



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:55 AM UTC

PDB ID : 7PFO / pdb_00007pfo
EMDB ID : EMD-13375
Title : Core human replisome
Authors : Jones, M.J.; Yeeles, J.T.P.
Deposited on : 2021-08-11
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

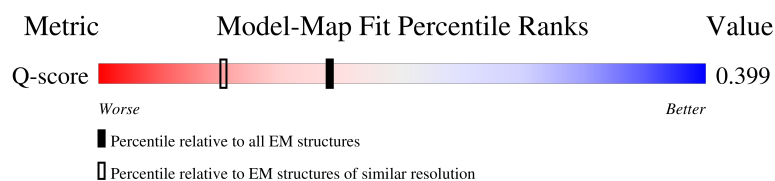
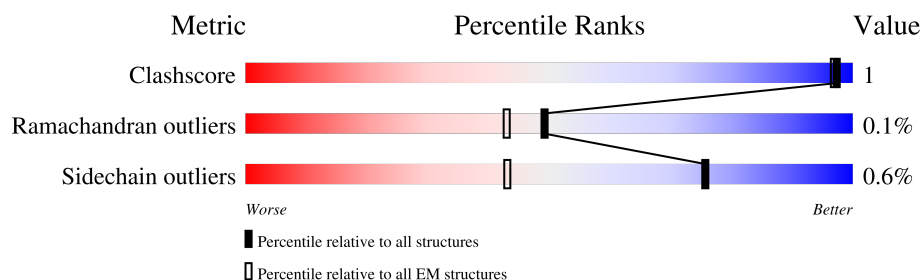
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 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.



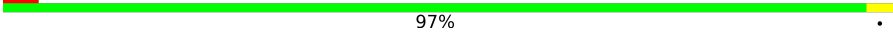
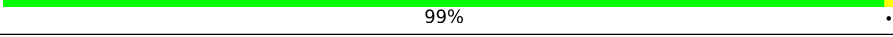
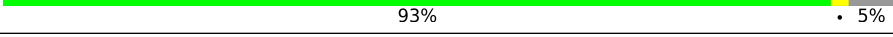
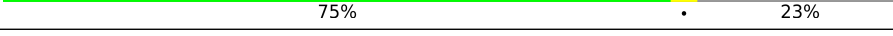
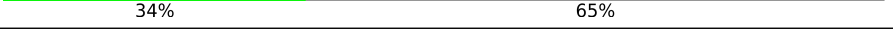
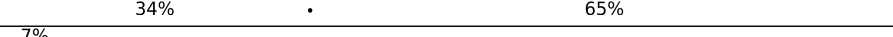
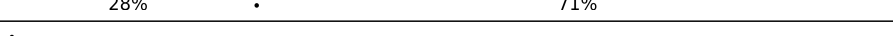
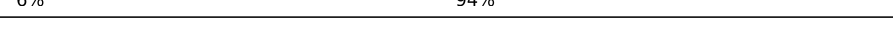
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	2	904	
2	3	808	
3	4	863	
4	5	734	

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Mol	Chain	Length	Quality of chain
5	6	821	
6	7	719	
7	A	527	
8	B	2286	
9	C	569	
10	D	196	
11	E	185	
12	F	216	
13	G	262	
14	H	1161	
14	I	1161	
14	J	1161	
15	K	1209	
16	L	301	
17	M	85	
18	N	54	
19	Q	1371	

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 136660 atoms, of which 68143 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	703	Total	C	H	N	O	S	0	0
			11177	3511	5597	994	1043	32		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	3	620	Total	C	H	N	O	S	0	0
			9770	3037	4912	859	936	26		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	4	619	Total	C	H	N	O	S	0	0
			9922	3103	4993	873	926	27		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	5	605	Total	C	H	N	O	S	0	0
			9544	2968	4809	841	891	35		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	6	632	Total	C	H	N	O	S	0	0
			10065	3150	5051	890	948	26		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	7	598	Total	C	H	N	O	S	0	0
			9552	2983	4802	840	897	30		

- Molecule 7 is a protein called DNA polymerase epsilon subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A	527	Total	C	H	N	O	S	0	0
			8359	2702	4160	697	780	20		

- Molecule 8 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	B	804	Total	C	H	N	O	S	0	0
			12975	4162	6478	1116	1176	43		

- Molecule 9 is a protein called Cell division control protein 45 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	C	534	Total	C	H	N	O	S	0	0
			8647	2764	4300	745	807	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	135Z	ASP	-	linker	UNP O75419
C	136A	TYR	-	linker	UNP O75419
C	136B	LYS	-	linker	UNP O75419
C	136C	ASP	-	linker	UNP O75419
C	136D	ASP	-	linker	UNP O75419
C	136E	ASP	-	linker	UNP O75419

- Molecule 10 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	D	195	Total	C	H	N	O	S	0	0
			3207	1013	1601	289	292	12		

- Molecule 11 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	176	Total	C	H	N	O	S	0	0
			2887	916	1456	242	264	9		

- Molecule 12 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	F	194	Total	C	H	N	O	S	0	0
			3048	979	1502	268	293	6		

- Molecule 13 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	G	203	Total	C	H	N	O	S	0	0
			3381	1065	1702	290	314	10		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-38	MET	-	initiating methionine	UNP Q9BRT9
G	-37	TRP	-	expression tag	UNP Q9BRT9
G	-36	SER	-	expression tag	UNP Q9BRT9
G	-35	HIS	-	expression tag	UNP Q9BRT9
G	-34	PRO	-	expression tag	UNP Q9BRT9
G	-33	GLN	-	expression tag	UNP Q9BRT9
G	-32	PHE	-	expression tag	UNP Q9BRT9
G	-31	GLU	-	expression tag	UNP Q9BRT9
G	-30	LYS	-	expression tag	UNP Q9BRT9
G	-29	GLY	-	expression tag	UNP Q9BRT9
G	-28	GLY	-	expression tag	UNP Q9BRT9
G	-27	GLY	-	expression tag	UNP Q9BRT9
G	-26	SER	-	expression tag	UNP Q9BRT9
G	-25	GLY	-	expression tag	UNP Q9BRT9
G	-24	GLY	-	expression tag	UNP Q9BRT9
G	-23	GLY	-	expression tag	UNP Q9BRT9
G	-22	SER	-	expression tag	UNP Q9BRT9
G	-21	GLY	-	expression tag	UNP Q9BRT9
G	-20	GLY	-	expression tag	UNP Q9BRT9
G	-19	SER	-	expression tag	UNP Q9BRT9
G	-18	ALA	-	expression tag	UNP Q9BRT9
G	-17	TRP	-	expression tag	UNP Q9BRT9
G	-16	SER	-	expression tag	UNP Q9BRT9
G	-15	HIS	-	expression tag	UNP Q9BRT9
G	-14	PRO	-	expression tag	UNP Q9BRT9
G	-13	GLN	-	expression tag	UNP Q9BRT9
G	-12	PHE	-	expression tag	UNP Q9BRT9
G	-11	GLU	-	expression tag	UNP Q9BRT9
G	-10	LYS	-	expression tag	UNP Q9BRT9
G	-9	SER	-	expression tag	UNP Q9BRT9
G	-8	GLY	-	expression tag	UNP Q9BRT9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	LEU	-	expression tag	UNP Q9BRT9
G	-6	GLU	-	expression tag	UNP Q9BRT9
G	-5	VAL	-	expression tag	UNP Q9BRT9
G	-4	LEU	-	expression tag	UNP Q9BRT9
G	-3	PHE	-	expression tag	UNP Q9BRT9
G	-2	GLN	-	expression tag	UNP Q9BRT9
G	-1	GLY	-	expression tag	UNP Q9BRT9
G	0	PRO	-	expression tag	UNP Q9BRT9

- Molecule 14 is a protein called WD repeat and HMG-box DNA-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	H	401	Total	C	H	N	O	S	0	0
			6309	2011	3140	552	585	21		
14	I	401	Total	C	H	N	O	S	0	0
			6309	2011	3140	552	585	21		
14	J	401	Total	C	H	N	O	S	0	0
			6308	2011	3139	552	585	21		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-31	MET	-	initiating methionine	UNP O75717
H	-30	ASP	-	expression tag	UNP O75717
H	-29	TYR	-	expression tag	UNP O75717
H	-28	LYS	-	expression tag	UNP O75717
H	-27	ASP	-	expression tag	UNP O75717
H	-26	ASP	-	expression tag	UNP O75717
H	-25	ASP	-	expression tag	UNP O75717
H	-24	ASP	-	expression tag	UNP O75717
H	-23	LYS	-	expression tag	UNP O75717
H	-22	ASP	-	expression tag	UNP O75717
H	-21	TYR	-	expression tag	UNP O75717
H	-20	LYS	-	expression tag	UNP O75717
H	-19	ASP	-	expression tag	UNP O75717
H	-18	ASP	-	expression tag	UNP O75717
H	-17	ASP	-	expression tag	UNP O75717
H	-16	ASP	-	expression tag	UNP O75717
H	-15	LYS	-	expression tag	UNP O75717
H	-14	ASP	-	expression tag	UNP O75717
H	-13	TYR	-	expression tag	UNP O75717
H	-12	LYS	-	expression tag	UNP O75717

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-11	ASP	-	expression tag	UNP O75717
H	-10	ASP	-	expression tag	UNP O75717
H	-9	ASP	-	expression tag	UNP O75717
H	-8	ASP	-	expression tag	UNP O75717
H	-7	LYS	-	expression tag	UNP O75717
H	-6	GLU	-	expression tag	UNP O75717
H	-5	ASN	-	expression tag	UNP O75717
H	-4	LEU	-	expression tag	UNP O75717
H	-3	TYR	-	expression tag	UNP O75717
H	-2	PHE	-	expression tag	UNP O75717
H	-1	GLN	-	expression tag	UNP O75717
H	0	GLY	-	expression tag	UNP O75717
I	-31	MET	-	initiating methionine	UNP O75717
I	-30	ASP	-	expression tag	UNP O75717
I	-29	TYR	-	expression tag	UNP O75717
I	-28	LYS	-	expression tag	UNP O75717
I	-27	ASP	-	expression tag	UNP O75717
I	-26	ASP	-	expression tag	UNP O75717
I	-25	ASP	-	expression tag	UNP O75717
I	-24	ASP	-	expression tag	UNP O75717
I	-23	LYS	-	expression tag	UNP O75717
I	-22	ASP	-	expression tag	UNP O75717
I	-21	TYR	-	expression tag	UNP O75717
I	-20	LYS	-	expression tag	UNP O75717
I	-19	ASP	-	expression tag	UNP O75717
I	-18	ASP	-	expression tag	UNP O75717
I	-17	ASP	-	expression tag	UNP O75717
I	-16	ASP	-	expression tag	UNP O75717
I	-15	LYS	-	expression tag	UNP O75717
I	-14	ASP	-	expression tag	UNP O75717
I	-13	TYR	-	expression tag	UNP O75717
I	-12	LYS	-	expression tag	UNP O75717
I	-11	ASP	-	expression tag	UNP O75717
I	-10	ASP	-	expression tag	UNP O75717
I	-9	ASP	-	expression tag	UNP O75717
I	-8	ASP	-	expression tag	UNP O75717
I	-7	LYS	-	expression tag	UNP O75717
I	-6	GLU	-	expression tag	UNP O75717
I	-5	ASN	-	expression tag	UNP O75717
I	-4	LEU	-	expression tag	UNP O75717
I	-3	TYR	-	expression tag	UNP O75717
I	-2	PHE	-	expression tag	UNP O75717

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	GLN	-	expression tag	UNP O75717
I	0	GLY	-	expression tag	UNP O75717
J	-31	MET	-	initiating methionine	UNP O75717
J	-30	ASP	-	expression tag	UNP O75717
J	-29	TYR	-	expression tag	UNP O75717
J	-28	LYS	-	expression tag	UNP O75717
J	-27	ASP	-	expression tag	UNP O75717
J	-26	ASP	-	expression tag	UNP O75717
J	-25	ASP	-	expression tag	UNP O75717
J	-24	ASP	-	expression tag	UNP O75717
J	-23	LYS	-	expression tag	UNP O75717
J	-22	ASP	-	expression tag	UNP O75717
J	-21	TYR	-	expression tag	UNP O75717
J	-20	LYS	-	expression tag	UNP O75717
J	-19	ASP	-	expression tag	UNP O75717
J	-18	ASP	-	expression tag	UNP O75717
J	-17	ASP	-	expression tag	UNP O75717
J	-16	ASP	-	expression tag	UNP O75717
J	-15	LYS	-	expression tag	UNP O75717
J	-14	ASP	-	expression tag	UNP O75717
J	-13	TYR	-	expression tag	UNP O75717
J	-12	LYS	-	expression tag	UNP O75717
J	-11	ASP	-	expression tag	UNP O75717
J	-10	ASP	-	expression tag	UNP O75717
J	-9	ASP	-	expression tag	UNP O75717
J	-8	ASP	-	expression tag	UNP O75717
J	-7	LYS	-	expression tag	UNP O75717
J	-6	GLU	-	expression tag	UNP O75717
J	-5	ASN	-	expression tag	UNP O75717
J	-4	LEU	-	expression tag	UNP O75717
J	-3	TYR	-	expression tag	UNP O75717
J	-2	PHE	-	expression tag	UNP O75717
J	-1	GLN	-	expression tag	UNP O75717
J	0	GLY	-	expression tag	UNP O75717

- Molecule 15 is a protein called Protein timeless homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	K	636	Total	C	H	N	O	S	0	0
			10448	3324	5233	929	936	26		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLY	-	expression tag	UNP Q9UNS1

- Molecule 16 is a protein called TIMELESS-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	L	87	Total	C	H	N	O	S	0	0
			1502	471	767	140	121	3		

- Molecule 17 is a DNA chain called Leading strand DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	M	32	Total	C	H	N	O	P	0	0
			1032	320	370	106	204	32		

- Molecule 18 is a DNA chain called Lagging Strand DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	N	22	Total	C	H	N	O	P	0	0
			686	211	248	74	131	22		

- Molecule 19 is a protein called Claspin.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	Q	79	Total	C	H	N	O	S	0	0
			1387	431	704	133	117	2		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1340	LEU	-	expression tag	UNP Q9HAW4
Q	1341	GLU	-	expression tag	UNP Q9HAW4
Q	1342	VAL	-	expression tag	UNP Q9HAW4
Q	1343	LEU	-	expression tag	UNP Q9HAW4
Q	1344	PHE	-	expression tag	UNP Q9HAW4
Q	1345	GLN	-	expression tag	UNP Q9HAW4
Q	1346	GLY	-	expression tag	UNP Q9HAW4
Q	1347	PRO	-	expression tag	UNP Q9HAW4
Q	1348	ASP	-	expression tag	UNP Q9HAW4
Q	1349	TYR	-	expression tag	UNP Q9HAW4
Q	1350	LYS	-	expression tag	UNP Q9HAW4
Q	1351	ASP	-	expression tag	UNP Q9HAW4
Q	1352	ASP	-	expression tag	UNP Q9HAW4

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	1353	ASP	-	expression tag	UNP Q9HAW4
Q	1354	ASP	-	expression tag	UNP Q9HAW4
Q	1355	LYS	-	expression tag	UNP Q9HAW4
Q	1356	ASP	-	expression tag	UNP Q9HAW4
Q	1357	TYR	-	expression tag	UNP Q9HAW4
Q	1358	LYS	-	expression tag	UNP Q9HAW4
Q	1359	ASP	-	expression tag	UNP Q9HAW4
Q	1360	ASP	-	expression tag	UNP Q9HAW4
Q	1361	ASP	-	expression tag	UNP Q9HAW4
Q	1362	ASP	-	expression tag	UNP Q9HAW4
Q	1363	LYS	-	expression tag	UNP Q9HAW4
Q	1364	ASP	-	expression tag	UNP Q9HAW4
Q	1365	TYR	-	expression tag	UNP Q9HAW4
Q	1366	LYS	-	expression tag	UNP Q9HAW4
Q	1367	ASP	-	expression tag	UNP Q9HAW4
Q	1368	ASP	-	expression tag	UNP Q9HAW4
Q	1369	ASP	-	expression tag	UNP Q9HAW4
Q	1370	ASP	-	expression tag	UNP Q9HAW4
Q	1371	LYS	-	expression tag	UNP Q9HAW4

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
20	2	1	Total Zn 1 1	0
20	4	1	Total Zn 1 1	0
20	5	1	Total Zn 1 1	0
20	6	1	Total Zn 1 1	0
20	7	1	Total Zn 1 1	0

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

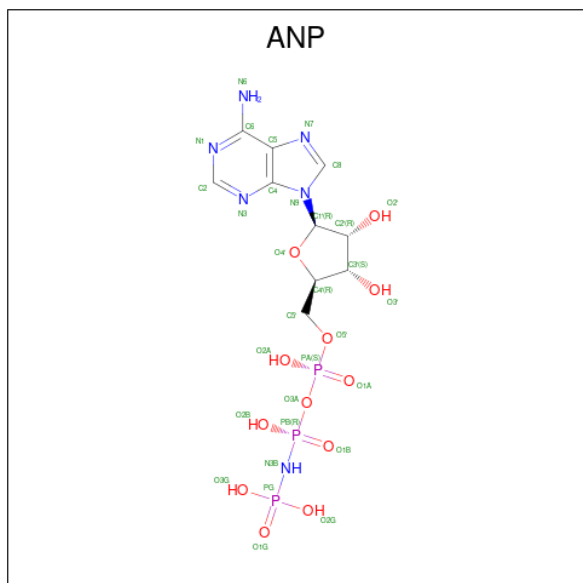
Mol	Chain	Residues	Atoms	AltConf
21	2	1	Total Mg 1 1	0

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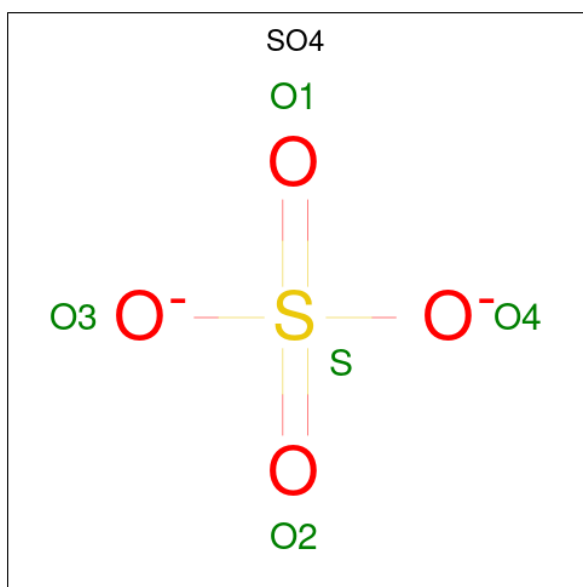
Mol	Chain	Residues	Atoms		AltConf
21	3	1	Total	Mg	0
			1	1	
21	5	1	Total	Mg	0
			1	1	

- Molecule 22 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).

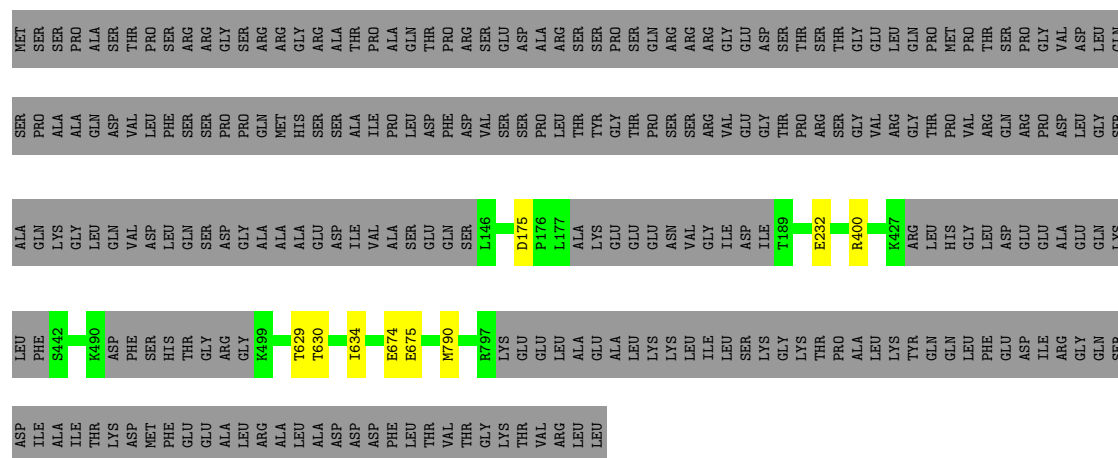


Mol	Chain	Residues	Atoms						AltConf
22	2	1	Total 44	C 10	H 13	N 6	O 12	P 3	0
22	3	1	Total 44	C 10	H 13	N 6	O 12	P 3	0
22	5	1	Total 44	C 10	H 13	N 6	O 12	P 3	0

- Molecule 23 is SULFATE ION (CCD ID: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).

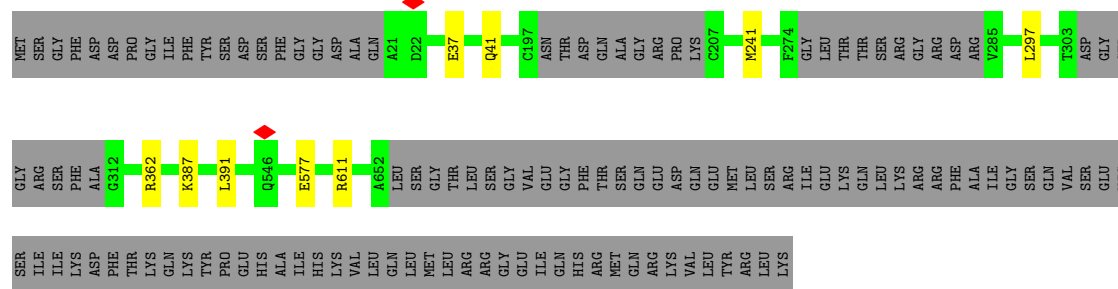


Mol	Chain	Residues	Atoms			AltConf
			Total	O	S	
23	A	1	5	4	1	0



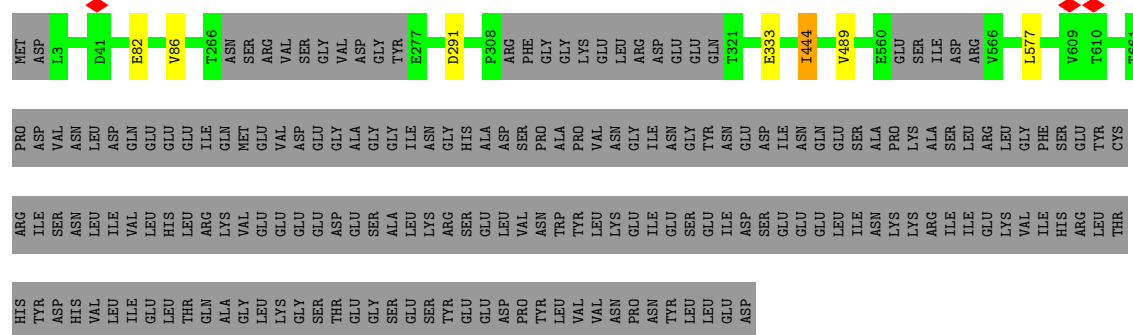
• Molecule 4: DNA replication licensing factor MCM5

Chain 5: 81% 18%



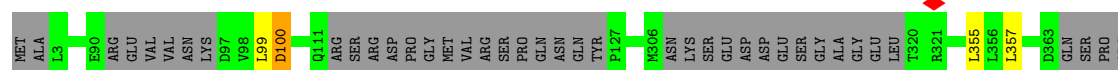
• Molecule 5: DNA replication licensing factor MCM6

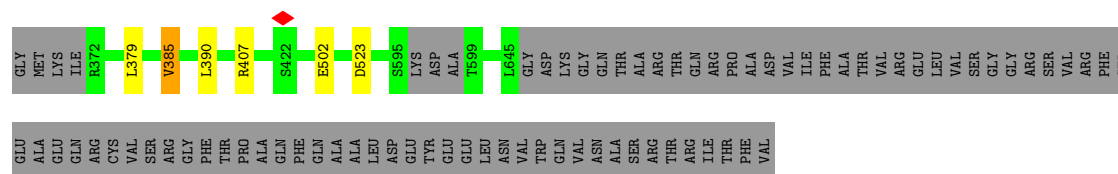
Chain 6: 76% 23%



• Molecule 6: DNA replication licensing factor MCM7

Chain 7: 82% 17%





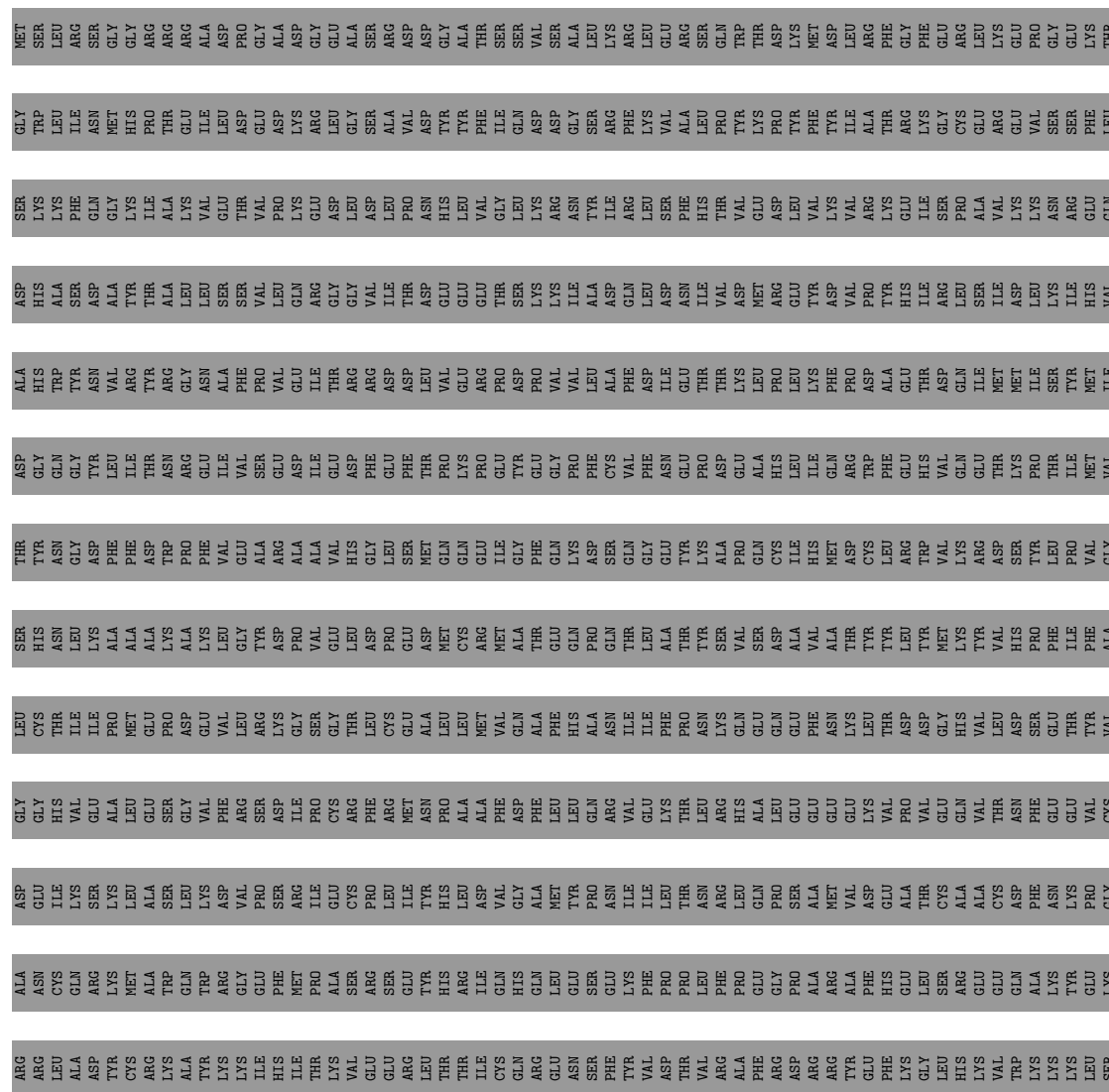
• Molecule 7: DNA polymerase epsilon subunit 2

Chain A: 97%



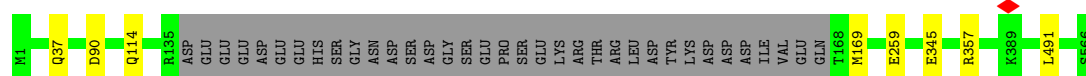
• Molecule 8: DNA polymerase epsilon catalytic subunit A

Chain B: 7%





- Molecule 9: Cell division control protein 45 homolog



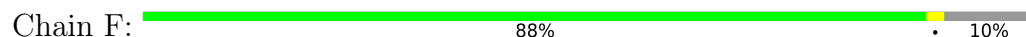
- Molecule 10: DNA replication complex GINS protein PSF1



- Molecule 11: DNA replication complex GINS protein PSF2



- Molecule 12: DNA replication complex GINS protein PSF3



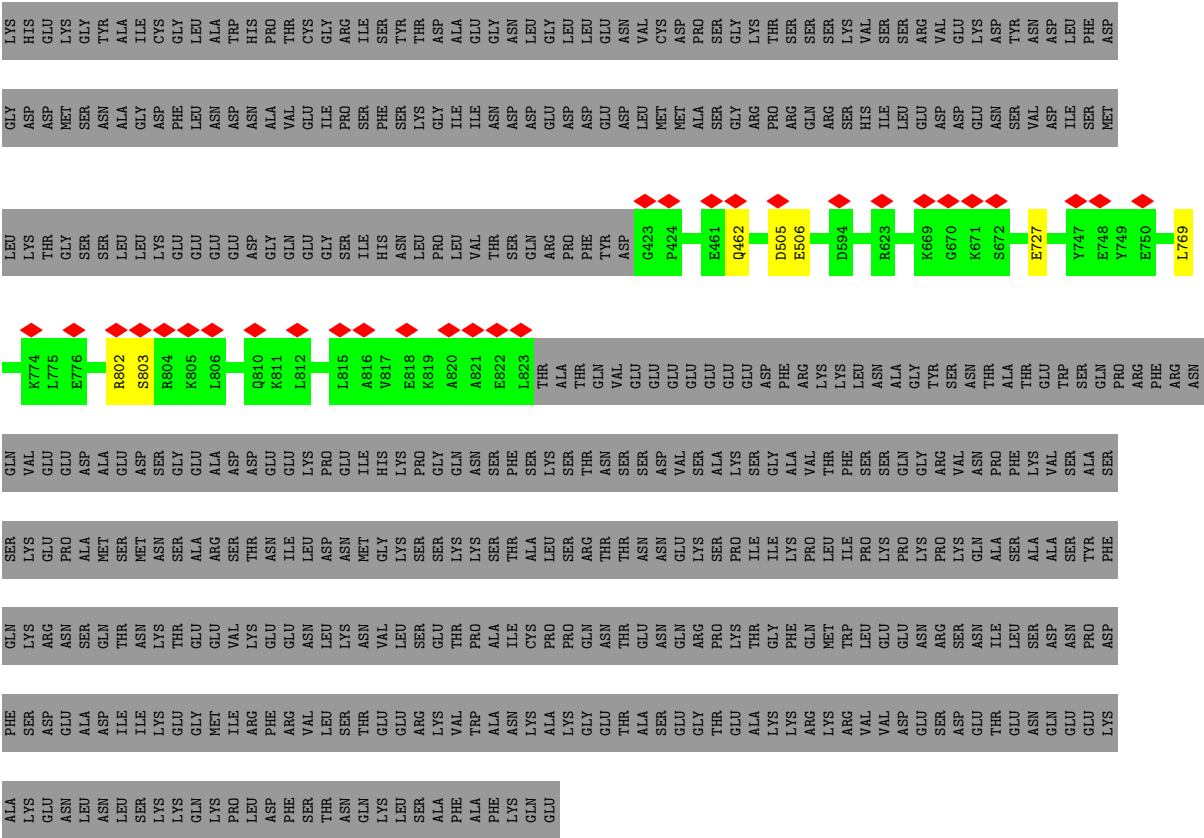
- Molecule 13: DNA replication complex GINS protein SLD5



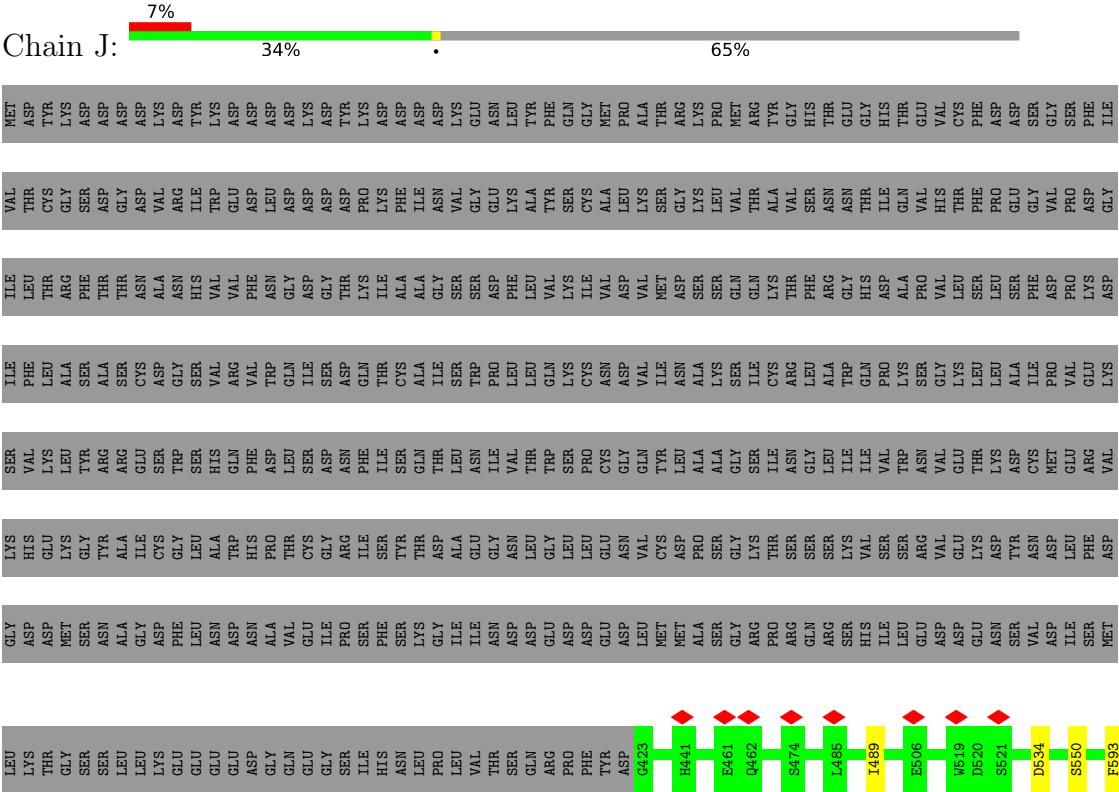
- Molecule 14: WD repeat and HMG-box DNA-binding protein 1

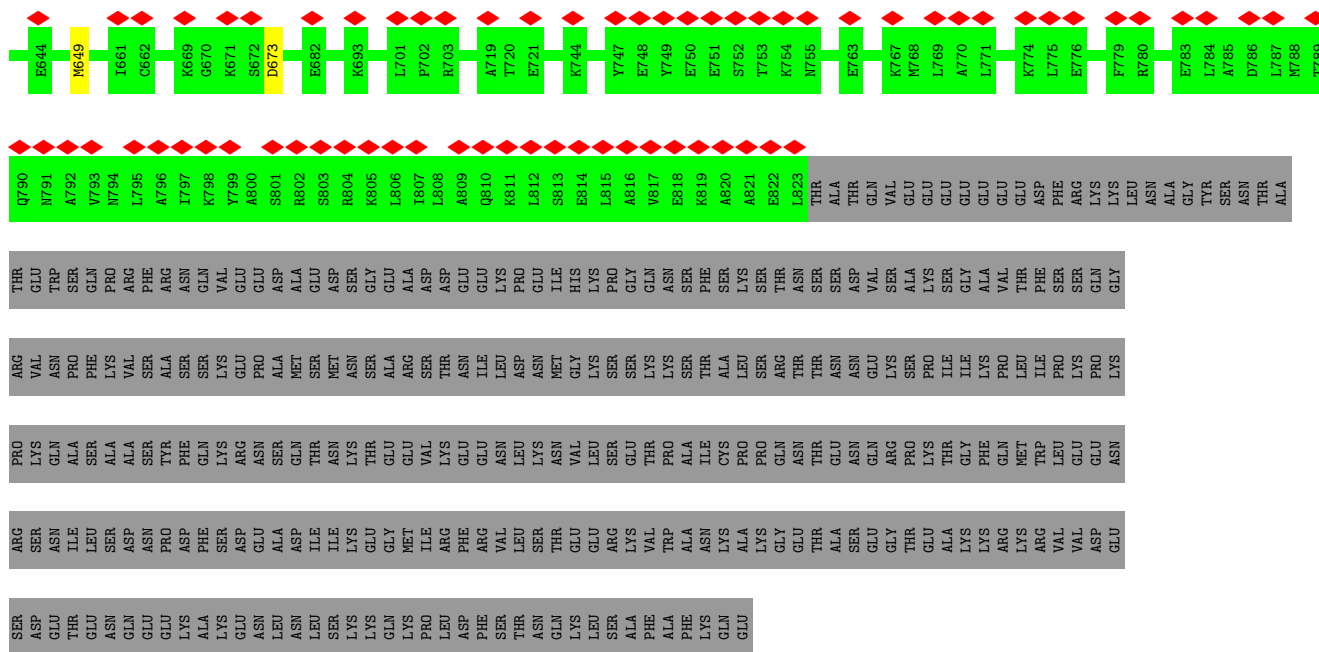




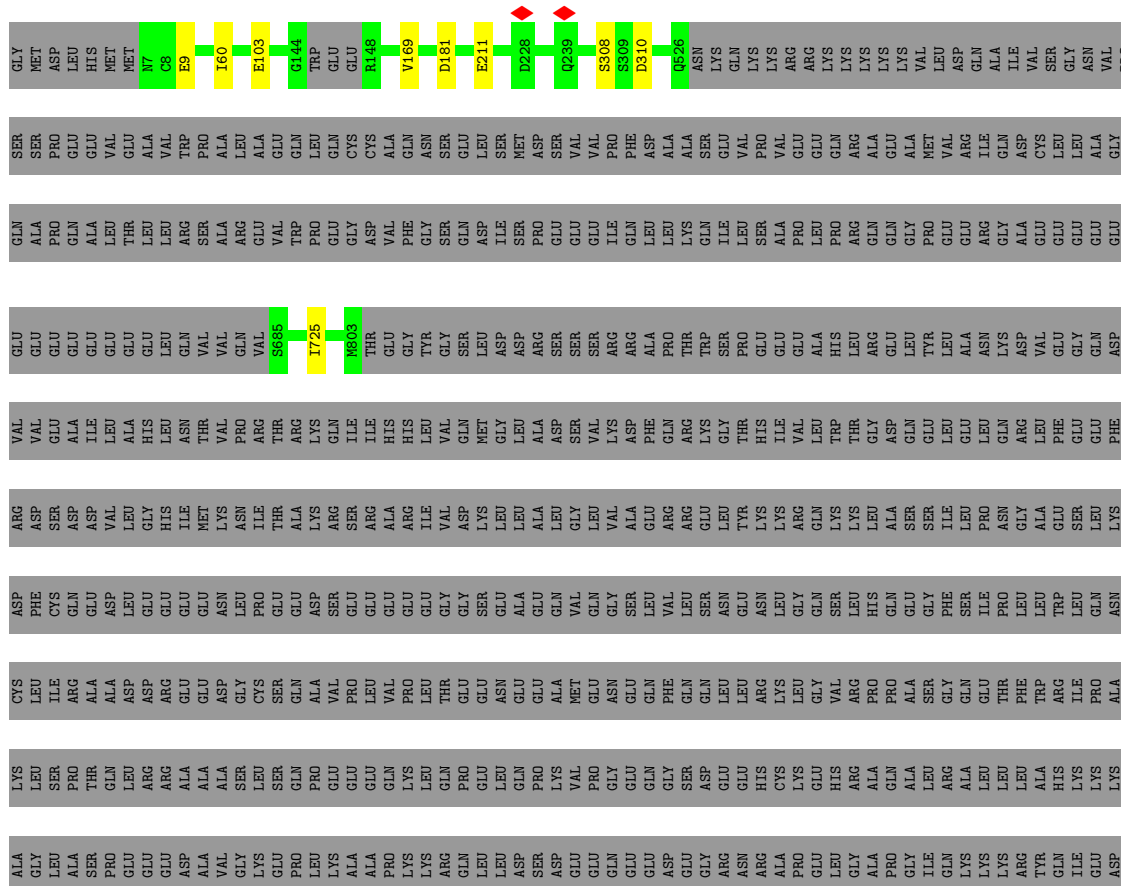


• Molecule 14: WD repeat and HMG-box DNA-binding protein 1





- Molecule 15: Protein timeless homolog





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110000	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 ($e^-/\text{\AA}^2$)	39.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.017	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0113	Depositor
Map size (Å)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, MG, ANP

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	0.25	0/5683	0.46	0/7675
2	3	0.23	0/4931	0.44	0/6653
3	4	0.22	0/5013	0.43	0/6776
4	5	0.21	0/4807	0.42	0/6468
5	6	0.22	0/5095	0.42	0/6876
6	7	0.27	0/4822	0.49	1/6507 (0.0%)
7	A	0.25	0/4310	0.49	0/5853
8	B	0.35	0/6647	0.67	1/9011 (0.0%)
9	C	0.19	0/4439	0.37	0/5992
10	D	0.22	0/1638	0.42	0/2202
11	E	0.20	0/1462	0.39	0/1981
12	F	0.19	0/1580	0.39	0/2133
13	G	0.20	0/1711	0.40	0/2305
14	H	0.24	0/3244	0.47	0/4395
14	I	0.23	0/3244	0.45	0/4395
14	J	0.21	0/3244	0.41	0/4395
15	K	0.22	0/5317	0.44	0/7162
16	L	0.22	0/750	0.41	0/999
17	M	0.33	0/738	0.60	0/1138
18	N	0.37	0/488	0.55	0/747
19	Q	0.22	0/693	0.42	0/919
All	All	0.24	0/69856	0.47	2/94582 (0.0%)

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
6	7	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	7	385	VAL	CA-CB-CG1	6.24	121.00	110.40
8	B	1397	LEU	N-CA-C	5.49	117.33	110.91

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	7	407	ARG	Peptide

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	5580	5597	5590	12	0
2	3	4858	4912	4908	12	0
3	4	4929	4993	4985	6	0
4	5	4735	4809	4800	7	0
5	6	5014	5051	5043	4	0
6	7	4750	4802	4793	6	0
7	A	4199	4160	4160	5	0
8	B	6497	6478	6471	13	0
9	C	4347	4300	4296	5	0
10	D	1606	1601	1601	1	0
11	E	1431	1456	1456	3	0
12	F	1546	1502	1500	2	0
13	G	1679	1702	1700	3	0
14	H	3169	3140	3138	3	0
14	I	3169	3140	3138	3	0
14	J	3169	3139	3138	2	0
15	K	5215	5233	5230	4	0
16	L	735	767	766	0	0
17	M	662	370	372	0	0
18	N	438	248	249	0	0
19	Q	683	704	701	1	0
20	2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	4	1	0	0	0	0
20	5	1	0	0	0	0
20	6	1	0	0	0	0
20	7	1	0	0	0	0
21	2	1	0	0	0	0
21	3	1	0	0	0	0
21	5	1	0	0	0	0
22	2	31	13	13	1	0
22	3	31	13	13	3	0
22	5	31	13	13	2	0
23	A	5	0	0	0	0
All	All	68517	68143	68074	83	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 1.

All (83) 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)
1:2:290:LEU:HD12	1:2:290:LEU:O	1.59	1.02
3:4:674:GLU:OE2	3:4:675:GLU:HG3	1.76	0.85
8:B:1813:TYR:CE1	8:B:1817:GLN:HG3	2.19	0.78
6:7:385:VAL:CG2	6:7:523:ASP:HB2	2.16	0.76
6:7:385:VAL:HG23	6:7:523:ASP:HB2	1.77	0.65
1:2:290:LEU:HD11	1:2:305:LEU:O	2.00	0.61
8:B:1852:LEU:HD22	8:B:1895:HIS:CD2	2.35	0.61
2:3:286:LYS:HA	2:3:289:LYS:HE3	1.82	0.61
1:2:290:LEU:O	1:2:290:LEU:CD1	2.42	0.60
2:3:289:LYS:HD3	2:3:633:MET:HB2	1.84	0.60
2:3:520:LEU:HD23	4:5:362:ARG:NH2	2.18	0.58
5:6:333:GLU:N	5:6:333:GLU:OE1	2.36	0.58
15:K:211:GLU:N	15:K:211:GLU:OE1	2.37	0.57
2:3:348:SER:H	22:3:1500:ANP:HNB1	1.52	0.56
6:7:385:VAL:HG23	6:7:523:ASP:CB	2.35	0.56
8:B:1813:TYR:CZ	8:B:1817:GLN:HG3	2.41	0.56
9:C:259:GLU:OE2	14:I:462:GLN:NE2	2.38	0.56
11:E:87:MET:HE3	11:E:88:PRO:HD2	1.88	0.56
8:B:1655:ILE:O	8:B:1659:ASN:ND2	2.38	0.56
2:3:289:LYS:CD	2:3:633:MET:HB2	2.36	0.55
15:K:9:GLU:N	15:K:9:GLU:OE1	2.37	0.55
2:3:417:MET:O	2:3:420:THR:OG1	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:102:GLU:OE1	7:A:102:GLU:N	2.39	0.55
6:7:385:VAL:HG22	6:7:523:ASP:HB2	1.89	0.55
4:5:577:GLU:OE1	4:5:577:GLU:N	2.40	0.54
2:3:348:SER:N	22:3:1500:ANP:HNB1	2.05	0.54
1:2:526:GLY:H	22:2:1003:ANP:HNB1	1.56	0.53
2:3:378:LEU:HB3	2:3:398:MET:HE2	1.90	0.53
14:I:802:ARG:O	14:I:803:SER:OG	2.28	0.52
15:K:103:GLU:N	15:K:103:GLU:OE1	2.43	0.52
8:B:1389:PRO:HG3	8:B:1683:LEU:HD13	1.91	0.51
7:A:387:ASN:OD1	7:A:388:GLU:N	2.45	0.50
3:4:175:ASP:N	3:4:175:ASP:OD1	2.43	0.50
13:G:175:VAL:HG12	13:G:220:VAL:HG12	1.94	0.50
9:C:345:GLU:OE1	9:C:357:ARG:NH1	2.46	0.49
8:B:2103:GLU:OE1	8:B:2103:GLU:N	2.46	0.48
8:B:1852:LEU:HD22	8:B:1895:HIS:CG	2.48	0.48
7:A:294:TRP:HA	7:A:325:PHE:O	2.13	0.48
6:7:502:GLU:OE1	6:7:502:GLU:N	2.47	0.48
7:A:259:ASN:ND2	7:A:265:SER:O	2.45	0.47
9:C:169:MET:N	9:C:169:MET:SD	2.87	0.47
2:3:593:GLU:HG2	2:3:646:VAL:HG21	1.96	0.47
14:H:740:ASP:OD2	14:H:744:LYS:NZ	2.45	0.47
9:C:37:GLN:NE2	10:D:149:GLU:OE2	2.48	0.47
8:B:1389:PRO:CG	8:B:1683:LEU:HD13	2.44	0.47
2:3:52:ASN:OD1	2:3:105:SER:OG	2.33	0.47
13:G:36:ASN:OD1	13:G:221:GLN:NE2	2.47	0.47
2:3:603:MET:SD	2:3:603:MET:N	2.86	0.46
1:2:620:LEU:HD13	4:5:241:MET:HE1	1.98	0.46
14:H:635:GLU:OE1	14:H:635:GLU:N	2.48	0.46
1:2:764:VAL:HG21	22:5:802:ANP:C4	2.46	0.45
5:6:444:ILE:HG23	5:6:489:VAL:HG21	1.98	0.45
3:4:629:THR:HG22	3:4:630:THR:H	1.81	0.45
11:E:7:GLU:OE1	12:F:189:TRP:NE1	2.46	0.45
15:K:308:SER:OG	15:K:310:ASP:OD1	2.33	0.45
3:4:400:ARG:NH2	5:6:291:ASP:OD2	2.48	0.45
5:6:82:GLU:O	5:6:86:VAL:HG22	2.17	0.45
22:3:1500:ANP:O2A	4:5:611:ARG:NH2	2.50	0.45
11:E:87:MET:HE2	11:E:92:TYR:CZ	2.52	0.44
1:2:225:GLU:N	1:2:225:GLU:OE1	2.50	0.44
1:2:307:ARG:NH1	1:2:413:GLU:OE2	2.47	0.44
3:4:790:MET:SD	3:4:790:MET:N	2.91	0.44
1:2:573:ALA:HB2	4:5:241:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:37:GLU:OE1	4:5:41:GLN:NE2	2.48	0.43
8:B:1431:VAL:HG21	8:B:1684:LEU:HD21	2.00	0.43
6:7:100:ASP:OD1	6:7:100:ASP:N	2.52	0.43
8:B:1802:TRP:CZ3	8:B:1817:GLN:HB3	2.54	0.43
13:G:96:ARG:NH2	13:G:121:SER:O	2.51	0.43
1:2:291:VAL:O	19:Q:593:LYS:NZ	2.52	0.42
2:3:527:LEU:HD12	12:F:99:VAL:HG22	2.01	0.42
14:H:534:ASP:O	14:H:550:SER:N	2.47	0.42
1:2:290:LEU:HD11	1:2:306:ILE:HA	2.01	0.42
14:J:635:GLU:OE1	14:J:635:GLU:N	2.53	0.42
4:5:387:LYS:NZ	22:5:802:ANP:O1G	2.53	0.41
8:B:1393:MET:O	8:B:1397:LEU:N	2.53	0.41
3:4:232:GLU:N	3:4:232:GLU:OE1	2.54	0.41
7:A:96:ARG:NH1	7:A:132:GLU:OE1	2.50	0.41
14:J:534:ASP:O	14:J:550:SER:N	2.54	0.41
14:I:505:ASP:OD1	14:I:506:GLU:N	2.53	0.41
1:2:746:MET:SD	1:2:799:LEU:HD21	2.62	0.40
8:B:1405:ASP:OD1	8:B:1406:MET:N	2.53	0.40
9:C:90:ASP:O	9:C:114:GLN:NE2	2.51	0.40
8:B:1388:LEU:HB3	8:B:1683:LEU:HB2	2.04	0.40

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	697/904 (77%)	671 (96%)	25 (4%)	1 (0%)	48	79
2	3	614/808 (76%)	594 (97%)	20 (3%)	0	100	100
3	4	611/863 (71%)	594 (97%)	17 (3%)	0	100	100
4	5	597/734 (81%)	580 (97%)	17 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	6	624/821 (76%)	607 (97%)	17 (3%)	0	100	100
6	7	586/719 (82%)	572 (98%)	14 (2%)	0	100	100
7	A	525/527 (100%)	503 (96%)	22 (4%)	0	100	100
8	B	792/2286 (35%)	706 (89%)	82 (10%)	4 (0%)	24	59
9	C	530/569 (93%)	522 (98%)	8 (2%)	0	100	100
10	D	193/196 (98%)	191 (99%)	2 (1%)	0	100	100
11	E	174/185 (94%)	172 (99%)	2 (1%)	0	100	100
12	F	190/216 (88%)	185 (97%)	5 (3%)	0	100	100
13	G	201/262 (77%)	200 (100%)	1 (0%)	0	100	100
14	H	399/1161 (34%)	385 (96%)	14 (4%)	0	100	100
14	I	399/1161 (34%)	392 (98%)	7 (2%)	0	100	100
14	J	399/1161 (34%)	390 (98%)	9 (2%)	0	100	100
15	K	630/1209 (52%)	615 (98%)	15 (2%)	0	100	100
16	L	85/301 (28%)	81 (95%)	4 (5%)	0	100	100
19	Q	73/1371 (5%)	73 (100%)	0	0	100	100
All	All	8319/15454 (54%)	8033 (97%)	281 (3%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	B	1431	VAL
8	B	1580	ARG
8	B	1656	PRO
1	2	713	GLU
8	B	1918	ASP

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	618/781 (79%)	613 (99%)	5 (1%)	73	82
2	3	534/707 (76%)	533 (100%)	1 (0%)	87	89
3	4	549/753 (73%)	548 (100%)	1 (0%)	87	89
4	5	515/625 (82%)	513 (100%)	2 (0%)	84	86
5	6	556/724 (77%)	554 (100%)	2 (0%)	84	86
6	7	518/619 (84%)	512 (99%)	6 (1%)	63	79
7	A	471/471 (100%)	466 (99%)	5 (1%)	65	79
8	B	725/2012 (36%)	717 (99%)	8 (1%)	65	79
9	C	487/520 (94%)	486 (100%)	1 (0%)	87	89
10	D	173/174 (99%)	173 (100%)	0	100	100
11	E	160/169 (95%)	160 (100%)	0	100	100
12	F	167/186 (90%)	165 (99%)	2 (1%)	63	79
13	G	188/233 (81%)	187 (100%)	1 (0%)	81	85
14	H	345/1018 (34%)	345 (100%)	0	100	100
14	I	345/1018 (34%)	343 (99%)	2 (1%)	78	84
14	J	345/1018 (34%)	341 (99%)	4 (1%)	63	79
15	K	561/1055 (53%)	557 (99%)	4 (1%)	76	83
16	L	78/274 (28%)	76 (97%)	2 (3%)	40	69
19	Q	72/1230 (6%)	72 (100%)	0	100	100
All	All	7407/13587 (54%)	7361 (99%)	46 (1%)	76	84

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	176	ASP
1	2	178	LYS
1	2	255	LEU
1	2	738	MET
1	2	874	ILE
2	3	527	LEU
3	4	634	ILE
4	5	297	LEU
4	5	391	LEU
5	6	444	ILE
5	6	577	LEU
6	7	99	LEU

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Mol	Chain	Res	Type
6	7	100	ASP
6	7	355	LEU
6	7	357	LEU
6	7	379	LEU
6	7	390	LEU
7	A	151	VAL
7	A	165	LEU
7	A	293	VAL
7	A	419	LEU
7	A	429	ARG
8	B	1366	PHE
8	B	1404	GLU
8	B	1588	GLN
8	B	1694	LEU
8	B	1903	LEU
8	B	1918	ASP
8	B	2182	LEU
8	B	2278	LEU
9	C	491	LEU
12	F	68	LEU
12	F	169	ASP
13	G	211	ILE
14	I	727	GLU
14	I	769	LEU
14	J	489	ILE
14	J	593	PHE
14	J	649	MET
14	J	673	ASP
15	K	60	ILE
15	K	169	VAL
15	K	181	ASP
15	K	725	ILE
16	L	70	GLN
16	L	140	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	344	ASN
1	2	421	ASN
1	2	443	HIS
1	2	781	HIS

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Mol	Chain	Res	Type
2	3	110	HIS
2	3	202	GLN
2	3	573	HIS
3	4	209	ASN
3	4	259	GLN
3	4	335	HIS
3	4	341	HIS
3	4	407	ASN
4	5	244	HIS
5	6	440	HIS
5	6	454	ASN
6	7	35	ASN
6	7	214	ASN
6	7	464	GLN
6	7	465	GLN
6	7	543	HIS
7	A	87	ASN
7	A	118	ASN
7	A	144	HIS
7	A	324	ASN
7	A	336	GLN
7	A	357	GLN
8	B	1810	HIS
8	B	1867	ASN
8	B	2098	ASN
9	C	261	ASN
9	C	287	HIS
9	C	312	GLN
9	C	330	GLN
9	C	408	ASN
9	C	414	HIS
9	C	427	GLN
9	C	472	HIS
10	D	72	ASN
10	D	100	ASN
11	E	51	ASN
12	F	115	HIS
12	F	205	ASN
13	G	191	GLN
14	H	464	ASN
14	H	486	ASN
14	H	790	GLN

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Mol	Chain	Res	Type
14	I	476	HIS
14	I	532	ASN
14	J	602	GLN
15	K	7	ASN
15	K	194	HIS
15	K	355	ASN
15	K	373	HIS
16	L	63	ASN
16	L	95	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 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	$\# Z > 2$
22	ANP	2	1003	21	33,33,33	1.04	5 (15%)	45,52,52	0.50	0
23	SO4	A	601	-	4,4,4	0.24	0	6,6,6	0.07	0
22	ANP	3	1500	21	33,33,33	0.96	3 (9%)	45,52,52	0.60	1 (2%)
22	ANP	5	802	21	33,33,33	0.97	4 (12%)	45,52,52	0.53	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
22	ANP	2	1003	21	-	3/18/38/38	0/3/3/3
22	ANP	3	1500	21	-	3/18/38/38	0/3/3/3
22	ANP	5	802	21	-	6/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	1500	ANP	PB-O3A	-3.46	1.54	1.59
22	2	1003	ANP	PB-O3A	-3.30	1.55	1.59
22	5	802	ANP	PB-O3A	-2.94	1.55	1.59
22	3	1500	ANP	PA-O3A	-2.71	1.56	1.59
22	5	802	ANP	PG-O1G	2.48	1.49	1.46
22	2	1003	ANP	PG-O1G	2.36	1.49	1.46
22	2	1003	ANP	PB-O1B	2.33	1.49	1.46
22	5	802	ANP	PG-N3B	2.31	1.69	1.63
22	2	1003	ANP	PG-N3B	2.27	1.69	1.63
22	5	802	ANP	PB-O1B	2.25	1.49	1.46
22	3	1500	ANP	PB-O1B	2.19	1.49	1.46
22	2	1003	ANP	PA-O3A	-2.09	1.57	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	1500	ANP	O1G-PG-N3B	-2.87	107.54	111.77

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	2	1003	ANP	PB-N3B-PG-O1G
22	2	1003	ANP	PA-O3A-PB-O2B
22	3	1500	ANP	PB-N3B-PG-O1G
22	3	1500	ANP	PA-O3A-PB-O2B
22	5	802	ANP	PG-N3B-PB-O1B
22	5	802	ANP	PG-N3B-PB-O3A
22	5	802	ANP	C5'-O5'-PA-O2A
22	5	802	ANP	C5'-O5'-PA-O3A

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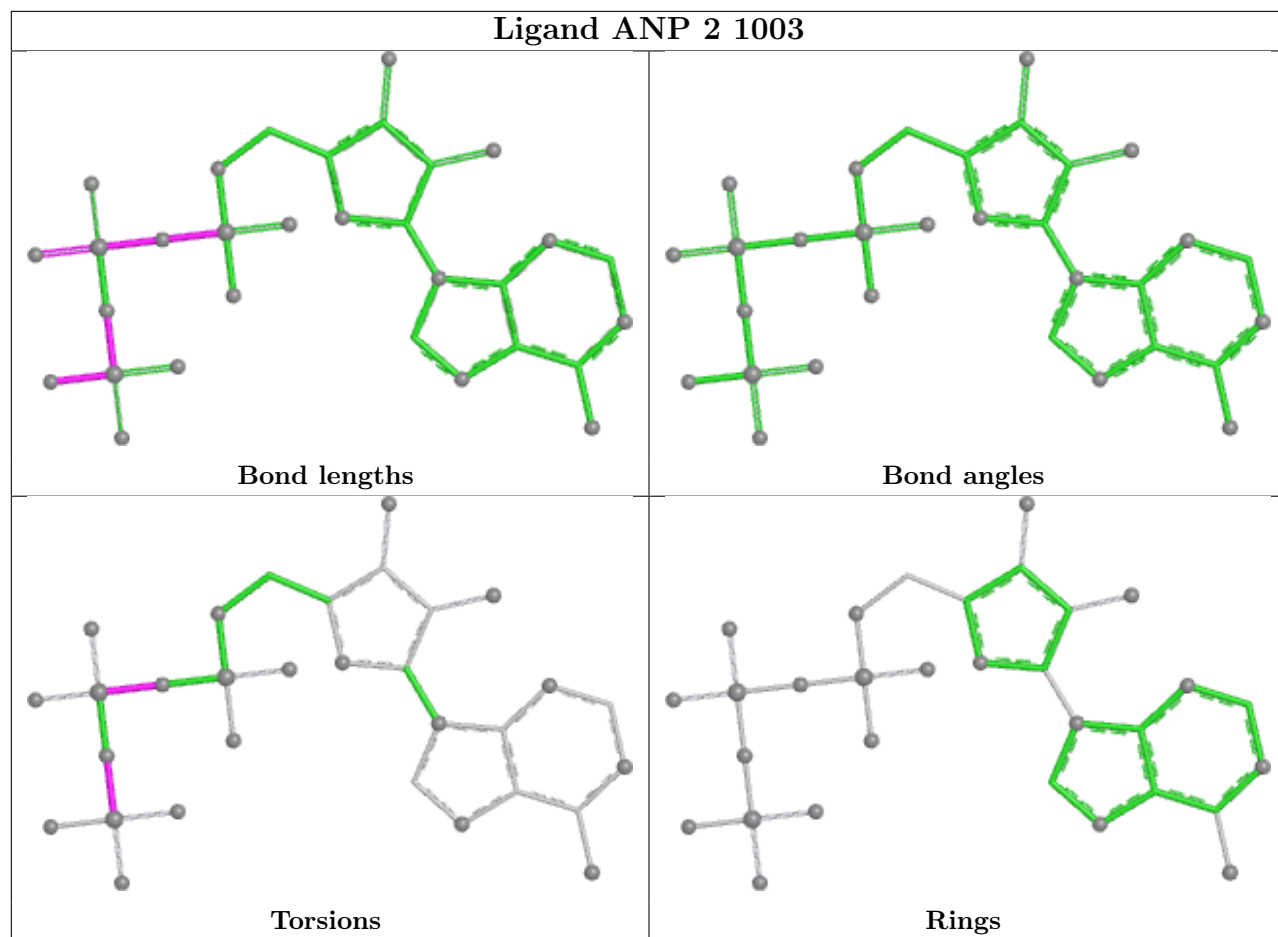
Mol	Chain	Res	Type	Atoms
22	5	802	ANP	C5'-O5'-PA-O1A
22	2	1003	ANP	PA-O3A-PB-O1B
22	3	1500	ANP	PA-O3A-PB-O1B
22	5	802	ANP	PA-O3A-PB-O1B

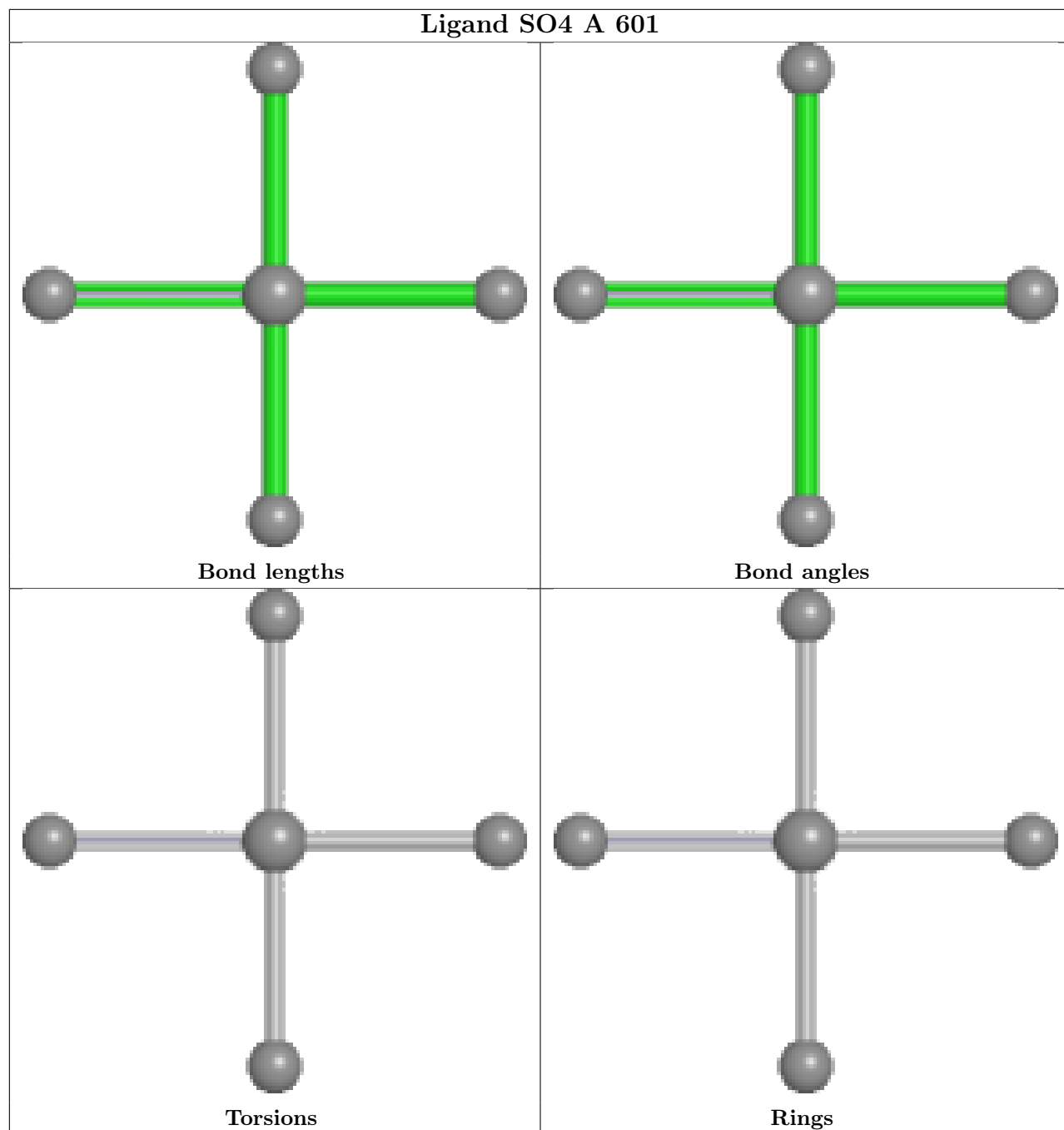
There are no ring outliers.

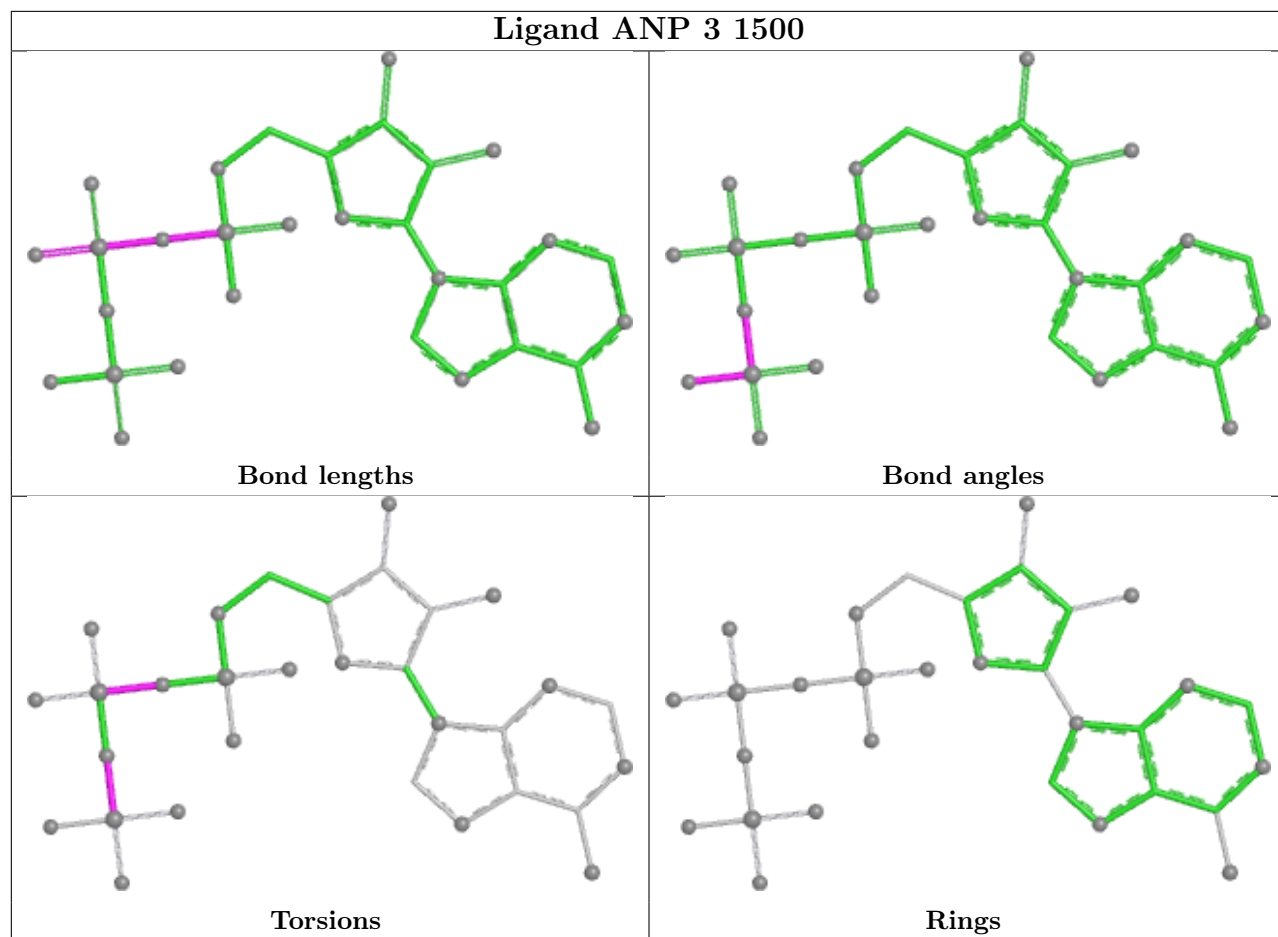
3 monomers are involved in 6 short contacts:

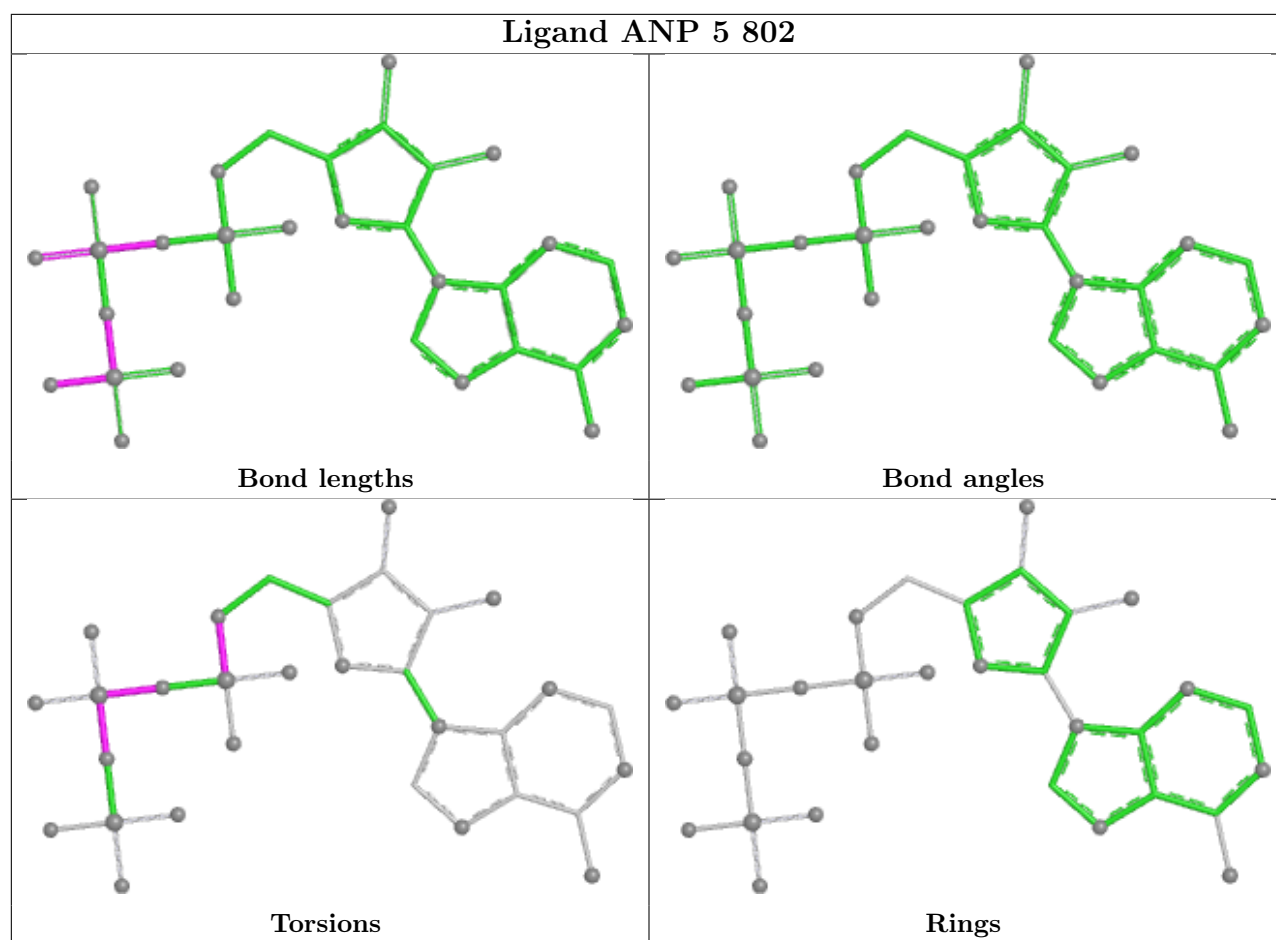
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	2	1003	ANP	1	0
22	3	1500	ANP	3	0
22	5	802	ANP	2	0

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.

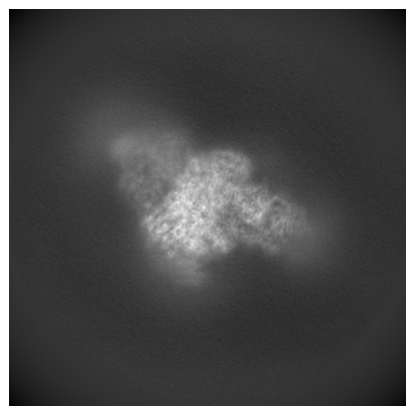
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13375. These allow visual inspection of the internal detail of the map and identification of artifacts.

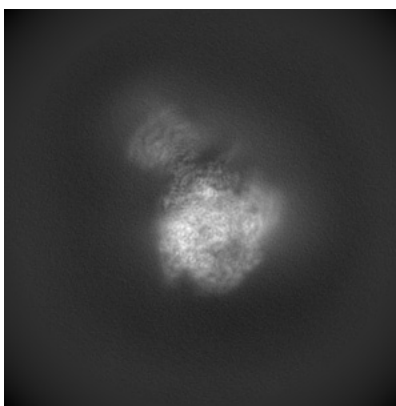
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

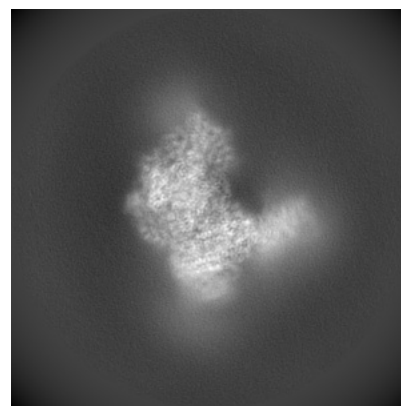
6.1.1 Primary map



X

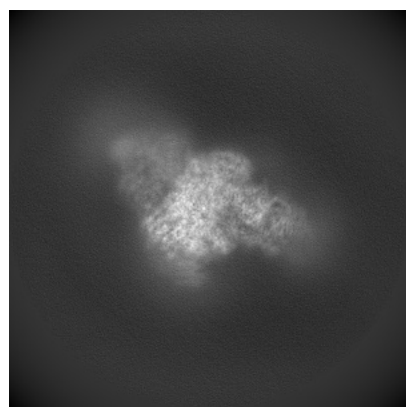


Y

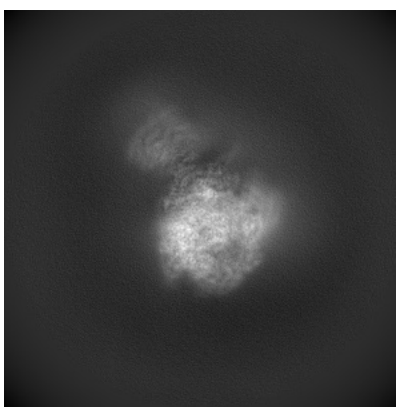


Z

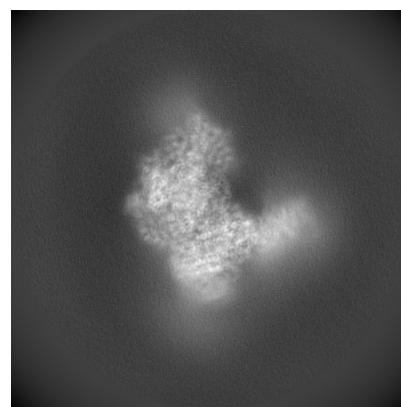
6.1.2 Raw map



X



Y

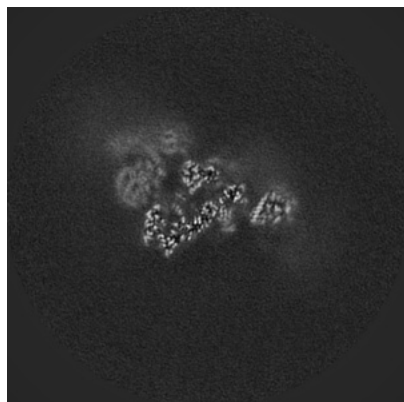


Z

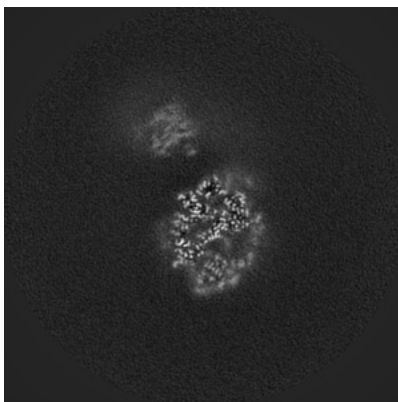
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

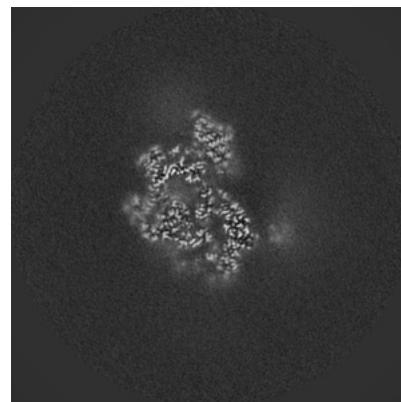
6.2.1 Primary map



X Index: 220

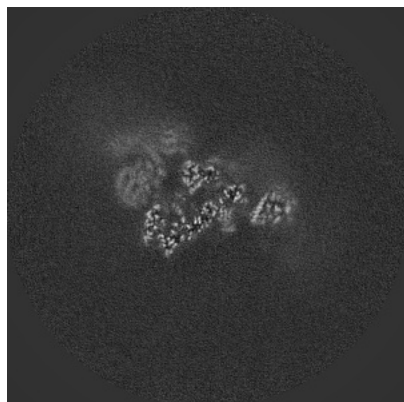


Y Index: 220

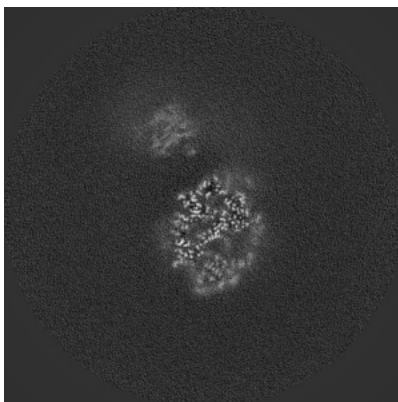


Z Index: 220

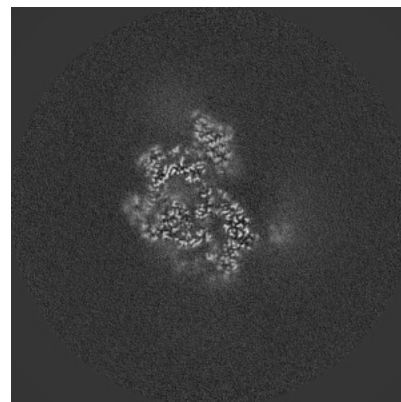
6.2.2 Raw map



X Index: 220



Y Index: 220

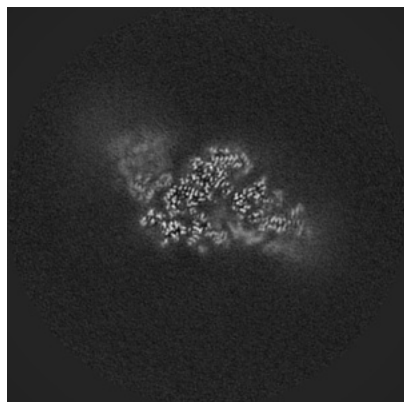


Z Index: 220

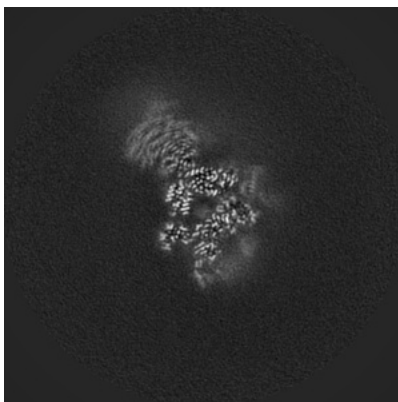
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

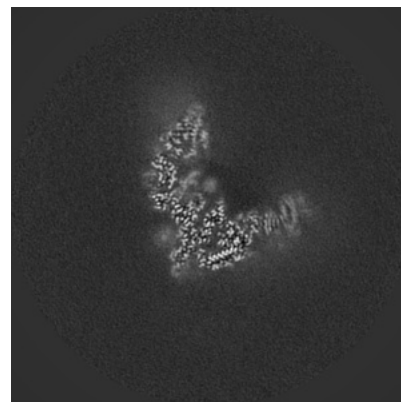
6.3.1 Primary map



X Index: 200

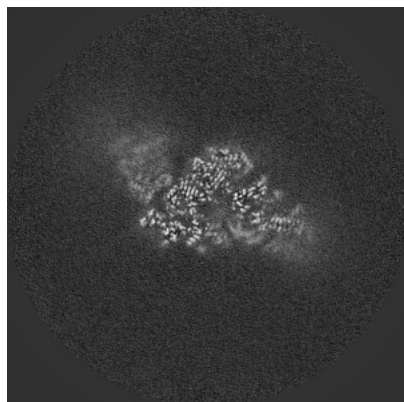


Y Index: 202

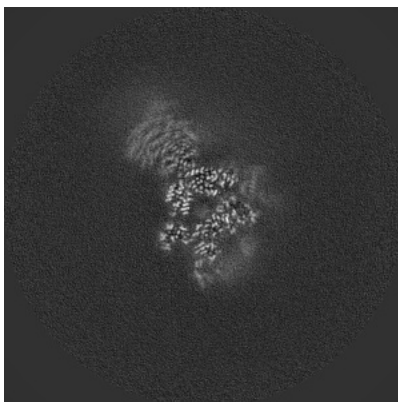


Z Index: 196

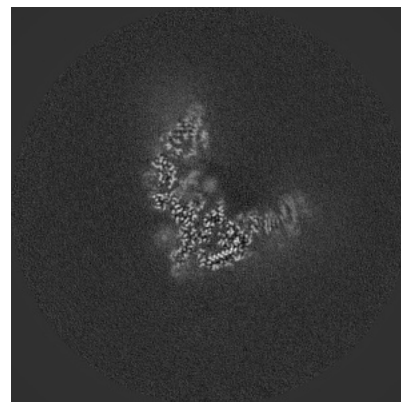
6.3.2 Raw map



X Index: 199



Y Index: 202



Z Index: 196

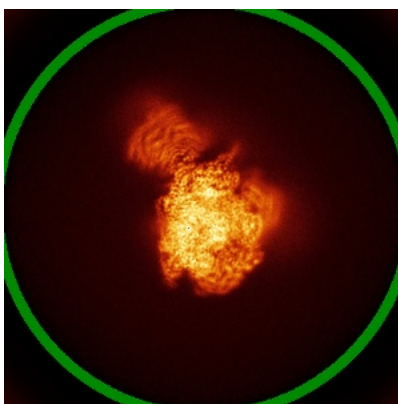
The images above show the largest variance slices of the map in three orthogonal directions.

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

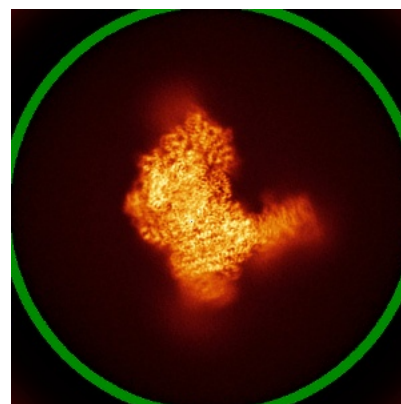
6.4.1 Primary map



X

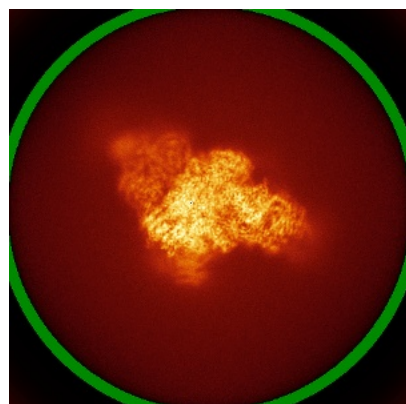


Y

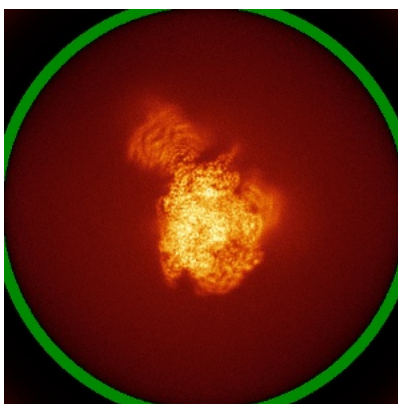


Z

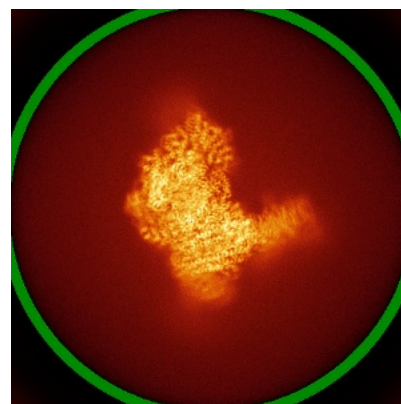
6.4.2 Raw map



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](#)

This section was not generated.

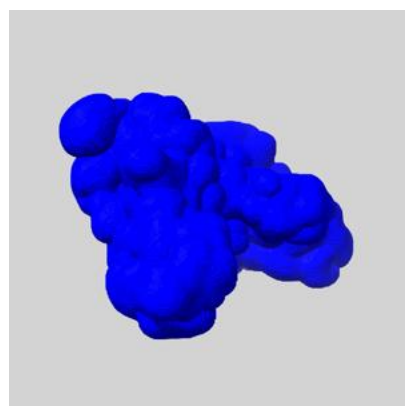
6.6 Mask visualisation [i](#)

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

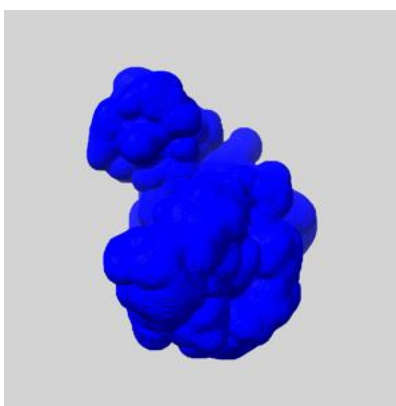
A mask typically either:

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

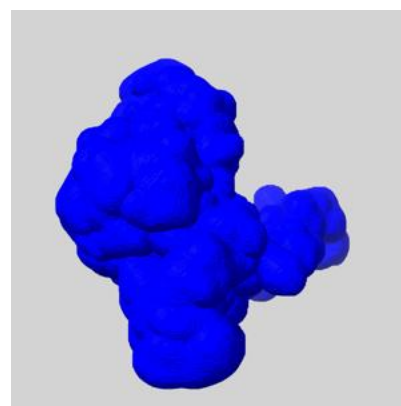
6.6.1 emd_13375_msk_1.map [i](#)



X



Y

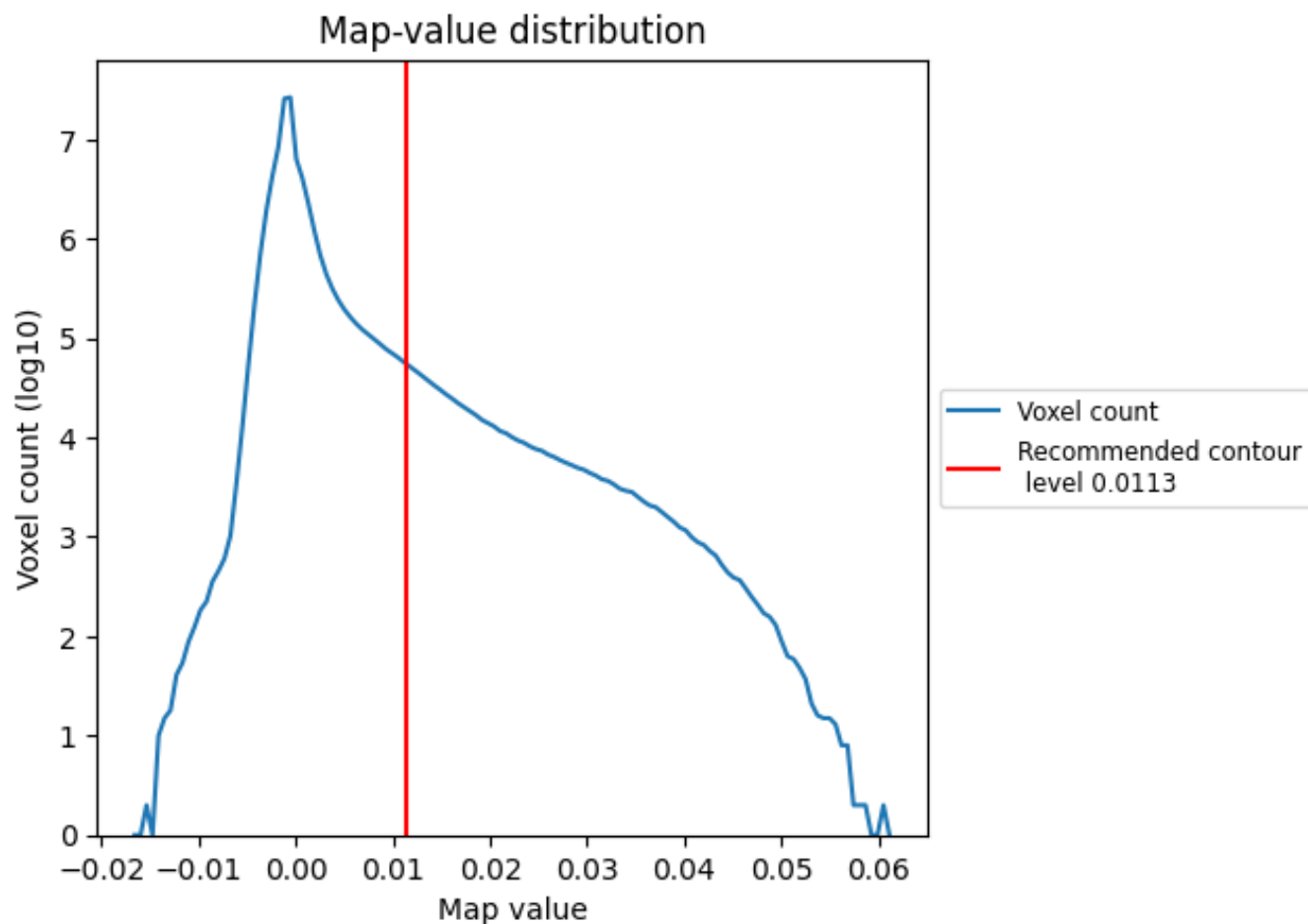


Z

7 Map analysis [i](#)

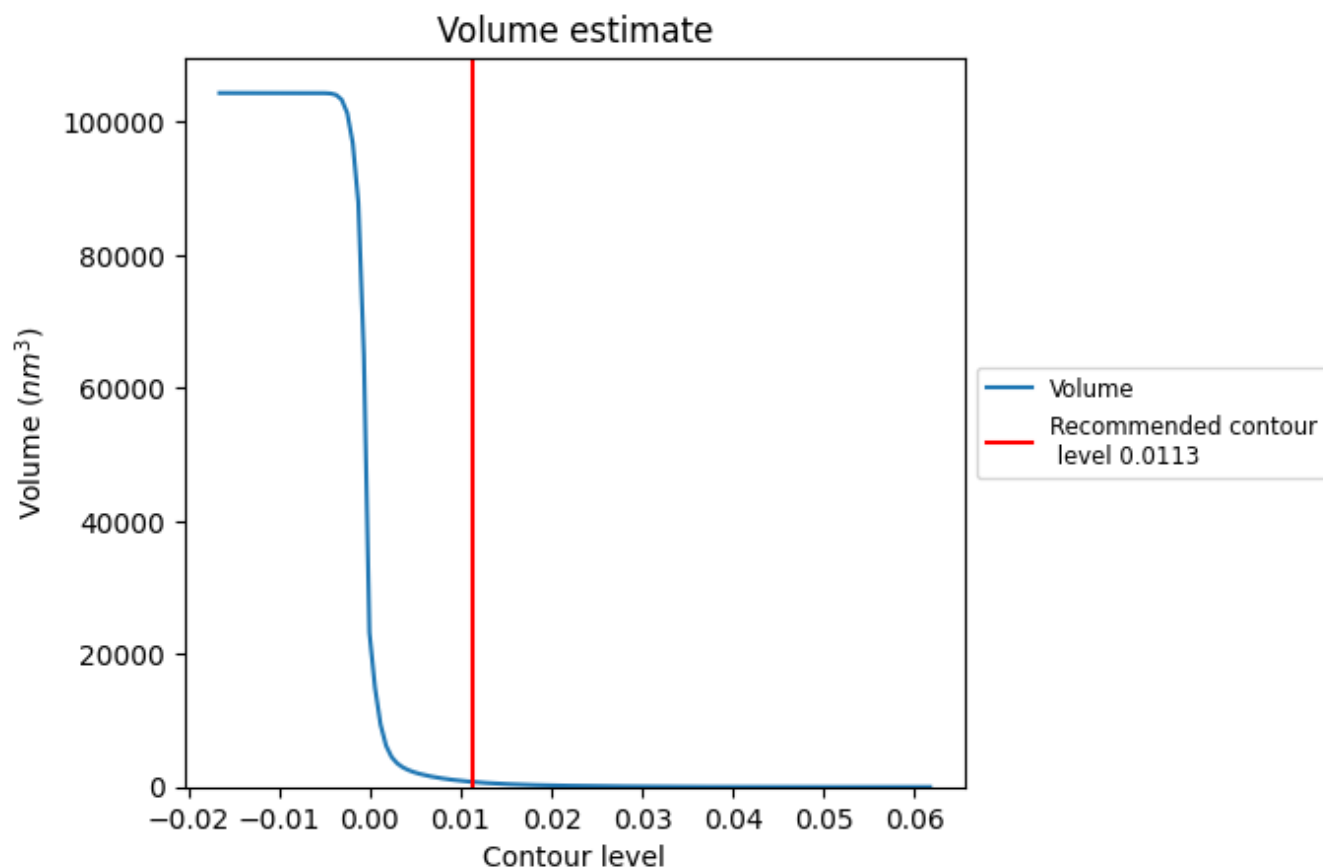
This section contains the results of statistical analysis of the map.

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.

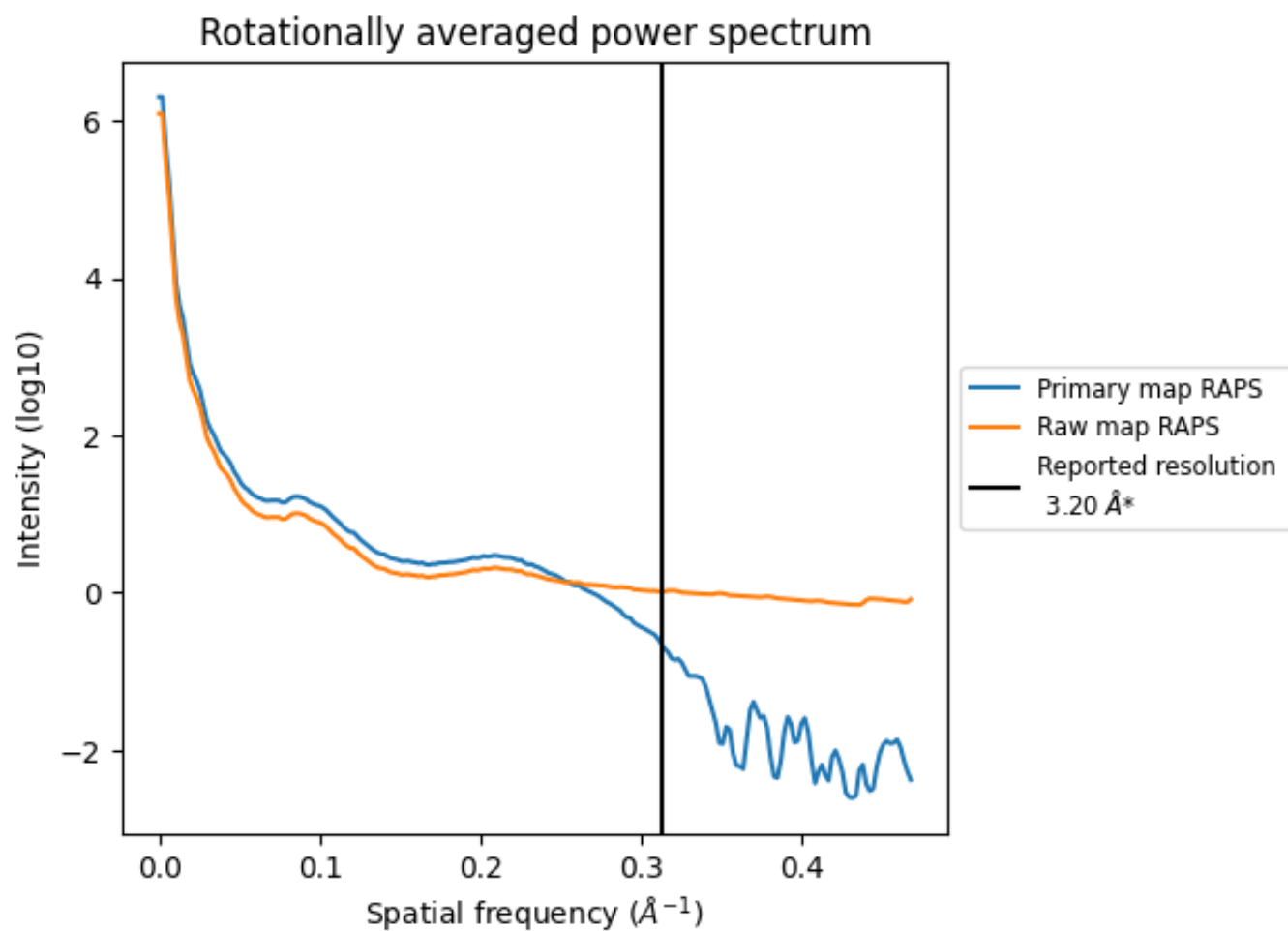
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 763 nm^3 ; this corresponds to an approximate mass of 689 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 [i](#)

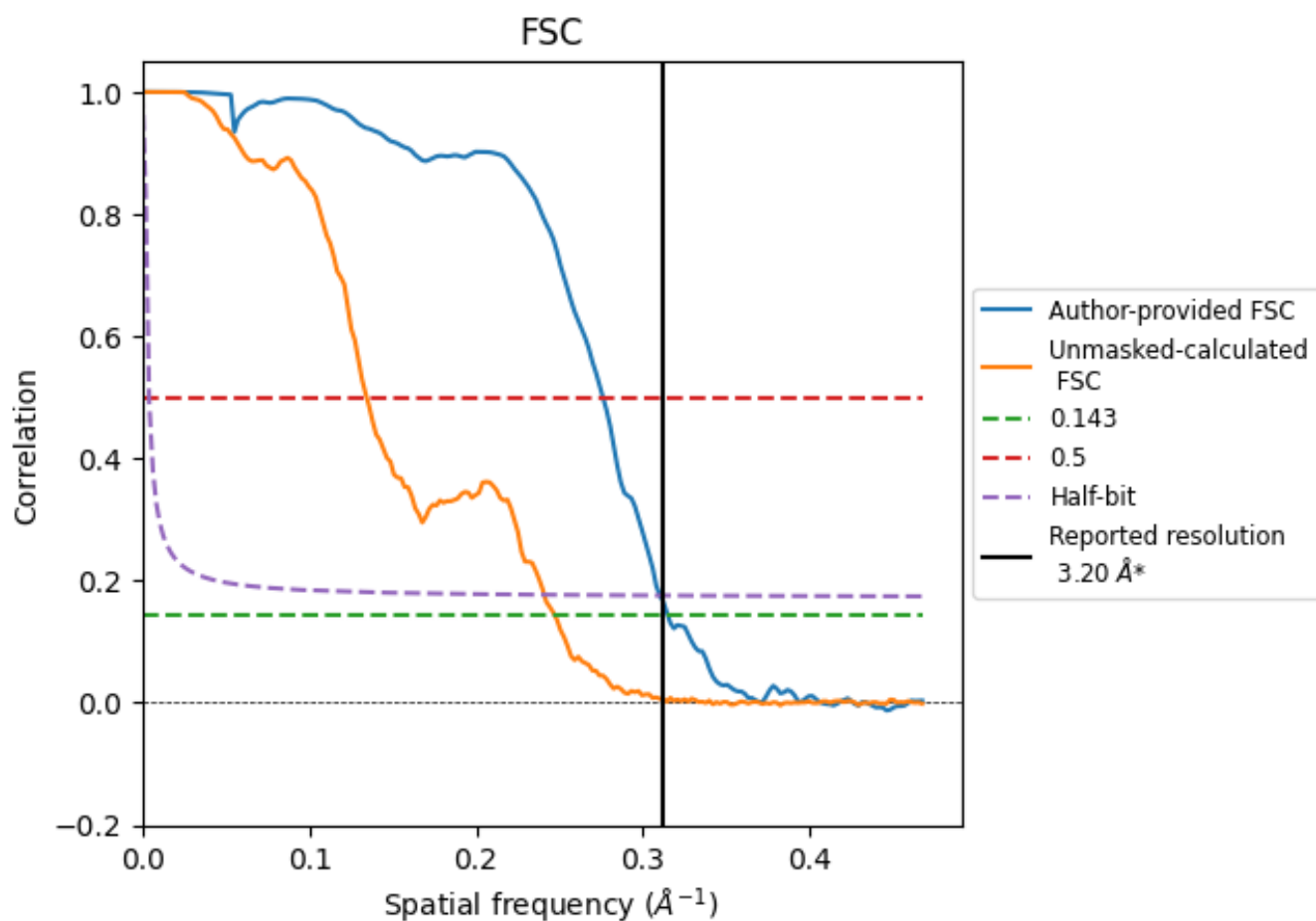


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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

8.2 Resolution estimates [i](#)

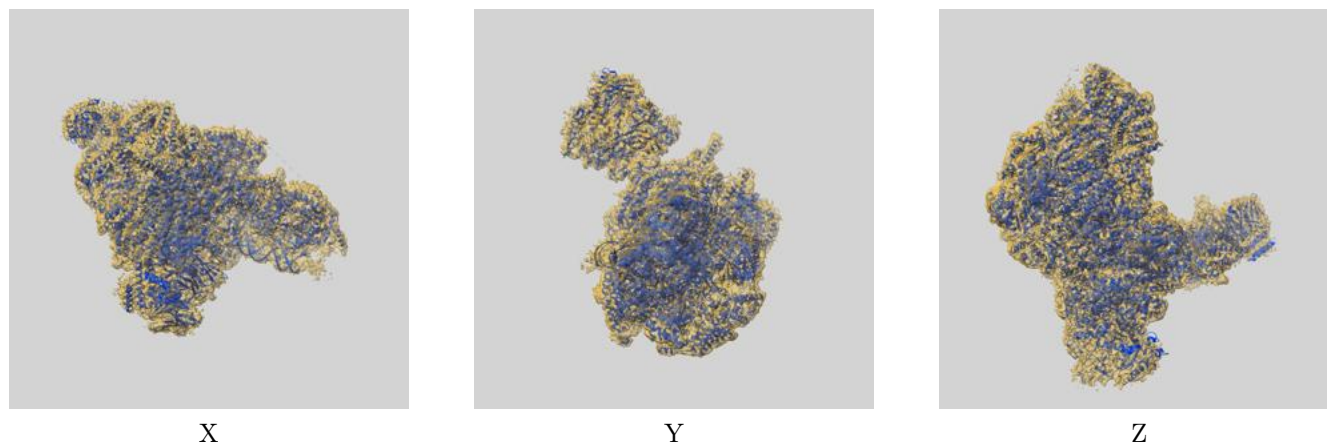
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.62	3.22
Unmasked-calculated*	4.05	7.43	4.15

*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 4.05 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

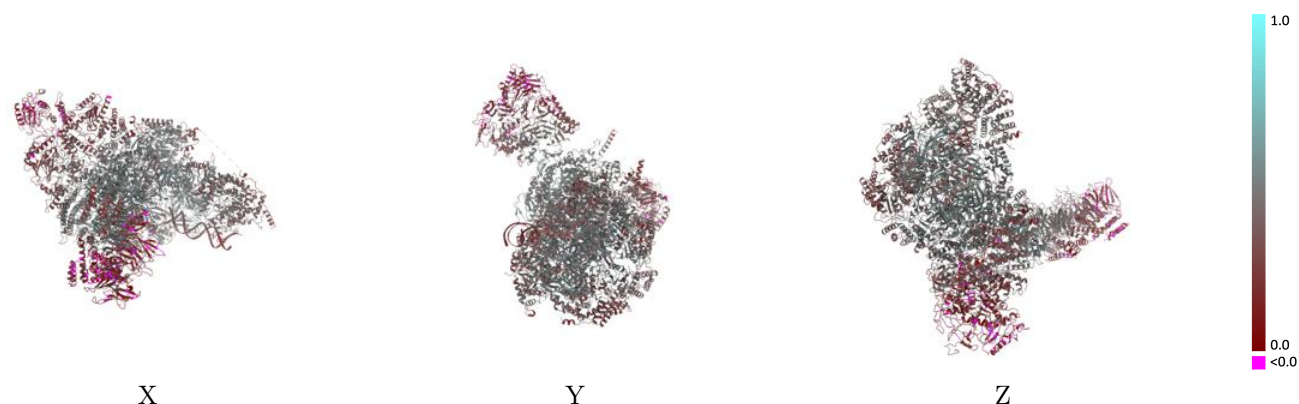
This section contains information regarding the fit between EMDB map EMD-13375 and PDB model 7PFO. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



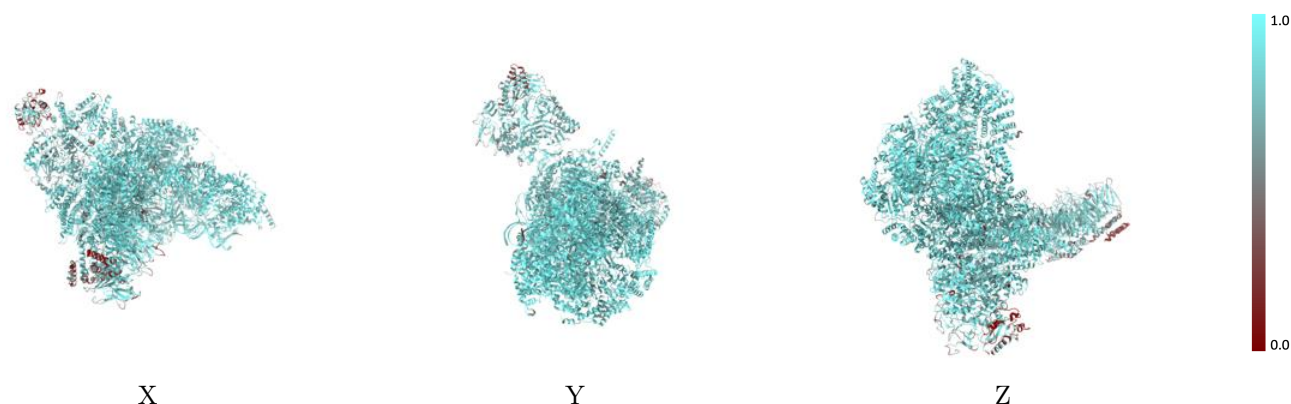
The images above show the 3D surface view of the map at the recommended contour level 0.0113 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



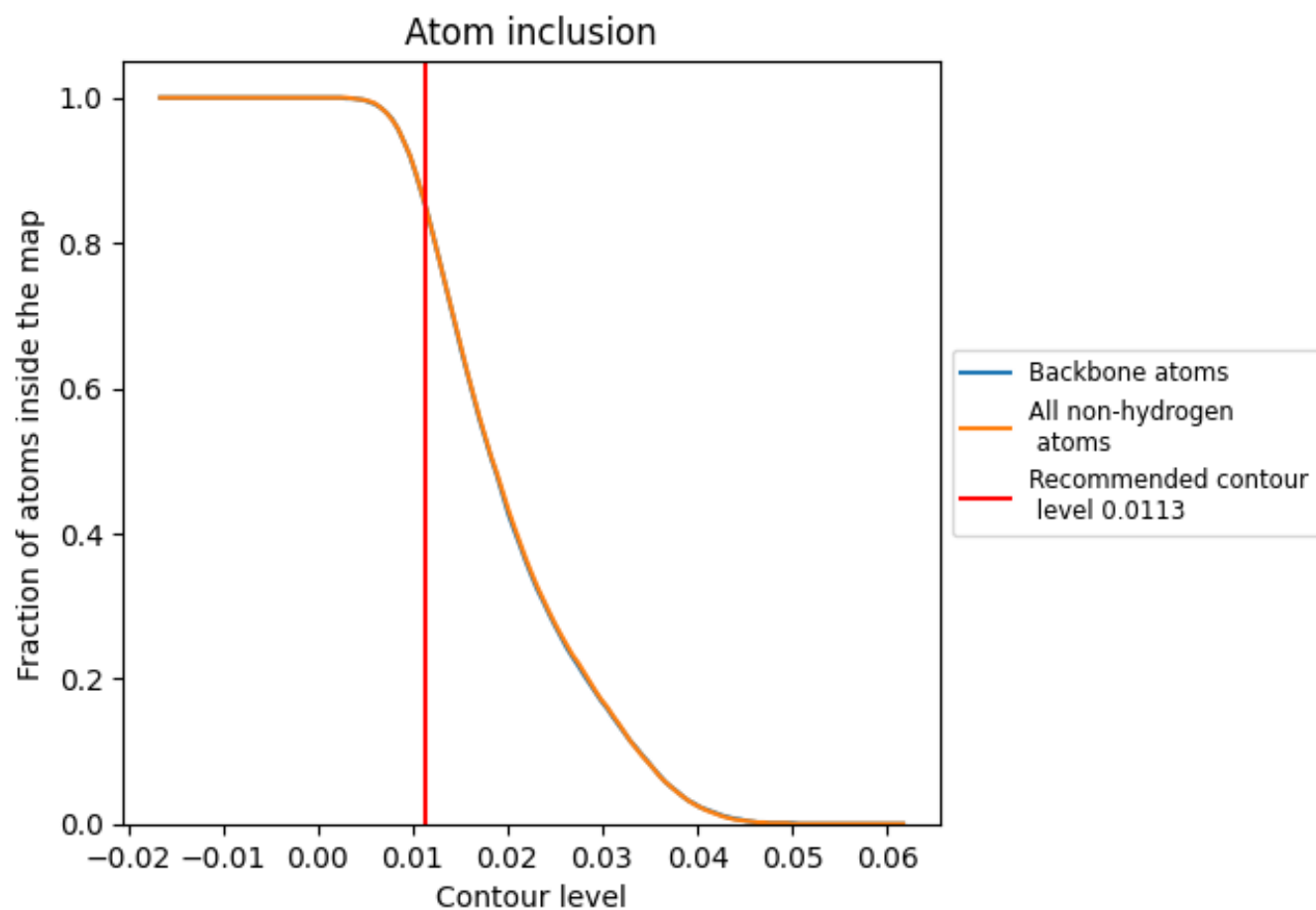
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0113).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 86% 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 (0.0113) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.3990
2	 0.8940	 0.4650
3	 0.9210	 0.4690
4	 0.9260	 0.4440
5	 0.9050	 0.4930
6	 0.9250	 0.4650
7	 0.9150	 0.4240
A	 0.8090	 0.3140
B	 0.6880	 0.2300
C	 0.9150	 0.4820
D	 0.9110	 0.4700
E	 0.9230	 0.5120
F	 0.9370	 0.4900
G	 0.9050	 0.4760
H	 0.7360	 0.2340
I	 0.7870	 0.3680
J	 0.6880	 0.2050
K	 0.9140	 0.4170
L	 0.8940	 0.4220
M	 0.8820	 0.3500
N	 0.9040	 0.2830
Q	 0.7500	 0.3280

