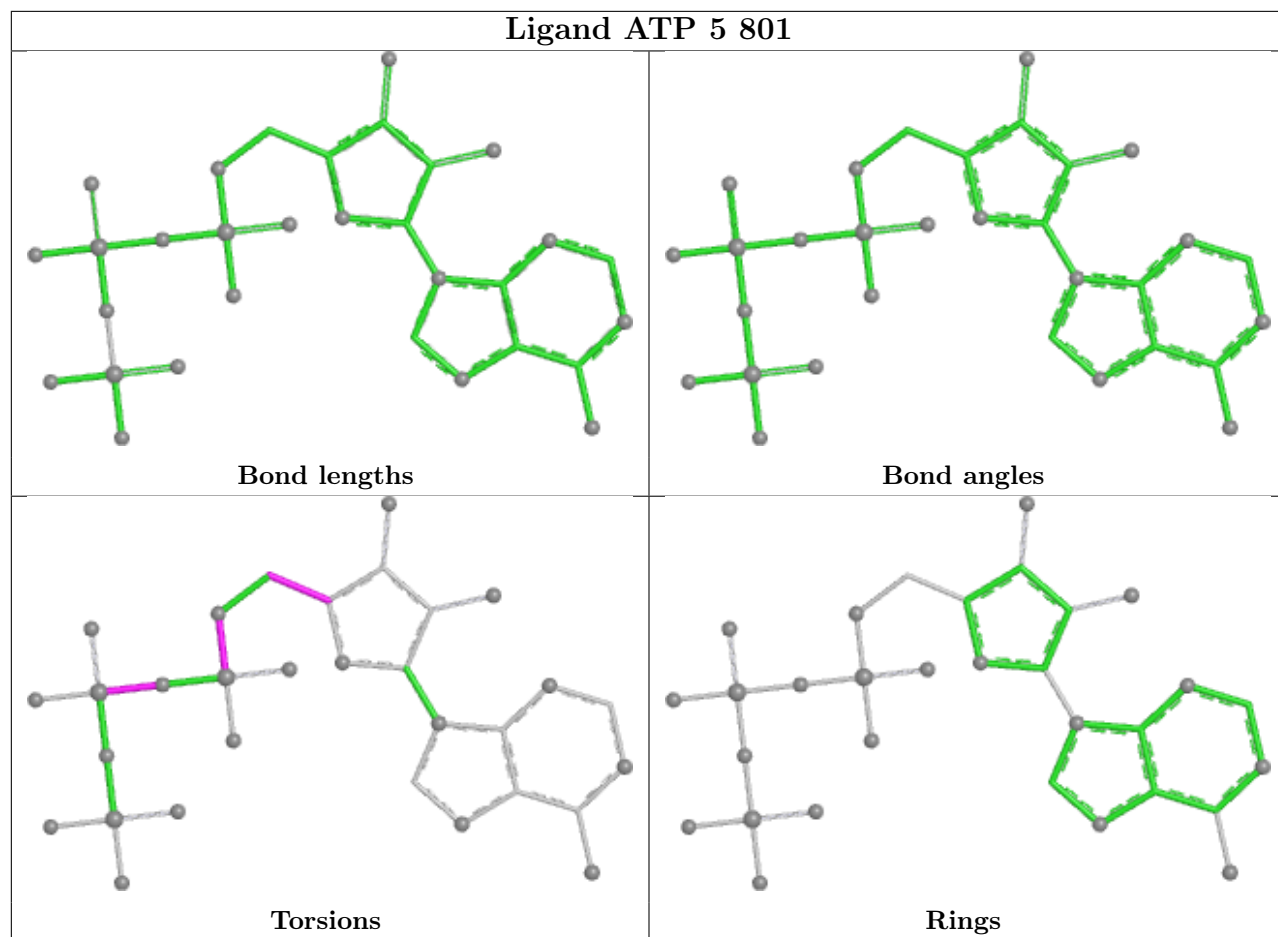
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

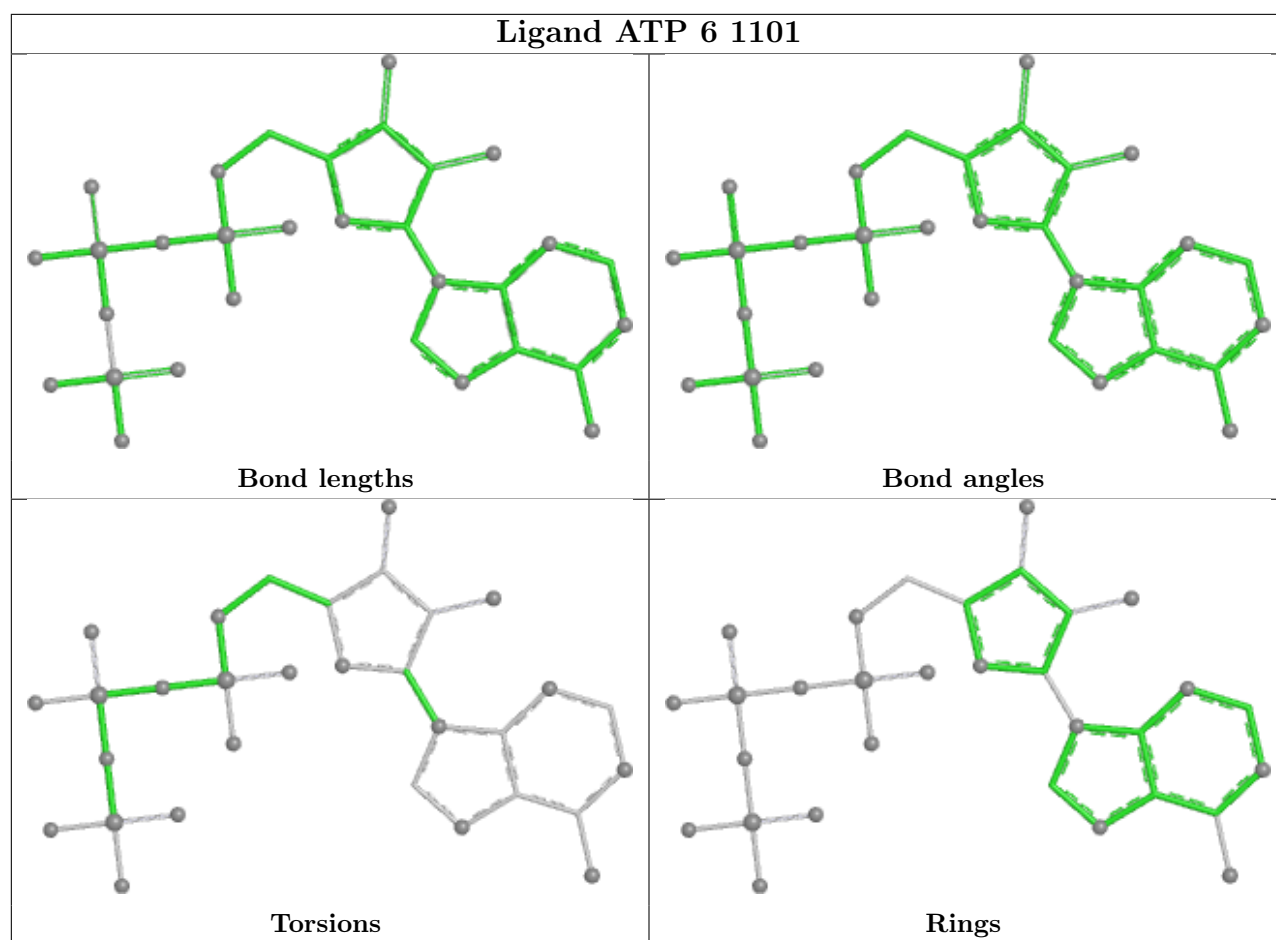
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

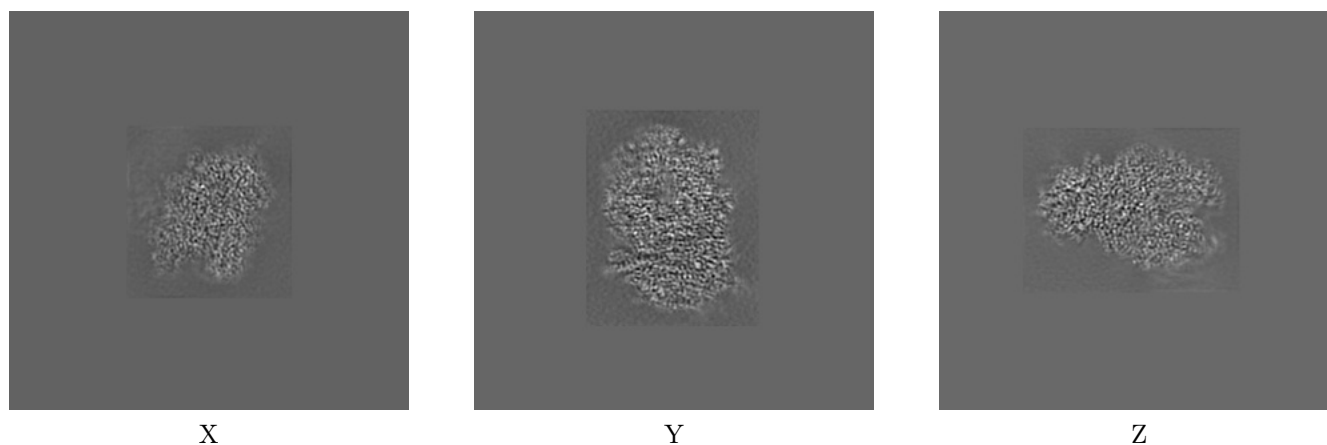
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47472. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

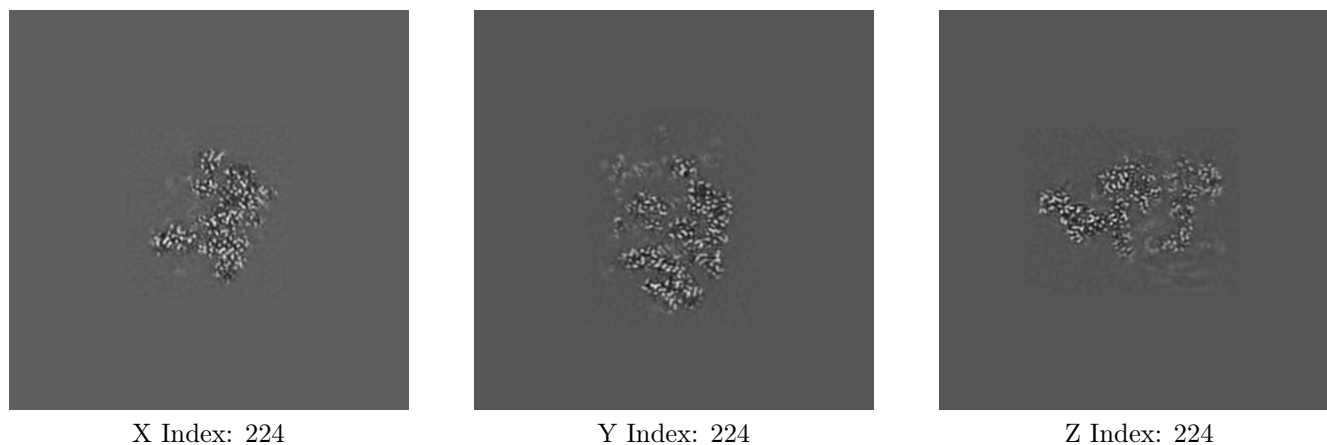
6.1.1 Primary map



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

6.2 Central slices [i](#)

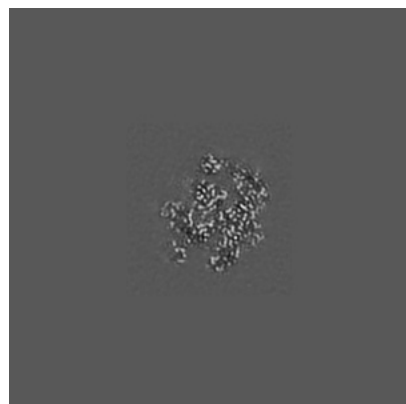
6.2.1 Primary map



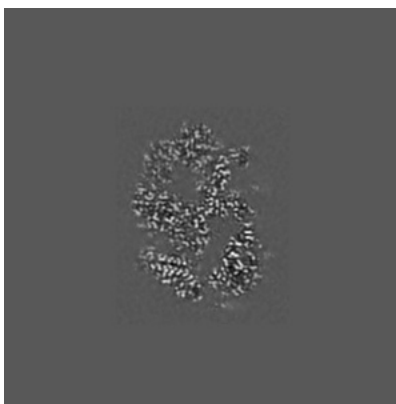
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

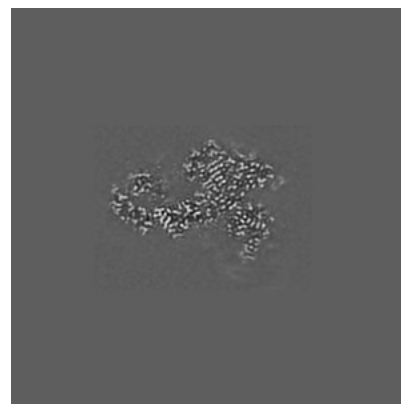
6.3.1 Primary map



X Index: 209



Y Index: 248

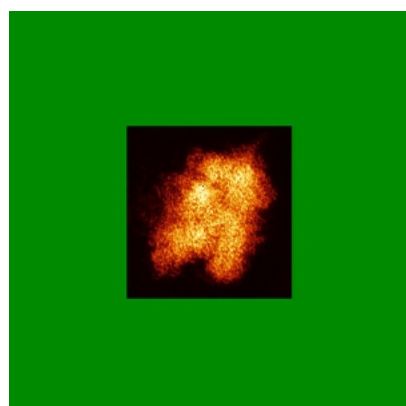


Z Index: 243

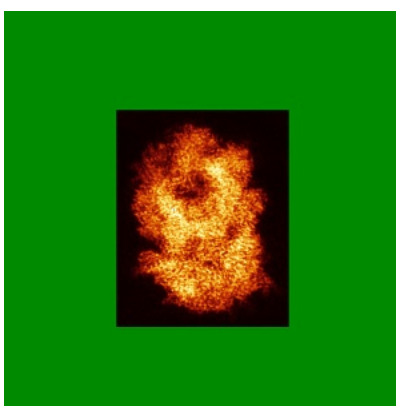
The images above show the largest variance slices of the map in three orthogonal directions.

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

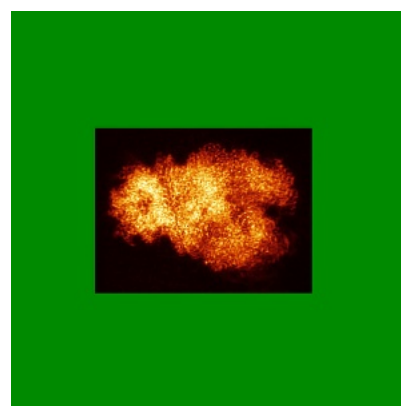
6.4.1 Primary map



X



Y

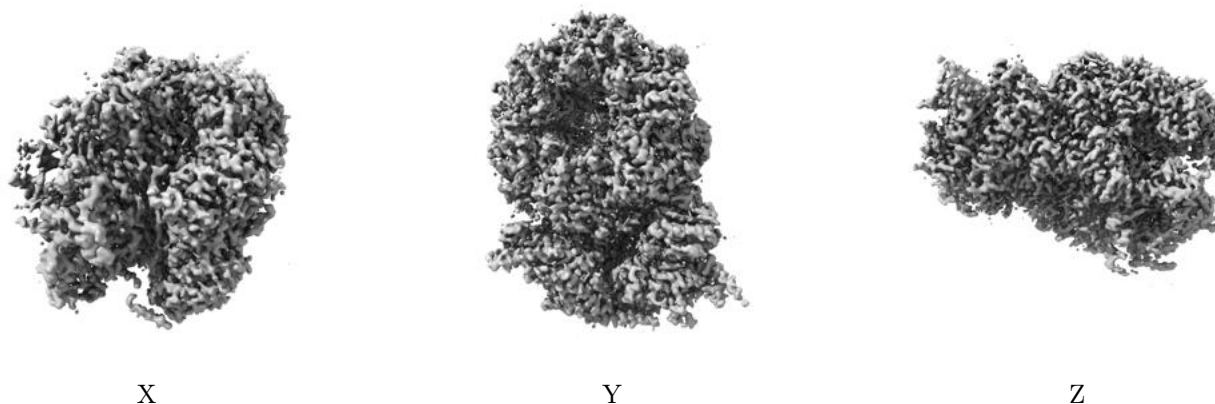


Z

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 0.841. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

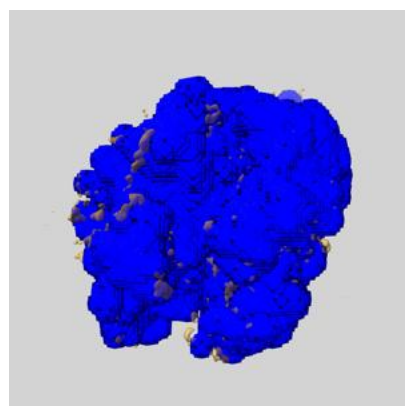
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

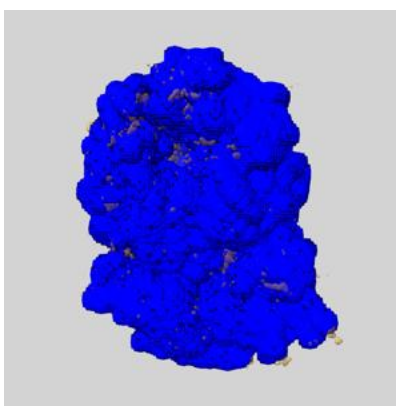
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

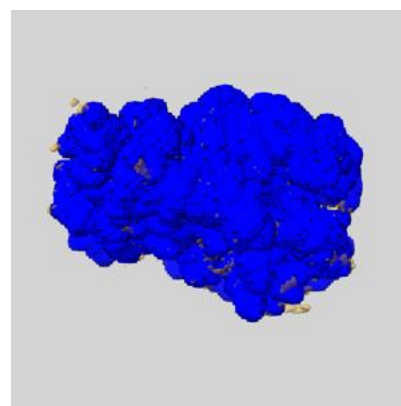
6.6.1 emd_47472_msk_1.map [i](#)



X



Y

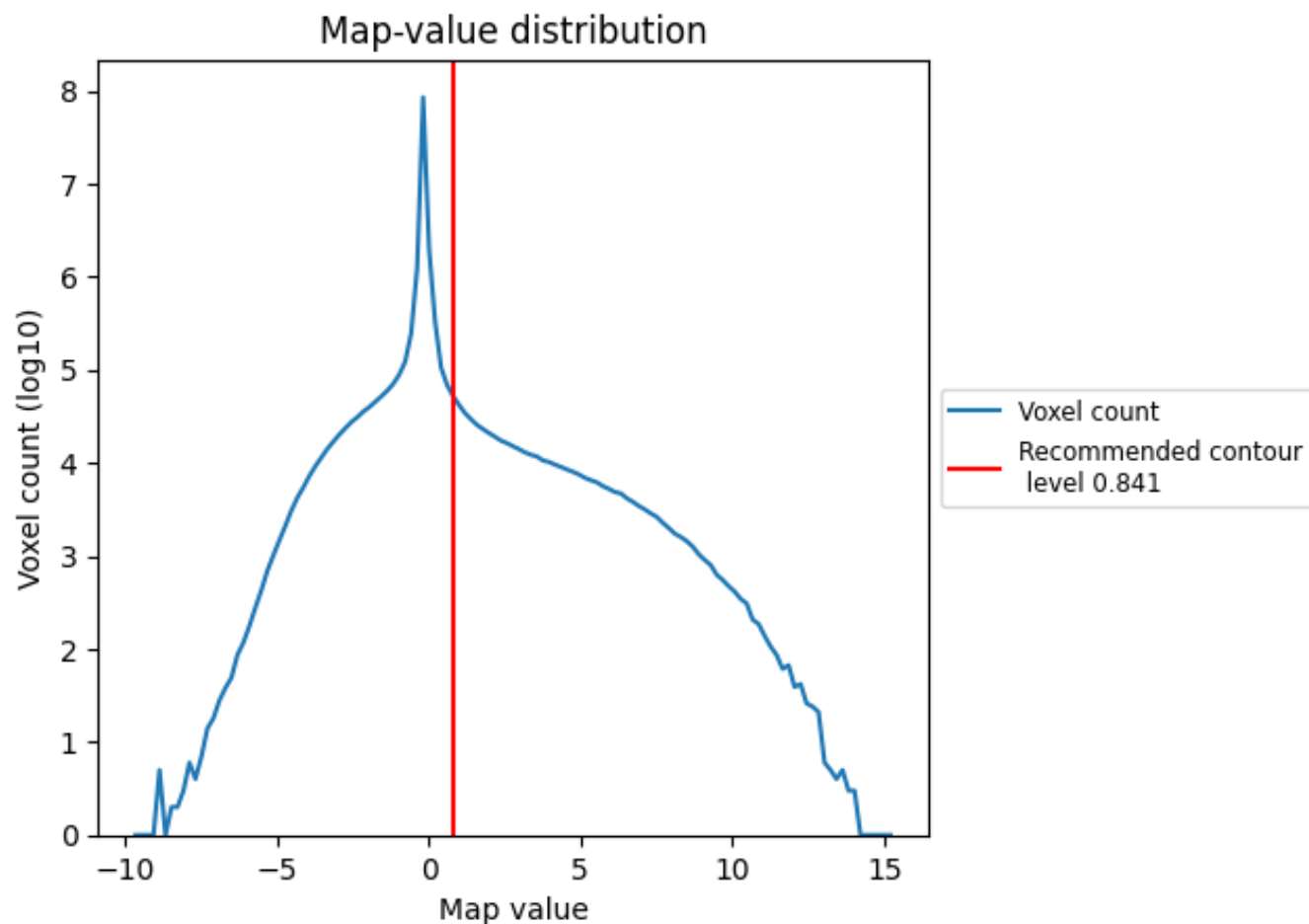


Z

7 Map analysis [i](#)

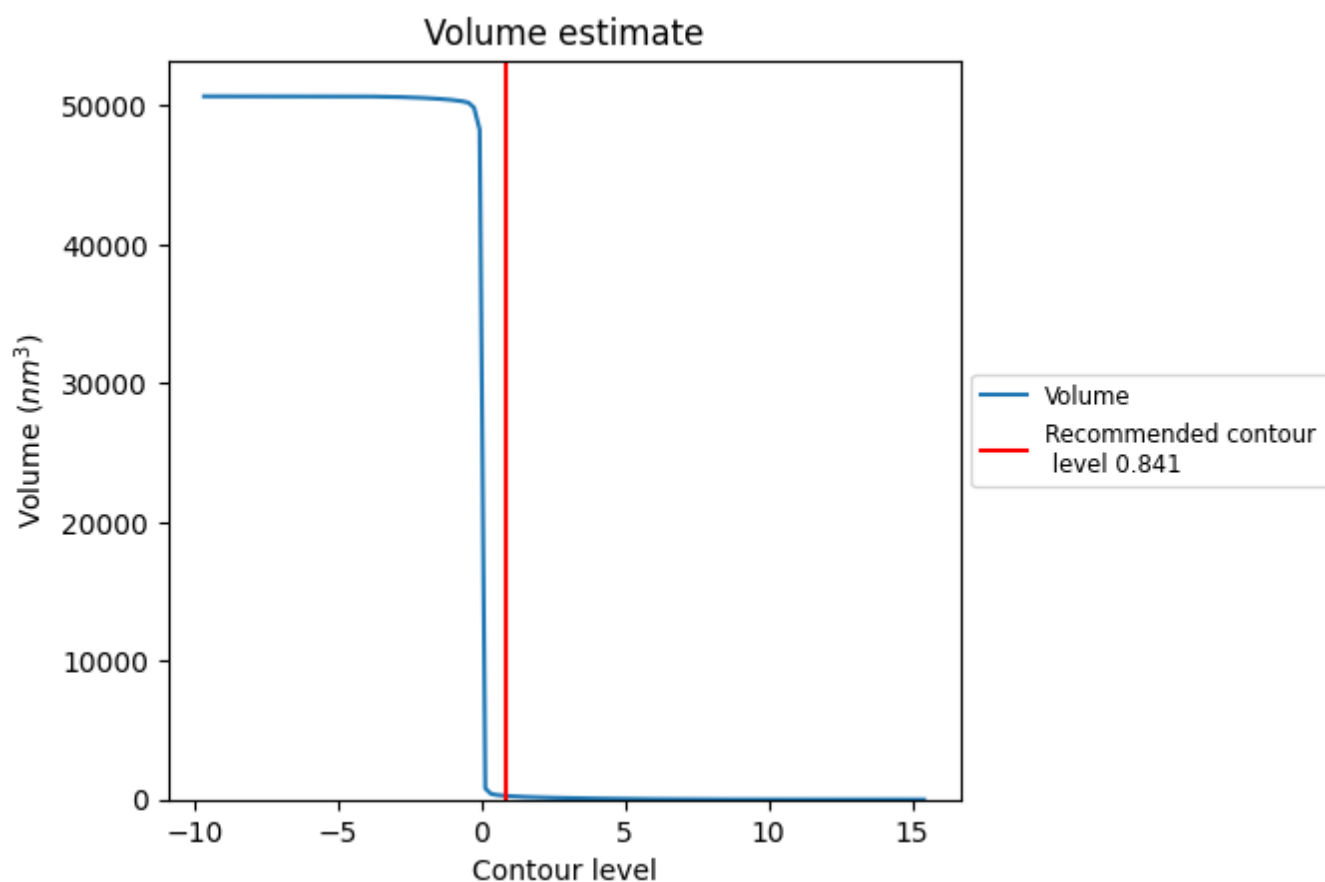
This section contains the results of statistical analysis of the map.

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.

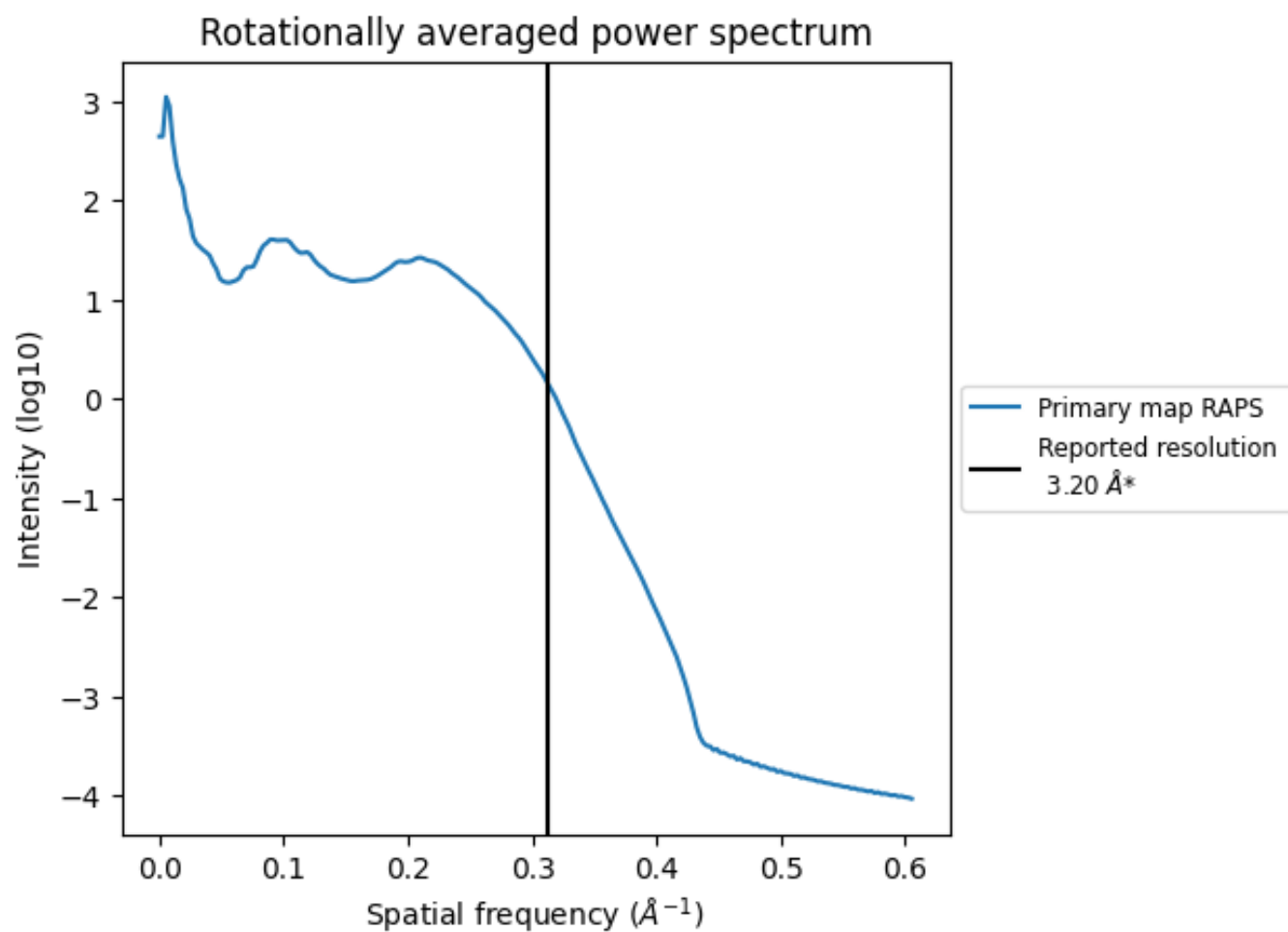
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm³; this corresponds to an approximate mass of 243 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 ⓘ

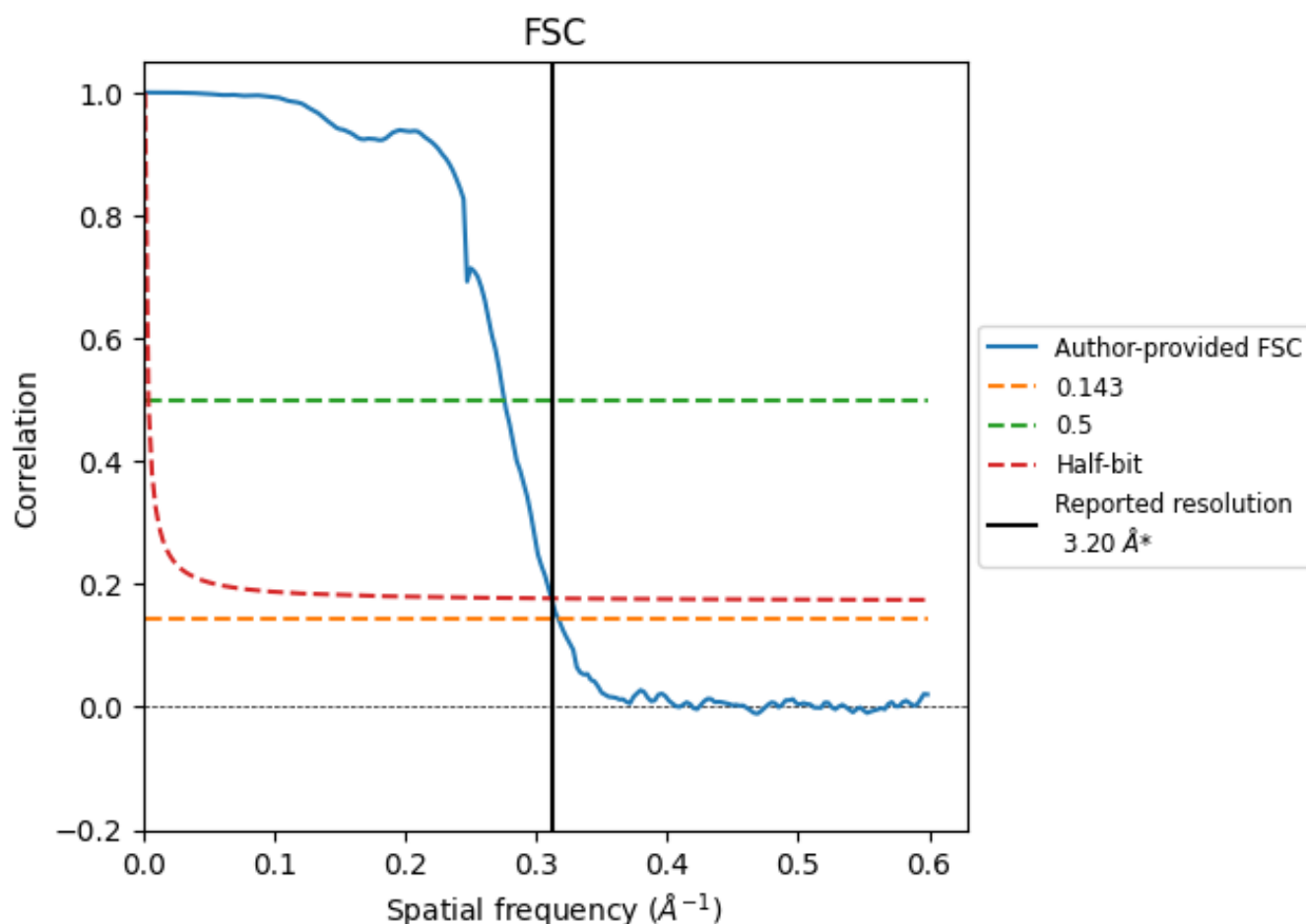


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

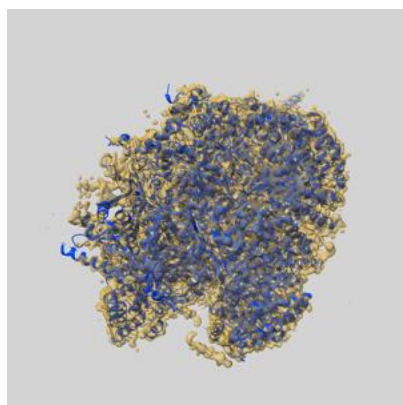
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.63	3.21
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

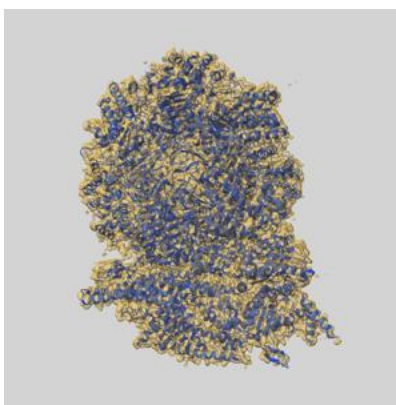
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47472 and PDB model 9E2Y. Per-residue inclusion information can be found in section [3](#) on page [9](#).

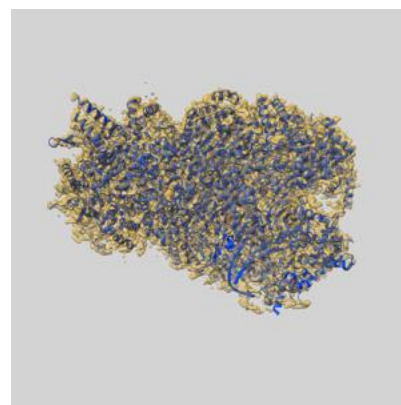
9.1 Map-model overlay [i](#)



X



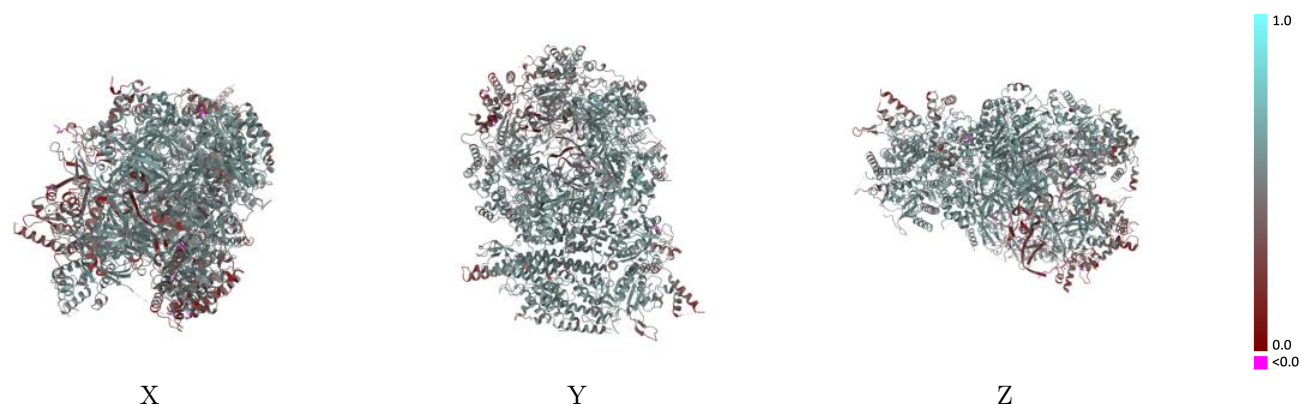
Y



Z

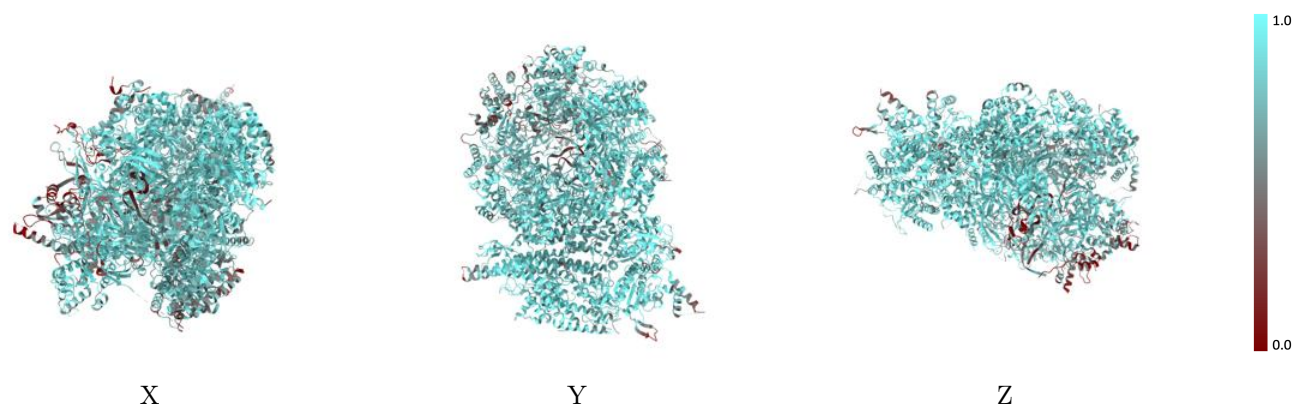
The images above show the 3D surface view of the map at the recommended contour level 0.841 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



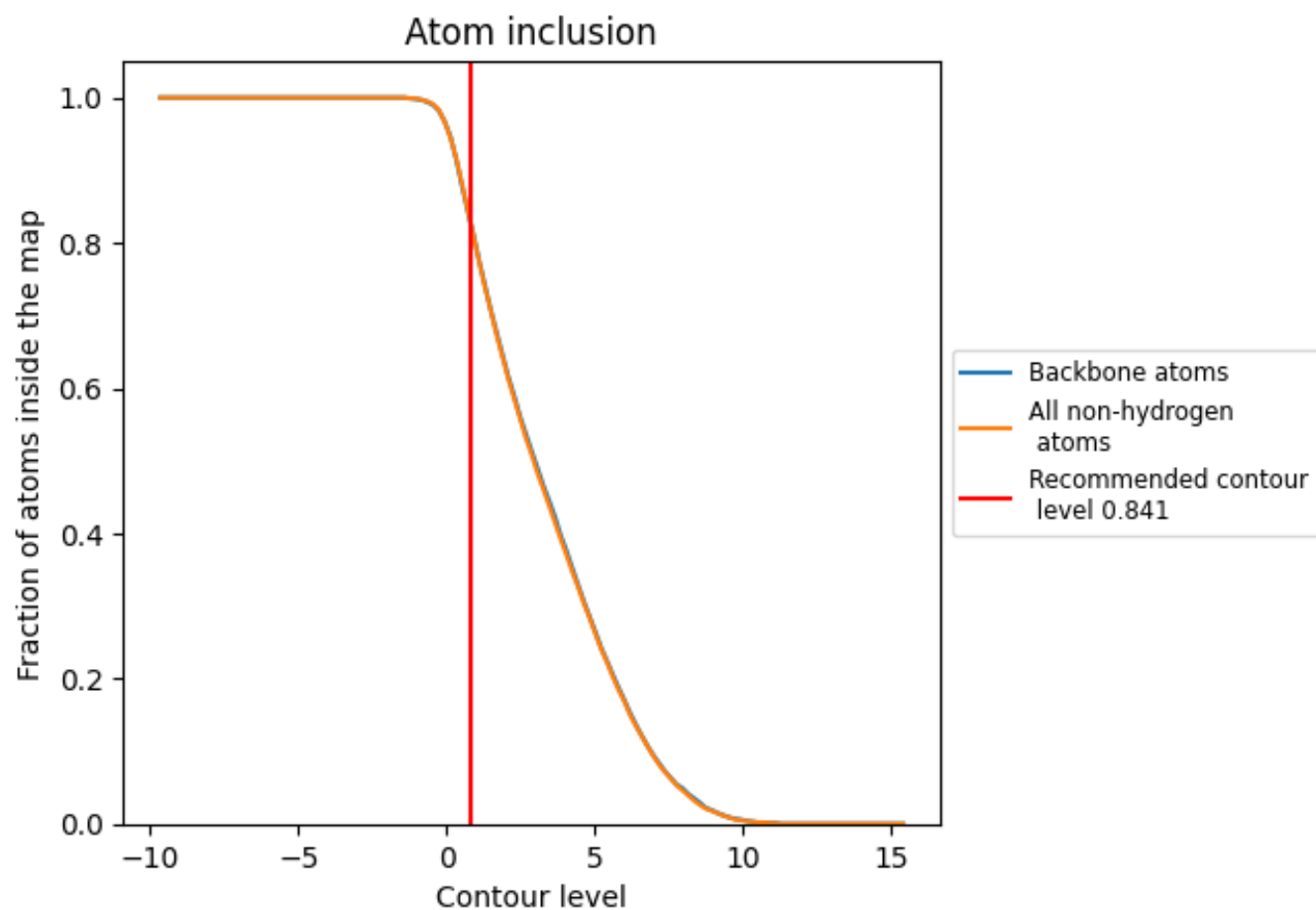
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.841).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (0.841) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8230	0.5130
2	0.8510	0.5450
3	0.8860	0.5530
4	0.7590	0.4600
5	0.8930	0.5620
6	0.8330	0.5130
7	0.7290	0.4480
A	0.8540	0.5100
B	0.9170	0.5660
C	0.9120	0.5530
D	0.8890	0.5390
E	0.8580	0.5220
F	0.5060	0.3350
G	0.5820	0.3040
X	0.3240	0.3250

1.0

0.0

<0.0