



wwPDB EM Validation Summary Report ⓘ

Mar 14, 2026 – 01:40 AM UTC

PDB ID : 8KG9 / pdb_00008kg9
EMDB ID : EMD-37215
Title : Yeast replisome in state III
Authors : Dang, S.; Zhai, Y.; Feng, J.; Yu, D.; Xu, Z.
Deposited on : 2023-08-17
Resolution : 4.52 Å (reported)
Based on initial model : 6SKL

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

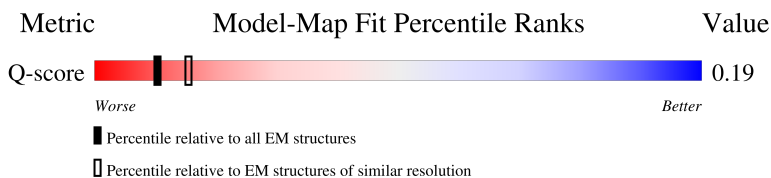
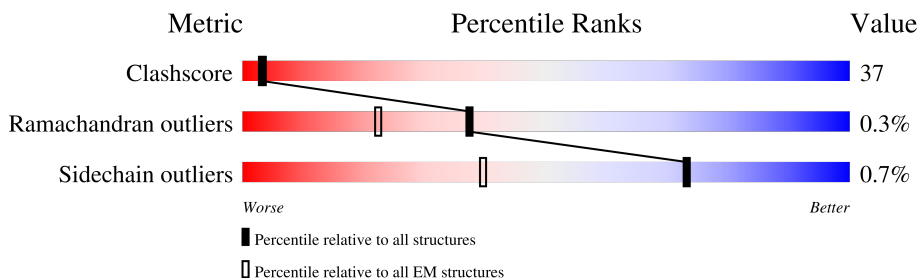
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.52 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.



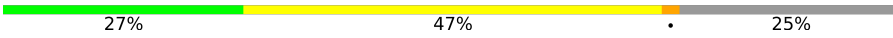
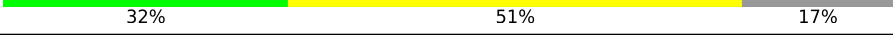
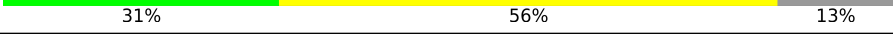
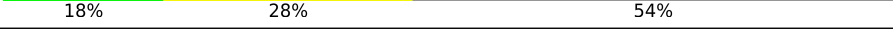
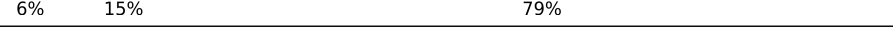
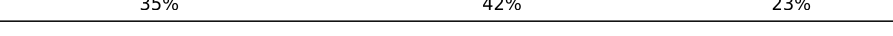
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2506 (4.02 - 5.02)

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	868	
2	3	971	
3	4	933	
4	5	775	

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Mol	Chain	Length	Quality of chain
5	6	1017	
6	7	845	
7	A	208	
8	B	213	
9	C	194	
10	D	294	
11	E	650	
12	F	927	
12	G	927	
12	H	927	
13	I	71	
14	J	61	
15	M	2222	
16	N	689	

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
18	ADP	2	902	-	-	X	-
18	ADP	3	1001	-	-	X	-
20	AGS	5	803	-	-	X	-
20	AGS	7	903	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 63507 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 MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	668	Total	C	N	O	S	0	0
			5270	3310	948	993	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	637	Total	C	N	O	S	0	0
			4948	3116	881	938	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	676	Total	C	N	O	S	0	0
			5390	3386	937	1036	31		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	676	Total	C	N	O	S	0	0
			5325	3347	919	1035	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	629	Total	C	N	O	S	0	0
			4955	3124	868	938	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	636	Total	C	N	O	S	0	0
			4945	3125	861	933	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	200	Total	C	N	O	S	0	0
			1633	1024	282	318	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	193	Total	C	N	O	S	0	0
			1617	1039	286	287	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	172	Total	C	N	O	S	0	0
			1387	904	223	253	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	243	Total	C	N	O	S	0	0
			2004	1276	327	389	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	568	Total	C	N	O	S	0	0
			4599	2935	778	872	14		

- Molecule 12 is a protein called DNA polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	424	Total	C	N	O	S	0	0
			3404	2188	564	637	15		
12	G	422	Total	C	N	O	S	0	0
			3380	2172	557	636	15		
12	H	425	Total	C	N	O	S	0	0
			3411	2193	565	638	15		

- Molecule 13 is a DNA chain called DNA (70-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	15	Total	C	N	O	P	0	0
			307	150	42	100	15		

- Molecule 14 is a DNA chain called DNA (61-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	8	Total	C	N	O	P	0	0
			159	76	29	46	8		

- Molecule 15 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	812	Total	C	N	O	S	0	0
			6447	4162	1059	1192	34		

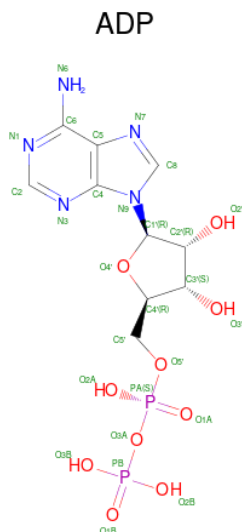
- Molecule 16 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	529	Total	C	N	O	S	0	0
			4199	2684	716	782	17		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

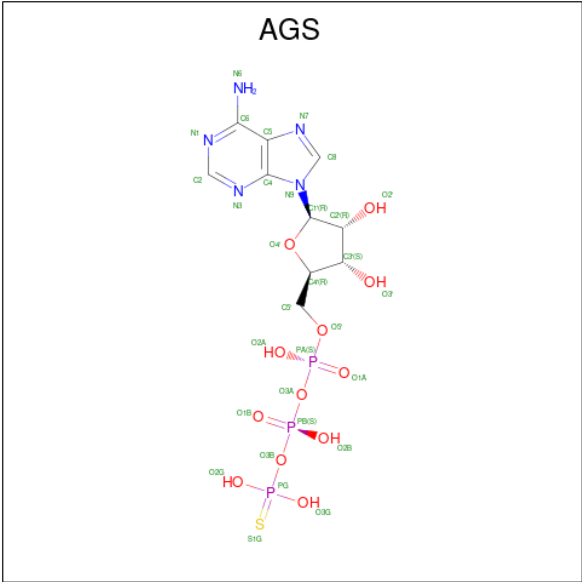


Mol	Chain	Residues	Atoms					AltConf
18	2	1	Total 27	C 10	N 5	O 10	P 2	0
18	3	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

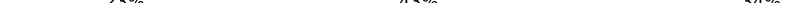
Mol	Chain	Residues	Atoms	AltConf
19	2	1	Total Mg 1 1	0
19	5	2	Total Mg 2 2	0
19	7	1	Total Mg 1 1	0

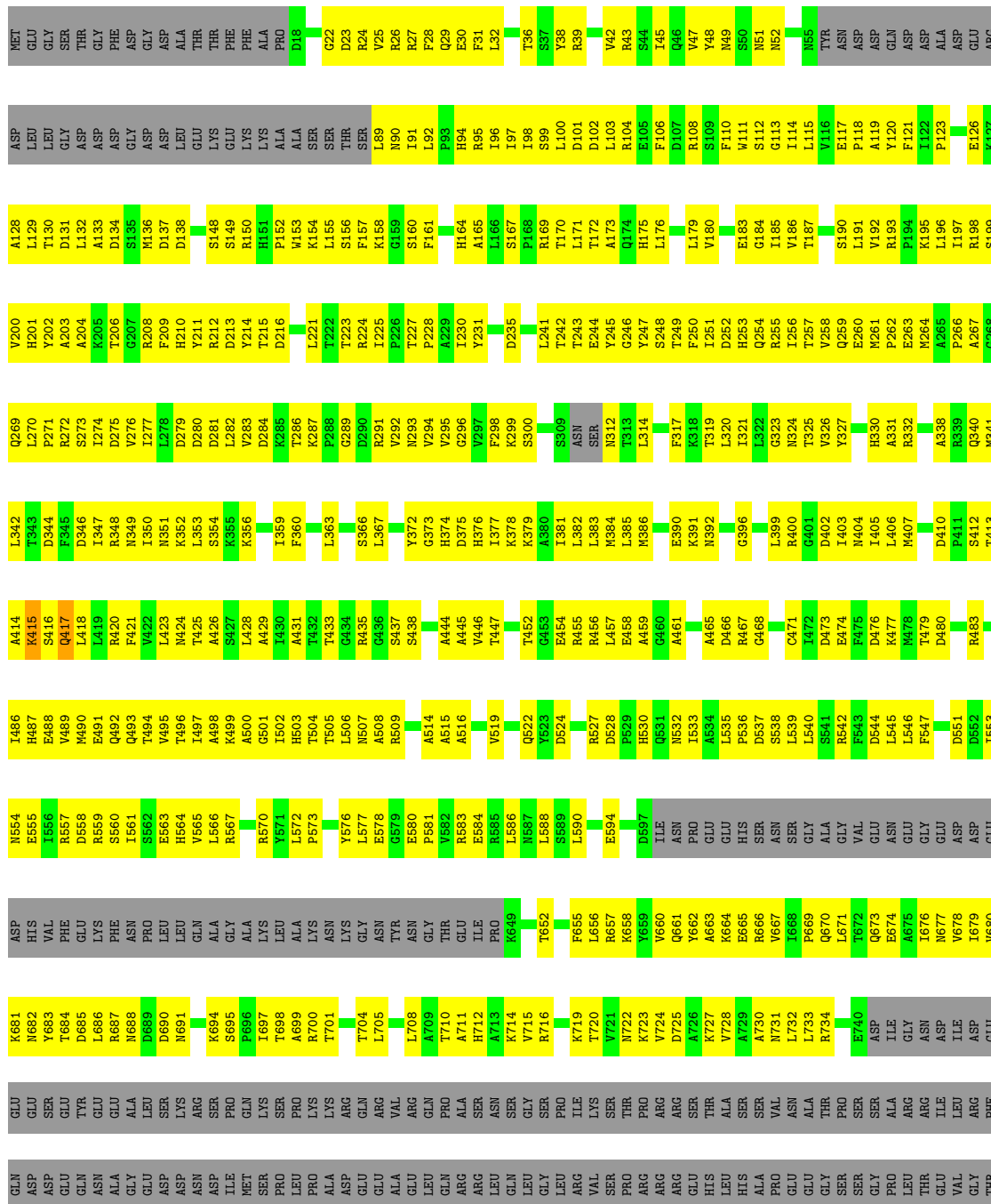
- Molecule 20 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{12}\text{P}_3\text{S}$) (labeled as "Ligand of Interest" by depositor).

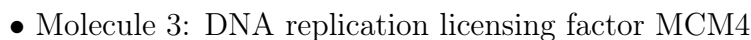


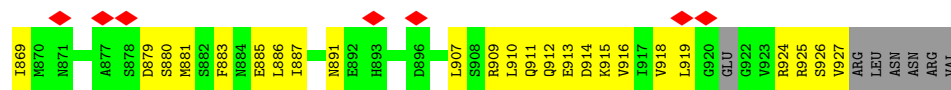
Mol	Chain	Residues	Atoms						AltConf
20	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
20	7	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 2: DNA replication licensing factor MCM3

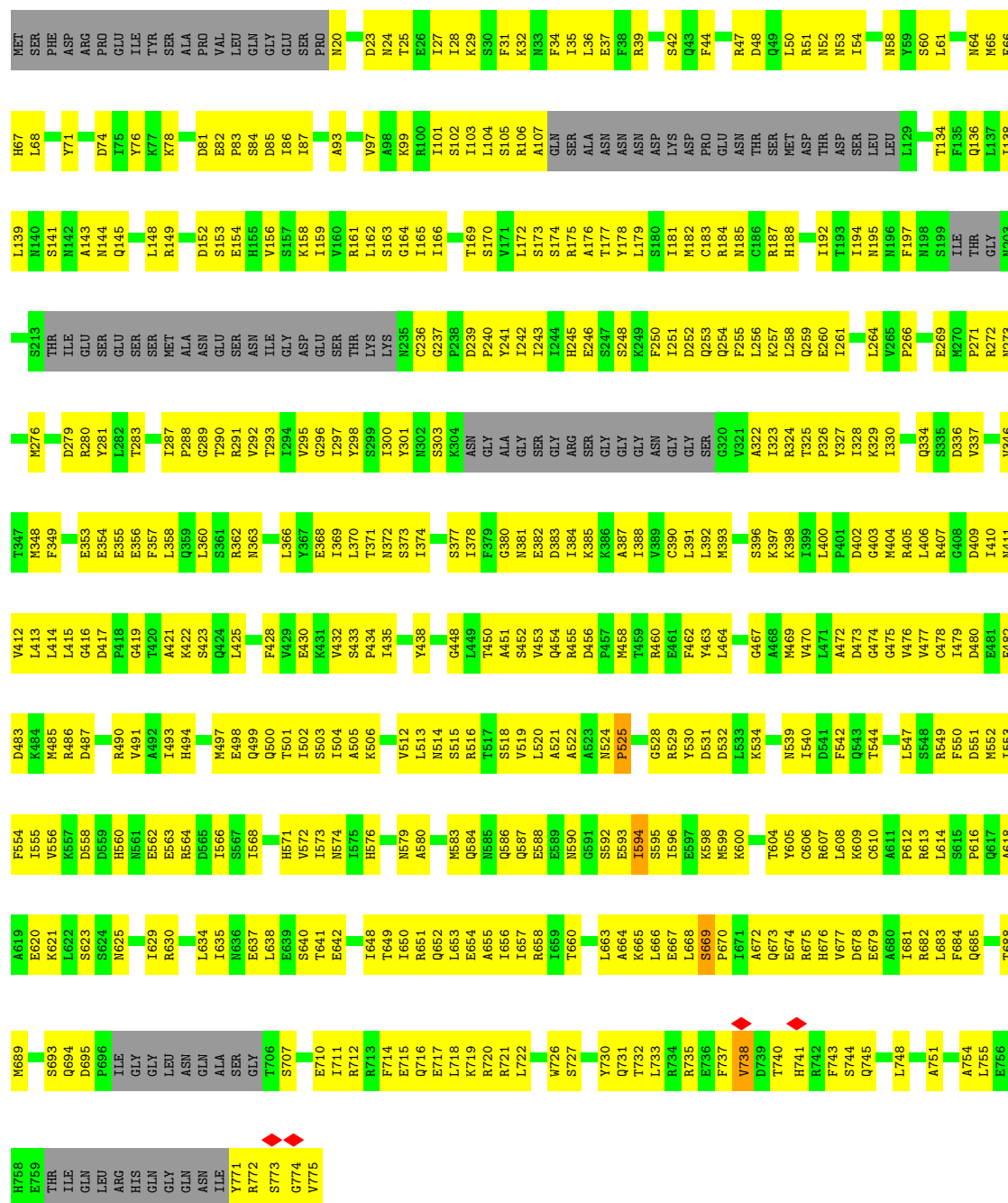
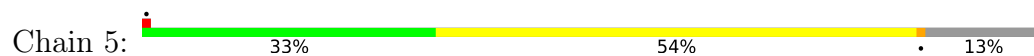
Chain 3:  23% 43% 34%



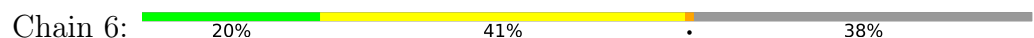




• Molecule 4: Minichromosome maintenance protein 5

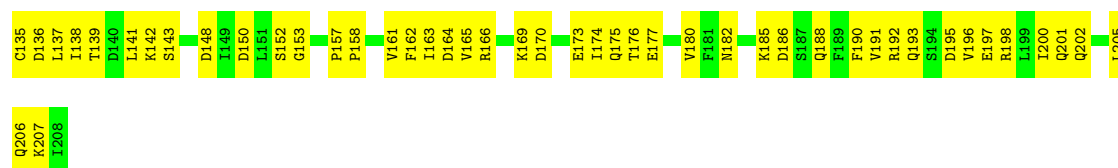


• Molecule 5: DNA replication licensing factor MCM6



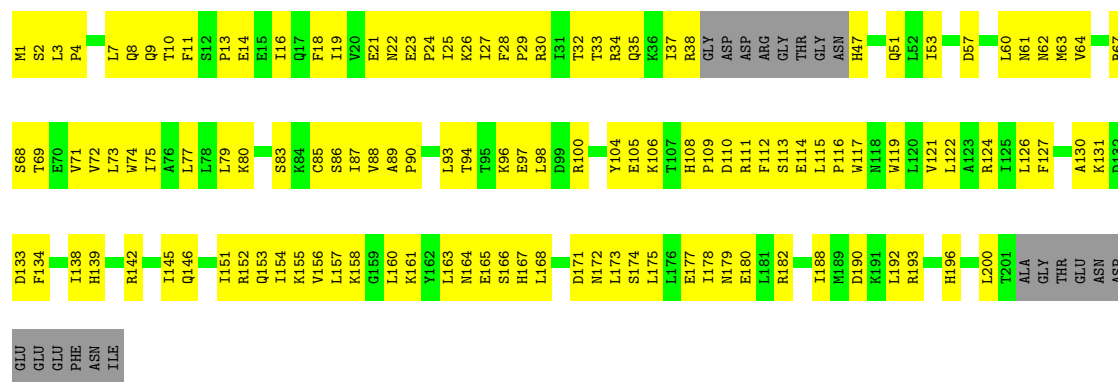
- Molecule 6: DNA replication licensing factor MCM7





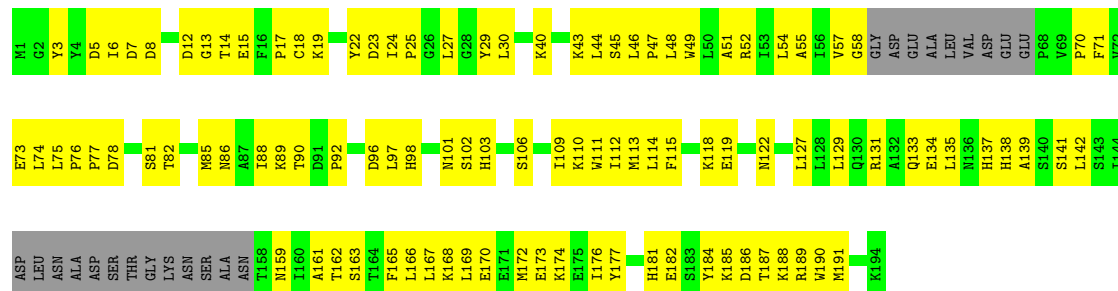
• Molecule 8: DNA replication complex GINS protein PSF2

Chain B: 33% 58% 9%



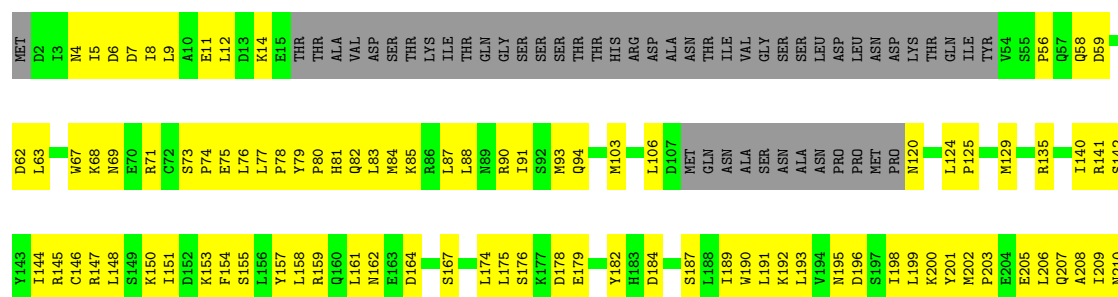
• Molecule 9: DNA replication complex GINS protein PSF3

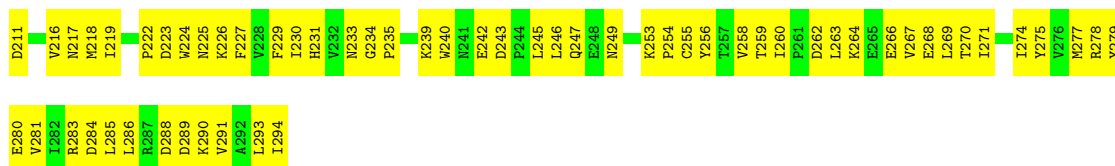
Chain C: 36% 53% 11%



• Molecule 10: DNA replication complex GINS protein SLD5

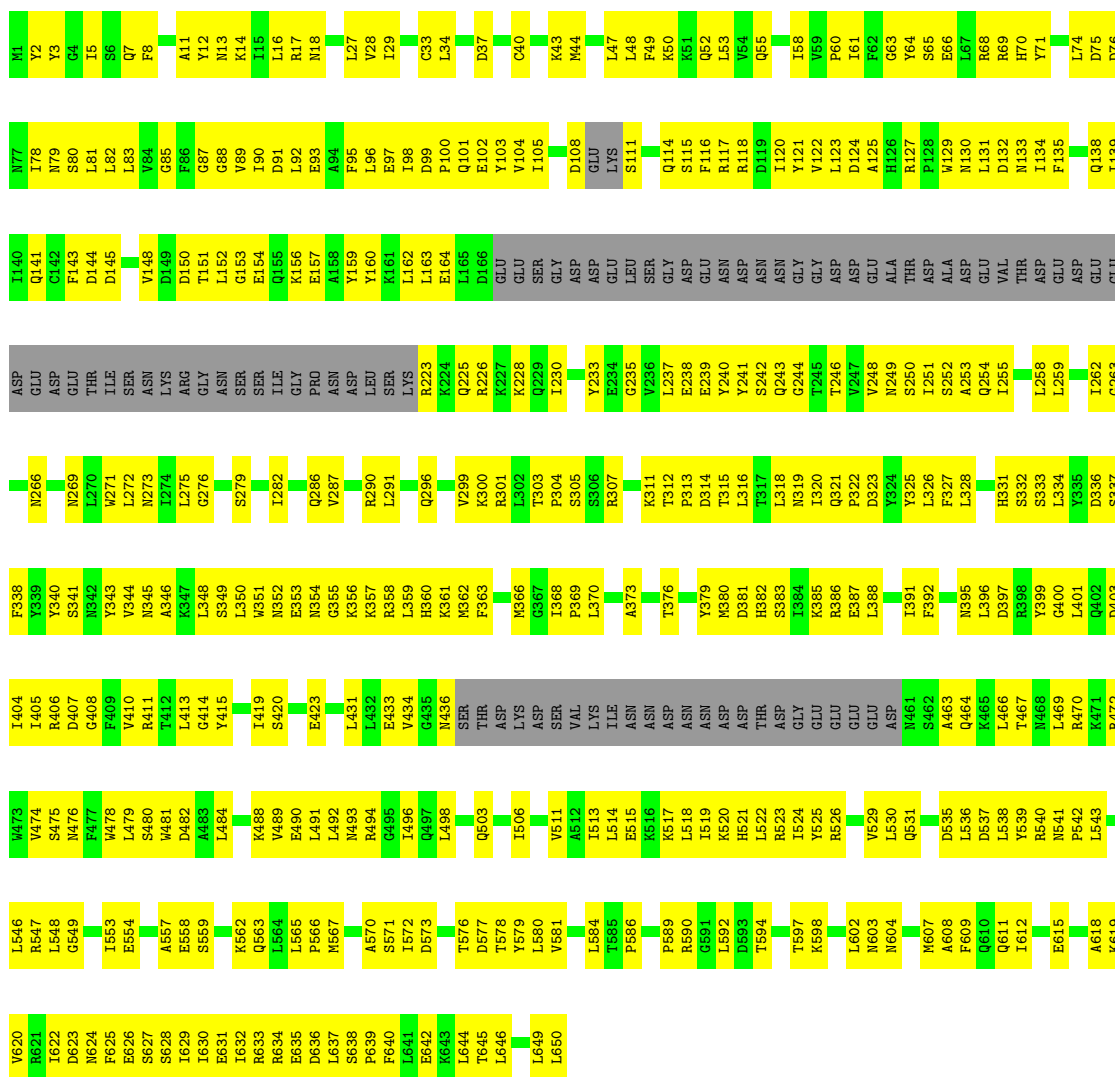
Chain D: 32% 51% 17%





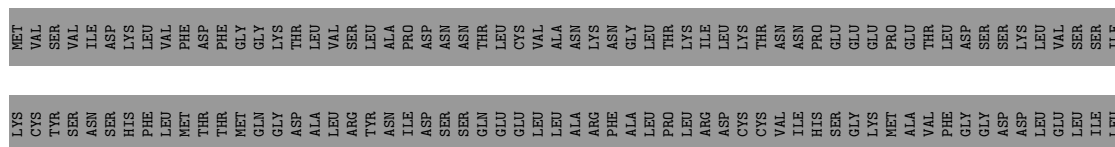
• Molecule 11: Cell division control protein 45

Chain E: 31% 56% 13%



• Molecule 12: DNA polymerase alpha-binding protein

Chain F: 20% 26% 54%



- Molecule 12: DNA polymerase alpha-binding protein

[illegible]

- Molecule 12: DNA polymerase alpha-binding protein



WORLD WIDE
PDB
PROTEIN DATA BANK

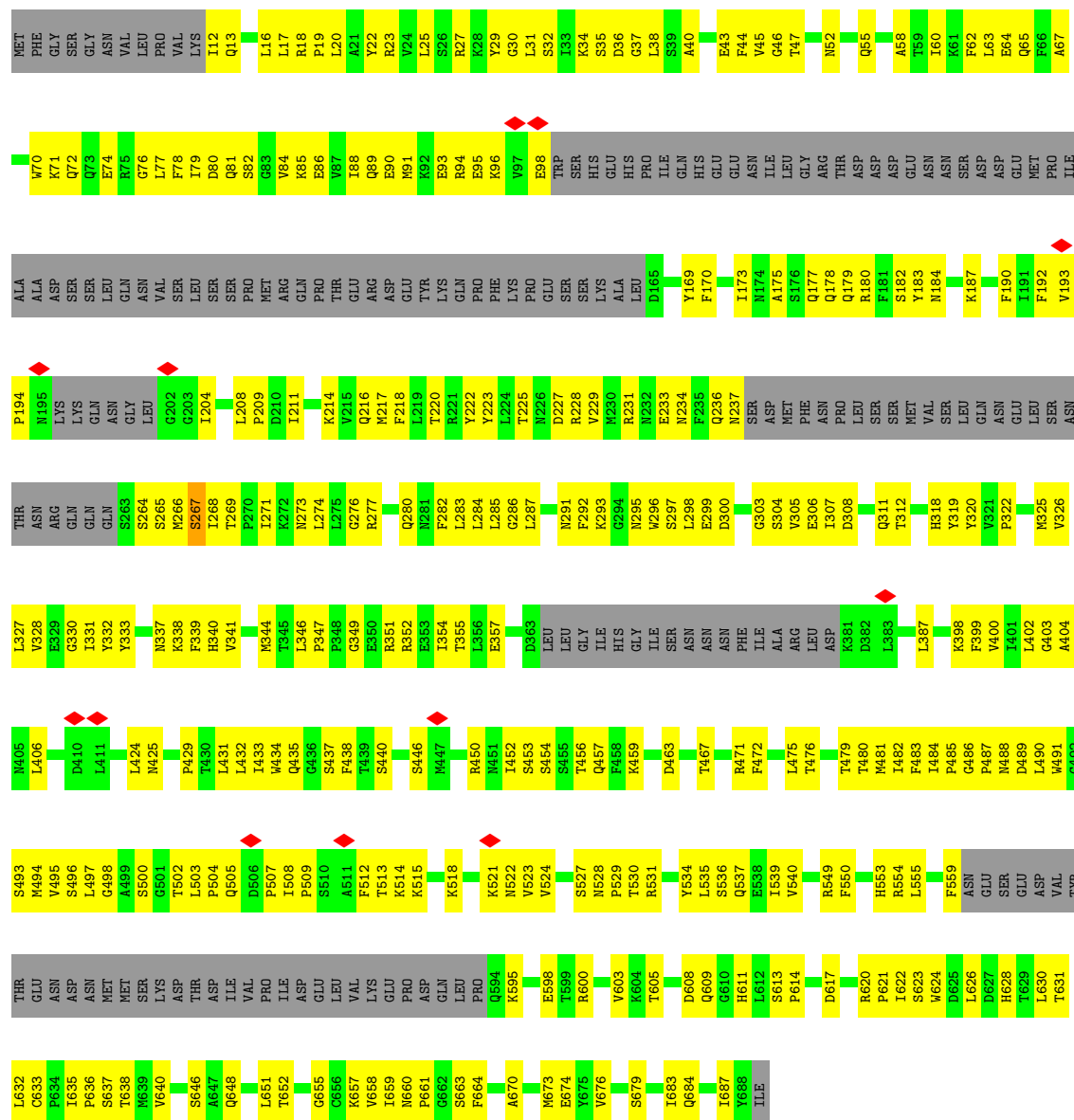






● Molecule 16: DNA polymerase epsilon subunit B

Chain N: 35% 42% 23%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17199	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.030	Depositor
Minimum map value	-0.192	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	466.39996, 466.39996, 466.39996	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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, AGS, 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	0.20	0/5360	0.47	0/7241
2	3	0.22	0/5032	0.46	0/6827
3	4	0.15	0/5459	0.41	0/7363
4	5	0.20	1/5402 (0.0%)	0.47	0/7300
5	6	0.25	0/5036	0.58	2/6799 (0.0%)
6	7	0.27	0/5019	0.51	4/6789 (0.1%)
7	A	0.42	1/1653 (0.1%)	0.66	1/2224 (0.0%)
8	B	0.18	0/1650	0.35	0/2231
9	C	0.17	0/1420	0.37	0/1918
10	D	0.19	0/2040	0.40	0/2755
11	E	0.17	0/4685	0.37	0/6343
12	F	0.17	0/3489	0.39	1/4724 (0.0%)
12	G	0.16	0/3465	0.41	0/4696
12	H	0.15	0/3496	0.38	0/4735
13	I	0.16	0/339	0.42	0/520
14	J	0.13	0/177	0.23	0/269
15	M	0.28	1/6586 (0.0%)	0.47	0/8926
16	N	0.19	0/4290	0.41	0/5811
All	All	0.22	3/64598 (0.0%)	0.45	8/87471 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	525	PRO	N-CD	-5.60	1.40	1.47
7	A	61	GLY	C-O	5.28	1.31	1.23
15	M	1941	LEU	C-O	5.22	1.30	1.24

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	57	GLN	CA-C-O	-5.69	114.81	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
12	F	762	ILE	N-CA-C	-5.15	107.32	111.91
5	6	116	GLU	CA-C-N	-5.14	112.13	120.72
5	6	116	GLU	C-N-CA	-5.14	112.13	120.72
6	7	620	HIS	CA-C-N	5.12	131.31	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	5270	0	5304	455	0
2	3	4948	0	4991	440	0
3	4	5390	0	5467	432	0
4	5	5325	0	5351	449	0
5	6	4955	0	4959	523	0
6	7	4945	0	4987	421	0
7	A	1633	0	1631	161	0
8	B	1617	0	1674	130	0
9	C	1387	0	1405	106	0
10	D	2004	0	2001	152	0
11	E	4599	0	4584	337	0
12	F	3404	0	3352	231	0
12	G	3380	0	3310	233	0
12	H	3411	0	3355	235	0
13	I	307	0	178	12	0
14	J	159	0	90	2	0
15	M	6447	0	6368	410	0
16	N	4199	0	4163	260	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
17	M	2	0	0	0	0
18	2	27	0	12	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	3	27	0	12	16	0
19	2	1	0	0	0	0
19	5	2	0	0	0	0
19	7	1	0	0	0	0
20	5	31	0	12	12	0
20	7	31	0	12	9	0
All	All	63507	0	63218	4674	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 37.

The worst 5 of 4674 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:802:ILE:HG13	5:6:736:MET:SD	1.57	1.44
5:6:735:HIS:O	5:6:736:MET:HG2	1.28	1.32
3:4:802:ILE:CG1	5:6:736:MET:SD	2.21	1.28
3:4:802:ILE:CD1	5:6:736:MET:SD	2.27	1.22
2:3:499:LYS:HA	6:7:490:GLY:HA2	1.19	1.16

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	664/868 (76%)	621 (94%)	42 (6%)	1 (0%)	43	77
2	3	629/971 (65%)	580 (92%)	49 (8%)	0	100	100
3	4	658/933 (70%)	616 (94%)	40 (6%)	2 (0%)	36	71
4	5	662/775 (85%)	609 (92%)	50 (8%)	3 (0%)	24	63
5	6	619/1017 (61%)	547 (88%)	67 (11%)	5 (1%)	16	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	7	622/845 (74%)	570 (92%)	47 (8%)	5 (1%)	16	53
7	A	196/208 (94%)	183 (93%)	12 (6%)	1 (0%)	24	63
8	B	189/213 (89%)	184 (97%)	5 (3%)	0	100	100
9	C	166/194 (86%)	164 (99%)	2 (1%)	0	100	100
10	D	237/294 (81%)	230 (97%)	7 (3%)	0	100	100
11	E	560/650 (86%)	548 (98%)	12 (2%)	0	100	100
12	F	418/927 (45%)	404 (97%)	14 (3%)	0	100	100
12	G	416/927 (45%)	408 (98%)	8 (2%)	0	100	100
12	H	419/927 (45%)	410 (98%)	9 (2%)	0	100	100
15	M	800/2222 (36%)	725 (91%)	72 (9%)	3 (0%)	30	67
16	N	517/689 (75%)	490 (95%)	27 (5%)	0	100	100
All	All	7772/12660 (61%)	7289 (94%)	463 (6%)	20 (0%)	37	71

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	6	178	LEU
5	6	714	VAL
15	M	1945	LEU
4	5	669	SER
5	6	744	PRO

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	2	578/770 (75%)	577 (100%)	1 (0%)	87	85
2	3	541/835 (65%)	539 (100%)	2 (0%)	84	82
3	4	614/848 (72%)	614 (100%)	0	100	100
4	5	602/688 (88%)	602 (100%)	0	100	100
5	6	543/886 (61%)	535 (98%)	8 (2%)	57	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	7	544/753 (72%)	535 (98%)	9 (2%)	53	67
7	A	184/193 (95%)	168 (91%)	16 (9%)	9	29
8	B	183/198 (92%)	183 (100%)	0	100	100
9	C	155/173 (90%)	155 (100%)	0	100	100
10	D	234/279 (84%)	234 (100%)	0	100	100
11	E	510/586 (87%)	510 (100%)	0	100	100
12	F	375/825 (46%)	375 (100%)	0	100	100
12	G	372/825 (45%)	372 (100%)	0	100	100
12	H	375/825 (46%)	375 (100%)	0	100	100
15	M	713/2014 (35%)	698 (98%)	15 (2%)	47	65
16	N	467/629 (74%)	466 (100%)	1 (0%)	87	85
All	All	6990/11327 (62%)	6938 (99%)	52 (1%)	73	79

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A	66	LYS
7	A	119	ASP
15	M	2016	LYS
7	A	69	LYS
7	A	108	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
12	G	563	HIS
15	M	1931	GLN
12	G	629	HIS
12	H	877	GLN
15	M	2030	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 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 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	ADP	3	1001	19	28,29,29	0.55	0	43,45,45	0.50	0
20	AGS	7	903	-	32,33,33	0.65	1 (3%)	45,52,52	0.55	0
18	ADP	2	902	19	28,29,29	0.47	0	43,45,45	0.60	0
20	AGS	5	803	19	32,33,33	0.64	1 (3%)	45,52,52	0.52	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	ADP	3	1001	19	-	5/16/32/32	0/3/3/3
20	AGS	7	903	-	-	6/21/38/38	0/3/3/3
18	ADP	2	902	19	-	5/16/32/32	0/3/3/3
20	AGS	5	803	19	-	7/21/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	903	AGS	PG-S1G	2.13	1.95	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	803	AGS	PG-S1G	2.08	1.95	1.90

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

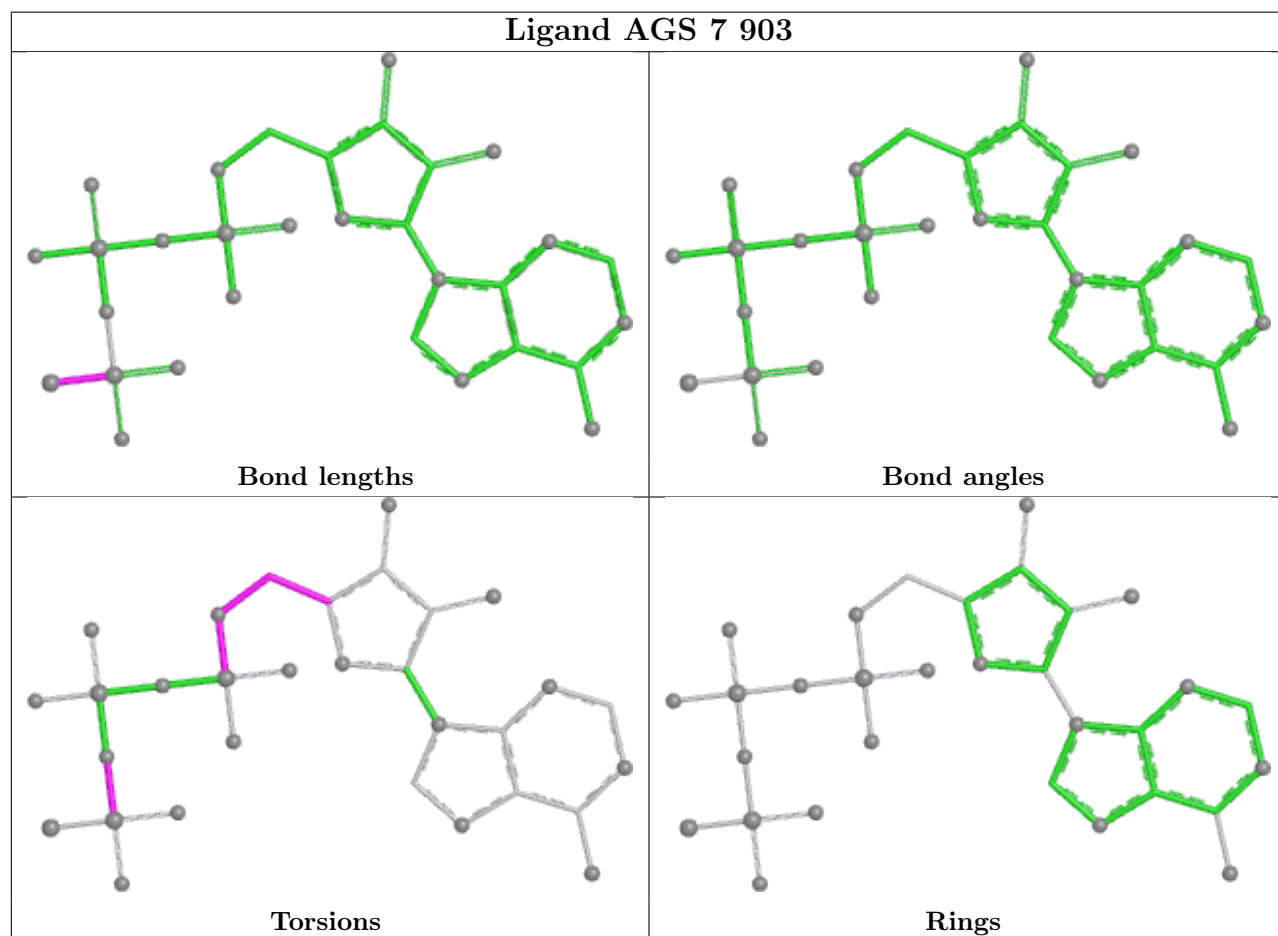
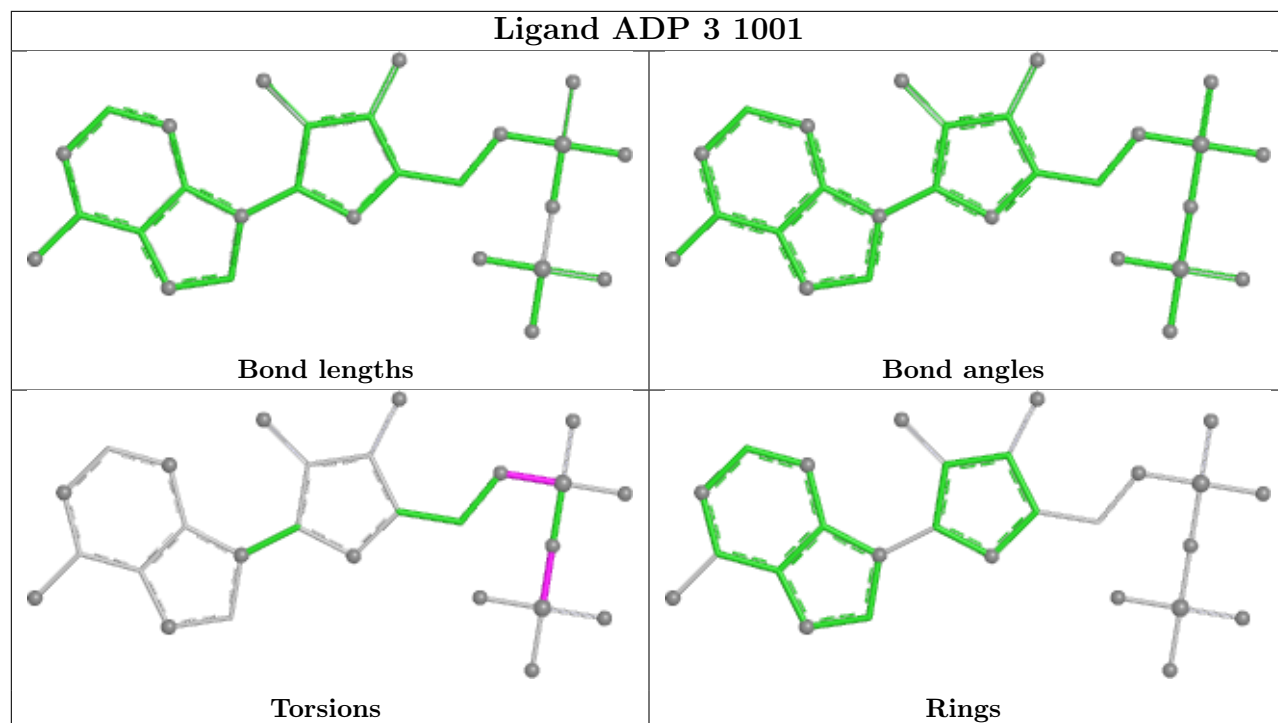
Mol	Chain	Res	Type	Atoms
18	2	902	ADP	PA-O3A-PB-O3B
18	3	1001	ADP	PA-O3A-PB-O2B
18	3	1001	ADP	C5'-O5'-PA-O1A
18	3	1001	ADP	C5'-O5'-PA-O3A
20	5	803	AGS	C5'-O5'-PA-O3A

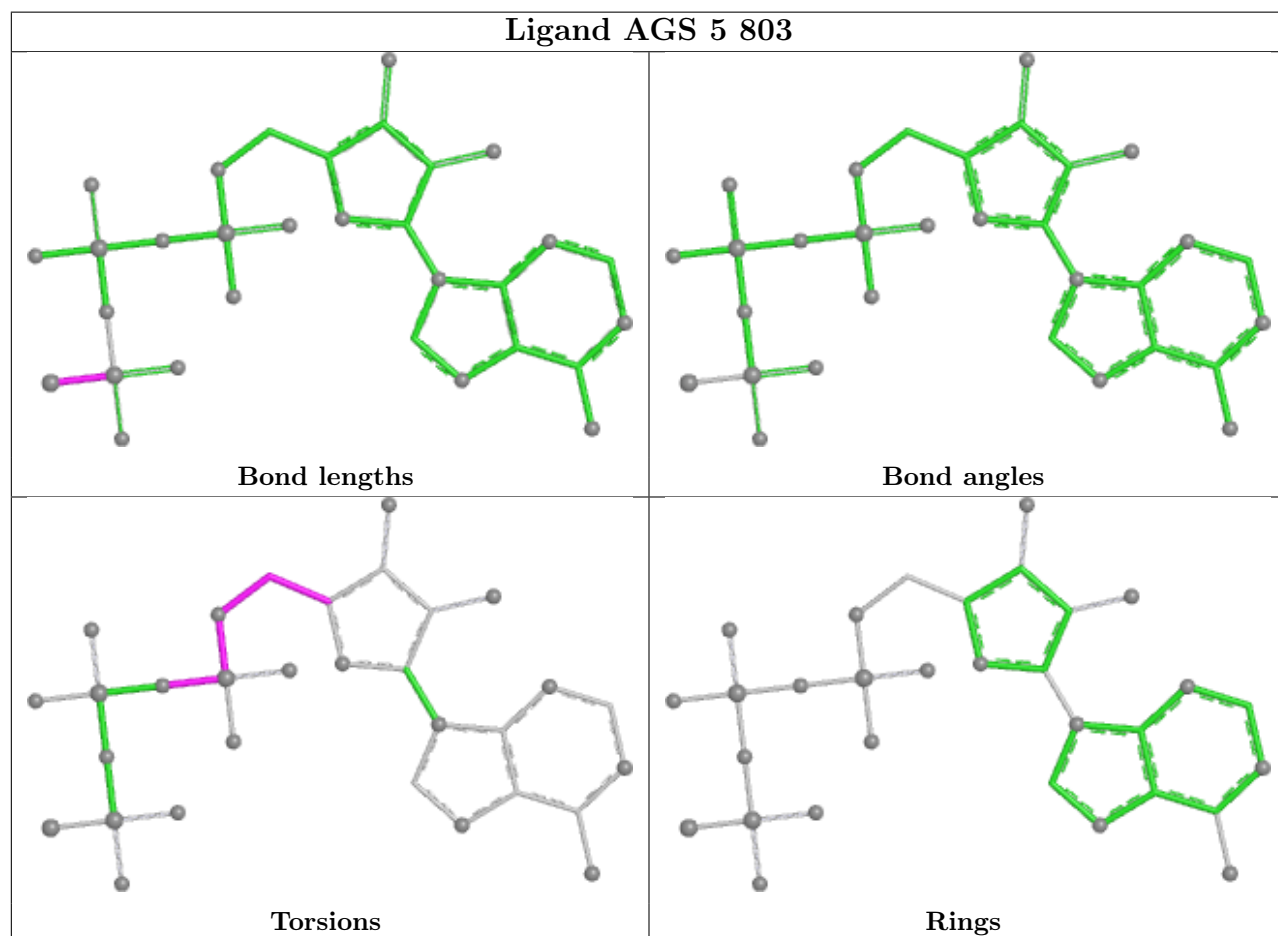
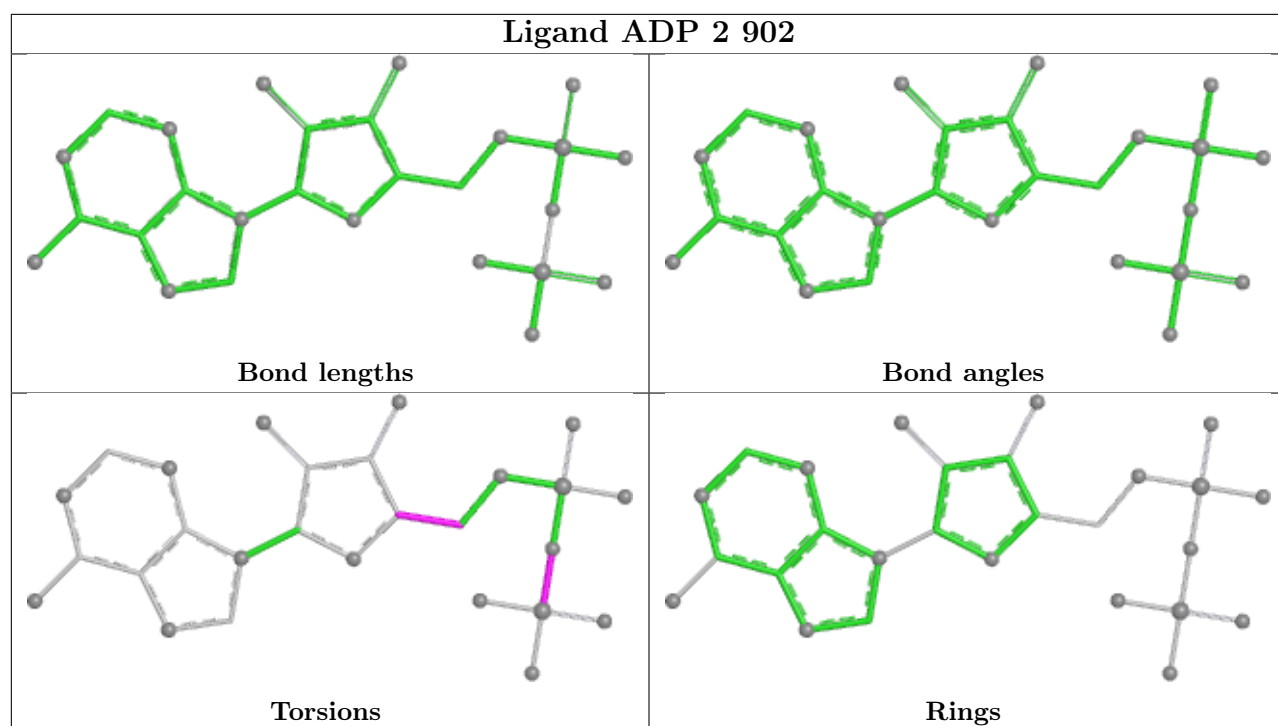
There are no ring outliers.

4 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3	1001	ADP	16	0
20	7	903	AGS	9	0
18	2	902	ADP	20	0
20	5	803	AGS	12	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.

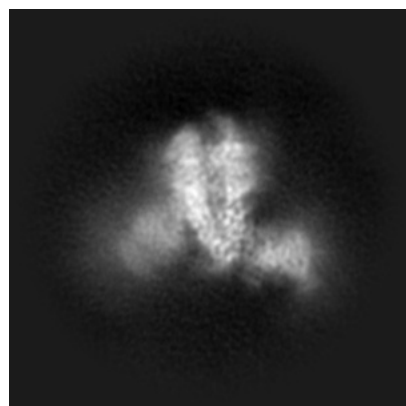
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37215. These allow visual inspection of the internal detail of the map and identification of artifacts.

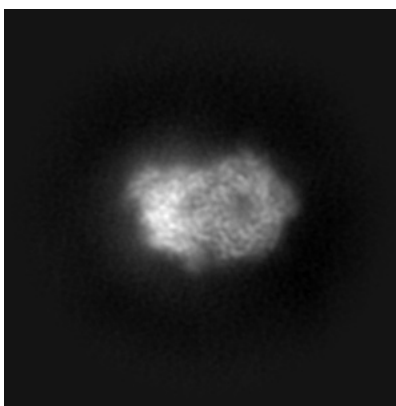
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

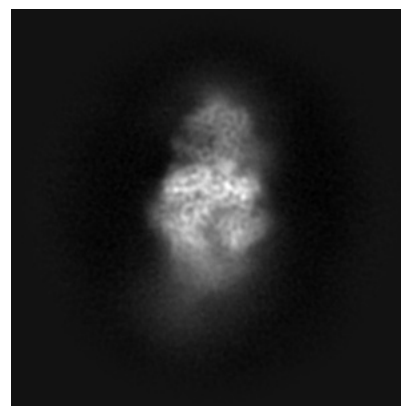
6.1.1 Primary map



X

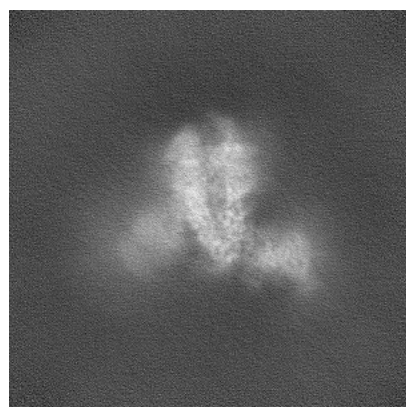


Y

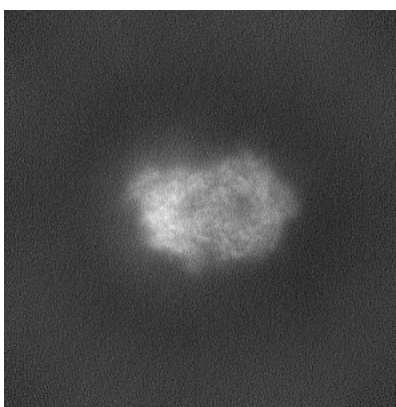


Z

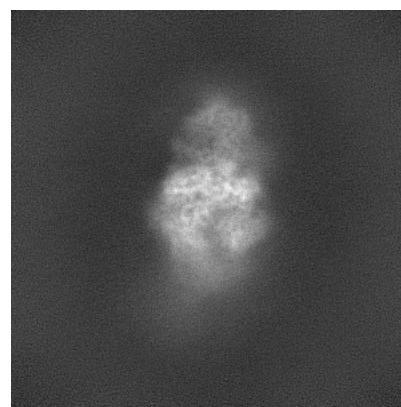
6.1.2 Raw map



X



Y

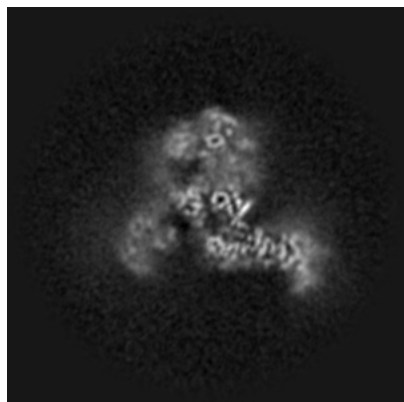


Z

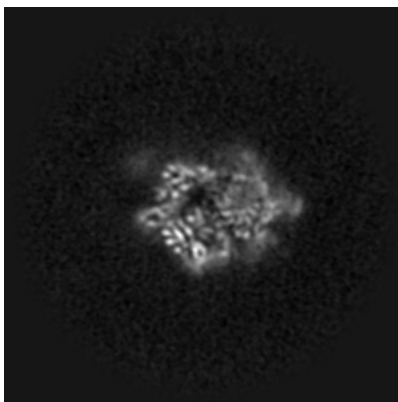
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

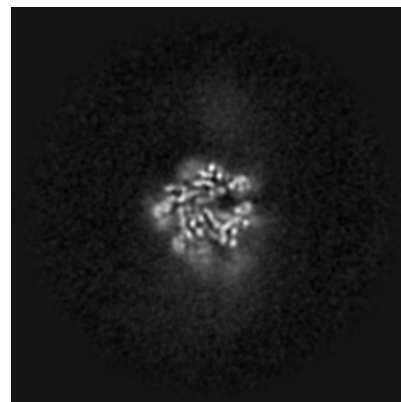
6.2.1 Primary map



X Index: 220

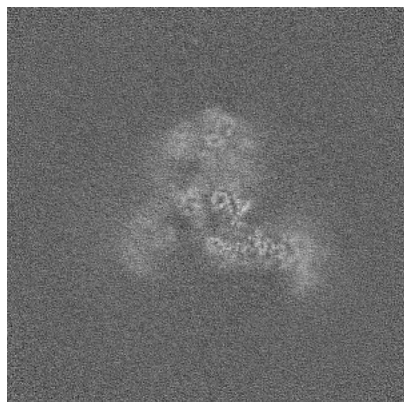


Y Index: 220

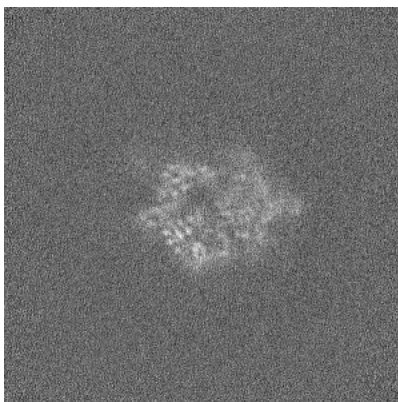


Z Index: 220

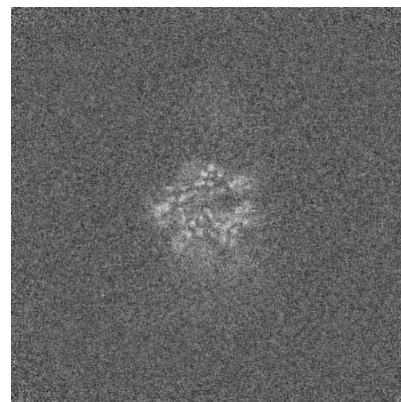
6.2.2 Raw map



X Index: 220



Y Index: 220

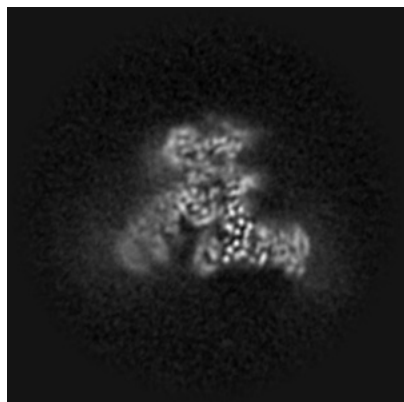


Z Index: 220

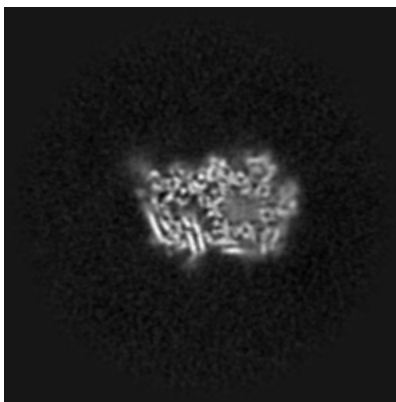
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

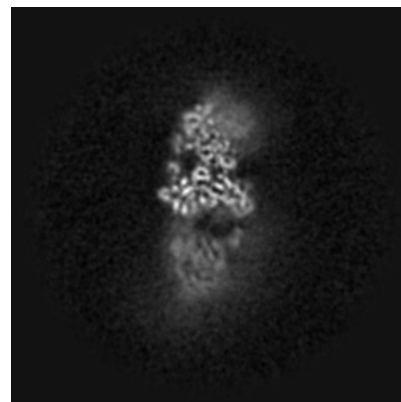
6.3.1 Primary map



X Index: 207

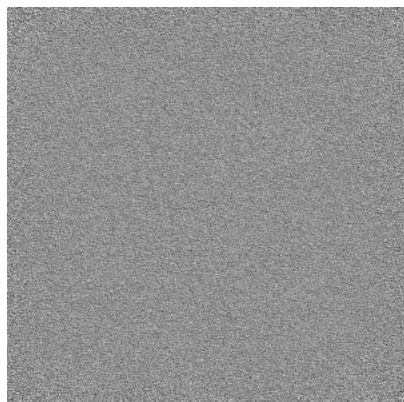


Y Index: 241

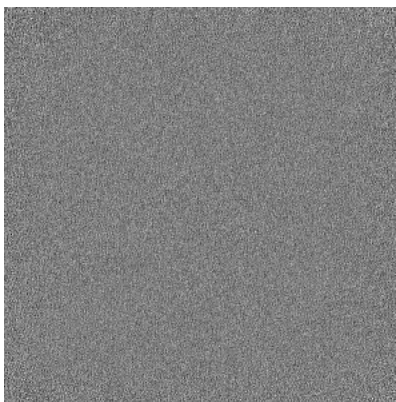


Z Index: 181

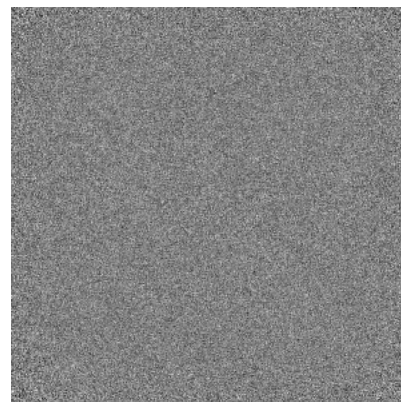
6.3.2 Raw map



X Index: 0



Y Index: 0

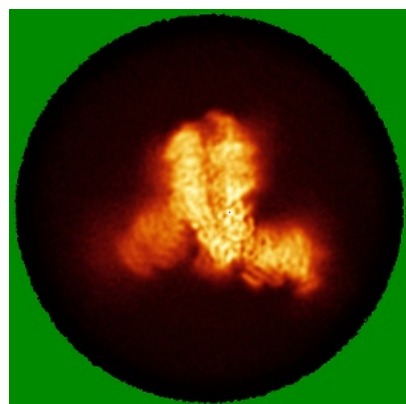


Z Index: 0

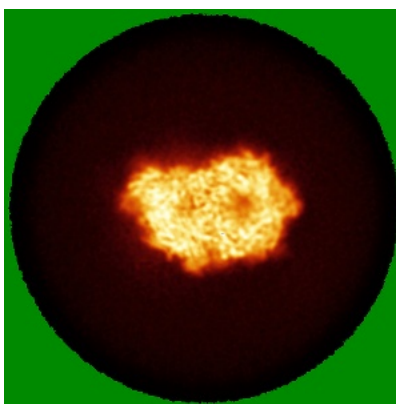
The images above show the largest variance slices of the map in three orthogonal directions.

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

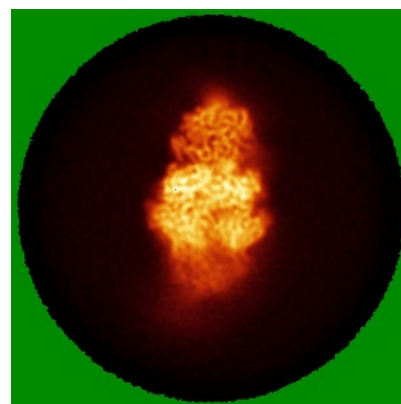
6.4.1 Primary map



X

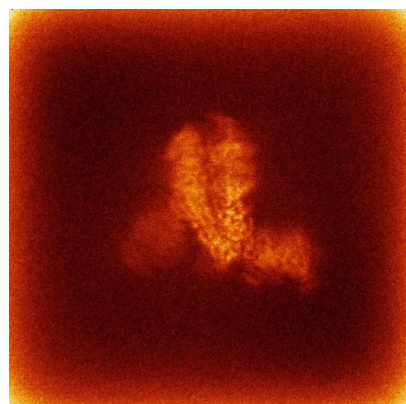


Y

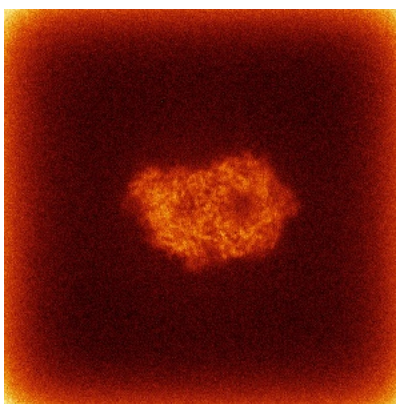


Z

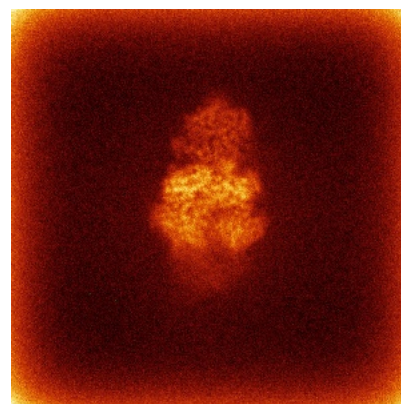
6.4.2 Raw map



X



Y



Z

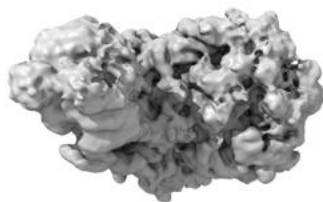
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



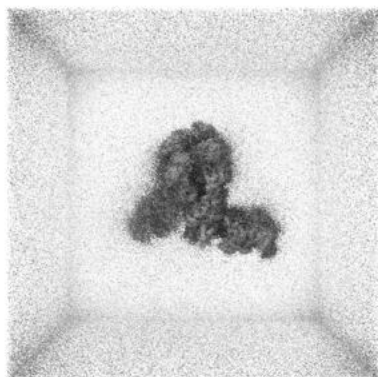
Y



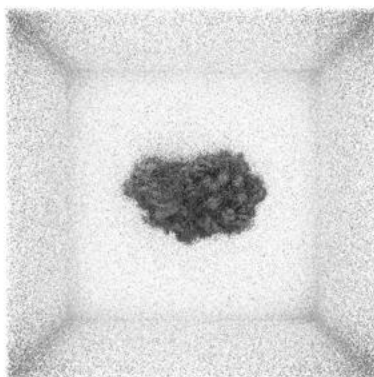
Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

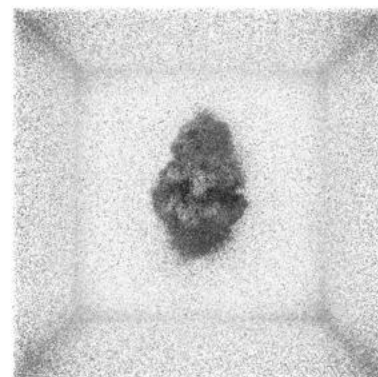
6.5.2 Raw map



X



Y



Z

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.

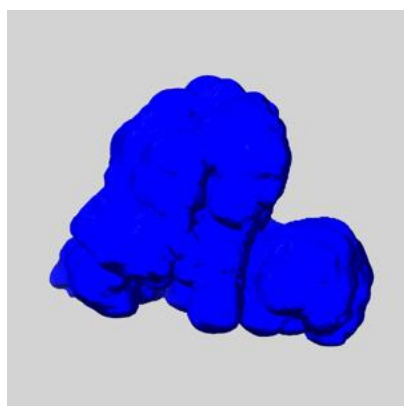
6.6 Mask visualisation [i](#)

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

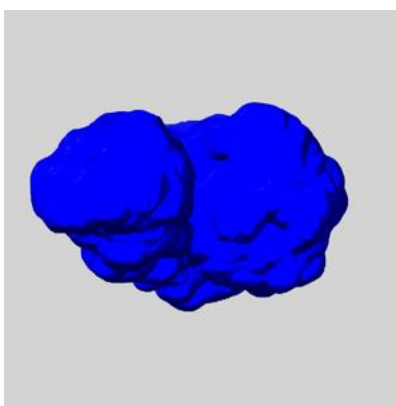
A mask typically either:

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

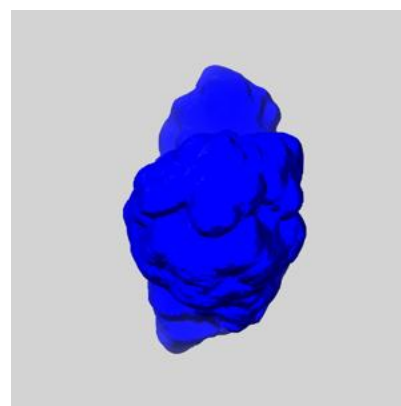
6.6.1 emd_37215_msk_1.map [i](#)



X



Y

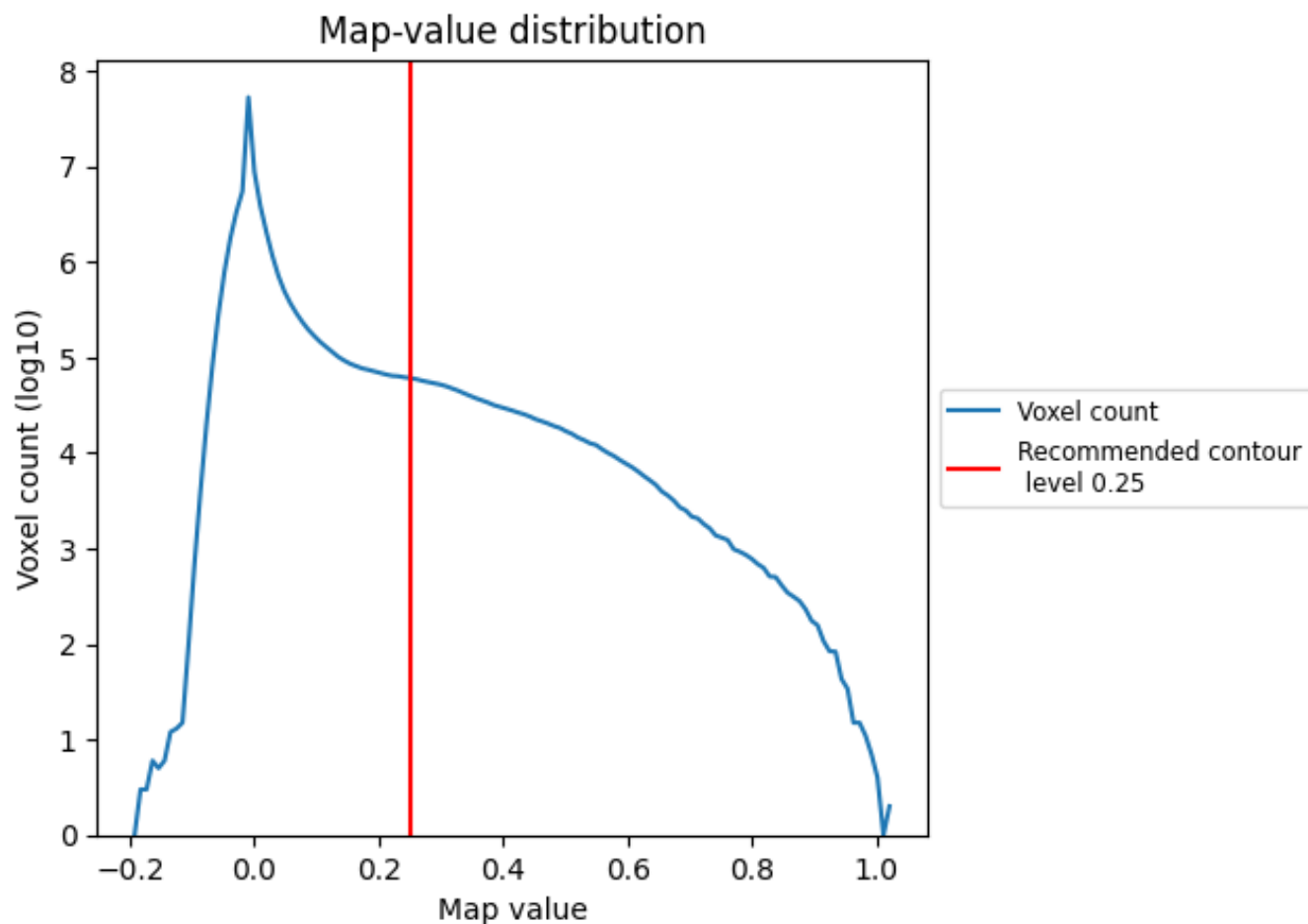


Z

7 Map analysis [i](#)

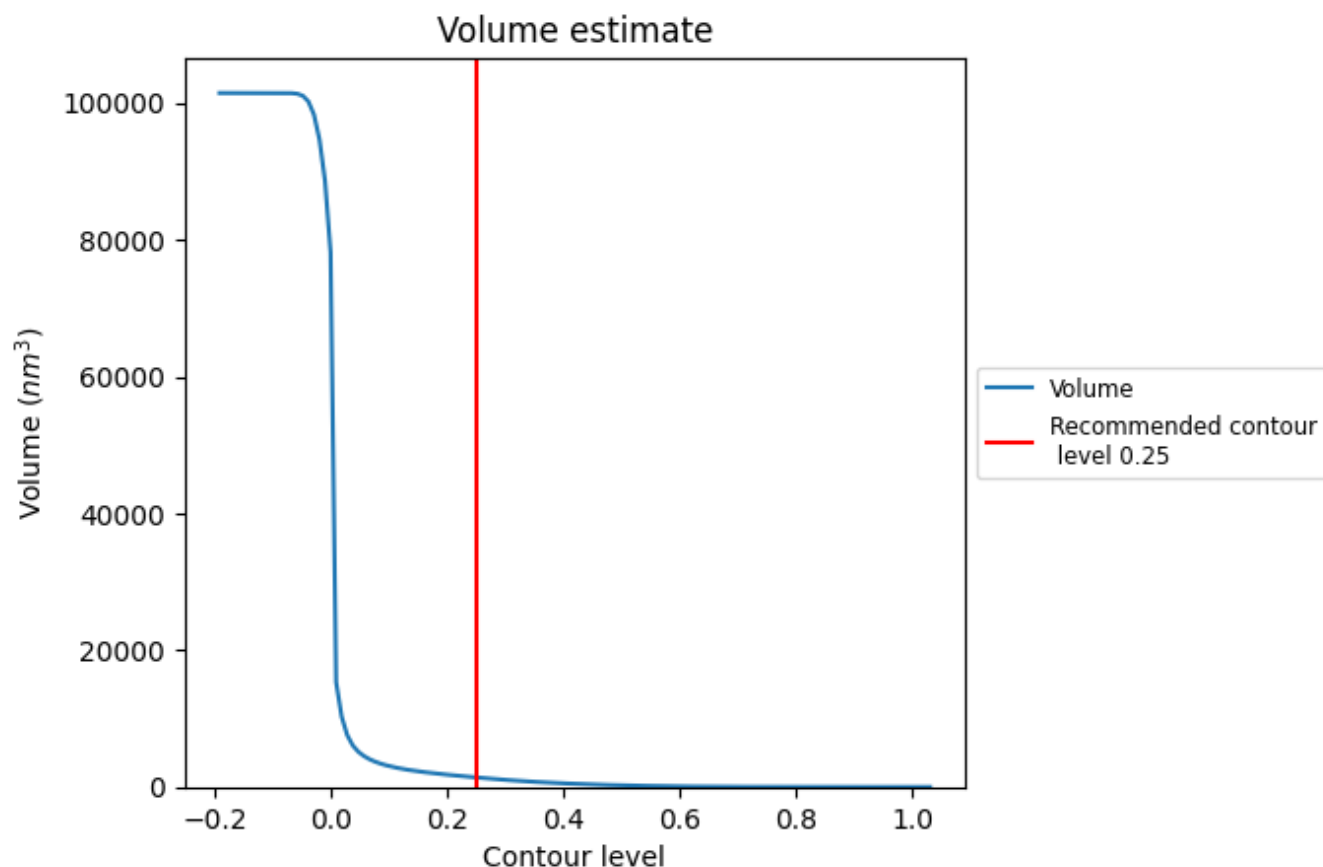
This section contains the results of statistical analysis of the map.

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.

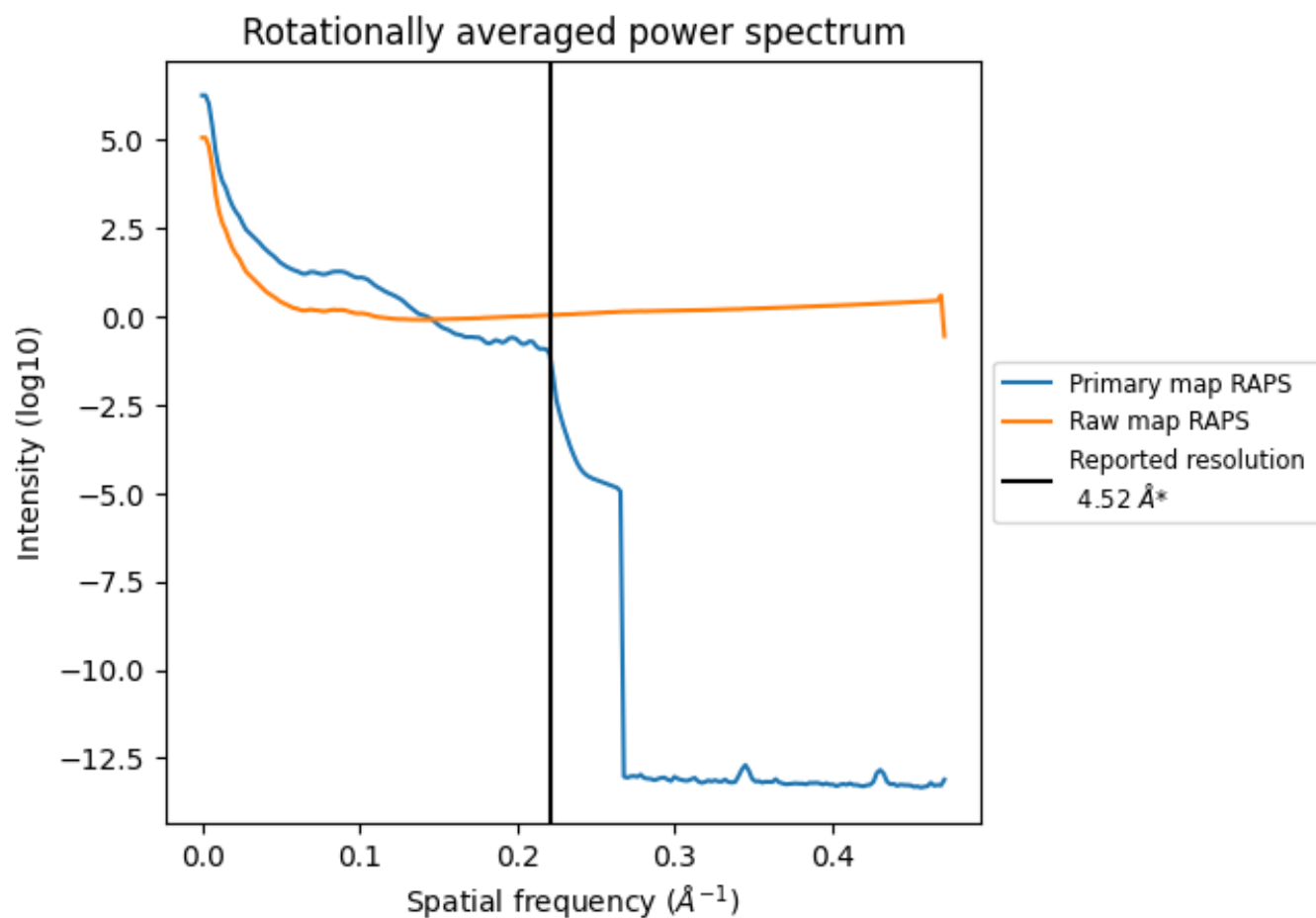
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1385 nm³; this corresponds to an approximate mass of 1251 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 ⓘ

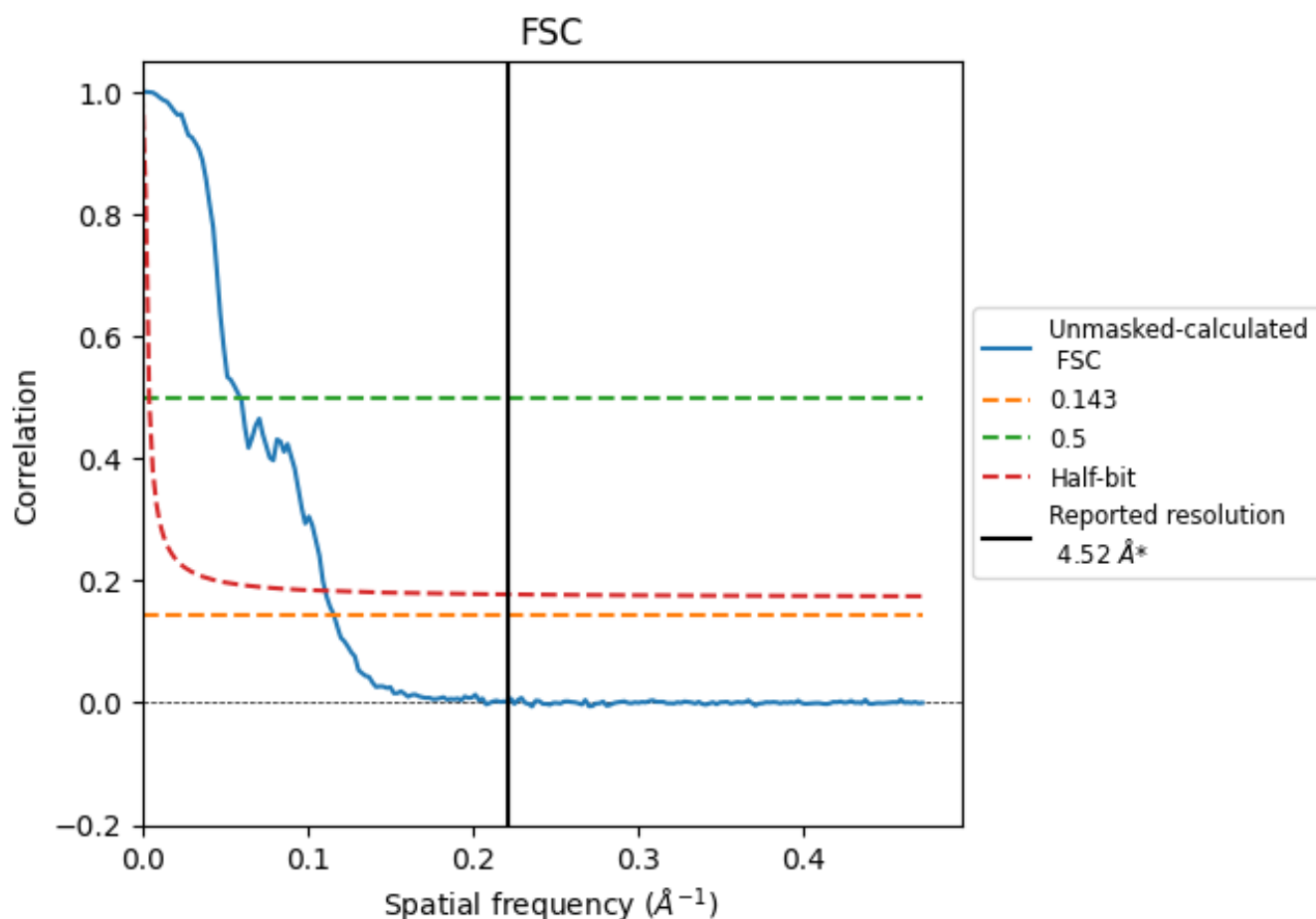


*Reported resolution corresponds to spatial frequency of 0.221 Å⁻¹

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 0.221 Å⁻¹

8.2 Resolution estimates [i](#)

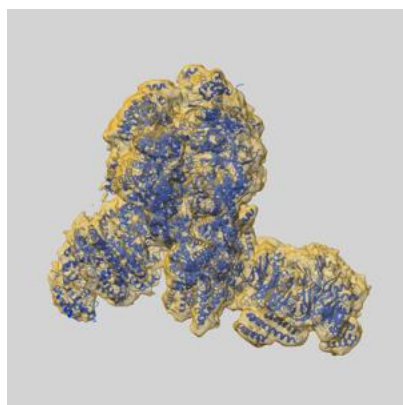
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.62	16.92	9.03

*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 8.62 differs from the reported value 4.52 by more than 10 %

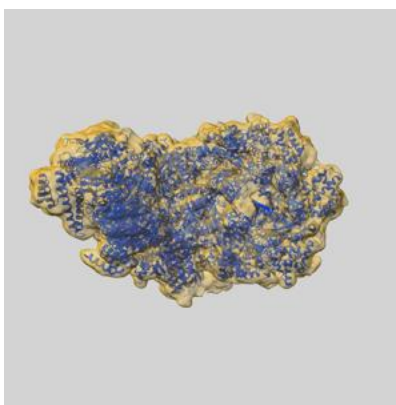
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37215 and PDB model 8KG9. Per-residue inclusion information can be found in section [3](#) on page [9](#).

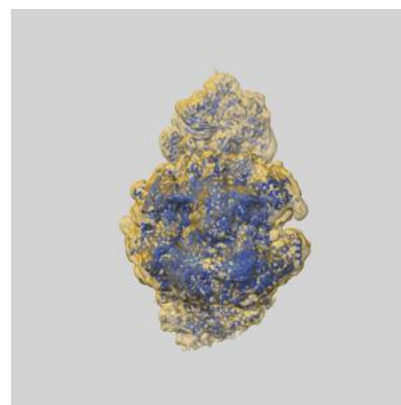
9.1 Map-model overlay [i](#)



X



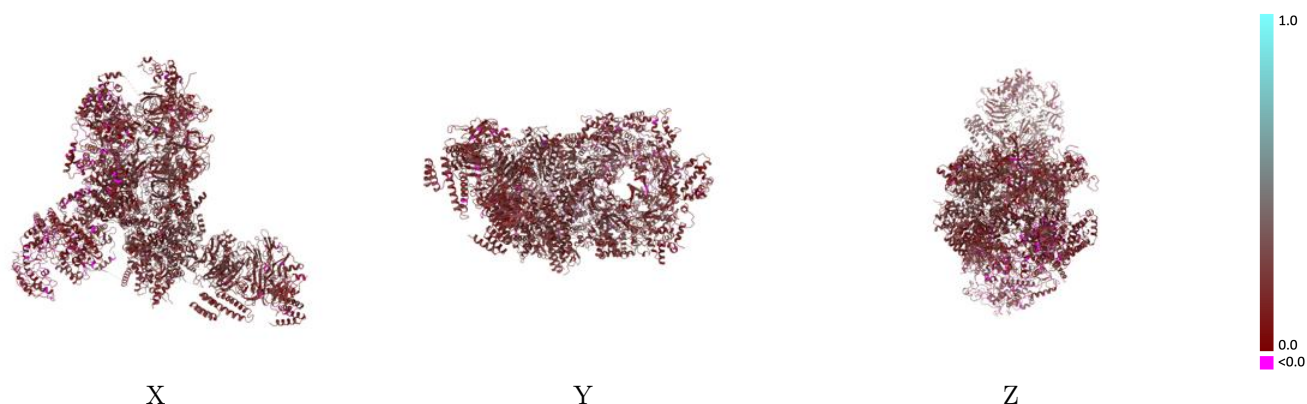
Y



Z

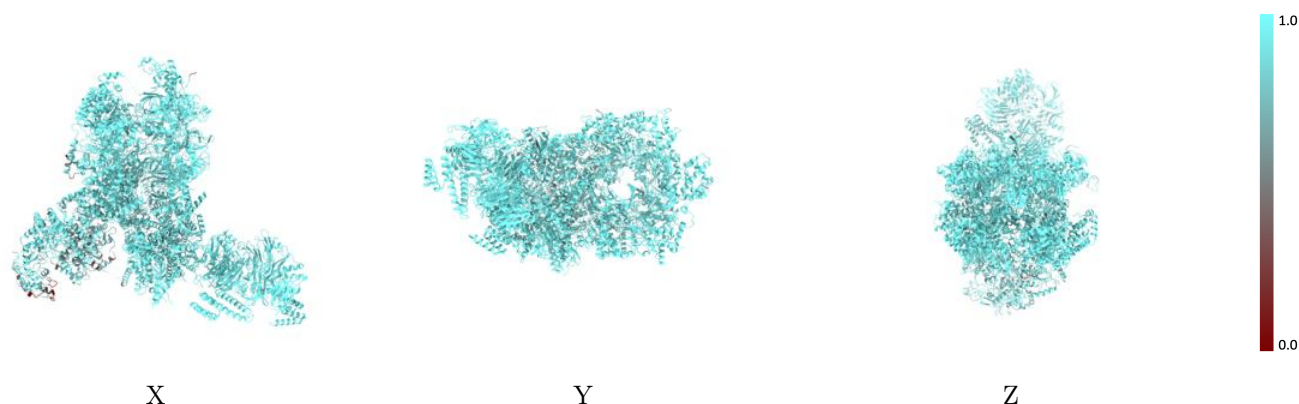
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



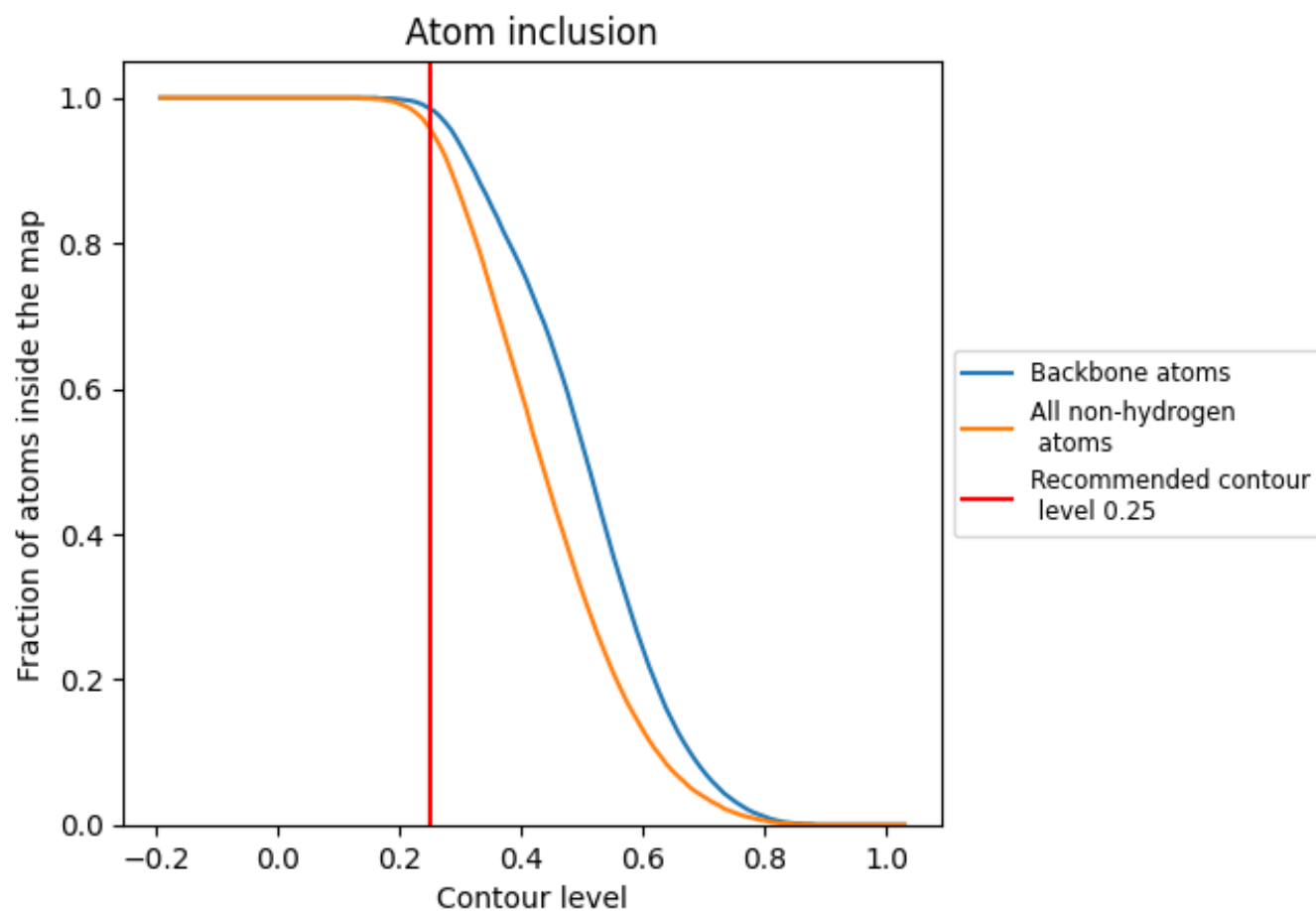
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9580	0.1900
2	0.9700	0.1940
3	0.9880	0.2150
4	0.9710	0.1590
5	0.9620	0.1950
6	0.9880	0.1660
7	0.9900	0.1930
A	0.9760	0.2100
B	0.9740	0.2370
C	0.9800	0.2200
D	0.9800	0.2310
E	0.9740	0.2230
F	0.9820	0.2270
G	0.9940	0.1930
H	0.9910	0.2000
I	0.9380	0.1820
J	0.8110	0.1360
M	0.8210	0.1410
N	0.9070	0.1640

1.0

0.0

<0.0