



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 04:07 PM UTC

PDB ID : 9E2Z / pdb_00009e2z
EMDB ID : EMD-47473
Title : Cryo-EM structure of human CMG helicase stalled at G4-containing DNA template
Authors : Allwein, B.; Batra, S.; Remus, D.; Hite, R.
Deposited on : 2024-10-23
Resolution : 2.60 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 EMD 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

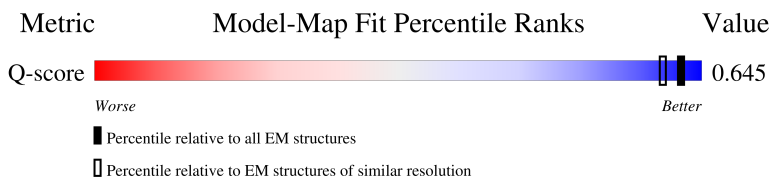
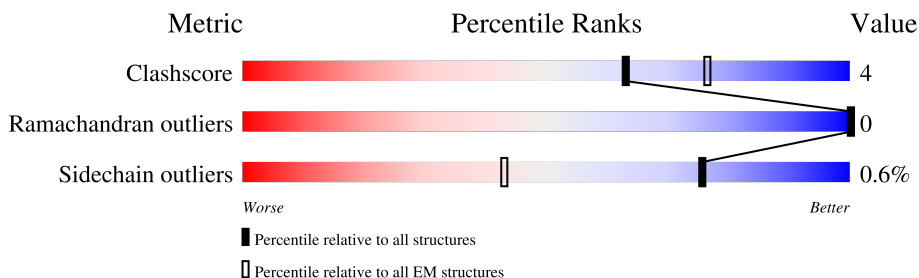
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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.



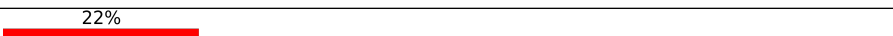
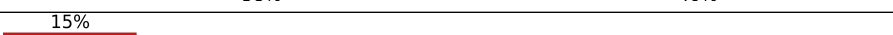
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	2	904	
2	3	853	
3	4	883	
4	5	734	

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Mol	Chain	Length	Quality of chain
5	6	821	
6	7	719	
7	A	196	
8	B	222	
9	C	216	
10	D	223	
11	E	566	
12	F	40	
13	G	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
17	ZN	7	1003	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 81491 atoms, of which 40474 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 MCM2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	2	616	Total	C	H	N	O	S	0	0
			9714	3062	4849	866	911	26		

- Molecule 2 is a protein called Isoform 2 of DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	3	639	Total	C	H	N	O	S	0	0
			10064	3138	5047	884	969	26		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	4	607	Total	C	H	N	O	S	0	0
			9711	3055	4864	855	911	26		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	-19	MET	-	initiating methionine	UNP P33991
4	-18	HIS	-	expression tag	UNP P33991
4	-17	HIS	-	expression tag	UNP P33991
4	-16	HIS	-	expression tag	UNP P33991
4	-15	HIS	-	expression tag	UNP P33991
4	-14	HIS	-	expression tag	UNP P33991
4	-13	HIS	-	expression tag	UNP P33991
4	-12	HIS	-	expression tag	UNP P33991
4	-11	HIS	-	expression tag	UNP P33991
4	-10	GLU	-	expression tag	UNP P33991
4	-9	ASN	-	expression tag	UNP P33991
4	-8	LEU	-	expression tag	UNP P33991
4	-7	TYR	-	expression tag	UNP P33991
4	-6	PHE	-	expression tag	UNP P33991
4	-5	GLN	-	expression tag	UNP P33991

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Chain	Residue	Modelled	Actual	Comment	Reference
4	-4	GLY	-	expression tag	UNP P33991
4	-3	SER	-	expression tag	UNP P33991
4	-2	SER	-	expression tag	UNP P33991
4	-1	ALA	-	expression tag	UNP P33991
4	0	THR	-	expression tag	UNP P33991

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	5	624	Total	C	H	N	O	S	0	0
			9825	3055	4938	875	922	35		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	6	617	Total	C	H	N	O	S	0	0
			9881	3100	4949	875	931	26		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	7	565	Total	C	H	N	O	S	0	0
			9030	2830	4531	794	847	28		

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A	195	Total	C	H	N	O	S	0	0
			3193	1011	1589	289	293	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	B	176	Total	C	H	N	O	S	0	0
			2883	916	1452	242	264	9		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	186	GLU	-	expression tag	UNP Q9Y248
B	187	ASN	-	expression tag	UNP Q9Y248

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Chain	Residue	Modelled	Actual	Comment	Reference
B	188	LEU	-	expression tag	UNP Q9Y248
B	189	TYR	-	expression tag	UNP Q9Y248
B	190	PHE	-	expression tag	UNP Q9Y248
B	191	GLN	-	expression tag	UNP Q9Y248
B	192	GLY	-	expression tag	UNP Q9Y248
B	193	SER	-	expression tag	UNP Q9Y248
B	194	ALA	-	expression tag	UNP Q9Y248
B	195	TRP	-	expression tag	UNP Q9Y248
B	196	SER	-	expression tag	UNP Q9Y248
B	197	HIS	-	expression tag	UNP Q9Y248
B	198	PRO	-	expression tag	UNP Q9Y248
B	199	GLN	-	expression tag	UNP Q9Y248
B	200	PHE	-	expression tag	UNP Q9Y248
B	201	GLU	-	expression tag	UNP Q9Y248
B	202	LYS	-	expression tag	UNP Q9Y248
B	203	GLY	-	expression tag	UNP Q9Y248
B	204	GLY	-	expression tag	UNP Q9Y248
B	205	GLY	-	expression tag	UNP Q9Y248
B	206	SER	-	expression tag	UNP Q9Y248
B	207	GLY	-	expression tag	UNP Q9Y248
B	208	GLY	-	expression tag	UNP Q9Y248
B	209	GLY	-	expression tag	UNP Q9Y248
B	210	SER	-	expression tag	UNP Q9Y248
B	211	GLY	-	expression tag	UNP Q9Y248
B	212	GLY	-	expression tag	UNP Q9Y248
B	213	SER	-	expression tag	UNP Q9Y248
B	214	ALA	-	expression tag	UNP Q9Y248
B	215	TRP	-	expression tag	UNP Q9Y248
B	216	SER	-	expression tag	UNP Q9Y248
B	217	HIS	-	expression tag	UNP Q9Y248
B	218	PRO	-	expression tag	UNP Q9Y248
B	219	GLN	-	expression tag	UNP Q9Y248
B	220	PHE	-	expression tag	UNP Q9Y248
B	221	GLU	-	expression tag	UNP Q9Y248
B	222	LYS	-	expression tag	UNP Q9Y248

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	C	196	Total	C	H	N	O	S	0	0
			3106	998	1534	275	293	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	D	204	Total	C	H	N	O	S	0	0
			3389	1070	1704	291	314	10		

- Molecule 11 is a protein called Cell division control protein 45 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	533	Total	C	H	N	O	S	0	0
			8607	2760	4268	744	804	31		

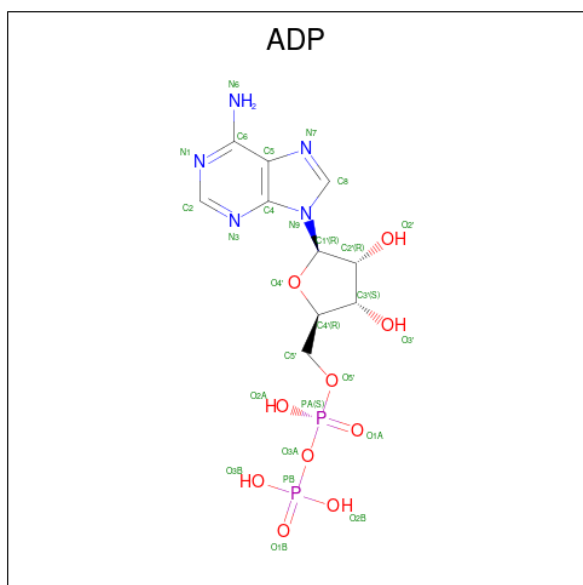
- Molecule 12 is a DNA chain called Leading strand DNA template.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	F	40	Total	C	H	N	O	P	0	0
			1292	397	453	155	247	40		

- Molecule 13 is a DNA chain called Lagging strand DNA template.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	G	13	Total	C	H	N	O	P	0	0
			413	127	146	53	74	13		

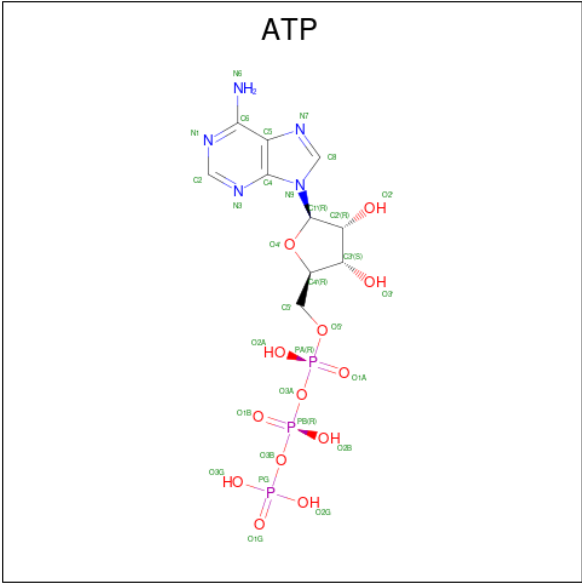
- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
15	2	1	Total	Mg	0
			1	1	
15	3	1	Total	Mg	0
			1	1	
15	4	1	Total	Mg	0
			1	1	
15	5	1	Total	Mg	0
			1	1	
15	6	1	Total	Mg	0
			1	1	
15	7	1	Total	Mg	0
			1	1	

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms						AltConf
16	7	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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

Mol	Chain	Residues	Atoms		AltConf
17	4	1	Total	Zn	0
			1	1	
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 POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
18	F	2	Total	K	0
			2	2	

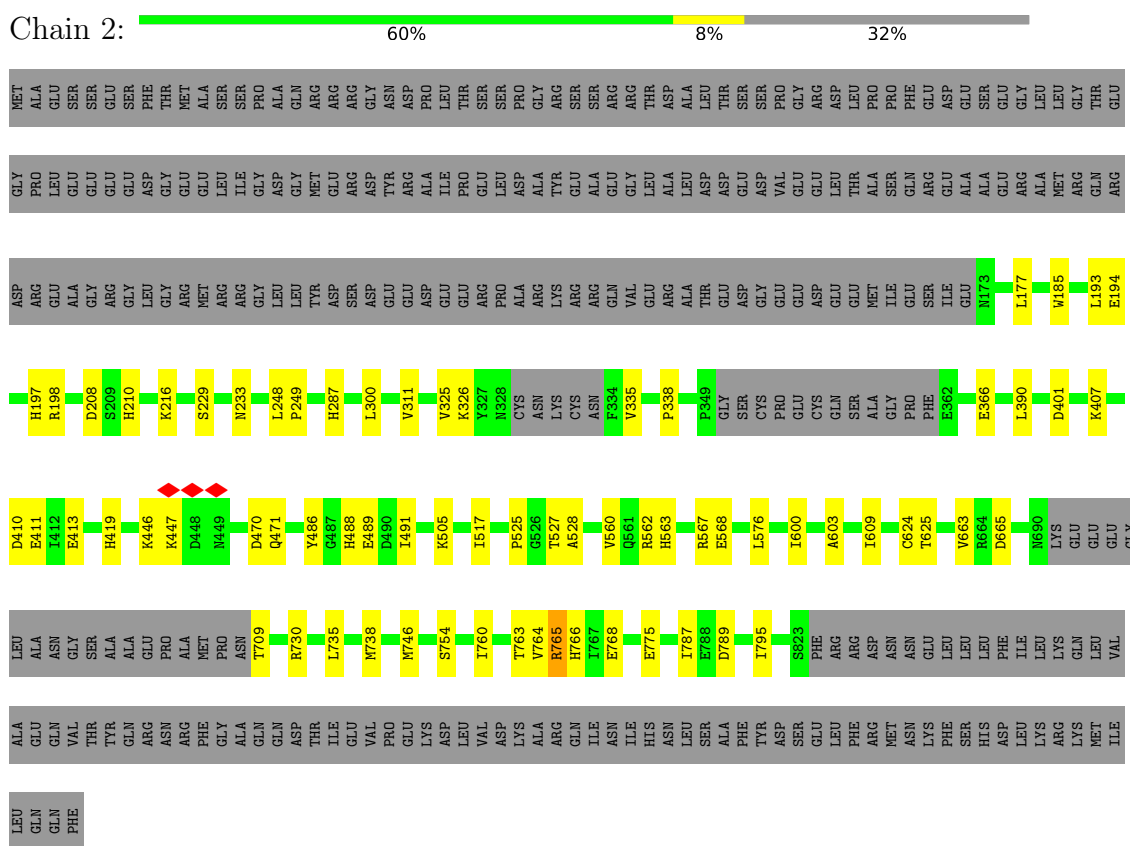
- Molecule 19 is water.

Mol	Chain	Residues	Atoms			AltConf
19	2	7	Total	H	O	0
			21	14	7	
19	3	8	Total	H	O	0
			24	16	8	
19	4	4	Total	H	O	0
			12	8	4	
19	5	8	Total	H	O	0
			24	16	8	
19	6	7	Total	H	O	0
			21	14	7	
19	7	5	Total	H	O	0
			15	10	5	

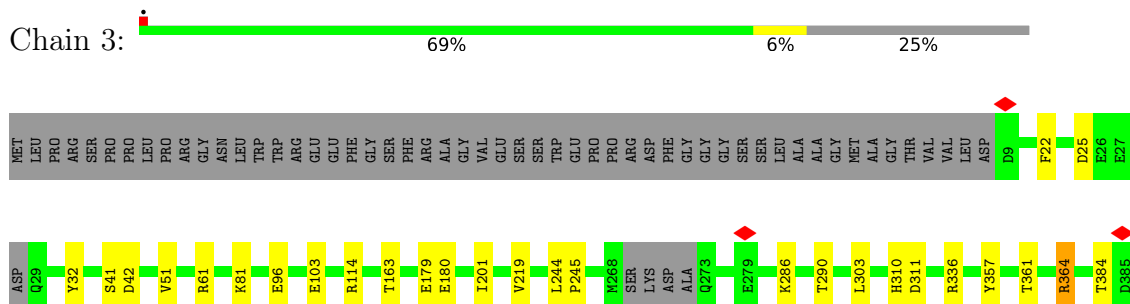
3 Residue-property plots

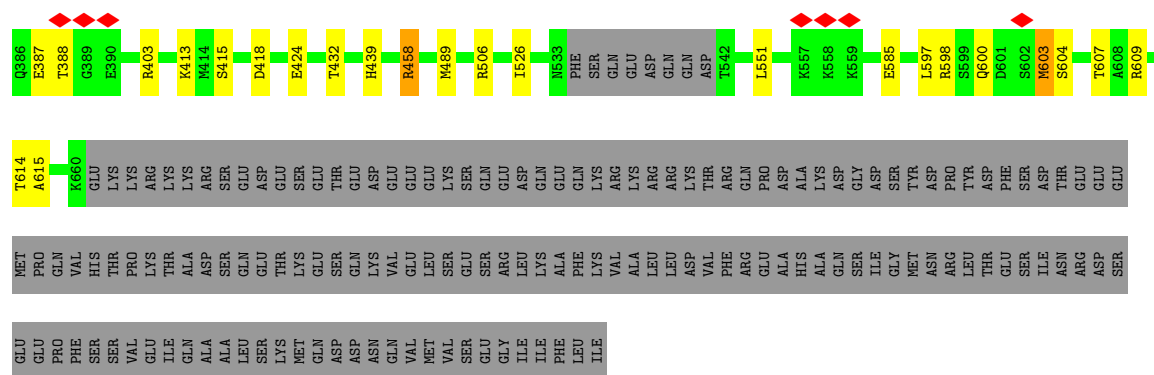
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 licensing factor MCM2

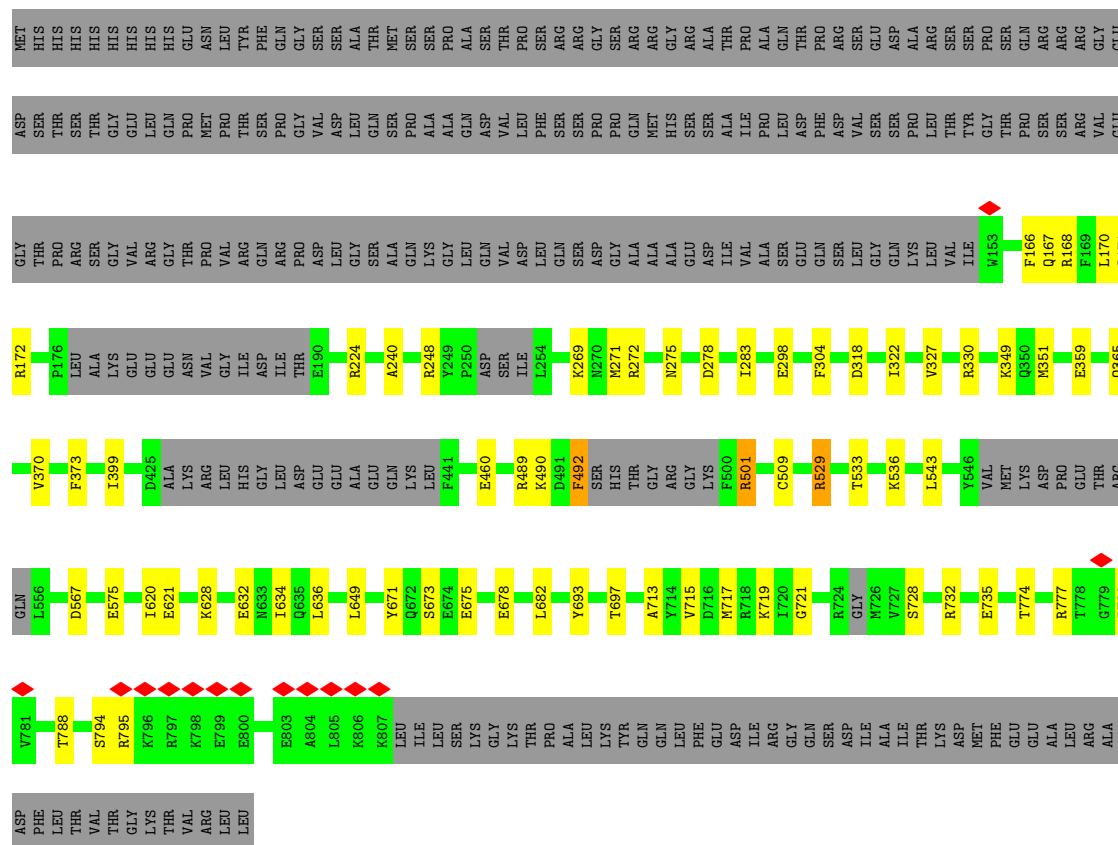


• Molecule 2: Isoform 2 of DNA replication licensing factor MCM3

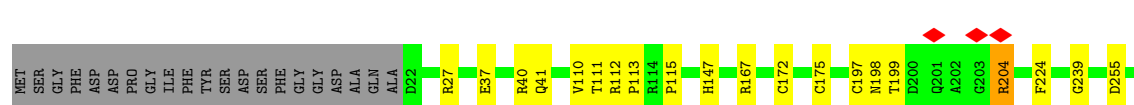
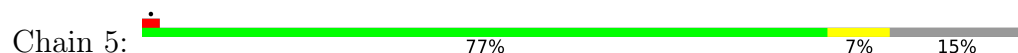


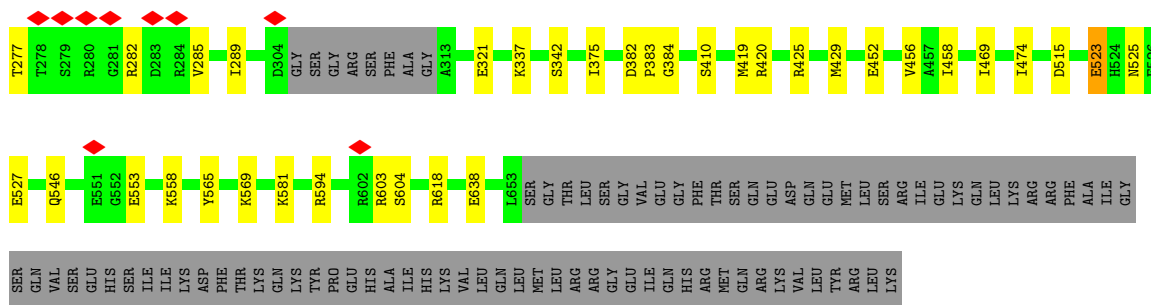


• Molecule 3: DNA replication licensing factor MCM4



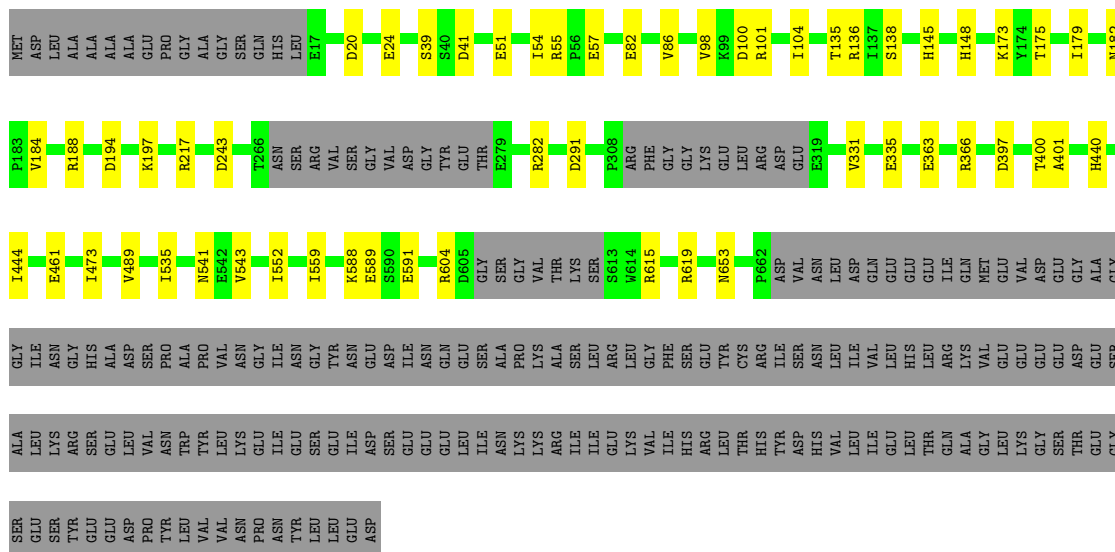
• Molecule 4: DNA replication licensing factor MCM5





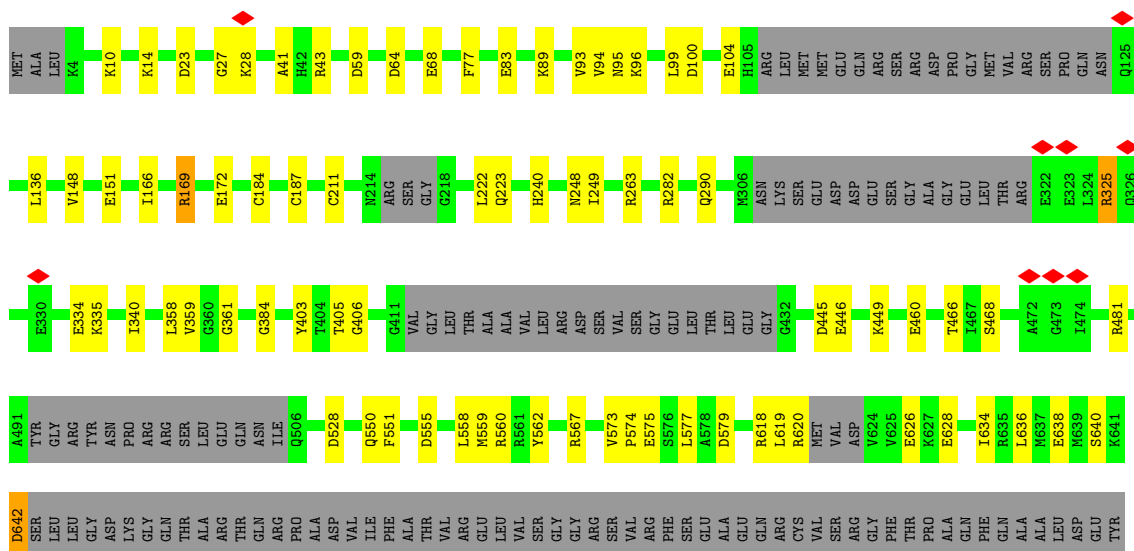
• Molecule 5: DNA replication licensing factor MCM6

Chain 6: 68% 7% 25%



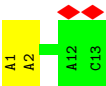
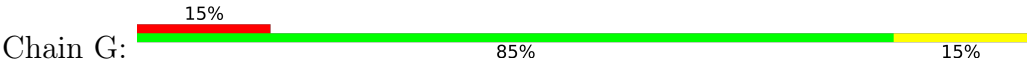
• Molecule 6: DNA replication licensing factor MCM7

Chain 7: 68% 11% 21%





● Molecule 13: Lagging strand DNA template



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	187345	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	100.950	Depositor
Minimum map value	-39.675	Depositor
Average map value	0.007	Depositor
Map value standard deviation	1.331	Depositor
Recommended contour level	3	Depositor
Map size (Å)	370.04797, 370.04797, 370.04797	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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, ATP, K, MG, 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	2	0.79	5/4954 (0.1%)	0.90	10/6695 (0.1%)
2	3	0.62	3/5093 (0.1%)	0.81	13/6872 (0.2%)
3	4	0.35	1/4929 (0.0%)	0.51	1/6657 (0.0%)
4	5	0.99	5/4962 (0.1%)	0.98	8/6679 (0.1%)
5	6	0.56	6/5012 (0.1%)	0.59	0/6763
6	7	0.42	0/4569	0.56	2/6164 (0.0%)
7	A	0.17	0/1636	0.29	0/2200
8	B	0.16	0/1462	0.26	0/1981
9	C	0.20	0/1607	0.32	0/2167
10	D	0.18	0/1717	0.32	0/2315
11	E	0.26	2/4431 (0.0%)	0.43	2/5982 (0.0%)
12	F	0.65	0/942	1.20	5/1458 (0.3%)
13	G	0.66	0/300	0.98	0/460
All	All	0.58	22/41614 (0.1%)	0.69	41/56393 (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
1	2	0	1
2	3	0	5
3	4	0	5
4	5	0	8
6	7	0	3
10	D	0	1
11	E	0	1
12	F	0	7
13	G	0	2
All	All	0	33

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	115	PRO	N-CD	-38.24	0.94	1.47
1	2	765	ARG	C-O	-8.71	1.14	1.24
4	5	383	PRO	C-O	-7.53	1.14	1.23
4	5	384	GLY	C-O	-7.40	1.16	1.24
4	5	382	ASP	C-O	-6.09	1.15	1.23

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	115	PRO	N-CD-CG	15.49	126.44	103.20
3	4	492	PHE	CA-CB-CG	9.68	123.48	113.80
2	3	310	HIS	N-CA-C	-9.23	93.26	108.49
4	5	115	PRO	CB-CG-CD	-8.55	78.75	106.10
4	5	115	PRO	N-CA-CB	-8.40	94.56	103.38

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	765	ARG	Sidechain
2	3	114	ARG	Sidechain
2	3	336	ARG	Sidechain
2	3	364	ARG	Sidechain
2	3	458	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	2	4865	4849	4881	38	0
2	3	5017	5047	5055	42	0
3	4	4847	4864	4878	61	0
4	5	4887	4938	4954	33	0
5	6	4932	4949	4958	37	0
6	7	4499	4531	4535	69	0
7	A	1604	1589	1594	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	1431	1452	1456	8	0
9	C	1572	1534	1537	9	0
10	D	1685	1704	1709	11	0
11	E	4339	4268	4289	40	0
12	F	839	453	447	5	0
13	G	267	146	140	0	0
14	2	27	12	12	1	0
15	2	1	0	0	0	0
15	3	1	0	0	0	0
15	4	1	0	0	0	0
15	5	1	0	0	0	0
15	6	1	0	0	0	0
15	7	1	0	0	0	0
16	3	31	12	12	1	0
16	4	31	12	12	0	0
16	5	31	12	12	2	0
16	6	31	12	12	3	0
16	7	31	12	12	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	2	0
18	F	2	0	0	0	0
19	2	7	14	0	0	0
19	3	8	16	0	1	0
19	4	4	8	0	1	0
19	5	8	16	0	2	0
19	6	7	14	0	1	0
19	7	5	10	0	3	0
All	All	41017	40474	40505	339	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 339 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)
2:3:600:GLN:CG	2:3:603:MET:HB3	1.65	1.25
6:7:187:CYS:SG	17:7:1003:ZN:ZN	1.34	1.15
2:3:600:GLN:HG2	2:3:603:MET:HE3	1.32	1.12
3:4:269:LYS:HZ2	3:4:283:ILE:CG2	1.62	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:14:VAL:HG13	11:E:19:VAL:HG11	1.32	1.10

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	2	608/904 (67%)	596 (98%)	12 (2%)	0	100	100
2	3	631/853 (74%)	617 (98%)	14 (2%)	0	100	100
3	4	593/883 (67%)	586 (99%)	7 (1%)	0	100	100
4	5	620/734 (84%)	611 (98%)	9 (2%)	0	100	100
5	6	609/821 (74%)	595 (98%)	14 (2%)	0	100	100
6	7	551/719 (77%)	546 (99%)	5 (1%)	0	100	100
7	A	193/196 (98%)	188 (97%)	5 (3%)	0	100	100
8	B	174/222 (78%)	172 (99%)	2 (1%)	0	100	100
9	C	192/216 (89%)	187 (97%)	5 (3%)	0	100	100
10	D	202/223 (91%)	199 (98%)	3 (2%)	0	100	100
11	E	529/566 (94%)	519 (98%)	10 (2%)	0	100	100
All	All	4902/6337 (77%)	4816 (98%)	86 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	2	537/781 (69%)	534 (99%)	3 (1%)	78	91
2	3	552/742 (74%)	549 (100%)	3 (0%)	81	92
3	4	538/771 (70%)	534 (99%)	4 (1%)	76	89
4	5	532/625 (85%)	526 (99%)	6 (1%)	65	84
5	6	550/724 (76%)	549 (100%)	1 (0%)	87	95
6	7	490/619 (79%)	484 (99%)	6 (1%)	63	83
7	A	173/174 (99%)	173 (100%)	0	100	100
8	B	160/195 (82%)	160 (100%)	0	100	100
9	C	169/186 (91%)	169 (100%)	0	100	100
10	D	189/205 (92%)	188 (100%)	1 (0%)	81	92
11	E	486/517 (94%)	485 (100%)	1 (0%)	87	95
All	All	4376/5539 (79%)	4351 (99%)	25 (1%)	76	91

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	5	419	MET
6	7	169	ARG
11	E	395	LYS
5	6	473	ILE
6	7	249	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
4	5	464	GLN
11	E	355	ASN
6	7	238	GLN
11	E	314	GLN
10	D	186	HIS

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 18 ligands modelled in this entry, 12 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$
16	ATP	6	1001	15	32,33,33	0.56	0	48,52,52	0.70	0
16	ATP	7	1001	15	32,33,33	0.46	0	48,52,52	0.69	1 (2%)
16	ATP	5	1001	15	32,33,33	0.49	0	48,52,52	0.65	0
14	ADP	2	1001	15	28,29,29	1.37	5 (17%)	43,45,45	1.88	10 (23%)
16	ATP	3	1001	15	32,33,33	0.45	0	48,52,52	0.67	0
16	ATP	4	1001	15	32,33,33	0.44	0	48,52,52	0.69	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
16	ATP	6	1001	15	-	8/22/38/38	0/3/3/3
16	ATP	7	1001	15	-	2/22/38/38	0/3/3/3
16	ATP	5	1001	15	-	1/22/38/38	0/3/3/3
14	ADP	2	1001	15	-	2/16/32/32	0/3/3/3
16	ATP	3	1001	15	-	2/22/38/38	0/3/3/3
16	ATP	4	1001	15	-	8/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	1001	ADP	C5-C4	4.35	1.46	1.39
14	2	1001	ADP	C5-N7	-2.56	1.34	1.39
14	2	1001	ADP	C5-C6	2.53	1.48	1.41
14	2	1001	ADP	C8-N7	2.06	1.35	1.31
14	2	1001	ADP	C4-N9	-2.02	1.33	1.37

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	1001	ADP	C5-C4-N3	-6.01	118.45	126.72
14	2	1001	ADP	N3-C4-N9	4.80	135.34	127.17
14	2	1001	ADP	C2-N3-C4	3.88	121.30	111.83
14	2	1001	ADP	N3-C2-N1	-3.59	123.14	128.58
14	2	1001	ADP	C4-C5-N7	-3.48	106.60	110.58

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	2	1001	ADP	C5'-O5'-PA-O3A
16	4	1001	ATP	C5'-O5'-PA-O1A
16	4	1001	ATP	C5'-O5'-PA-O2A
16	4	1001	ATP	C5'-O5'-PA-O3A
16	6	1001	ATP	C5'-O5'-PA-O1A

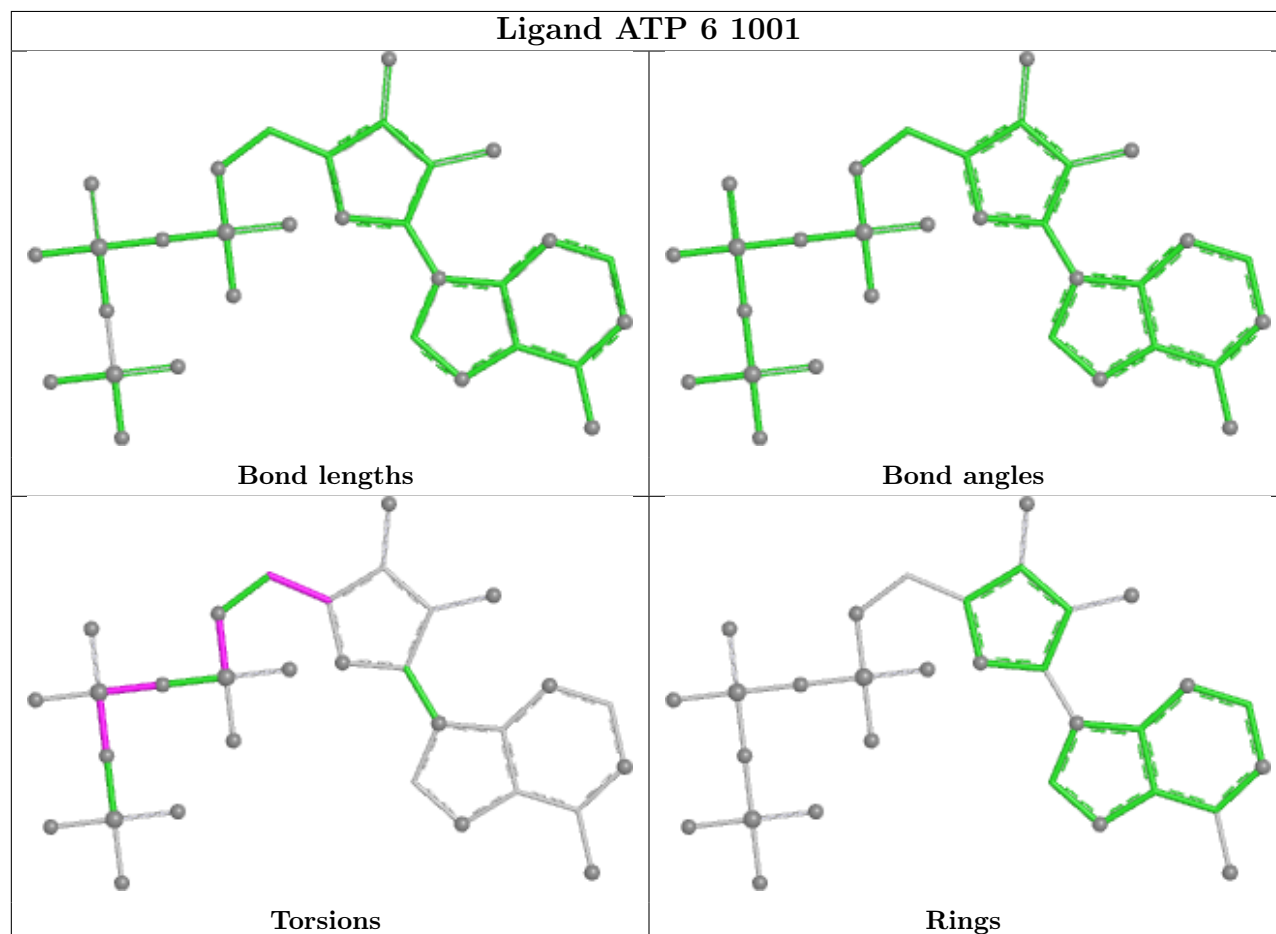
There are no ring outliers.

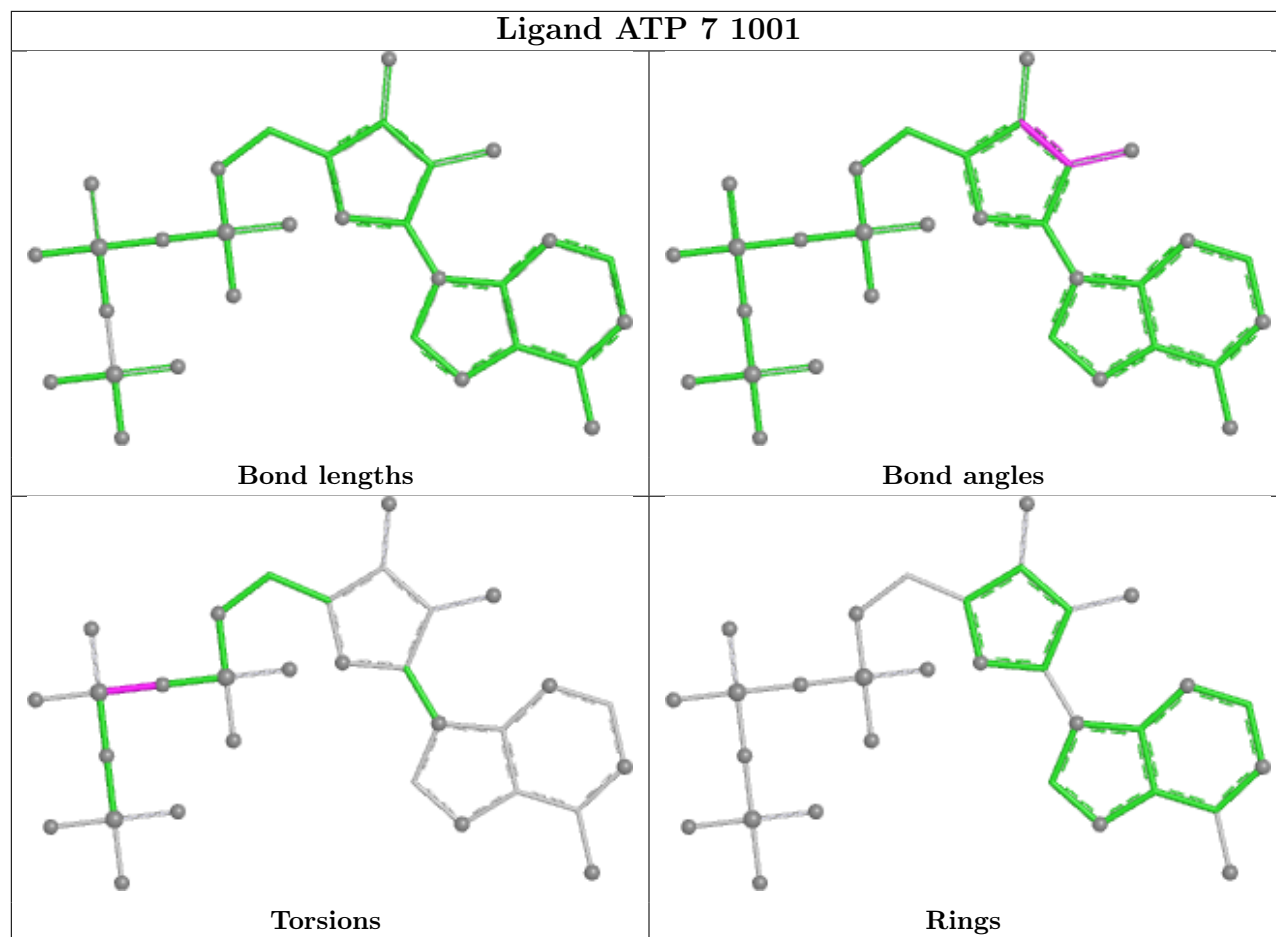
4 monomers are involved in 7 short contacts:

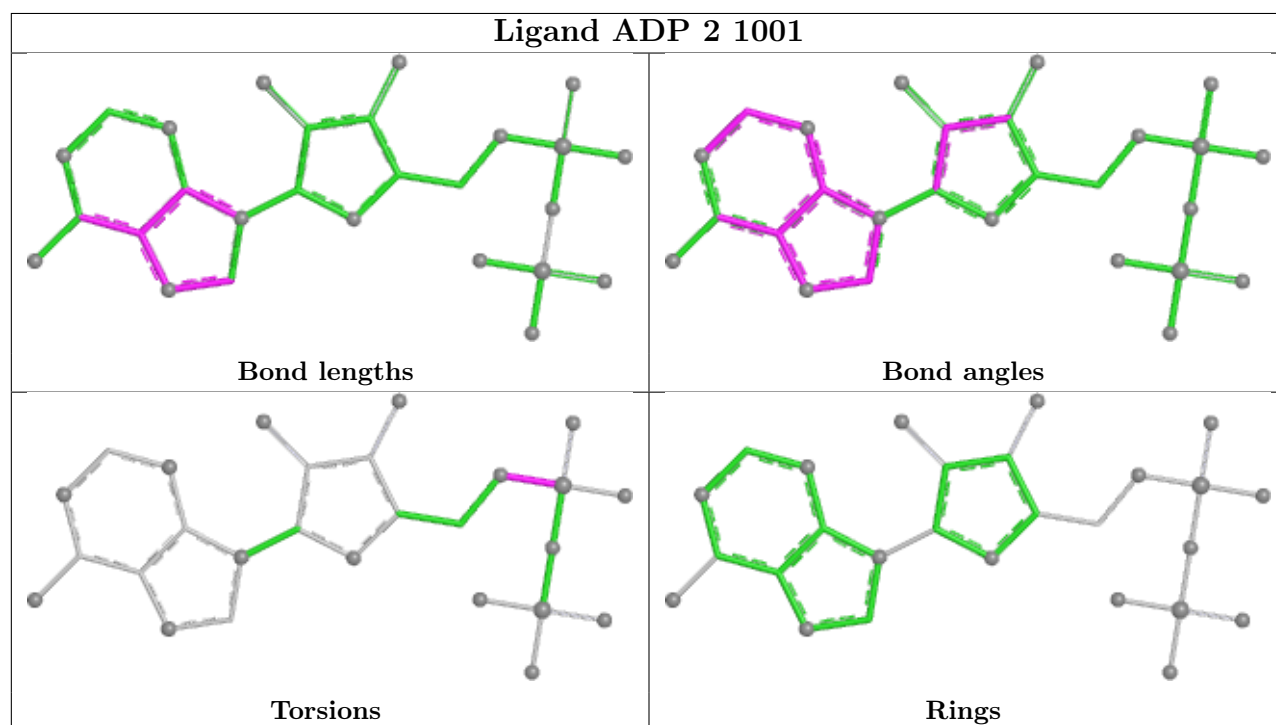
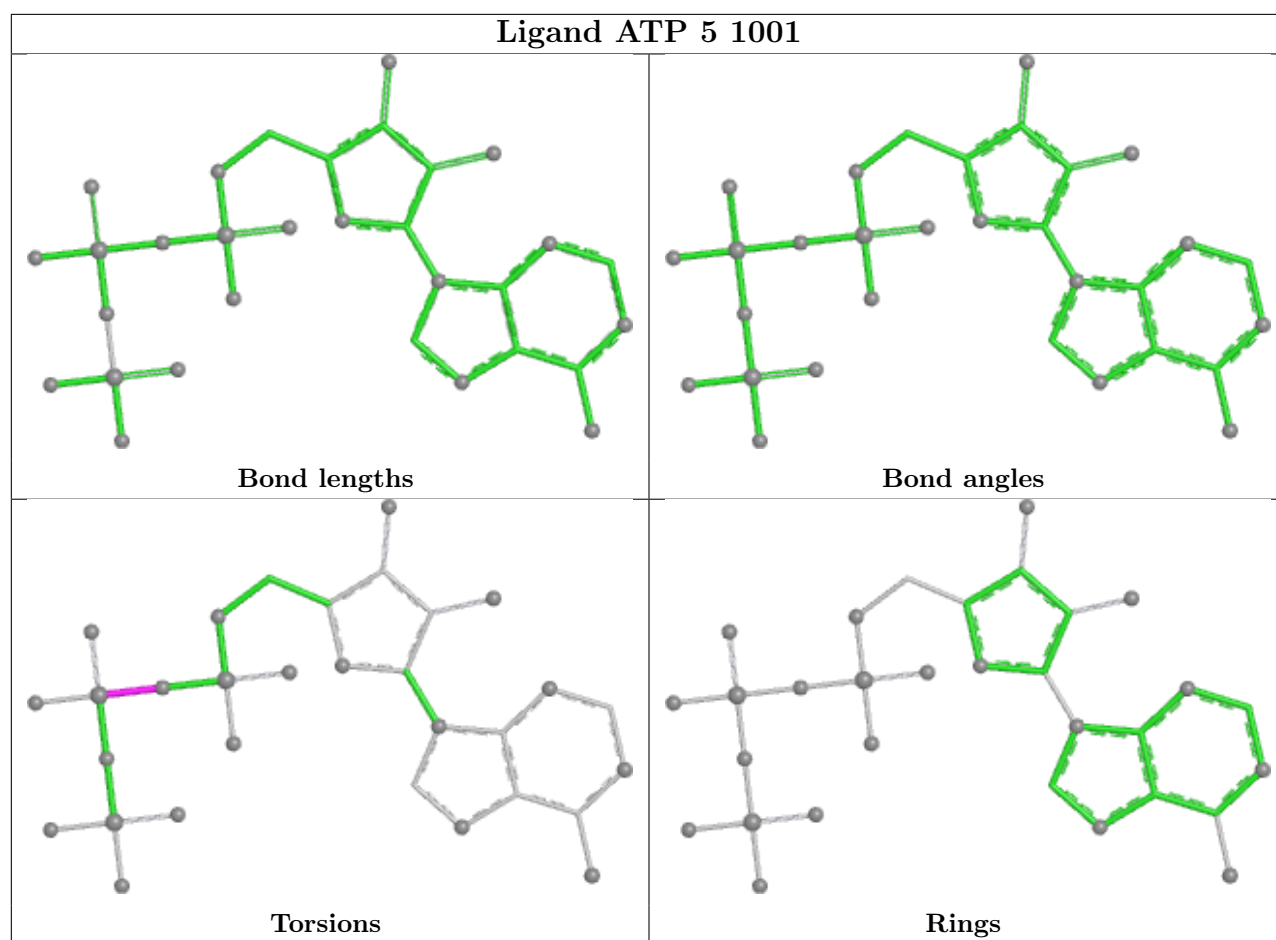
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	6	1001	ATP	3	0
16	5	1001	ATP	2	0
14	2	1001	ADP	1	0
16	3	1001	ATP	1	0

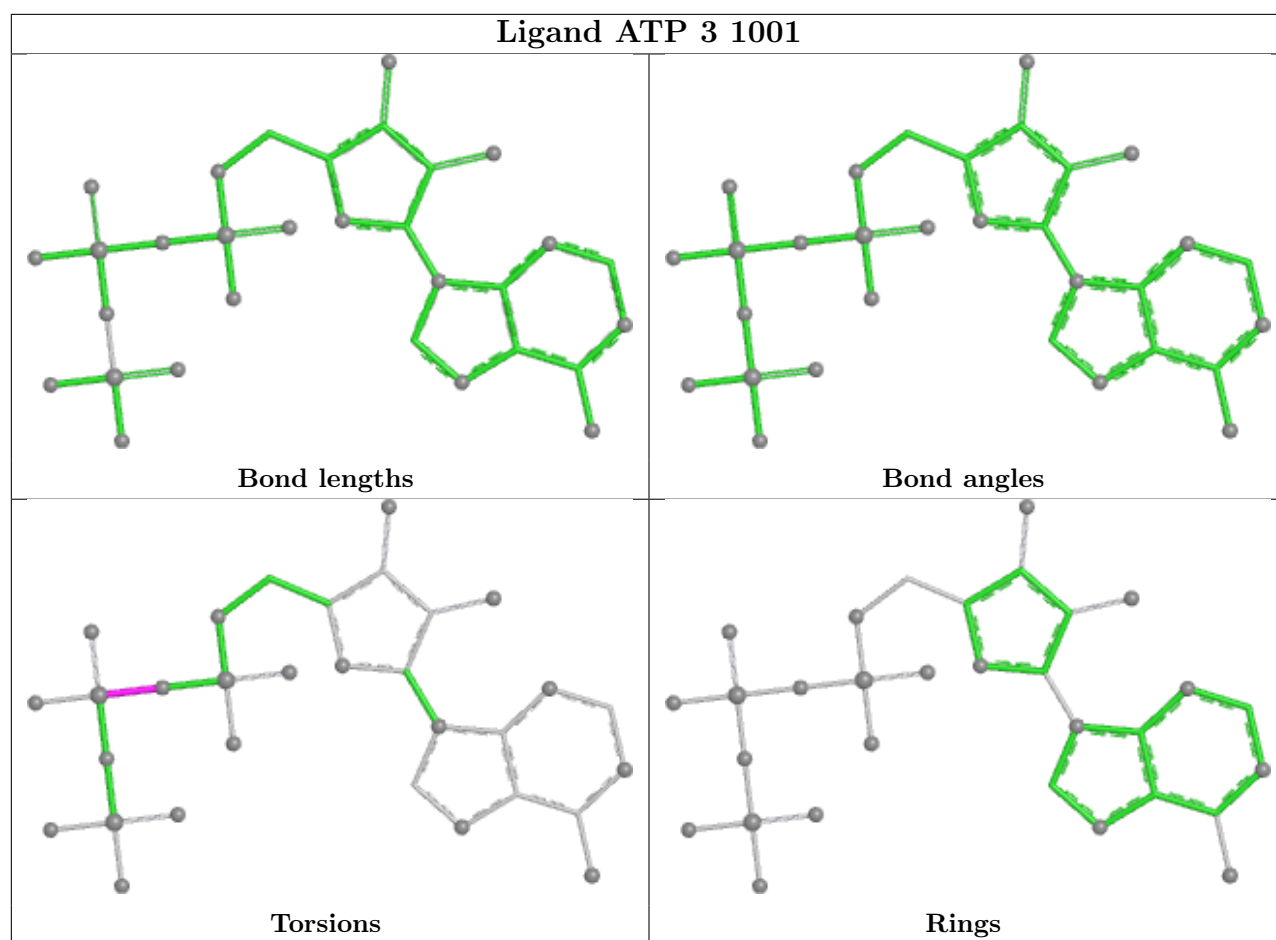
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

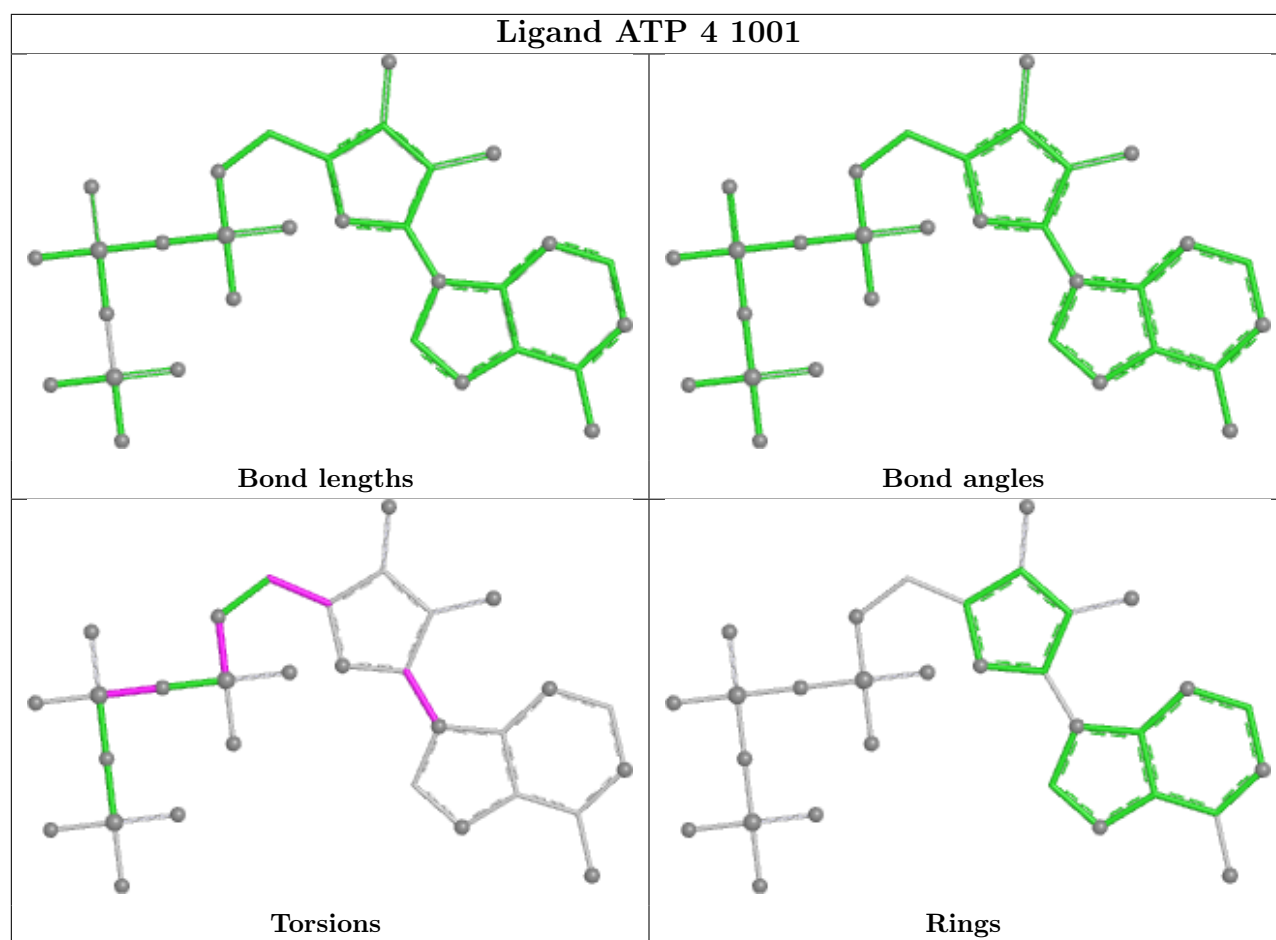
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

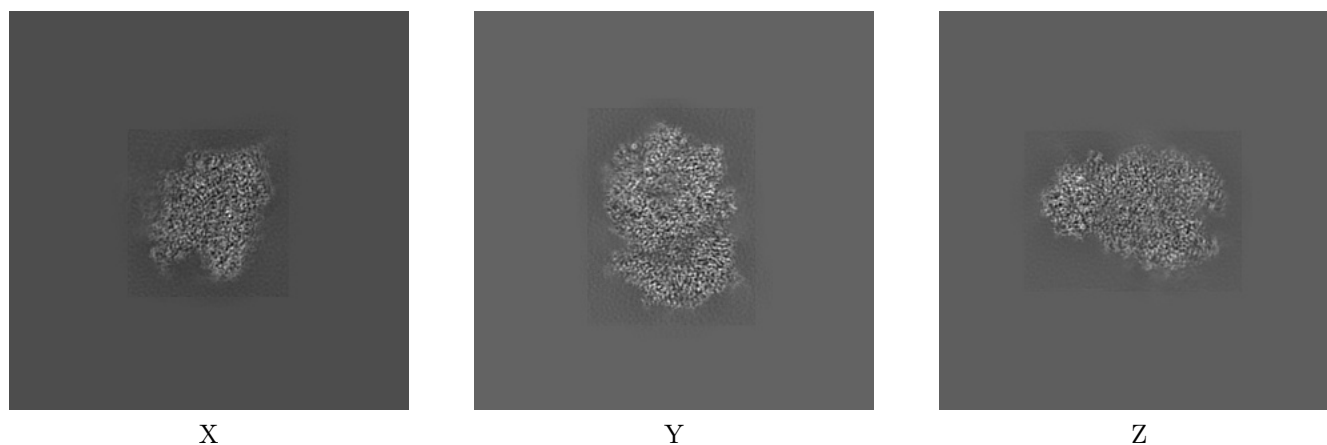
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47473. 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](#)

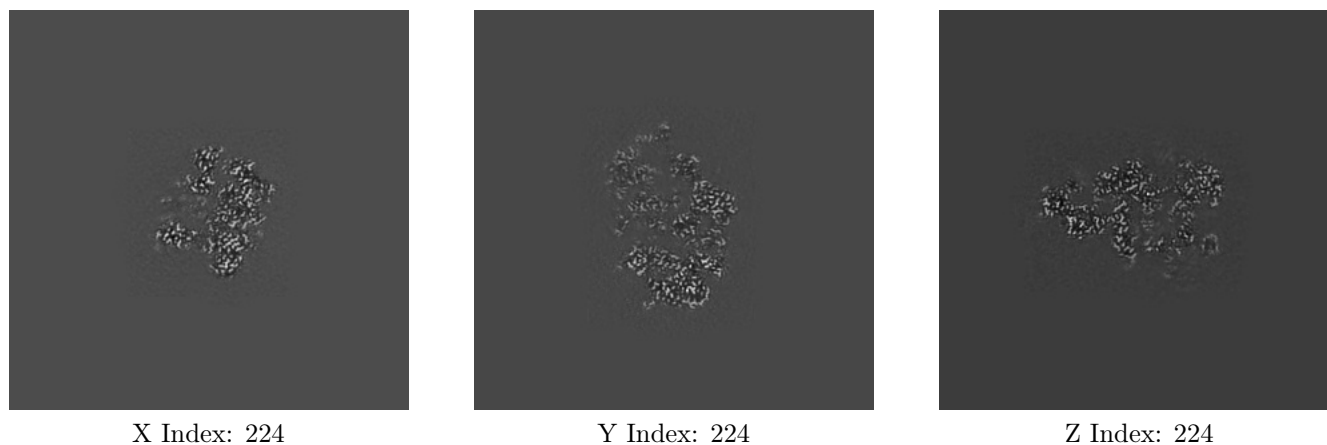
6.1.1 Primary map



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

6.2 Central slices [i](#)

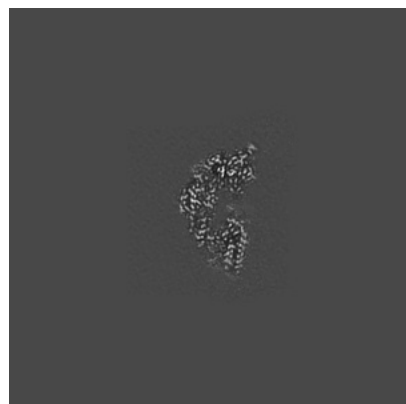
6.2.1 Primary map



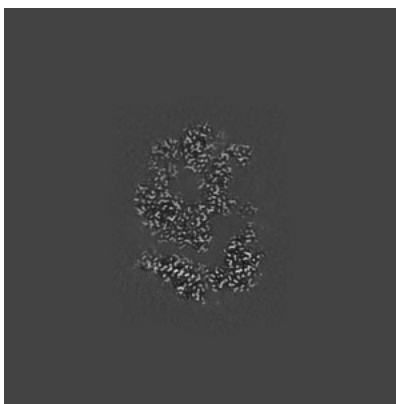
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

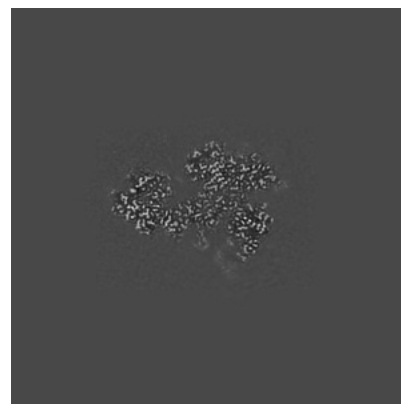
6.3.1 Primary map



X Index: 158



Y Index: 247

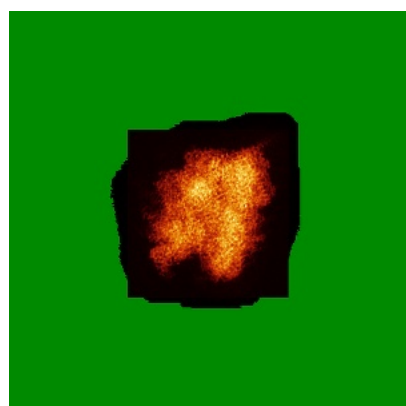


Z Index: 246

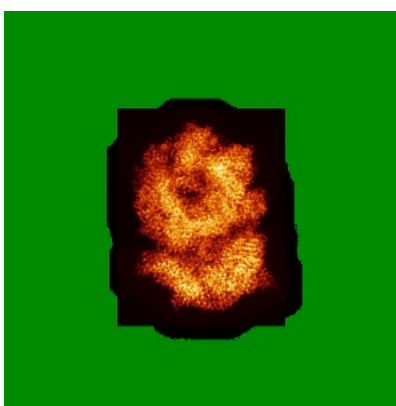
The images above show the largest variance slices of the map in three orthogonal directions.

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

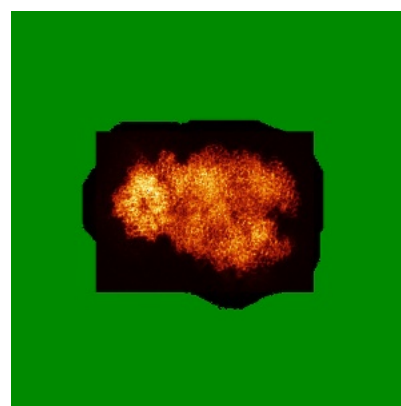
6.4.1 Primary map



X



Y

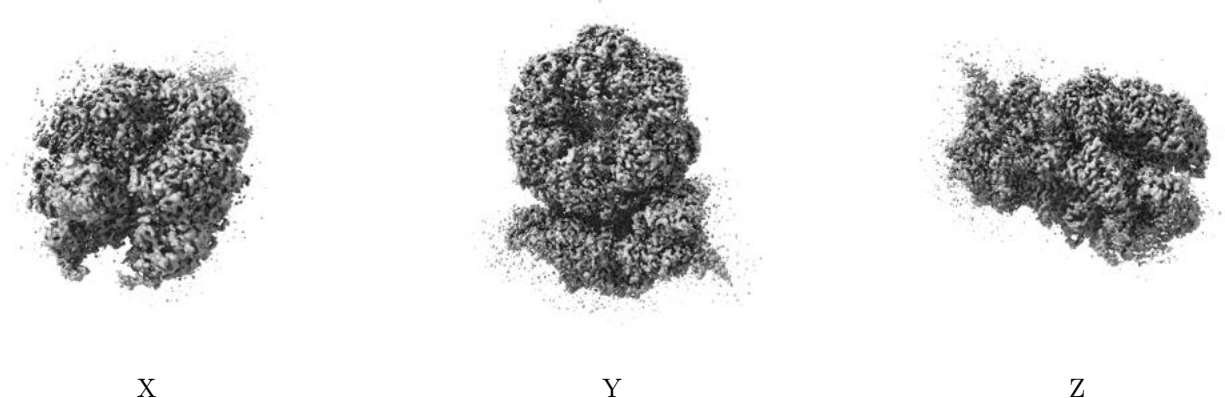


Z

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

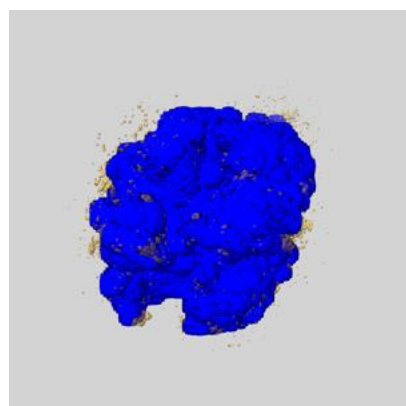
6.6 Mask visualisation [i](#)

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

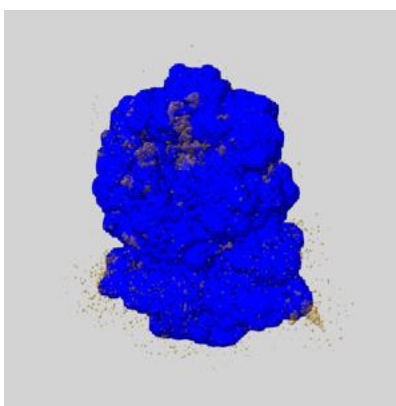
A mask typically either:

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

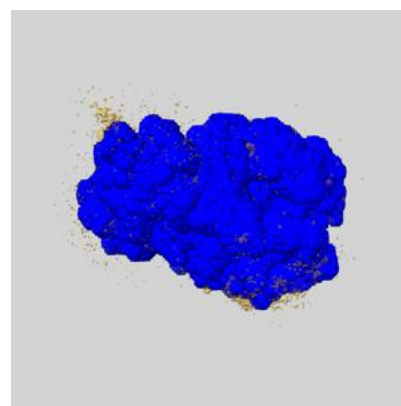
6.6.1 emd_47473_msk_1.map [i](#)



X



Y

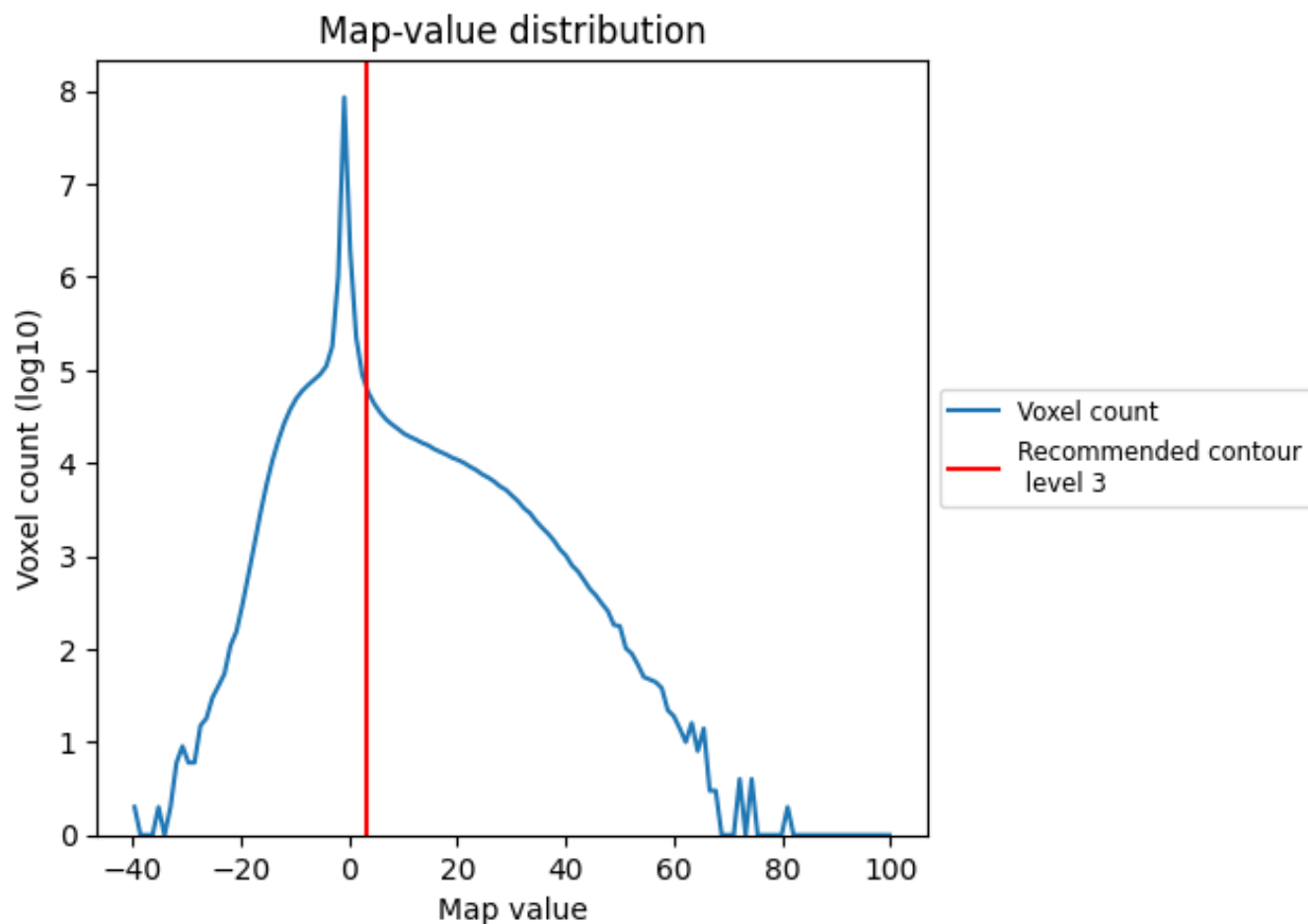


Z

7 Map analysis [i](#)

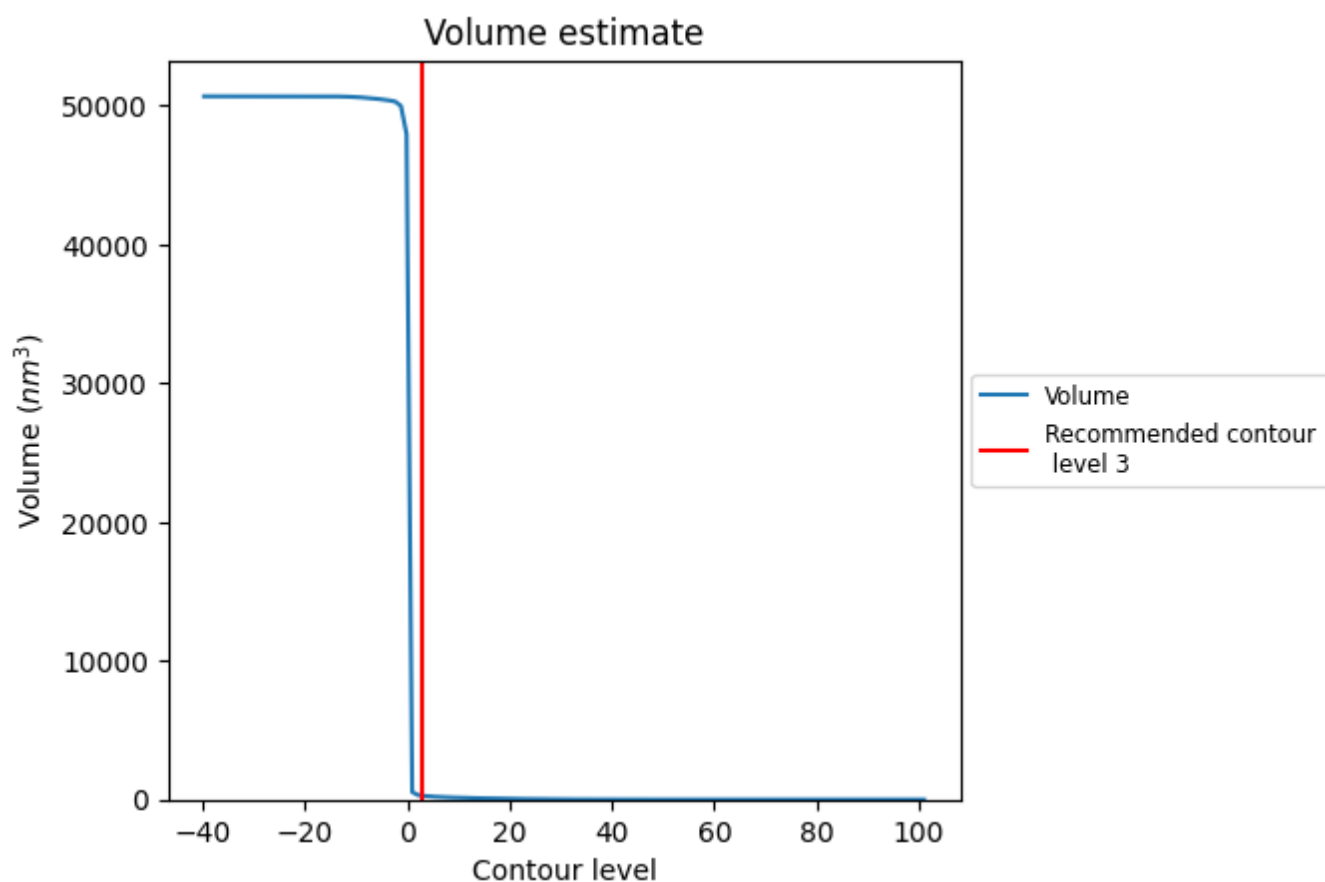
This section contains the results of statistical analysis of the map.

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.

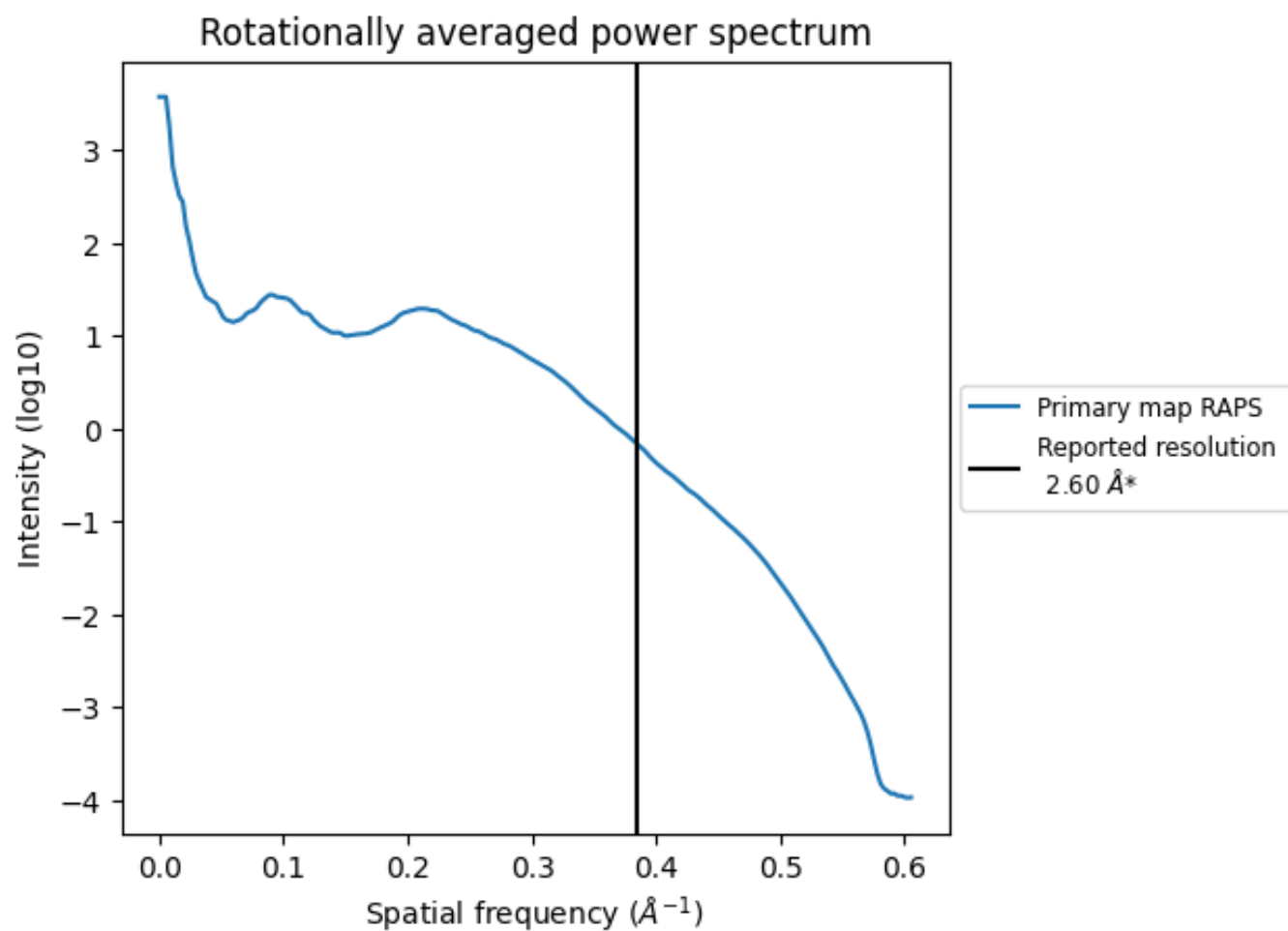
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 278 nm^3 ; this corresponds to an approximate mass of 251 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 ⓘ

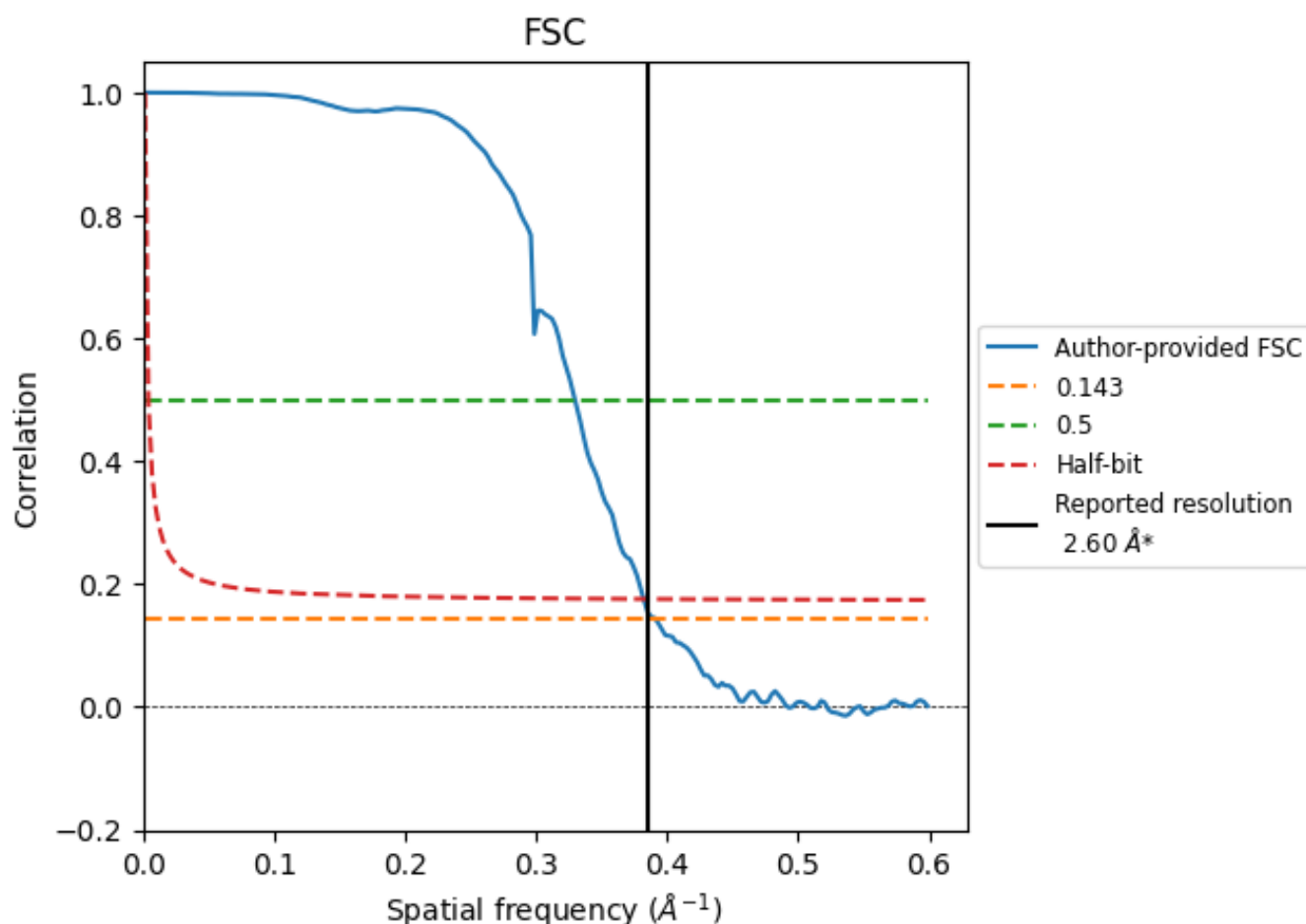


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

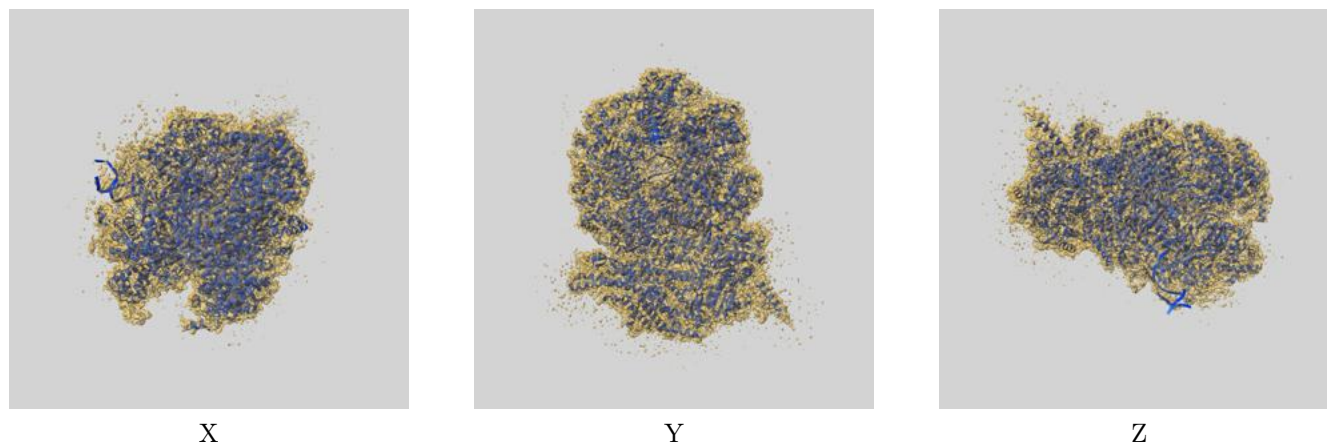
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.56	3.03	2.62
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

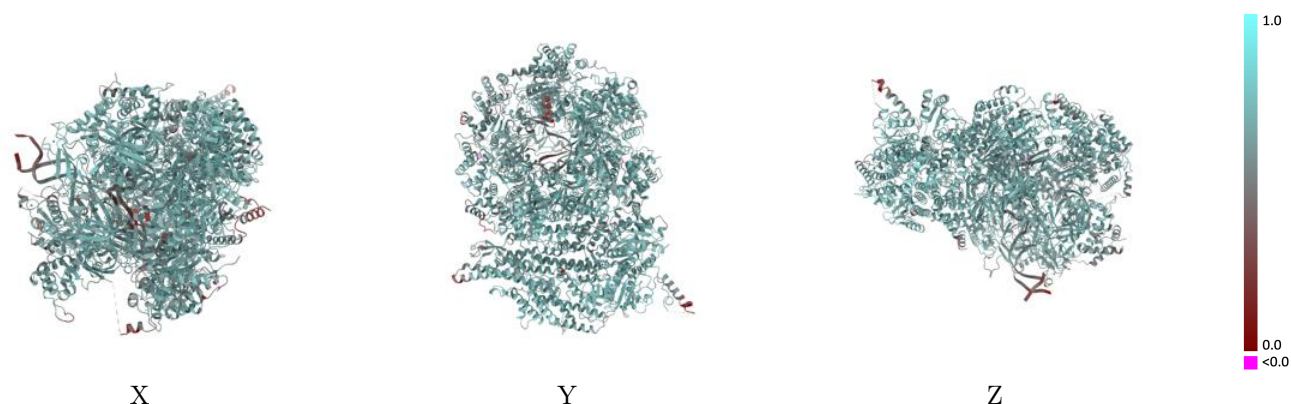
This section contains information regarding the fit between EMDB map EMD-47473 and PDB model 9E2Z. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



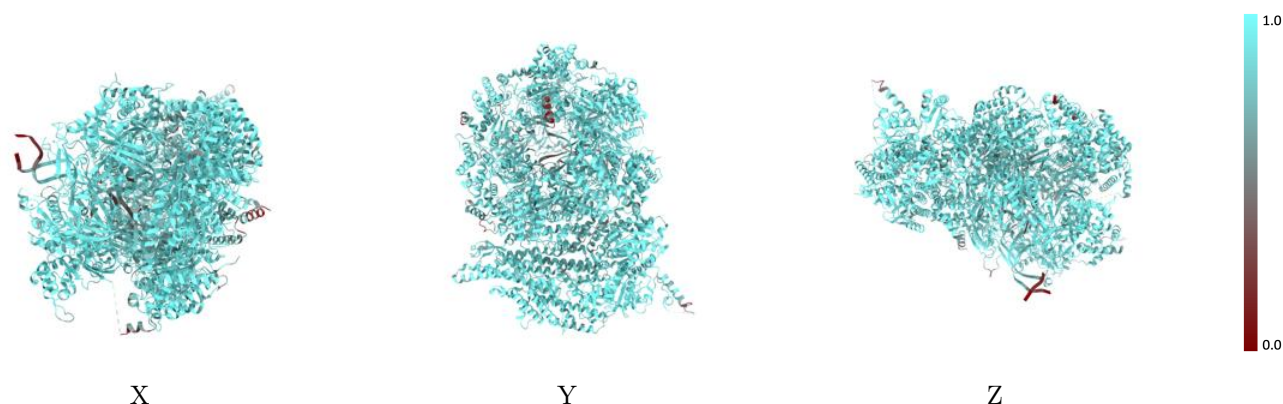
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



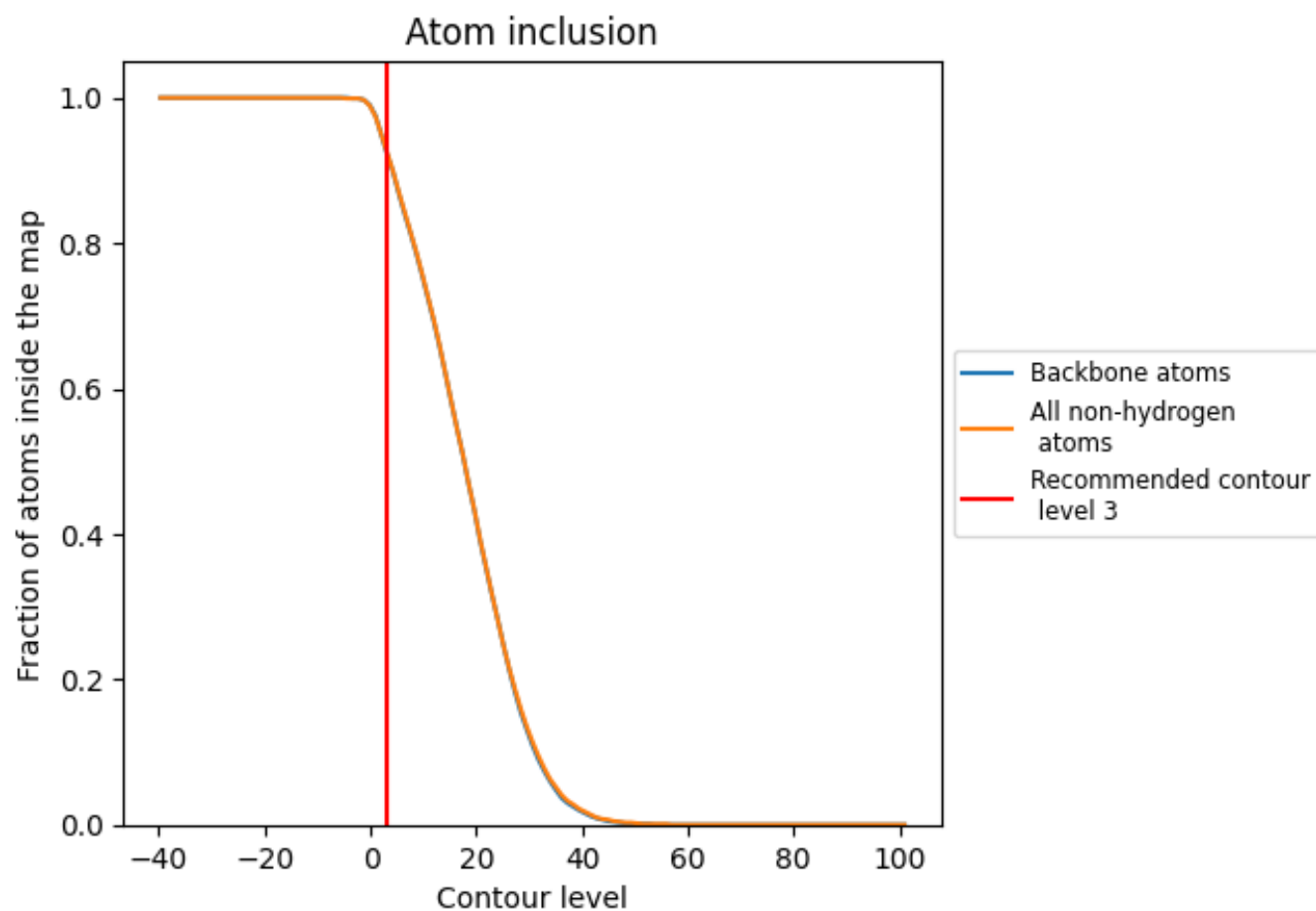
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9280	0.6450
2	0.9540	0.6690
3	0.9260	0.6420
4	0.9150	0.6220
5	0.9450	0.6710
6	0.9520	0.6530
7	0.9090	0.6040
A	0.9530	0.6530
B	0.9840	0.6980
C	0.9400	0.6590
D	0.9650	0.6720
E	0.9490	0.6600
F	0.6970	0.4830
G	0.7450	0.4880

1.0

0.0

<0.0