



Full wwPDB EM Validation Report ⓘ

Jun 27, 2022 – 05:10 pm BST

PDB ID : 7PLO
EMDB ID : EMD-13494
Title : H. sapiens replisome-CUL2/LRR1 complex
Authors : Jones, M.J.; Yeeles, J.T.P.; Deegan, T.D.; Jenkyn-Bedford, M.
Deposited on : 2021-09-01
Resolution : 2.80 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.dev8
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

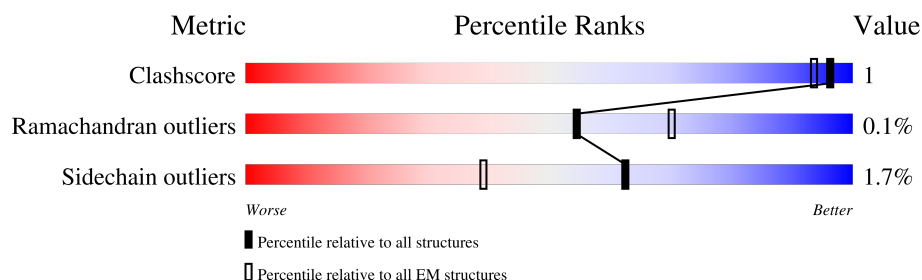
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	Q	1371	
2	2	904	
3	3	808	
4	4	863	
5	5	734	
6	6	821	
7	7	719	
8	A	527	

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Mol	Chain	Length	Quality of chain
9	B	2286	
10	C	569	
11	D	196	
12	E	185	
13	F	216	
14	G	262	
15	H	1161	
15	I	1161	
15	J	1161	
16	K	1209	
17	L	301	
18	M	85	
19	N	41	
20	O	414	
21	P	118	
22	R	112	
23	S	759	
24	T	108	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 78855 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 Claspin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	79	Total	C	N	O	S	0	0
			683	431	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 2 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	697	Total	C	N	O	S	0	0
			5527	3476	983	1037	31		

- Molecule 3 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	628	Total	C	N	O	S	0	0
			4908	3068	867	947	26		

- Molecule 4 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	619	Total	C	N	O	S	0	0
			4925	3100	873	925	27		

- Molecule 5 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	614	Total	C	N	O	S	0	0
			4803	3007	856	905	35		

- Molecule 6 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	631	Total	C	N	O	S	0	0
			5004	3143	889	946	26		

- Molecule 7 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	607	Total	C	N	O	S	0	0
			4818	3024	859	904	31		

- Molecule 8 is a protein called DNA polymerase epsilon subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	527	Total	C	N	O	S	0	0
			4195	2699	696	780	20		

- Molecule 9 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	759	Total	C	N	O	S	0	0
			6050	3826	1030	1150	44		

- Molecule 10 is a protein called Cell division control protein 45 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	534	Total	C	N	O	S	0	0
			4347	2764	745	807	31		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 11 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	196	Total	C	N	O	S	0	0
			1613	1016	290	295	12		

- Molecule 12 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	176	Total	C	N	O	S	0	0
			1431	916	242	264	9		

- Molecule 13 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	194	Total	C	N	O	S	0	0
			1546	979	268	293	6		

- Molecule 14 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	203	Total	C	N	O	S	0	0
			1679	1065	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 15 is a protein called WD repeat and HMG-box DNA-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	401	Total	C	N	O	S	1	0
			3178	2016	554	587	21		
15	I	451	Total	C	N	O	S	1	0
			3473	2209	606	637	21		
15	J	401	Total	C	N	O	S	2	0
			3183	2019	554	589	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 16 is a protein called Protein timeless homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	639	Total	C	N	O	S	0	0
			5247	3345	933	943	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 17 is a protein called TIMELESS-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	86	Total	C	N	O	S	0	0
			726	465	138	120	3		

- Molecule 18 is a DNA chain called Leading strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	33	Total	C	N	O	P	0	0
			682	330	108	211	33		

- Molecule 19 is a DNA chain called Lagging strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	22	Total	C	N	O	P	0	0
			438	211	74	131	22		

- Molecule 20 is a protein called Leucine-rich repeat protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	382	Total	C	N	O	S	0	0
			2888	1837	513	522	16		

- Molecule 21 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	82	Total	C	N	O	S	1	0
			629	399	105	122	3		

- Molecule 22 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	91	Total	C	N	O	S	1	0
			701	450	113	132	6		

- Molecule 23 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	671	Total	C	N	O	S	0	0
			5386	3404	921	1019	42		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-14	MET	-	initiating methionine	UNP Q13617
S	-13	ASP	-	expression tag	UNP Q13617
S	-12	TYR	-	expression tag	UNP Q13617
S	-11	LYS	-	expression tag	UNP Q13617
S	-10	ASP	-	expression tag	UNP Q13617
S	-9	ASP	-	expression tag	UNP Q13617
S	-8	ASP	-	expression tag	UNP Q13617
S	-7	GLY	-	expression tag	UNP Q13617
S	-6	ASP	-	expression tag	UNP Q13617
S	-5	TYR	-	expression tag	UNP Q13617
S	-4	LYS	-	expression tag	UNP Q13617
S	-3	ASP	-	expression tag	UNP Q13617
S	-2	ASP	-	expression tag	UNP Q13617
S	-1	ASP	-	expression tag	UNP Q13617
S	0	GLY	-	expression tag	UNP Q13617
S	?	-	LYS	deletion	UNP Q13617

- Molecule 24 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	86	Total	C	N	O	S	0	0
			685	429	127	120	9		

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
25	2	1	Total	Zn	0
			1	1	
25	4	1	Total	Zn	0
			1	1	
25	5	1	Total	Zn	0
			1	1	
25	6	1	Total	Zn	0
			1	1	
25	7	1	Total	Zn	0
			1	1	

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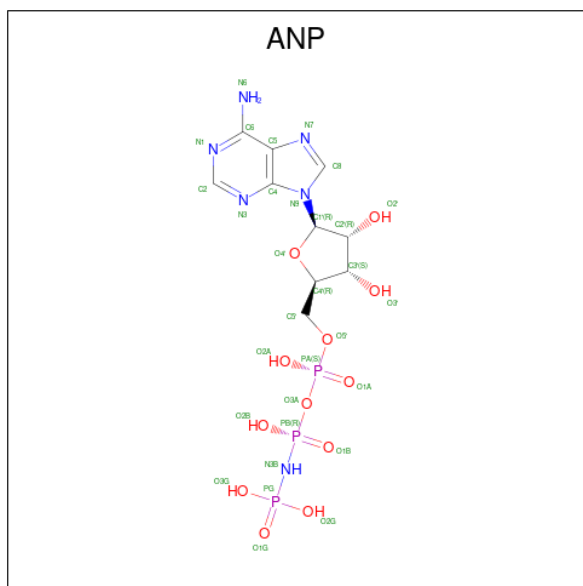
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Mol	Chain	Residues	Atoms		AltConf
25	B	1	Total	Zn	0
			1	1	
25	T	3	Total	Zn	0
			3	3	

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

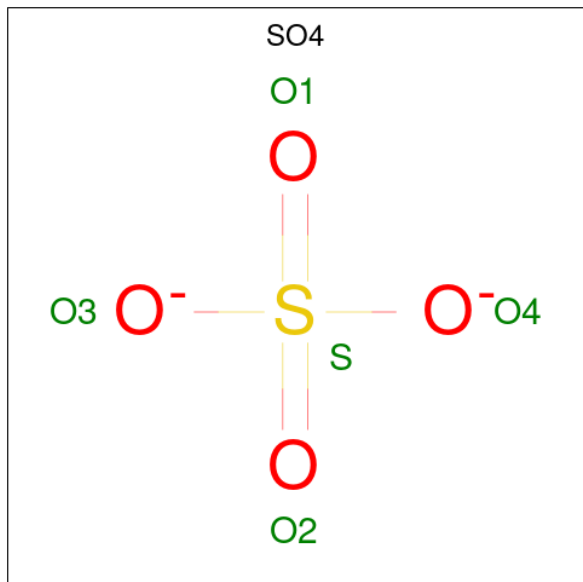
Mol	Chain	Residues	Atoms		AltConf
26	2	1	Total	Mg	0
			1	1	
26	3	1	Total	Mg	0
			1	1	
26	5	1	Total	Mg	0
			1	1	

- Molecule 27 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	2	1	Total	C	N	O	P	0
			31	10	6	12	3	
27	3	1	Total	C	N	O	P	0
			31	10	6	12	3	
27	5	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 28 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



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

[illegible]

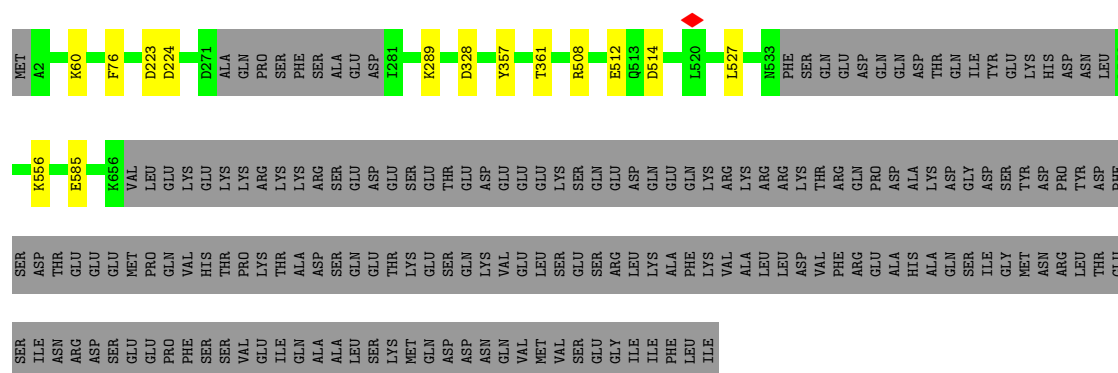
- Molecule 2: DNA replication licensing factor MCM2

Chain 2: 75% . 23%

Y246	ARG	ASP	GLY	MET
D894	LEU	GLU	PRO	ALA
	LYS	ALA	LEU	GLU
	ARG	GLY	GLU	SER
	LYS	ARG	GLU	GLU
	MET	GLY	GLU	SER
	LEU	GLY	GLY	PHE
	GLN	ARG	GLY	THR
	GLN	MET	GLY	MET
	PHE	ARG	LEU	ALA
		ARG	LEU	SER
		ARG	ILE	SER
		GLY	GLY	PRO
		LEU	ASP	ALA
		LEU	GLY	GLN
		TYR	MET	ARG
		ASP	GLU	ARG
		SER	ARG	ARG
		ASN	ASP	GLY
	LYS	GLU	TYR	ASN
	GLU	GLU	ARG	ASP
	GLU	GLU	ALA	PRO
	GLY	GLU	ILE	LEU
	LEU	ARG	GLU	THR
	ALA	PRO	LEU	SER
	ASN	ALA	ASP	SER
	GLY	ARG	ALA	GLY
	SER	LYS	TYR	ARG
	SER	ARG	GLU	SER
	ALA	ARG	ALA	SER
	GLU	GLN	GLU	ARG
	PRO	VAL	GLY	ARG
	ALA	GLU	LEU	THR
	MET	ARG	ALA	ASP
	PRO	ALA	LEU	ALA
	GLN	THR	ASP	LEU
	ASN	GLU	GLU	ASP
		T769	ASP	SER
		L735	GLY	SER
		T763	GLU	PRO
			GLU	GLY
			ASP	ARG
			GLU	THR
			GLU	ASP
			GLU	LEU
			GLU	THR
			GLU	PRO
			GLU	PRO
			ILE	SER
			E169	PHE
			D176	GLU
			L177	ASP
			K178	GLU
				SER
			S181	GLU
				GLY
			K200	LEU
				ARG
			E217	GLY
				THR
				GLN
				ARG
				GLU

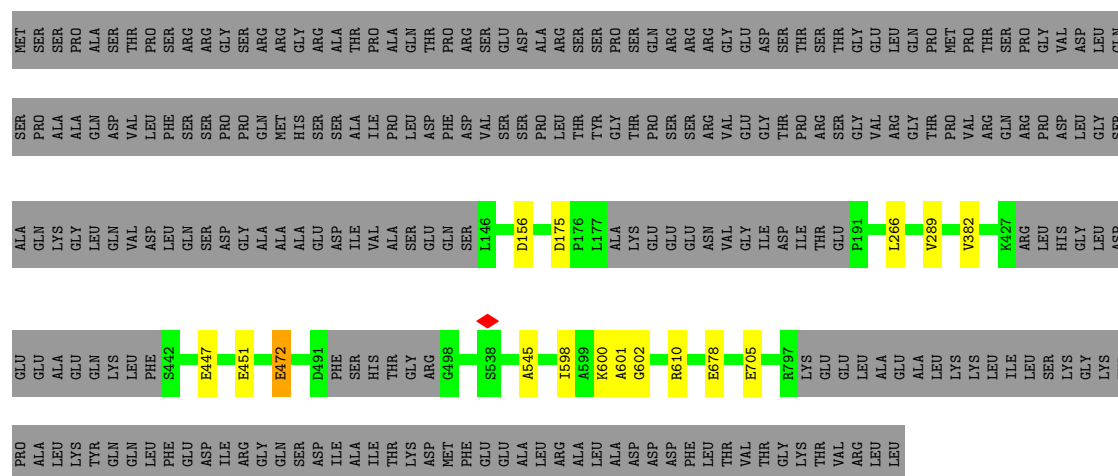
- Molecule 3: DNA replication licensing factor MCM3

Chain 3: 76% 22%



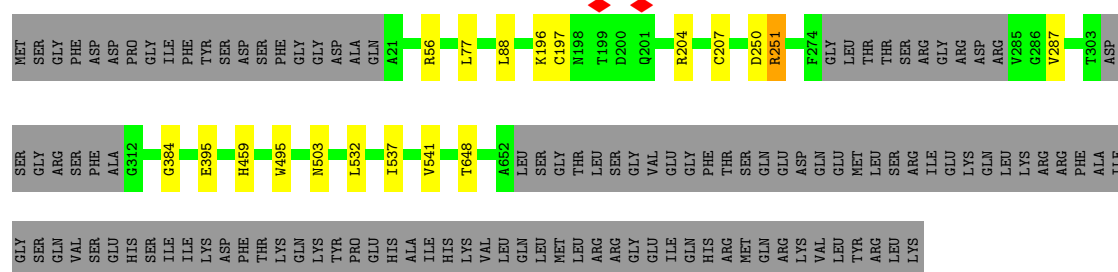
• Molecule 4: DNA replication licensing factor MCM4

Chain 4: 70% 28%



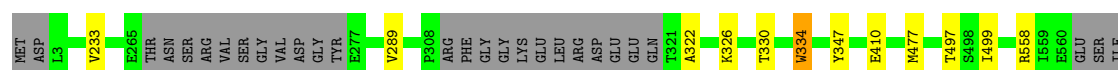
• Molecule 5: DNA replication licensing factor MCM5

Chain 5: 81% 16%

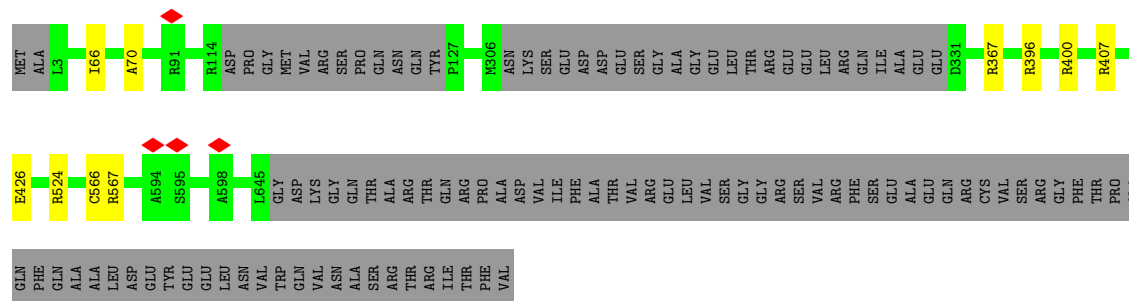
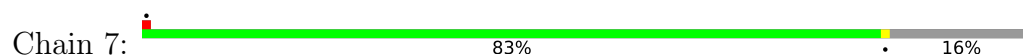


• Molecule 6: DNA replication licensing factor MCM6

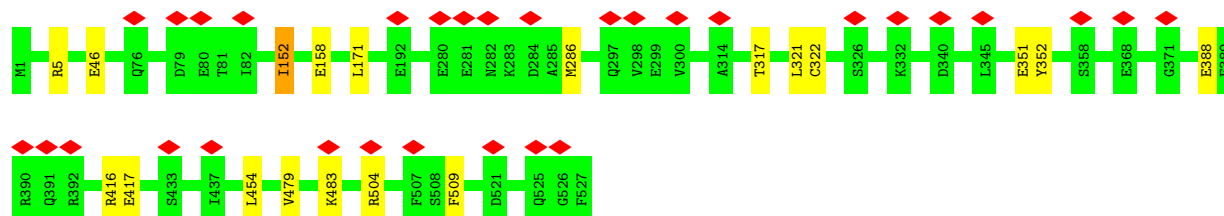
Chain 6: 75% 23%



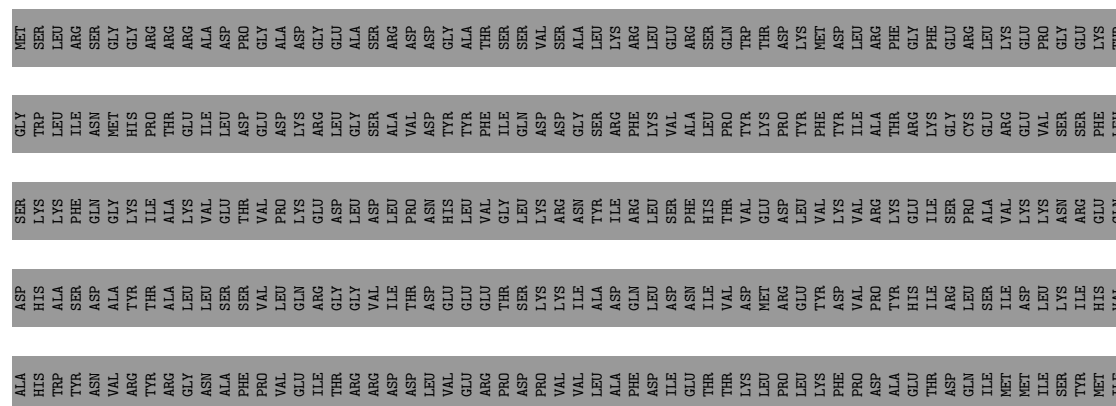
- Molecule 7: DNA replication licensing factor MCM7



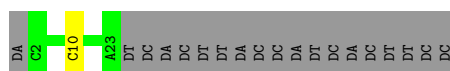
- Molecule 8: DNA polymerase epsilon subunit 2



- Molecule 9: DNA polymerase epsilon catalytic subunit A

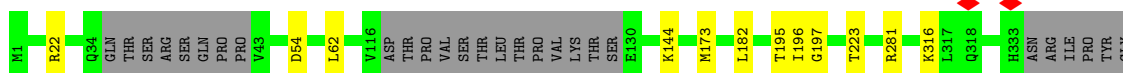


[illegible]



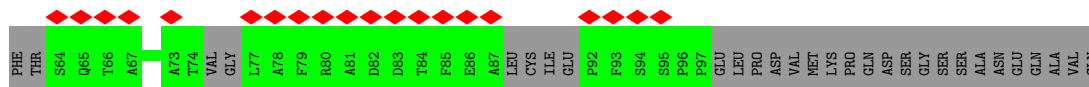
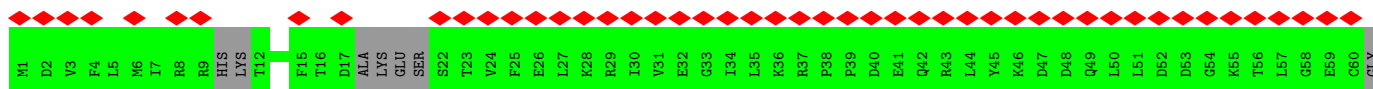
- Molecule 20: Leucine-rich repeat protein 1

Chain O: 88% 8%



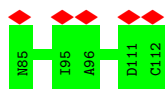
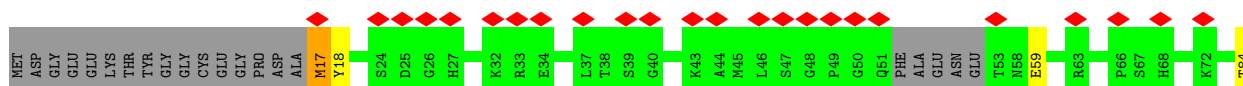
- Molecule 21: Elongin-B

Chain P: 58% 69% 31%



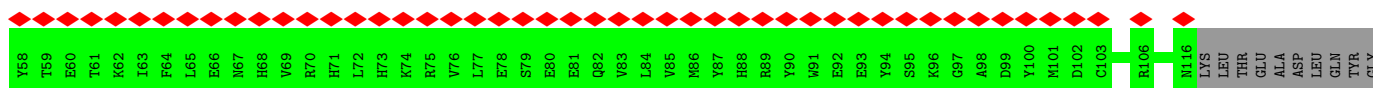
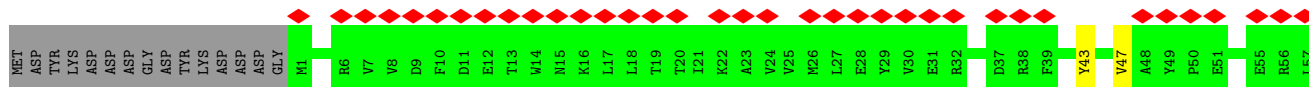
- Molecule 22: Elongin-C

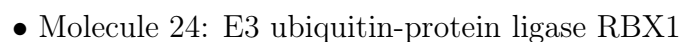
Chain R: 26% 78% 19%



- Molecule 23: Cullin-2

Chain S: 84% 87% 12%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	232000	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 ($e^-/\text{\AA}^2$)	38.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.336	Depositor
Minimum map value	-0.180	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0181	Depositor
Map size (\AA)	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, SO4, 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	Q	0.36	0/693	0.63	0/919
2	2	0.30	0/5630	0.65	0/7607
3	3	0.29	0/4981	0.65	0/6723
4	4	0.29	0/5009	0.65	1/6769 (0.0%)
5	5	0.30	0/4877	0.67	0/6564
6	6	0.30	0/5085	0.66	0/6862
7	7	0.29	0/4894	0.68	0/6605
8	A	0.32	0/4306	0.65	0/5849
9	B	0.33	0/6165	0.69	1/8331 (0.0%)
10	C	0.29	0/4439	0.61	0/5992
11	D	0.31	0/1645	0.67	0/2210
12	E	0.29	0/1462	0.58	0/1981
13	F	0.29	0/1580	0.59	0/2133
14	G	0.31	0/1711	0.64	0/2305
15	H	0.32	0/3253	0.65	0/4407
15	I	0.31	0/3555	0.61	0/4826
15	J	0.30	0/3261	0.64	0/4418
16	K	0.30	0/5352	0.64	0/7212
17	L	0.31	0/741	0.74	0/988
18	M	0.80	0/760	1.21	1/1172 (0.1%)
19	N	0.88	0/488	1.07	0/747
20	O	0.30	0/2933	0.66	1/3962 (0.0%)
21	P	0.28	0/639	0.65	0/858
22	R	0.31	0/717	0.56	0/965
23	S	0.31	0/5472	0.62	0/7361
24	T	0.30	0/702	0.65	0/952
All	All	0.32	0/80350	0.66	4/108718 (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
2	2	0	1
9	B	0	1
23	S	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	156	ASP	CB-CG-OD1	7.82	125.34	118.30
20	O	391	GLY	C-N-CA	6.05	136.83	121.70
9	B	2183	PRO	N-CA-CB	5.62	110.05	103.30
18	M	39	DG	O4'-C1'-N9	5.13	111.59	108.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	822	LEU	Peptide
9	B	1453	ARG	Peptide
23	S	614	ILE	Mainchain

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	Q	683	0	699	46	0
2	2	5527	0	5519	9	0
3	3	4908	0	4956	8	0
4	4	4925	0	4980	5	0
5	5	4803	0	4868	10	0
6	6	5004	0	5025	20	0
7	7	4818	0	4882	1	0
8	A	4195	0	4149	3	0
9	B	6050	0	5907	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	4347	0	4296	3	0
11	D	1613	0	1606	2	0
12	E	1431	0	1456	1	0
13	F	1546	0	1500	2	0
14	G	1679	0	1700	2	0
15	H	3178	0	3145	1	0
15	I	3473	0	3324	3	0
15	J	3183	0	3149	2	0
16	K	5247	0	5253	33	0
17	L	726	0	753	1	0
18	M	682	0	384	0	0
19	N	438	0	249	1	0
20	O	2888	0	2859	7	0
21	P	629	0	611	0	0
22	R	701	0	687	1	0
23	S	5386	0	5270	6	0
24	T	685	0	645	0	0
25	2	1	0	0	0	0
25	4	1	0	0	0	0
25	5	1	0	0	0	0
25	6	1	0	0	0	0
25	7	1	0	0	0	0
25	B	1	0	0	0	0
25	T	3	0	0	0	0
26	2	1	0	0	0	0
26	3	1	0	0	0	0
26	5	1	0	0	0	0
27	2	31	0	13	1	0
27	3	31	0	13	1	0
27	5	31	0	13	2	0
28	A	5	0	0	0	0
All	All	78855	0	77911	128	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 (128) 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:Q:613:ARG:NH1	16:K:21:GLU:HG3	1.44	1.29
1:Q:613:ARG:HH22	16:K:21:GLU:CG	1.47	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:613:ARG:HH22	16:K:21:GLU:CB	1.51	1.24
1:Q:613:ARG:CZ	16:K:21:GLU:HG3	1.81	1.11
1:Q:613:ARG:NH2	16:K:21:GLU:HB2	1.69	1.07
1:Q:613:ARG:NH2	16:K:21:GLU:CG	2.21	1.02
1:Q:613:ARG:NH2	16:K:21:GLU:CB	2.20	1.01
1:Q:613:ARG:HH22	16:K:21:GLU:HB2	1.20	1.01
1:Q:613:ARG:HH12	16:K:21:GLU:CG	1.74	0.98
1:Q:613:ARG:NH2	16:K:21:GLU:HG3	1.78	0.96
1:Q:535:PHE:CE1	6:6:326:LYS:HG3	2.06	0.90
1:Q:532:LYS:HE2	6:6:334:TRP:CZ2	2.08	0.89
1:Q:613:ARG:HH12	16:K:21:GLU:HG3	0.93	0.88
1:Q:309:PRO:HG3	16:K:351:GLU:O	1.74	0.87
1:Q:532:LYS:HE2	6:6:334:TRP:CE2	2.10	0.86
1:Q:305:PRO:CD	16:K:461:VAL:HG12	2.07	0.85
1:Q:532:LYS:HG2	6:6:334:TRP:CZ2	2.14	0.83
1:Q:305:PRO:HD3	16:K:461:VAL:HG12	1.60	0.83
1:Q:305:PRO:HD3	16:K:461:VAL:CG1	2.14	0.76
1:Q:535:PHE:CE1	6:6:326:LYS:CG	2.69	0.73
1:Q:305:PRO:CD	16:K:461:VAL:CG1	2.68	0.71
1:Q:535:PHE:CE1	6:6:322:ALA:O	2.43	0.70
6:6:596:GLU:OE1	6:6:597:GLN:NE2	2.25	0.70
14:G:22:THR:OG1	14:G:25:GLU:OE1	2.11	0.69
1:Q:532:LYS:HE2	6:6:334:TRP:CH2	2.28	0.68
5:5:495:TRP:O	5:5:503:ASN:ND2	2.26	0.68
1:Q:535:PHE:CZ	6:6:322:ALA:O	2.48	0.67
22:R:17:MET:SD	22:R:17:MET:N	2.70	0.63
1:Q:532:LYS:CE	6:6:334:TRP:CE2	2.82	0.63
1:Q:535:PHE:HE1	6:6:326:LYS:HG3	1.60	0.59
4:4:545:ALA:HB3	4:4:598:ILE:HD11	1.85	0.59
1:Q:613:ARG:NH2	16:K:26:HIS:CD2	2.71	0.58
1:Q:305:PRO:HD2	16:K:461:VAL:HG12	1.82	0.58
1:Q:315:HIS:CE1	16:K:142:GLN:HE22	2.19	0.58
1:Q:613:ARG:NE	16:K:26:HIS:CE1	2.71	0.58
23:S:170:ASP:OD1	23:S:249:ARG:NH2	2.37	0.58
5:5:197:CYS:N	5:5:207:CYS:SG	2.76	0.57
16:K:9:GLU:N	16:K:9:GLU:OE1	2.37	0.57
1:Q:532:LYS:HE2	6:6:334:TRP:CD2	2.40	0.56
16:K:451:ASN:ND2	16:K:512:MET:SD	2.78	0.56
1:Q:613:ARG:HD3	16:K:26:HIS:CE1	2.40	0.56
1:Q:528:LEU:HD21	6:6:334:TRP:CD1	2.42	0.55
9:B:1879:ARG:NH2	9:B:1881:GLU:OE2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:384:GLY:H	27:5:801:ANP:HNB1	1.54	0.55
20:O:197:GLY:O	20:O:223:THR:OG1	2.14	0.55
1:Q:609:ARG:NE	2:2:176:ASP:OD2	2.37	0.54
20:O:402:SER:OG	20:O:403:LEU:N	2.39	0.54
1:Q:535:PHE:HE1	6:6:322:ALA:O	1.91	0.54
9:B:2019:ALA:HB3	9:B:2020:PRO:HD3	1.91	0.53
19:N:10:DC:OP1	20:O:22:ARG:NH1	2.41	0.53
17:L:146:ASP:N	17:L:146:ASP:OD1	2.40	0.52
1:Q:593:LYS:NZ	2:2:291:VAL:O	2.31	0.52
16:K:52:ARG:NH1	16:K:88:ASN:O	2.44	0.51
9:B:2236:CYS:SG	9:B:2237:SER:N	2.82	0.51
4:4:600:LYS:O	4:4:602:GLY:N	2.44	0.50
3:3:527:LEU:HD12	13:F:99:VAL:HG22	1.93	0.49
4:4:472:GLU:N	4:4:472:GLU:OE1	2.46	0.49
20:O:387:ASP:O	20:O:391:GLY:HA3	2.11	0.49
15:I:1025:TRP:CD1	15:I:1057:LEU:HD11	2.48	0.49
10:C:499:MET:SD	10:C:499:MET:N	2.87	0.48
4:4:289:VAL:HG21	4:4:382:VAL:CG1	2.43	0.48
15:H:534:ASP:OD1	15:H:535:ILE:N	2.46	0.48
9:B:1957:GLU:N	9:B:1970:SER:O	2.47	0.48
8:A:152:ILE:HG21	13:F:45:ALA:HB1	1.96	0.48
8:A:286:MET:O	8:A:317:THR:N	2.47	0.48
1:Q:532:LYS:HG2	6:6:334:TRP:HZ2	1.73	0.47
6:6:477:MET:HG2	6:6:499:ILE:HD12	1.97	0.47
2:2:526:GLY:H	27:2:1003:ANP:HNB1	1.63	0.46
16:K:348:GLU:N	16:K:348:GLU:OE1	2.47	0.46
1:Q:613:ARG:CD	16:K:26:HIS:CE1	2.98	0.46
3:3:357:TYR:CZ	3:3:361:THR:HG21	2.51	0.46
3:3:508:ARG:NH2	3:3:514:ASP:O	2.49	0.46
27:3:1500:ANP:N3B	27:3:1500:ANP:O2A	2.49	0.45
1:Q:532:LYS:HG2	6:6:334:TRP:CE2	2.50	0.45
2:2:217:GLU:OE1	2:2:217:GLU:N	2.50	0.45
9:B:1959:ARG:NH1	9:B:1969:GLU:OE2	2.50	0.45
9:B:1859:LEU:O	9:B:1862:SER:OG	2.33	0.45
16:K:14:CYS:SG	16:K:60:ILE:HG21	2.57	0.44
9:B:1746:ASN:OD1	9:B:1747:ASP:N	2.50	0.44
2:2:763:THR:HG22	5:5:532:LEU:HD21	1.99	0.44
1:Q:539:ALA:HA	6:6:322:ALA:CB	2.48	0.44
1:Q:613:ARG:CZ	16:K:26:HIS:CD2	3.01	0.44
3:3:585:GLU:N	3:3:585:GLU:OE1	2.50	0.44
23:S:439:LEU:HD11	23:S:458:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:613:ARG:HE	16:K:26:HIS:CG	2.35	0.44
2:2:735:LEU:HD22	5:5:541:VAL:HG22	2.00	0.44
15:I:1044:ALA:HA	20:O:316:LYS:HE3	2.00	0.44
8:A:388:GLU:OE1	8:A:388:GLU:N	2.49	0.44
9:B:1490:TYR:CE1	9:B:1520:SER:HB2	2.53	0.44
3:3:328:ASP:N	3:3:328:ASP:OD1	2.51	0.43
15:J:603:LEU:HD23	15:J:614:LEU:HD13	2.00	0.43
9:B:1882:ASP:OD1	9:B:1883:ALA:N	2.50	0.43
1:Q:532:LYS:HE2	6:6:334:TRP:CZ3	2.53	0.43
4:4:175:ASP:OD1	4:4:175:ASP:N	2.51	0.43
5:5:77:LEU:CD2	5:5:88:LEU:HD12	2.48	0.43
23:S:43:TYR:O	23:S:47:VAL:HG23	2.19	0.43
7:7:66:ILE:O	7:7:70:ALA:HA	2.19	0.43
11:D:88:ARG:NE	14:G:101:GLU:OE1	2.51	0.43
16:K:140:LEU:HD21	16:K:152:ASP:HB3	2.01	0.42
1:Q:535:PHE:HZ	6:6:322:ALA:O	2.00	0.42
9:B:2102:LEU:CD2	9:B:2133:VAL:HG21	2.50	0.42
2:2:200:LYS:HG3	2:2:262:ALA:HB1	2.02	0.42
5:5:384:GLY:N	27:5:801:ANP:HNB1	2.17	0.42
23:S:487:ASN:ND2	23:S:508:GLN:OE1	2.53	0.42
20:O:54:ASP:N	20:O:54:ASP:OD1	2.53	0.42
5:5:250:ASP:OD2	5:5:251:ARG:NE	2.51	0.41
9:B:1466:GLU:N	9:B:1469:GLU:OE2	2.53	0.41
16:K:393:SER:O	16:K:395:ARG:NE	2.51	0.41
3:3:508:ARG:NH1	3:3:512:GLU:OE2	2.50	0.41
1:Q:601:LEU:HD22	2:2:246:TYR:HB2	2.02	0.41
5:5:537:ILE:O	5:5:541:VAL:HG23	2.20	0.41
10:C:37:GLN:NE2	11:D:149:GLU:OE2	2.53	0.41
20:O:182:LEU:HD23	20:O:196:ILE:HD11	2.02	0.41
1:Q:613:ARG:NH1	16:K:21:GLU:CG	2.40	0.41
9:B:1407:TYR:CD2	9:B:1452:VAL:HG11	2.56	0.41
15:I:717:GLN:NE2	15:J:528:ASP:OD1	2.52	0.41
3:3:223:ASP:N	3:3:223:ASP:OD1	2.53	0.41
9:B:1756:ILE:O	9:B:1760:VAL:HG23	2.20	0.41
9:B:2169:LEU:HD23	9:B:2169:LEU:H	1.86	0.41
3:3:357:TYR:CE1	3:3:361:THR:HG21	2.56	0.41
9:B:1600:ILE:H	9:B:1600:ILE:HD12	1.86	0.40
10:C:276:LEU:HD22	10:C:344:ILE:HG21	2.03	0.40
5:5:56:ARG:NH2	12:E:119:ASP:OD1	2.52	0.40
16:K:46:ASP:OD1	16:K:47:GLU:N	2.54	0.40
2:2:385:VAL:O	2:2:387:ALA:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1664:ILE:HG22	9:B:1664:ILE:O	2.21	0.40
23:S:622:MET:SD	23:S:622:MET:N	2.90	0.40
23:S:684:ILE:HD12	23:S:722:ILE:HD11	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	Q	73/1371 (5%)	73 (100%)	0	0	100	100
2	2	691/904 (76%)	653 (94%)	38 (6%)	0	100	100
3	3	622/808 (77%)	595 (96%)	26 (4%)	1 (0%)	47	78
4	4	611/863 (71%)	585 (96%)	25 (4%)	1 (0%)	47	78
5	5	608/734 (83%)	590 (97%)	18 (3%)	0	100	100
6	6	623/821 (76%)	597 (96%)	26 (4%)	0	100	100
7	7	601/719 (84%)	576 (96%)	25 (4%)	0	100	100
8	A	525/527 (100%)	488 (93%)	35 (7%)	2 (0%)	34	66
9	B	731/2286 (32%)	648 (89%)	78 (11%)	5 (1%)	22	53
10	C	530/569 (93%)	521 (98%)	9 (2%)	0	100	100
11	D	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
12	E	174/185 (94%)	171 (98%)	3 (2%)	0	100	100
13	F	190/216 (88%)	186 (98%)	4 (2%)	0	100	100
14	G	201/262 (77%)	195 (97%)	6 (3%)	0	100	100
15	H	400/1161 (34%)	382 (96%)	18 (4%)	0	100	100
15	I	448/1161 (39%)	434 (97%)	14 (3%)	0	100	100
15	J	401/1161 (34%)	384 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	K	635/1209 (52%)	606 (95%)	29 (5%)	0	100	100
17	L	84/301 (28%)	78 (93%)	6 (7%)	0	100	100
20	O	374/414 (90%)	340 (91%)	34 (9%)	0	100	100
21	P	71/118 (60%)	65 (92%)	6 (8%)	0	100	100
22	R	87/112 (78%)	86 (99%)	1 (1%)	0	100	100
23	S	640/759 (84%)	607 (95%)	33 (5%)	0	100	100
24	T	84/108 (78%)	75 (89%)	8 (10%)	1 (1%)	13	39
All	All	9598/16965 (57%)	9124 (95%)	464 (5%)	10 (0%)	54	81

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	A	152	ILE
9	B	1394	VAL
9	B	1905	ILE
9	B	1775	ALA
3	3	556	LYS
24	T	43	ALA
4	4	601	ALA
8	A	158	GLU
9	B	1384	VAL
9	B	1470	MET

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	Q	72/1230 (6%)	67 (93%)	5 (7%)	15	41
2	2	612/781 (78%)	606 (99%)	6 (1%)	76	93
3	3	539/707 (76%)	535 (99%)	4 (1%)	84	95
4	4	548/753 (73%)	541 (99%)	7 (1%)	69	91
5	5	522/625 (84%)	515 (99%)	7 (1%)	69	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	6	554/724 (76%)	545 (98%)	9 (2%)	62	88
7	7	526/619 (85%)	518 (98%)	8 (2%)	65	89
8	A	470/471 (100%)	456 (97%)	14 (3%)	41	75
9	B	672/2012 (33%)	643 (96%)	29 (4%)	29	62
10	C	487/520 (94%)	482 (99%)	5 (1%)	76	93
11	D	174/174 (100%)	173 (99%)	1 (1%)	86	96
12	E	160/169 (95%)	160 (100%)	0	100	100
13	F	167/186 (90%)	165 (99%)	2 (1%)	71	92
14	G	188/233 (81%)	187 (100%)	1 (0%)	88	96
15	H	346/1018 (34%)	338 (98%)	8 (2%)	50	82
15	I	355/1018 (35%)	349 (98%)	6 (2%)	60	87
15	J	347/1018 (34%)	341 (98%)	6 (2%)	60	87
16	K	564/1055 (54%)	550 (98%)	14 (2%)	47	80
17	L	77/274 (28%)	76 (99%)	1 (1%)	69	91
20	O	303/380 (80%)	298 (98%)	5 (2%)	60	87
21	P	67/103 (65%)	67 (100%)	0	100	100
22	R	77/96 (80%)	73 (95%)	4 (5%)	23	55
23	S	590/693 (85%)	588 (100%)	2 (0%)	92	98
24	T	72/90 (80%)	72 (100%)	0	100	100
All	All	8489/14949 (57%)	8345 (98%)	144 (2%)	62	87

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	315	HIS
1	Q	525	ASN
1	Q	536	TRP
1	Q	593	LYS
1	Q	602	GLN
2	2	178	LYS
2	2	181	SER
2	2	352	CYS
2	2	356	GLN
2	2	457	THR
2	2	821	TYR

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Mol	Chain	Res	Type
3	3	60	LYS
3	3	76	PHE
3	3	224	ASP
3	3	289	LYS
4	4	266	LEU
4	4	447	GLU
4	4	451	GLU
4	4	472	GLU
4	4	610	ARG
4	4	678	GLU
4	4	705	GLU
5	5	196	LYS
5	5	204	ARG
5	5	251	ARG
5	5	287	VAL
5	5	395	GLU
5	5	459	HIS
5	5	648	THR
6	6	233	VAL
6	6	289	VAL
6	6	330	THR
6	6	334	TRP
6	6	347	TYR
6	6	410	GLU
6	6	497	THR
6	6	558	ARG
6	6	597	GLN
7	7	367	ARG
7	7	396	ARG
7	7	400	ARG
7	7	407	ARG
7	7	426	GLU
7	7	524	ARG
7	7	566	CYS
7	7	567	ARG
8	A	5	ARG
8	A	46	GLU
8	A	171	LEU
8	A	321	LEU
8	A	322	CYS
8	A	351	GLU
8	A	352	TYR

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Mol	Chain	Res	Type
8	A	416	ARG
8	A	417	GLU
8	A	454	LEU
8	A	479	VAL
8	A	483	LYS
8	A	504	ARG
8	A	509	PHE
9	B	1376	GLU
9	B	1412	ASN
9	B	1453	ARG
9	B	1492	HIS
9	B	1559	THR
9	B	1562	LYS
9	B	1593	LEU
9	B	1595	ARG
9	B	1660	LEU
9	B	1691	ARG
9	B	1715	GLU
9	B	1732	GLN
9	B	1837	LEU
9	B	1870	ARG
9	B	1876	LYS
9	B	1888	GLU
9	B	1909	ARG
9	B	1932	ARG
9	B	1935	CYS
9	B	1939	ASP
9	B	1959	ARG
9	B	1985	PHE
9	B	2058	GLU
9	B	2078	ARG
9	B	2158	CYS
9	B	2187	CYS
9	B	2205	GLU
9	B	2225	ARG
9	B	2269	TYR
10	C	170	ARG
10	C	275	ASP
10	C	284	TRP
10	C	299	ARG
10	C	499	MET
11	D	156	TYR

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Mol	Chain	Res	Type
13	F	68	LEU
13	F	169	ASP
14	G	81	GLU
15	H	456	ARG
15	H	499	LEU
15	H	669	LYS
15	H	688	ARG
15	H	741	TYR
15	H	744	LYS
15	H	812	LEU
15	H	815	LEU
15	I	459	ASN
15	I	525	TRP
15	I	558	THR
15	I	727	GLU
15	I	756	GLN
15	I	762	GLN
15	J	497	ILE
15	J	555	ARG
15	J	558	THR
15	J	652	ARG
15	J	741	TYR
15	J	766	MET
16	K	21	GLU
16	K	106	PHE
16	K	124	PHE
16	K	137	LEU
16	K	139	GLU
16	K	157	GLU
16	K	179	ILE
16	K	201	LEU
16	K	348	GLU
16	K	395	ARG
16	K	466	ARG
16	K	520	ARG
16	K	525	VAL
16	K	692	LEU
17	L	87	LYS
20	O	62	LEU
20	O	144	LYS
20	O	173	MET
20	O	195	THR

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Mol	Chain	Res	Type
20	O	281	ARG
22	R	17	MET
22	R	18	TYR
22	R	59	GLU
22	R	84	THR
23	S	270	MET
23	S	622	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
16	K	26	HIS
16	K	142	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 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
28	SO4	A	601	-	4,4,4	0.13	0	6,6,6	0.05	0
27	ANP	3	1500	26	29,33,33	1.07	4 (13%)	31,52,52	1.13	2 (6%)
27	ANP	2	1003	26	29,33,33	1.07	4 (13%)	31,52,52	0.99	2 (6%)
27	ANP	5	801	26	29,33,33	1.07	4 (13%)	31,52,52	1.00	2 (6%)

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
27	ANP	3	1500	26	-	6/14/38/38	0/3/3/3
27	ANP	2	1003	26	-	2/14/38/38	0/3/3/3
27	ANP	5	801	26	-	5/14/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	3	1500	ANP	PB-O3A	-2.80	1.55	1.59
27	2	1003	ANP	PB-O3A	-2.58	1.55	1.59
27	5	801	ANP	PB-O3A	-2.50	1.55	1.59
27	2	1003	ANP	PG-N3B	2.36	1.69	1.63
27	5	801	ANP	PG-O1G	2.34	1.49	1.46
27	5	801	ANP	PG-N3B	2.34	1.69	1.63
27	2	1003	ANP	PG-O1G	2.29	1.49	1.46
27	3	1500	ANP	PG-N3B	2.27	1.69	1.63
27	5	801	ANP	PB-O1B	2.21	1.49	1.46
27	2	1003	ANP	PB-O1B	2.17	1.49	1.46
27	3	1500	ANP	PG-O1G	2.15	1.49	1.46
27	3	1500	ANP	PB-O1B	2.11	1.49	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	1500	ANP	PB-O3A-PA	-4.28	117.53	132.62
27	5	801	ANP	PB-O3A-PA	-3.34	120.85	132.62
27	2	1003	ANP	PB-O3A-PA	-3.31	120.97	132.62
27	3	1500	ANP	C5-C6-N6	2.32	123.88	120.35
27	2	1003	ANP	C5-C6-N6	2.31	123.87	120.35
27	5	801	ANP	C5-C6-N6	2.26	123.79	120.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

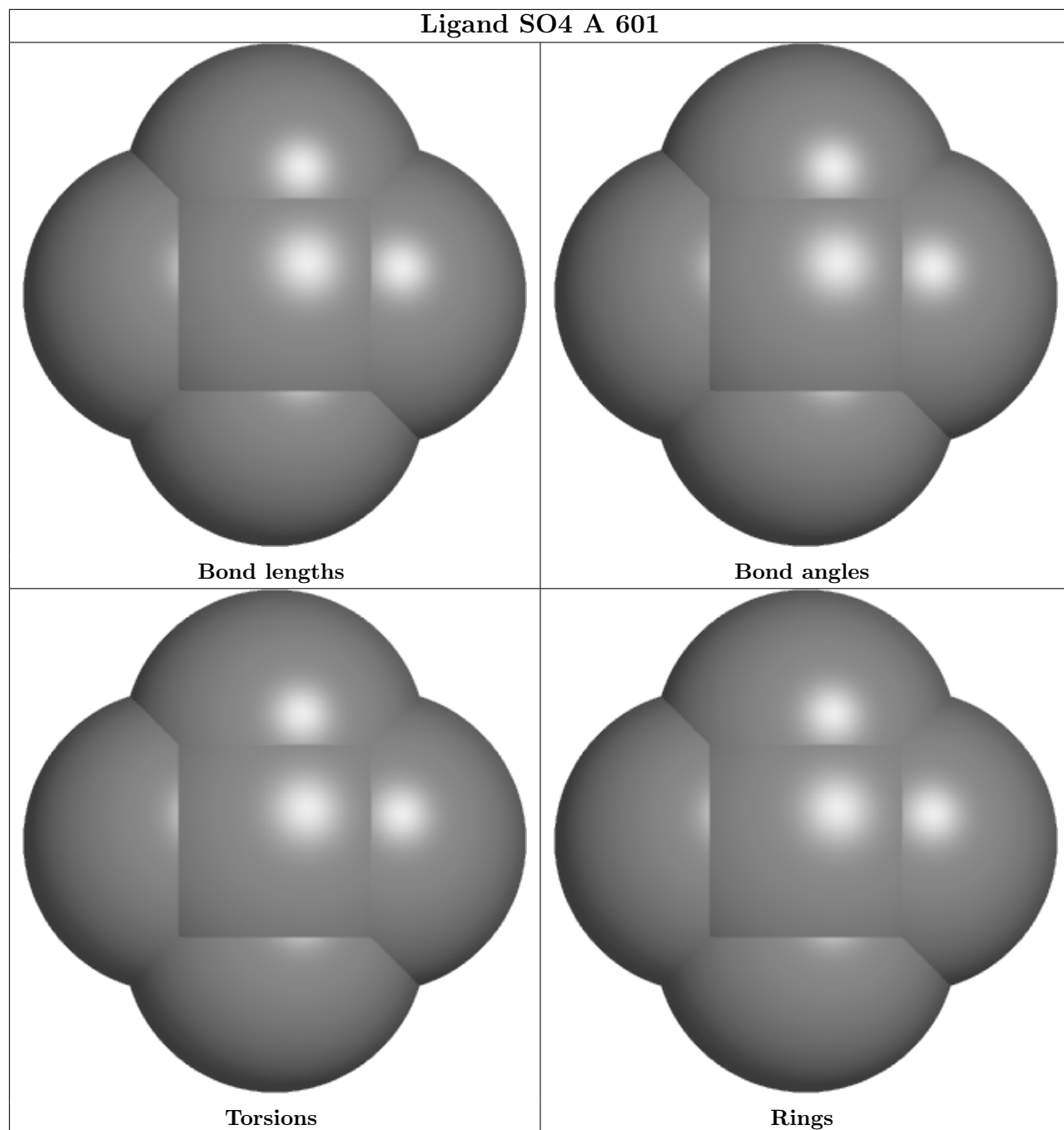
Mol	Chain	Res	Type	Atoms
27	2	1003	ANP	PB-N3B-PG-O1G
27	2	1003	ANP	PA-O3A-PB-O1B
27	3	1500	ANP	PB-N3B-PG-O1G
27	3	1500	ANP	PG-N3B-PB-O1B
27	3	1500	ANP	PG-N3B-PB-O3A
27	3	1500	ANP	C5'-O5'-PA-O1A
27	3	1500	ANP	C5'-O5'-PA-O2A
27	5	801	ANP	PB-N3B-PG-O1G
27	5	801	ANP	PA-O3A-PB-O1B
27	5	801	ANP	PA-O3A-PB-O2B
27	5	801	ANP	O4'-C4'-C5'-O5'
27	5	801	ANP	C3'-C4'-C5'-O5'
27	3	1500	ANP	C5'-O5'-PA-O3A

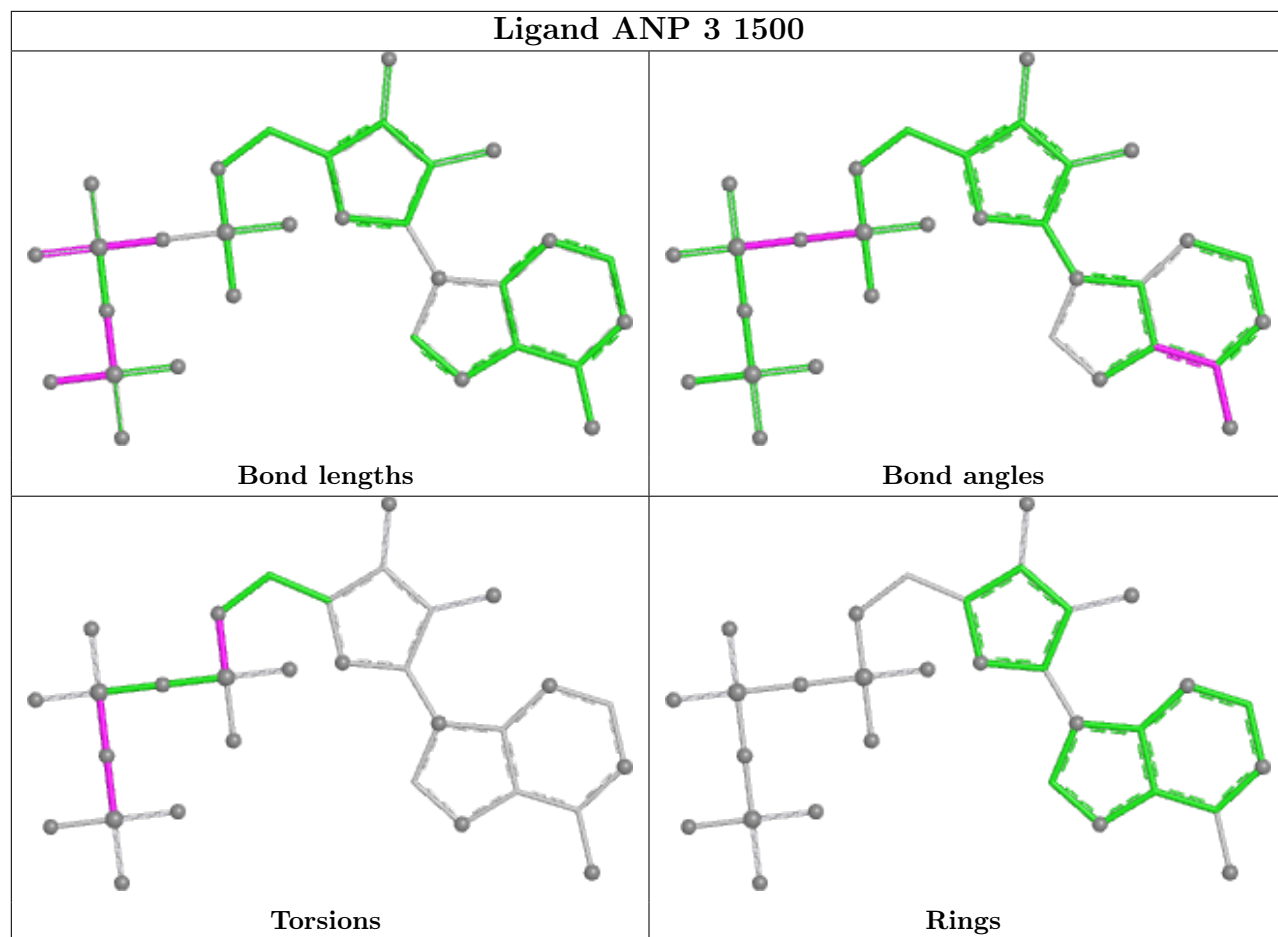
There are no ring outliers.

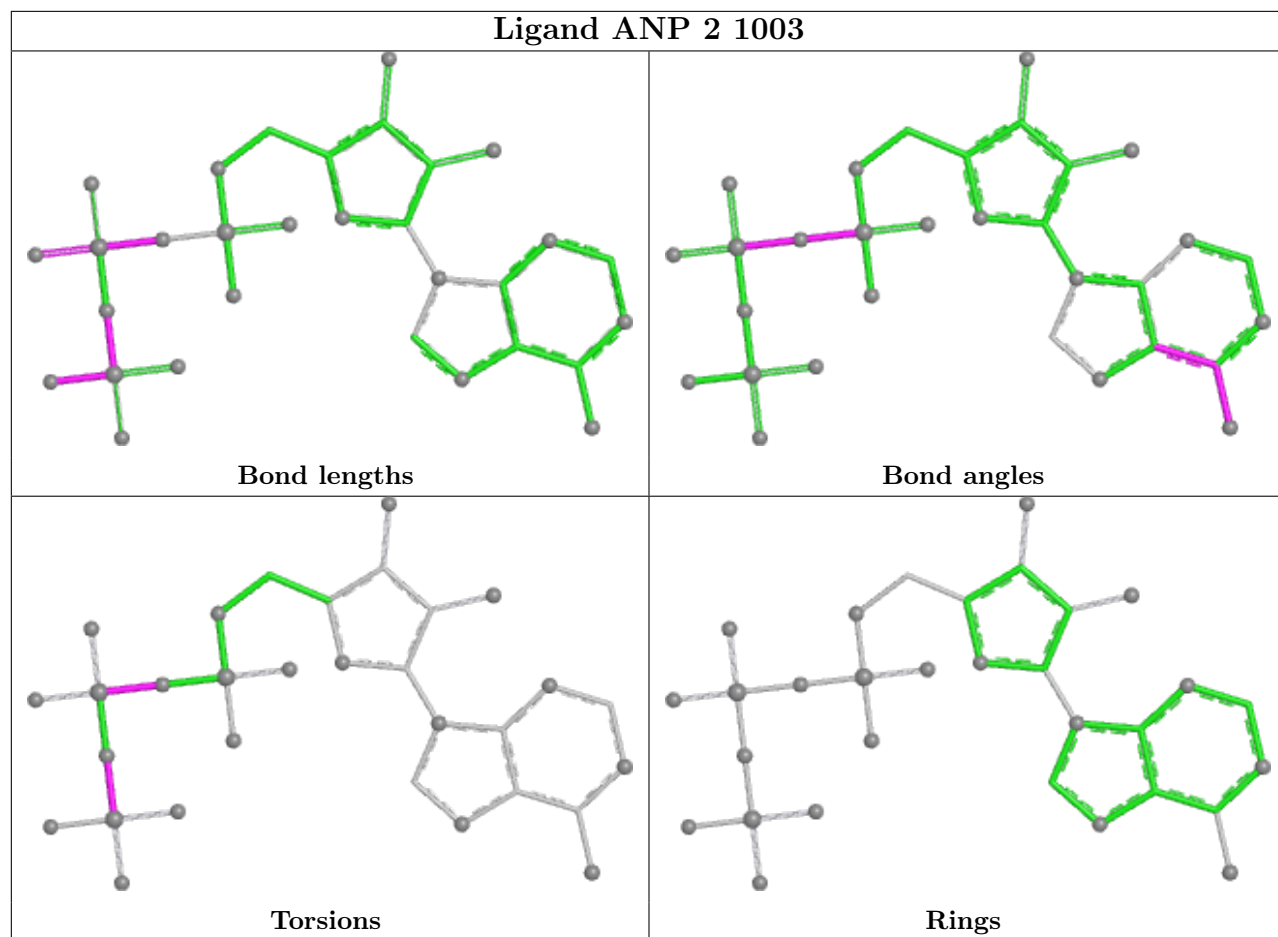
3 monomers are involved in 4 short contacts:

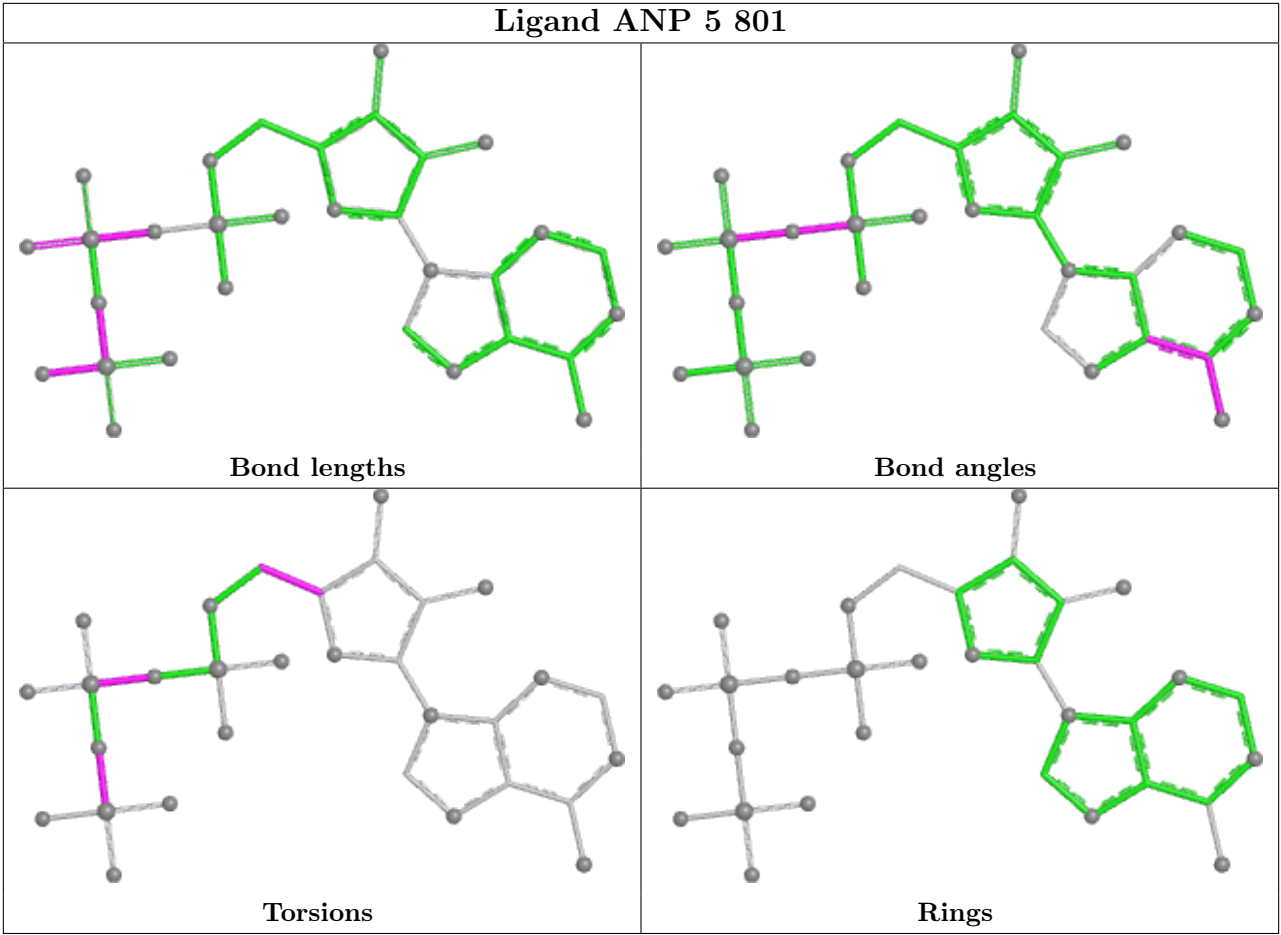
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	3	1500	ANP	1	0
27	2	1003	ANP	1	0
27	5	801	ANP	2	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	M	1
22	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	47:DT	O3'	51:DT	P	21.13
1	R	53:THR	C	58:ASN	N	8.39

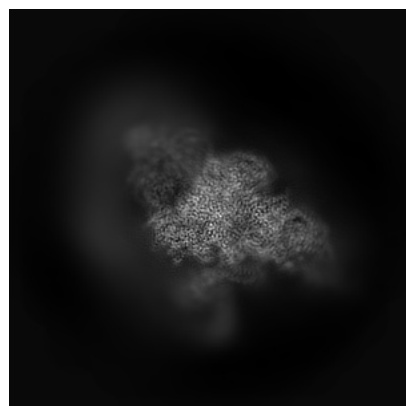
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13494. These allow visual inspection of the internal detail of the map and identification of artifacts.

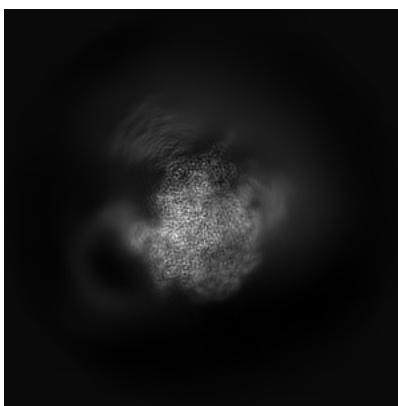
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

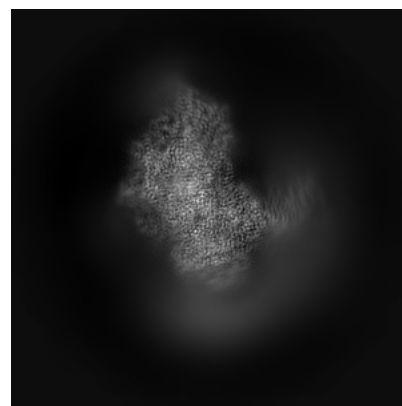
6.1.1 Primary map



X

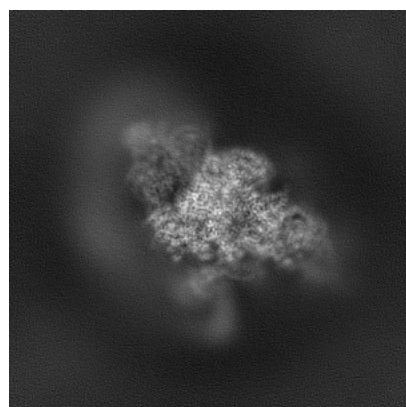


Y

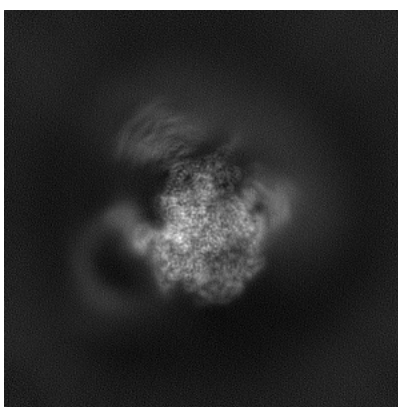


Z

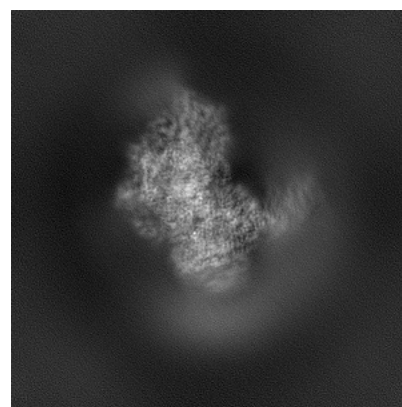
6.1.2 Raw map



X



Y

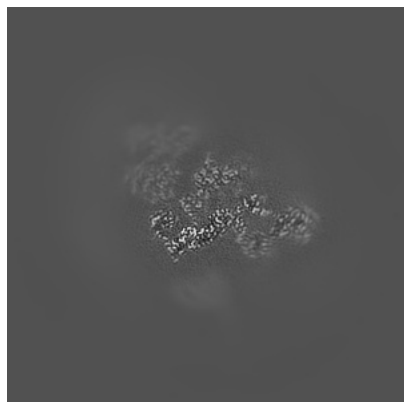


Z

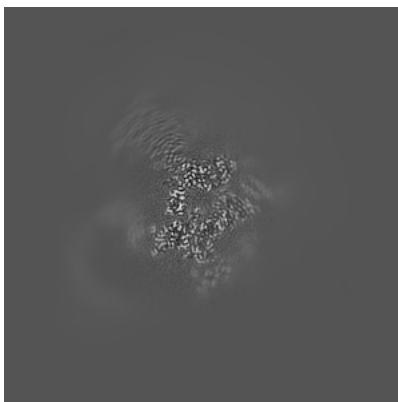
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

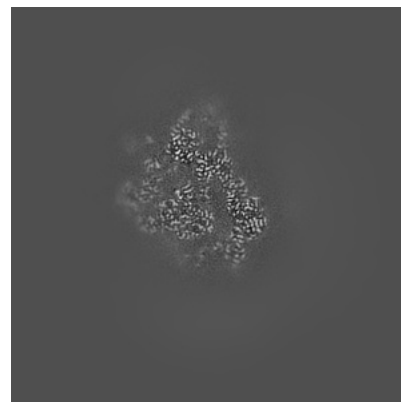
6.2.1 Primary map



X Index: 200

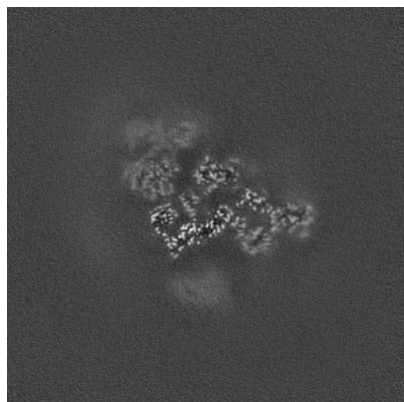


Y Index: 200

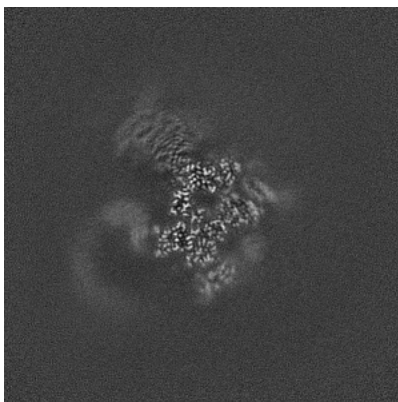


Z Index: 200

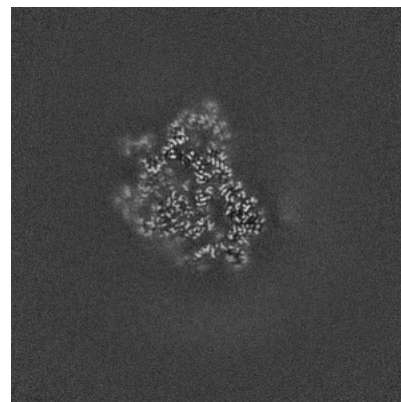
6.2.2 Raw map



X Index: 200



Y Index: 200

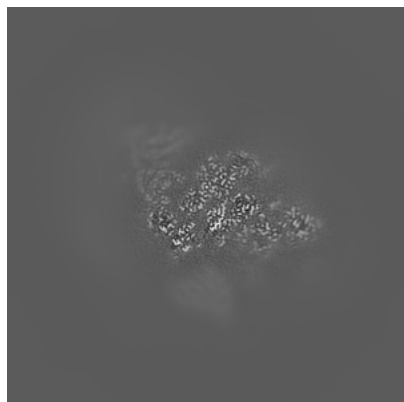


Z Index: 200

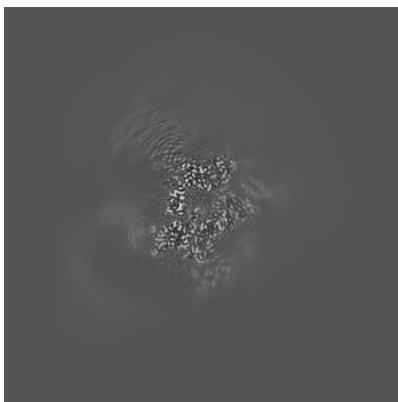
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

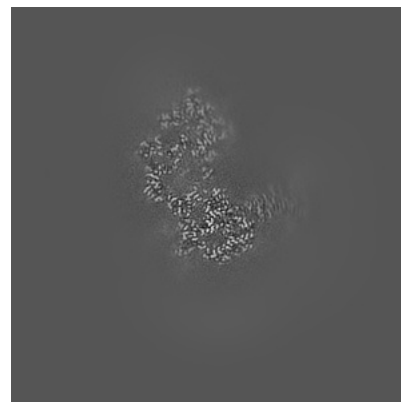
6.3.1 Primary map



X Index: 191

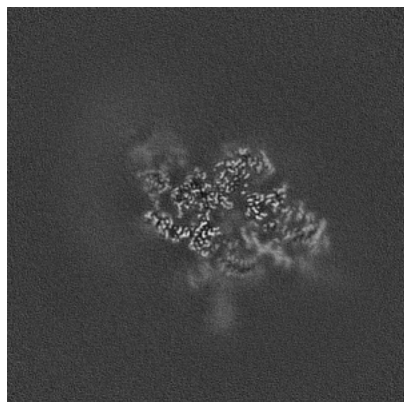


Y Index: 200

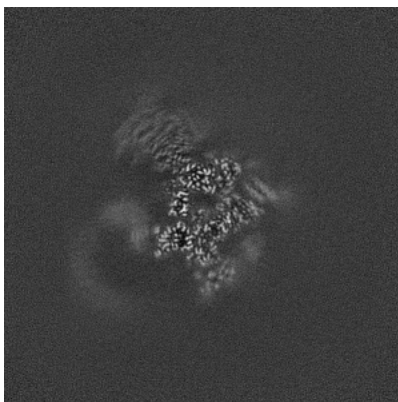


Z Index: 174

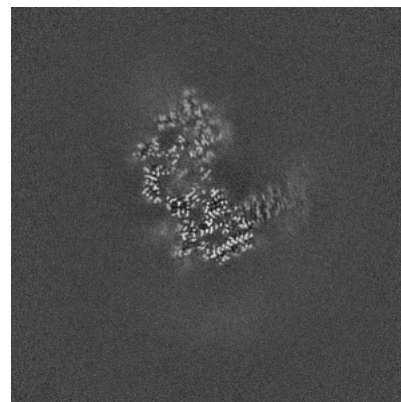
6.3.2 Raw map



X Index: 175



Y Index: 199

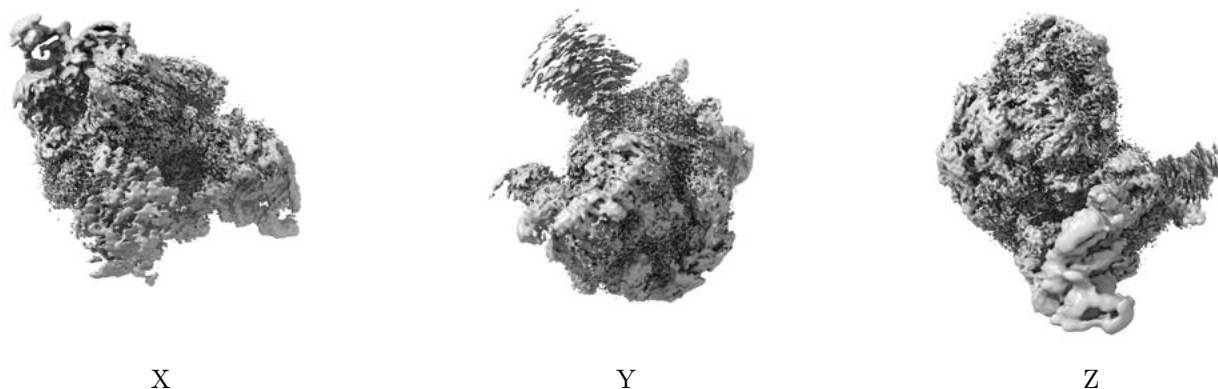


Z Index: 178

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

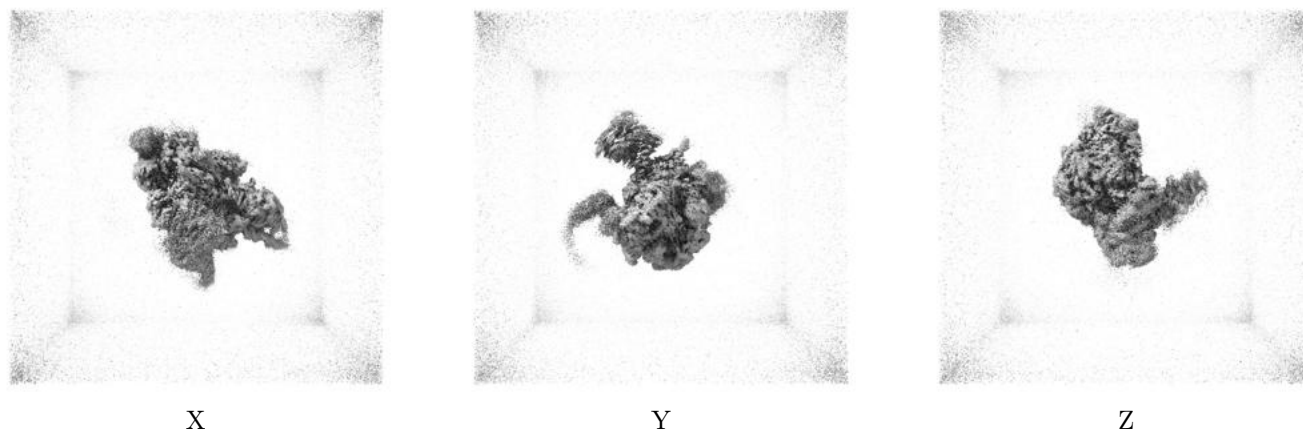
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0181. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

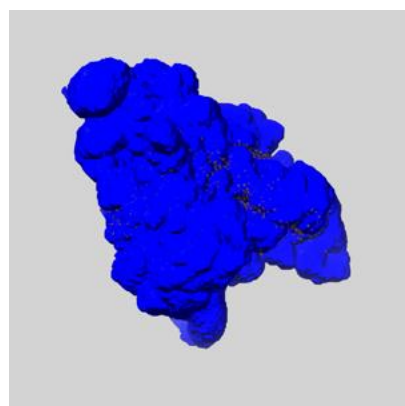
6.5 Mask visualisation [i](#)

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

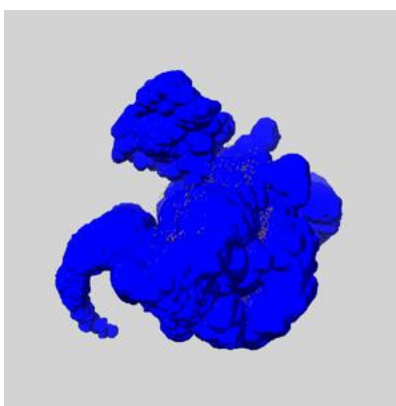
A mask typically either:

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

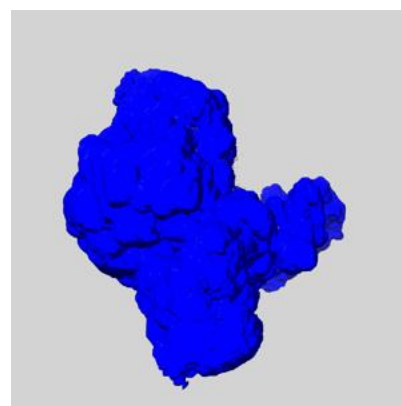
6.5.1 emd_13494_msk_1.map [i](#)



X



Y

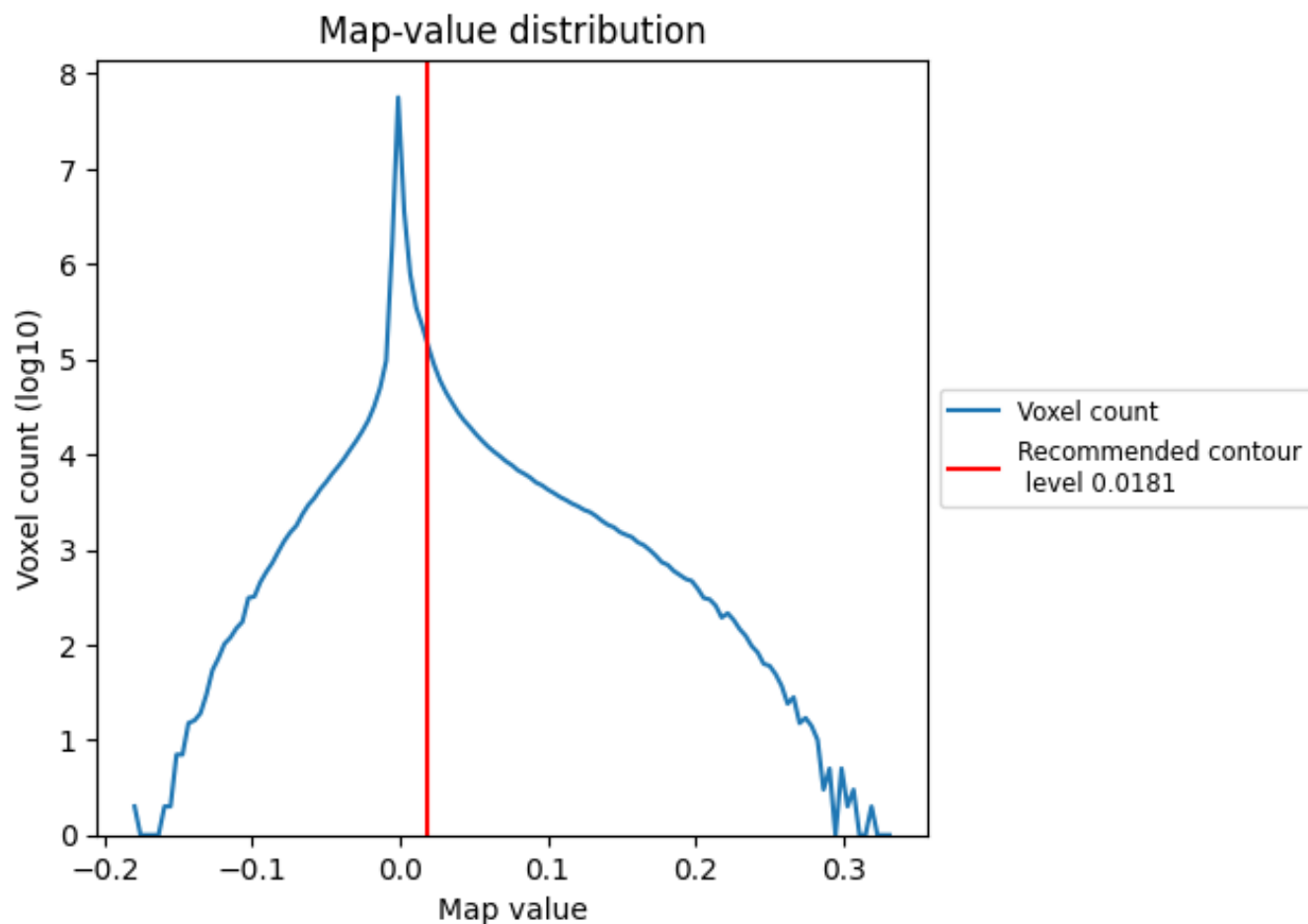


Z

7 Map analysis [i](#)

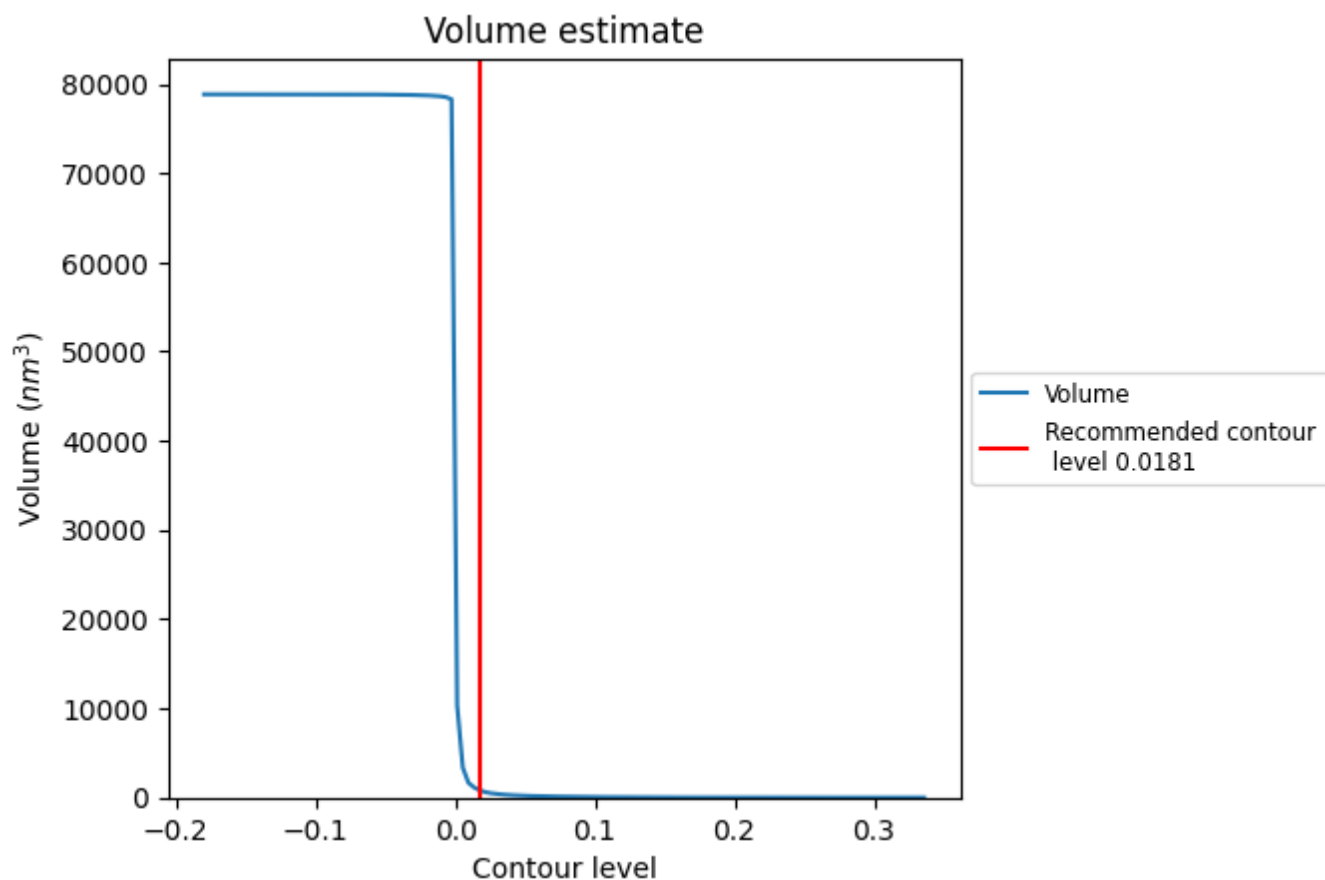
This section contains the results of statistical analysis of the map.

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.

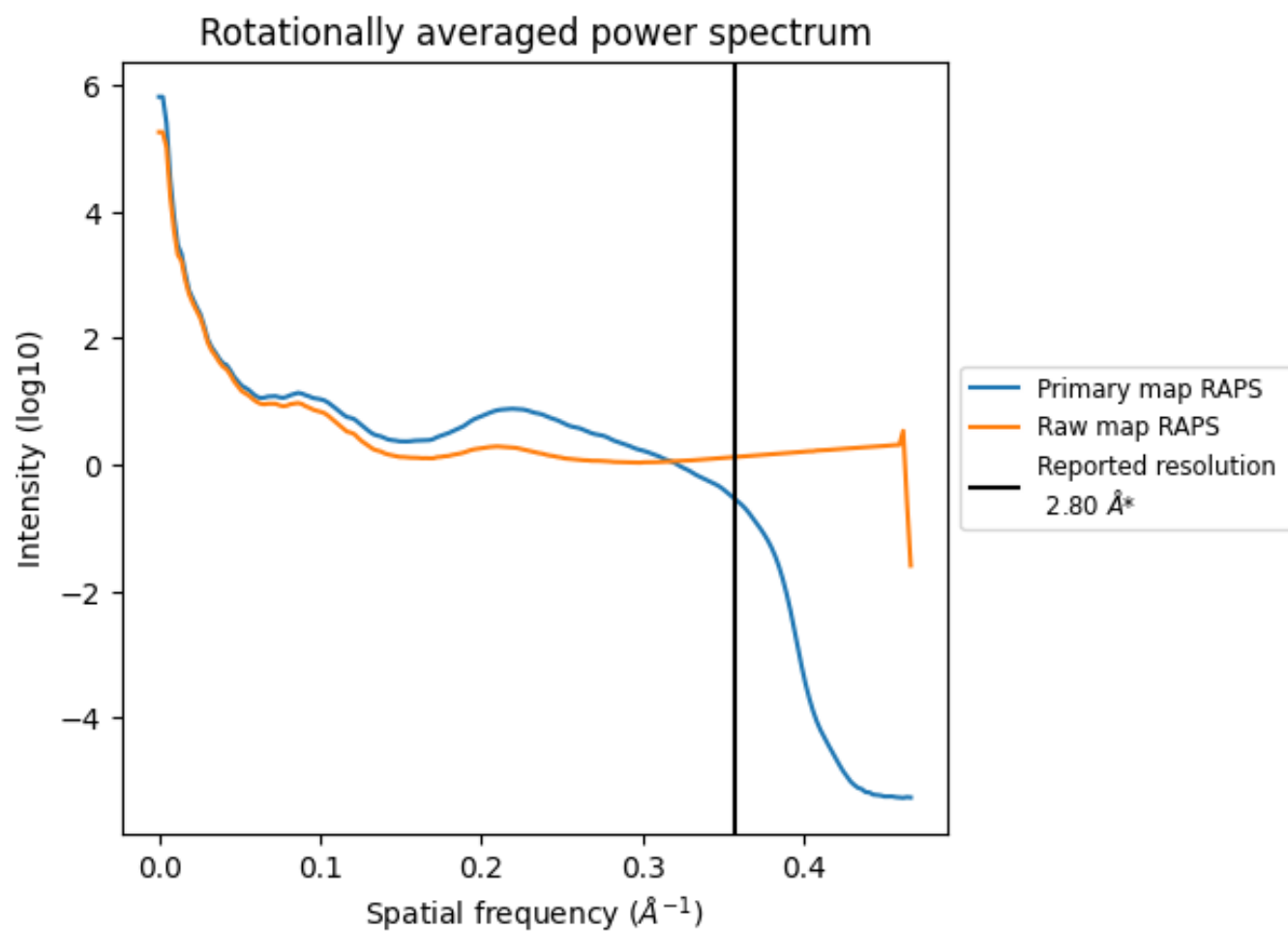
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 791 nm^3 ; this corresponds to an approximate mass of 714 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 ⓘ

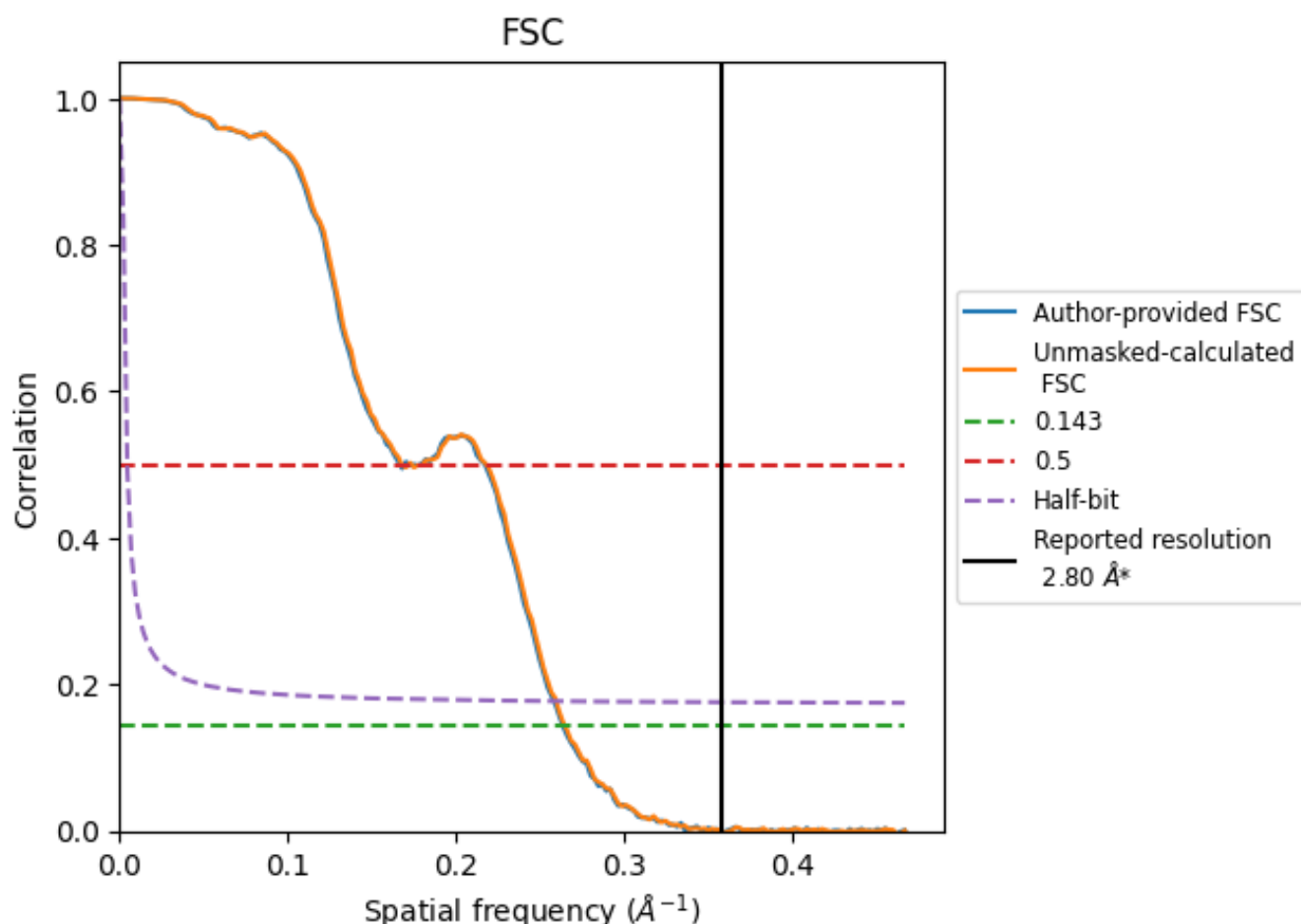


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	3.80	6.01	3.88
Unmasked-calculated*	3.78	5.97	3.86

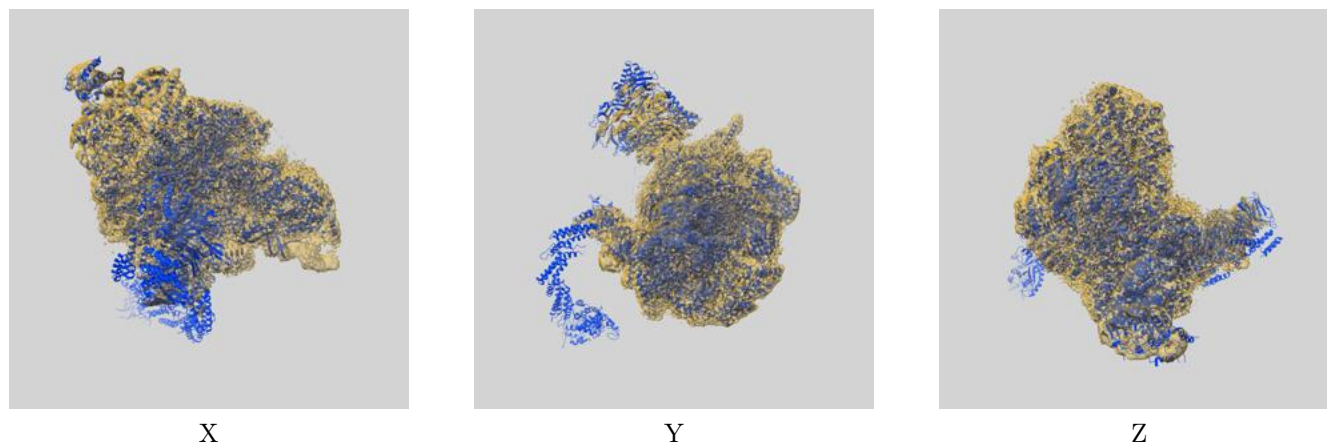
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 2.8 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

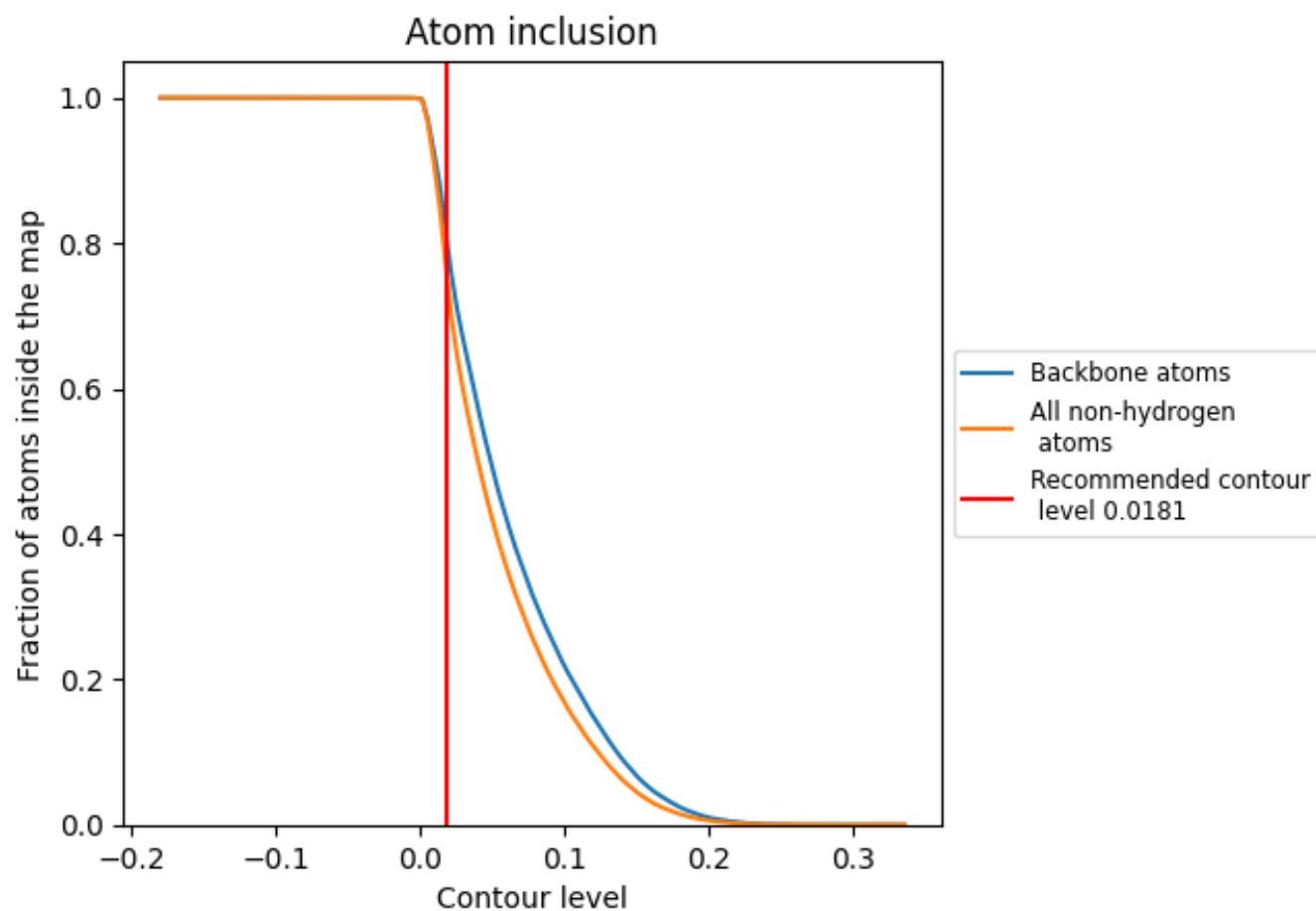
This section contains information regarding the fit between EMDB map EMD-13494 and PDB model 7PLO. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0181 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 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.