



Full wwPDB EM Validation Report ⓘ

Dec 13, 2021 – 12:23 pm GMT

PDB ID : 7PFO
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.0.dev97
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) : 2.24

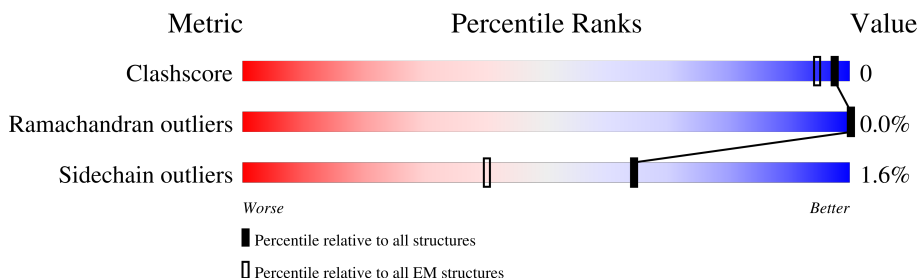
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


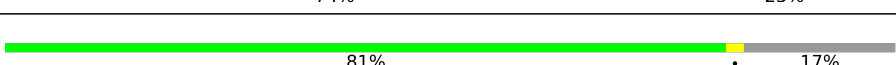

The reported resolution of this entry is 3.20 Å.

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.



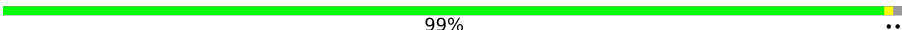
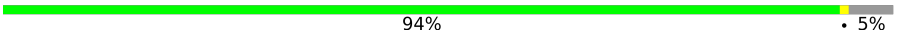










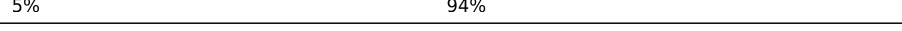
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	B	2286	
2	A	527	
3	4	863	
4	6	821	
5	7	719	
6	3	808	
7	2	904	
8	5	734	

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Mol	Chain	Length	Quality of chain
9	D	196	 99% ..
10	E	185	 94% • 5%
11	F	216	 88% • 10%
12	G	261	 76% • 22%
13	C	572	 92% • 7%
14	K	1208	 52% • 47%
15	L	338	 25% .. 74%
16	M	85	 35% • 62%
17	H	1160	 34% 65%
17	I	1160	 33% • 65%
17	J	1160	 7% 34% • 65%
18	N	54	 41% 59%
19	Q	1403	 5% 94%

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 68086 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	759	Total	C	N	O	S	0	0
			6061	3834	1030	1153	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	527	Total	C	N	O	S	0	0
			4199	2702	697	780	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	619	Total	C	N	O	S	0	0
			4929	3103	873	926	27		

- Molecule 4 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	632	Total	C	N	O	S	0	0
			5014	3150	890	948	26		

- Molecule 5 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	595	Total	C	N	O	S	0	0
			4722	2965	841	885	31		

- Molecule 6 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3	620	Total	C	N	O	S	0	0
			4858	3037	859	936	26		

- Molecule 7 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2	703	Total	C	N	O	S	0	0
			5580	3511	994	1043	32		

- Molecule 8 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	5	605	Total	C	N	O	S	0	0
			4735	2968	841	891	35		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	195	Total	C	N	O	S	0	0
			1606	1013	289	292	12		

- Molecule 10 is a protein called DNA replication complex GINS protein PSF2.

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

- Molecule 11 is a protein called DNA replication complex GINS protein PSF3.

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

- Molecule 12 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	203	Total	C	N	O	S	0	0
			1679	1065	290	314	10		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 13 is a protein called Cell division control protein 45 homolog, Cell division control protein 45 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	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	-	expression tag	UNP O75419
C	136A	TYR	-	expression tag	UNP O75419
C	136B	LYS	-	expression tag	UNP O75419
C	136C	ASP	-	expression tag	UNP O75419
C	136D	ASP	-	expression tag	UNP O75419
C	136E	ASP	-	expression tag	UNP O75419

- Molecule 14 is a protein called Protein timeless homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	636	Total	C	N	O	S	0	0
			5215	3324	929	936	26		

- Molecule 15 is a protein called TIMELESS-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	87	Total	C	N	O	S	0	0
			735	471	140	121	3		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-36	TRP	-	expression tag	UNP Q9BVW5
L	-35	SER	-	expression tag	UNP Q9BVW5
L	-34	HIS	-	expression tag	UNP Q9BVW5
L	-33	PRO	-	expression tag	UNP Q9BVW5
L	-32	GLN	-	expression tag	UNP Q9BVW5
L	-31	PHE	-	expression tag	UNP Q9BVW5
L	-30	GLU	-	expression tag	UNP Q9BVW5
L	-29	LYS	-	expression tag	UNP Q9BVW5
L	-28	GLY	-	expression tag	UNP Q9BVW5
L	-27	GLY	-	expression tag	UNP Q9BVW5
L	-26	GLY	-	expression tag	UNP Q9BVW5
L	-25	SER	-	expression tag	UNP Q9BVW5
L	-24	GLY	-	expression tag	UNP Q9BVW5
L	-23	GLY	-	expression tag	UNP Q9BVW5
L	-22	GLY	-	expression tag	UNP Q9BVW5
L	-21	SER	-	expression tag	UNP Q9BVW5
L	-20	GLY	-	expression tag	UNP Q9BVW5
L	-19	GLY	-	expression tag	UNP Q9BVW5
L	-18	SER	-	expression tag	UNP Q9BVW5
L	-17	ALA	-	expression tag	UNP Q9BVW5
L	-16	TRP	-	expression tag	UNP Q9BVW5

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-15	SER	-	expression tag	UNP Q9BVW5
L	-14	HIS	-	expression tag	UNP Q9BVW5
L	-13	PRO	-	expression tag	UNP Q9BVW5
L	-12	GLN	-	expression tag	UNP Q9BVW5
L	-11	PHE	-	expression tag	UNP Q9BVW5
L	-10	GLU	-	expression tag	UNP Q9BVW5
L	-9	LYS	-	expression tag	UNP Q9BVW5
L	-8	SER	-	expression tag	UNP Q9BVW5
L	-7	GLY	-	expression tag	UNP Q9BVW5
L	-6	GLU	-	expression tag	UNP Q9BVW5
L	-5	ASN	-	expression tag	UNP Q9BVW5
L	-4	LEU	-	expression tag	UNP Q9BVW5
L	-3	TYR	-	expression tag	UNP Q9BVW5
L	-2	PHE	-	expression tag	UNP Q9BVW5
L	-1	GLN	-	expression tag	UNP Q9BVW5
L	0	GLY	-	expression tag	UNP Q9BVW5

- Molecule 16 is a DNA chain called Leading strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	32	Total	C	N	O	P	0	0
			662	320	106	204	32		

- Molecule 17 is a protein called WD repeat and HMG-box DNA-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	401	Total	C	N	O	S	1	0
			3178	2016	554	587	21		
17	I	401	Total	C	N	O	S	1	0
			3178	2016	554	587	21		
17	J	401	Total	C	N	O	S	2	0
			3183	2019	554	589	21		

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	-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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
I	-1	GLN	-	expression tag	UNP O75717
I	0	GLY	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-2	PHE	-	expression tag	UNP O75717
J	-1	GLN	-	expression tag	UNP O75717
J	0	GLY	-	expression tag	UNP O75717

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

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

- Molecule 19 is a protein called Claspin.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	79	Total	C	N	O	S	0	0
			683	431	133	117	2		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	-31	LEU	-	expression tag	UNP Q9HAW4
Q	-30	GLU	-	expression tag	UNP Q9HAW4
Q	-29	VAL	-	expression tag	UNP Q9HAW4
Q	-28	LEU	-	expression tag	UNP Q9HAW4
Q	-27	PHE	-	expression tag	UNP Q9HAW4
Q	-26	GLN	-	expression tag	UNP Q9HAW4
Q	-25	GLY	-	expression tag	UNP Q9HAW4
Q	-24	PRO	-	expression tag	UNP Q9HAW4
Q	-23	ASP	-	expression tag	UNP Q9HAW4
Q	-22	TYR	-	expression tag	UNP Q9HAW4
Q	-21	LYS	-	expression tag	UNP Q9HAW4
Q	-20	ASP	-	expression tag	UNP Q9HAW4
Q	-19	ASP	-	expression tag	UNP Q9HAW4
Q	-18	ASP	-	expression tag	UNP Q9HAW4
Q	-17	ASP	-	expression tag	UNP Q9HAW4
Q	-16	LYS	-	expression tag	UNP Q9HAW4
Q	-15	ASP	-	expression tag	UNP Q9HAW4
Q	-14	TYR	-	expression tag	UNP Q9HAW4
Q	-13	LYS	-	expression tag	UNP Q9HAW4
Q	-12	ASP	-	expression tag	UNP Q9HAW4
Q	-11	ASP	-	expression tag	UNP Q9HAW4
Q	-10	ASP	-	expression tag	UNP Q9HAW4
Q	-9	ASP	-	expression tag	UNP Q9HAW4

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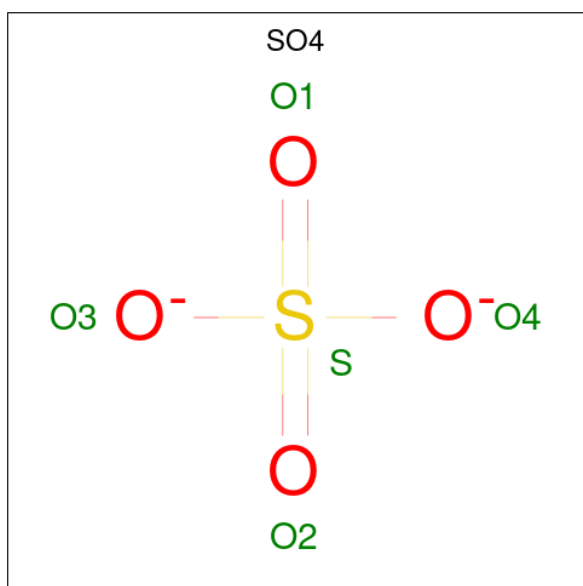
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-8	LYS	-	expression tag	UNP Q9HAW4
Q	-7	ASP	-	expression tag	UNP Q9HAW4
Q	-6	TYR	-	expression tag	UNP Q9HAW4
Q	-5	LYS	-	expression tag	UNP Q9HAW4
Q	-4	ASP	-	expression tag	UNP Q9HAW4
Q	-3	ASP	-	expression tag	UNP Q9HAW4
Q	-2	ASP	-	expression tag	UNP Q9HAW4
Q	-1	ASP	-	expression tag	UNP Q9HAW4
Q	0	LYS	-	expression tag	UNP Q9HAW4
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
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 (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of

Interest" by depositor).

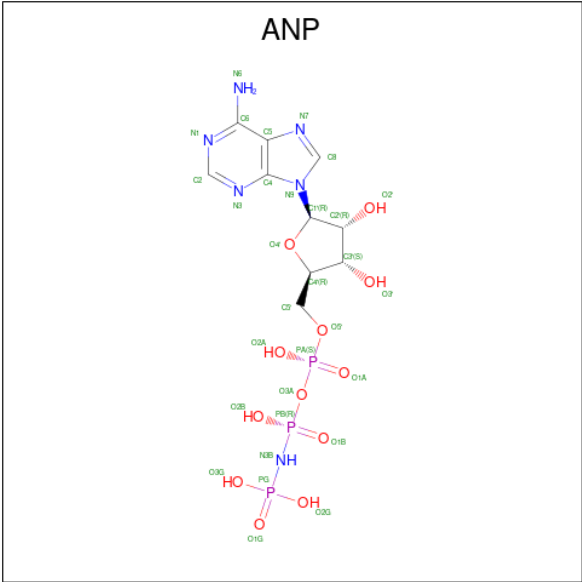
Mol	Chain	Residues	Atoms		AltConf
20	B	1	Total	Zn	0
			1	1	
20	4	1	Total	Zn	0
			1	1	
20	6	1	Total	Zn	0
			1	1	
20	7	1	Total	Zn	0
			1	1	
20	2	1	Total	Zn	0
			1	1	
20	5	1	Total	Zn	0
			1	1	

- Molecule 21 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).

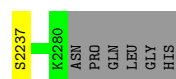


Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total	C	N	O	P	0
			31	10	6	12	3	
22	2	1	Total	C	N	O	P	0
			31	10	6	12	3	
22	5	1	Total	C	N	O	P	0
			31	10	6	12	3	

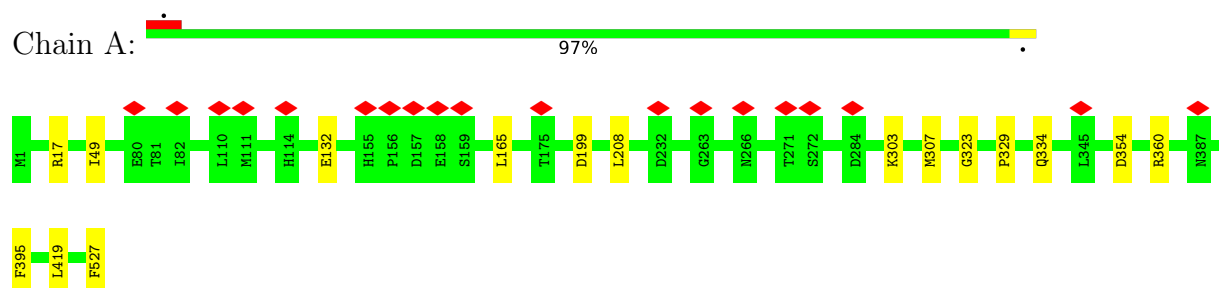
- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
23	3	1	Total	Mg	0
			1	1	
23	2	1	Total	Mg	0
			1	1	
23	5	1	Total	Mg	0
			1	1	

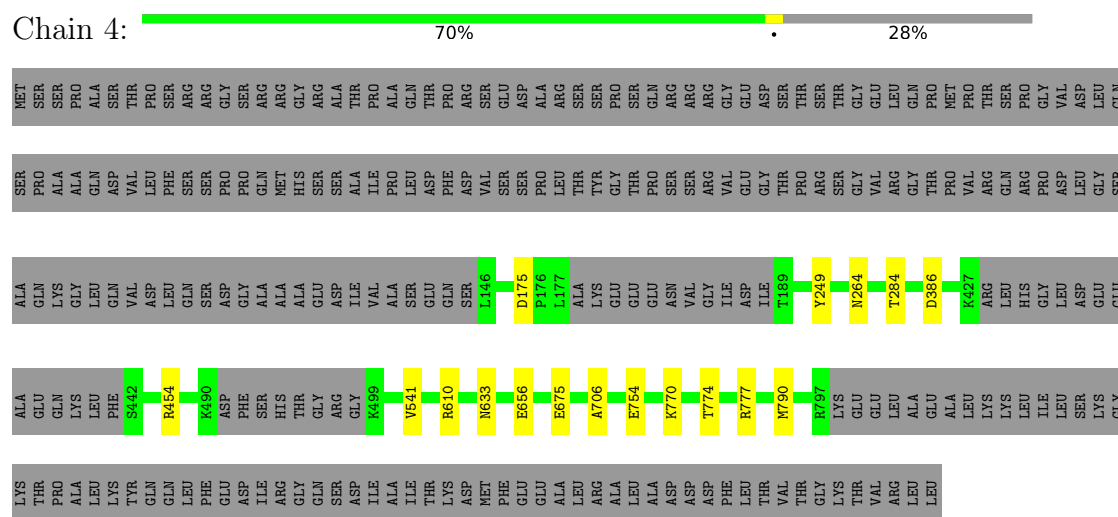




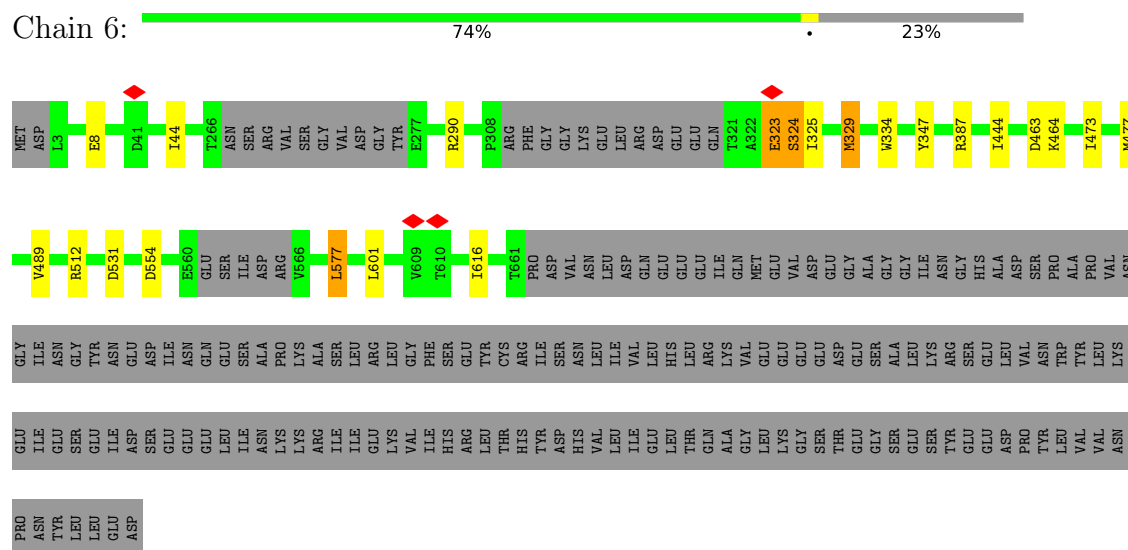
• Molecule 2: DNA polymerase epsilon subunit 2



• Molecule 3: DNA replication licensing factor MCM4



• Molecule 4: DNA replication licensing factor MCM6



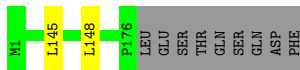
- Molecule 9: DNA replication complex GINS protein PSF1

Chain D:  99%



- Molecule 10: DNA replication complex GINS protein PSF2

Chain E: 94% . 5%

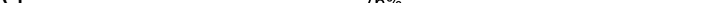


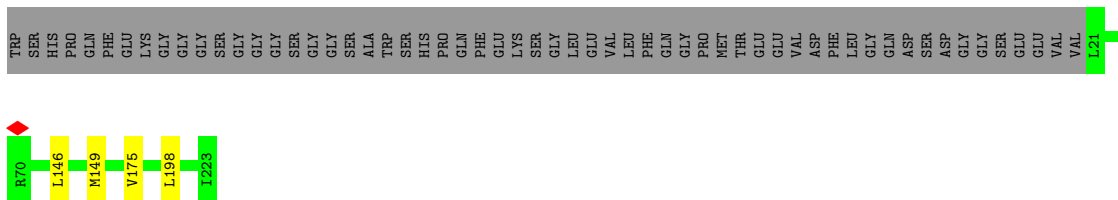
- Molecule 11: DNA replication complex GINS protein PSF3

Chain F: 88% 10%



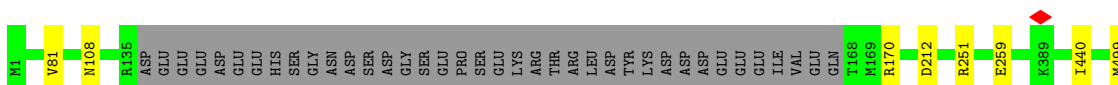
- Molecule 12: DNA replication complex GINS protein SLD5

Chain G:  76% 22%



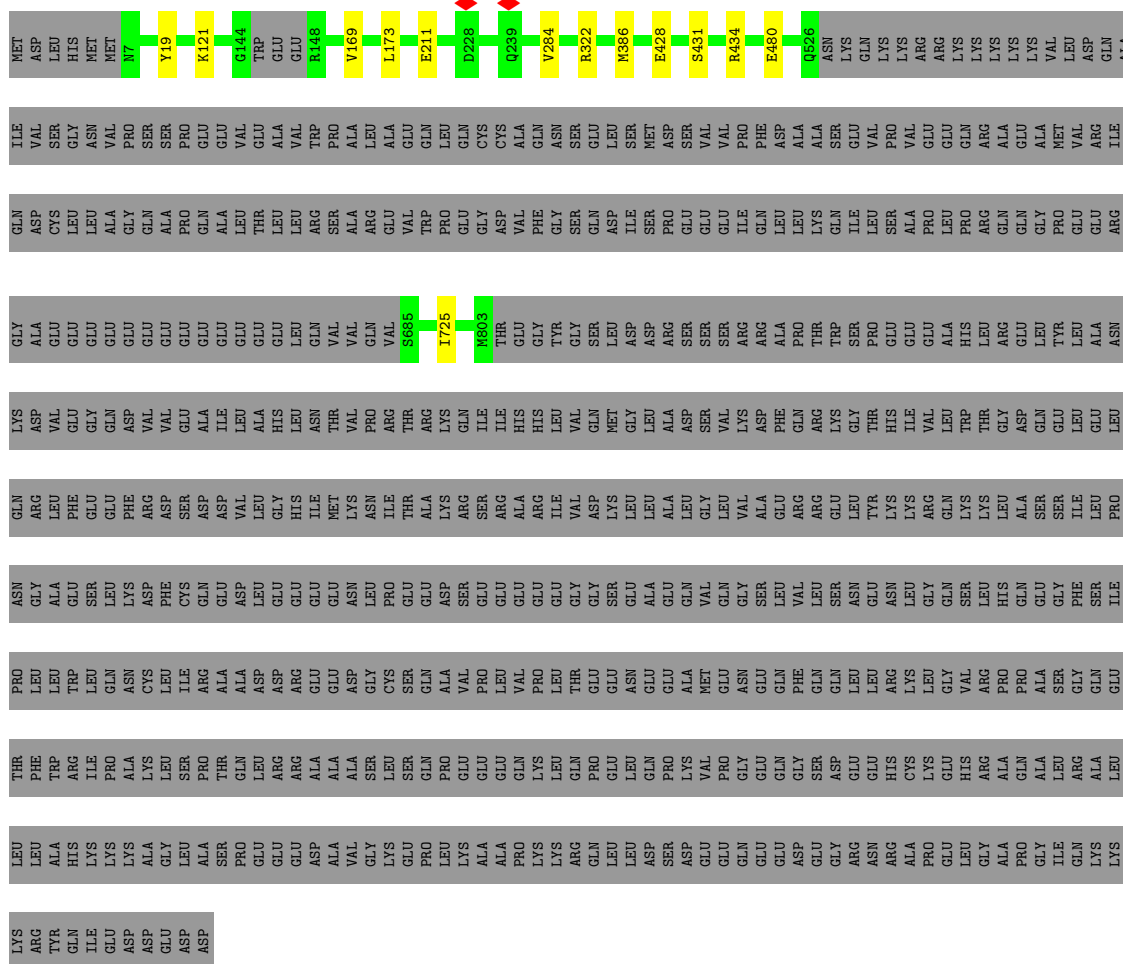
- Molecule 13: Cell division control protein 45 homolog,Cell division control protein 45 homolog

Chain C: 92% • 7%



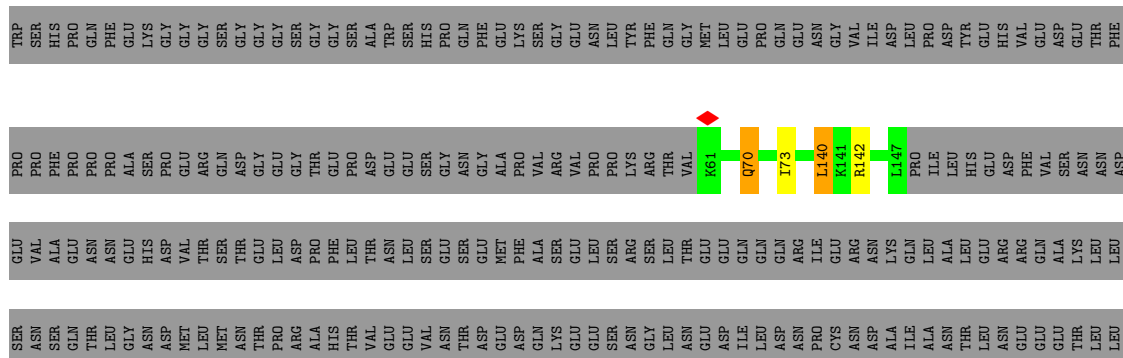
- Molecule 14: Protein timeless homolog

Chain K:



- Molecule 15: TIMELESS-interacting protein

Chain L:







[illegible]

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 (\AA)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: ANP, ZN, SO4, MG

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	B	0.37	0/6177	0.70	0/8348
2	A	0.37	0/4310	0.65	0/5853
3	4	0.33	0/5013	0.65	0/6776
4	6	0.34	0/5095	0.64	1/6876 (0.0%)
5	7	0.35	0/4796	0.67	0/6470
6	3	0.34	1/4931 (0.0%)	0.65	0/6653
7	2	0.35	0/5683	0.66	0/7675
8	5	0.35	0/4807	0.65	2/6468 (0.0%)
9	D	0.34	0/1638	0.62	0/2202
10	E	0.36	0/1462	0.60	0/1981
11	F	0.33	0/1580	0.59	0/2133
12	G	0.38	0/1711	0.61	0/2305
13	C	0.33	0/4439	0.59	0/5992
14	K	0.36	0/5317	0.64	1/7162 (0.0%)
15	L	0.35	0/750	0.70	1/999 (0.1%)
16	M	0.67	0/738	1.11	2/1138 (0.2%)
17	H	0.34	0/3253	0.65	0/4407
17	I	0.33	0/3253	0.62	0/4407
17	J	0.34	0/3261	0.65	0/4418
18	N	0.76	0/488	1.02	0/747
19	Q	0.36	0/693	0.64	0/919
All	All	0.36	1/69395 (0.0%)	0.66	7/93929 (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	A	0	1
5	7	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	3	0	1
7	2	0	1
9	D	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	3	531	ASP	C-N	5.08	1.43	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	M	51	DT	OP1-P-OP2	-6.24	110.24	119.60
8	5	391	LEU	CA-CB-CG	5.70	128.40	115.30
4	6	554	ASP	CB-CG-OD1	5.56	123.30	118.30
14	K	173	LEU	CA-CB-CG	5.40	127.72	115.30
16	M	56	DT	P-O3'-C3'	5.33	126.09	119.70
8	5	328	LEU	CA-CB-CG	5.12	127.07	115.30
15	L	140	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	2	762	ILE	Peptide
6	3	178	ASP	Peptide
5	7	245	PRO	Peptide
2	A	323	GLY	Peptide
9	D	2	PHE	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	B	6061	0	5934	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4199	0	4160	5	0
3	4	4929	0	4985	5	0
4	6	5014	0	5043	8	0
5	7	4722	0	4778	2	0
6	3	4858	0	4908	5	0
7	2	5580	0	5589	13	0
8	5	4735	0	4800	3	0
9	D	1606	0	1601	0	0
10	E	1431	0	1456	1	0
11	F	1546	0	1500	0	0
12	G	1679	0	1700	2	0
13	C	4347	0	4296	5	0
14	K	5215	0	5230	3	0
15	L	735	0	766	1	0
16	M	662	0	372	0	0
17	H	3178	0	3145	0	0
17	I	3178	0	3145	4	0
17	J	3183	0	3149	1	0
18	N	438	0	249	0	0
19	Q	683	0	701	3	0
20	2	1	0	0	0	0
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
20	B	1	0	0	0	0
21	A	5	0	0	0	0
22	2	31	0	13	2	0
22	3	31	0	13	1	0
22	5	31	0	13	1	0
23	2	1	0	0	0	0
23	3	1	0	0	0	0
23	5	1	0	0	0	0
All	All	68086	0	67546	61	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 0.

All (61) 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)
4:6:325:ILE:HD11	4:6:577:LEU:HD22	1.77	0.67
6:3:348:SER:H	22:3:1500:ANP:HNB1	1.46	0.63
12:G:175:VAL:HG11	12:G:198:LEU:HB3	1.88	0.55
7:2:526:GLY:H	22:2:1003:ANP:HNB1	1.55	0.53
4:6:329:MET:HB3	4:6:334:TRP:CE2	2.46	0.51
3:4:175:ASP:N	3:4:175:ASP:OD1	2.42	0.51
1:B:1579:ARG:HG2	1:B:1610:PRO:HD2	1.96	0.48
2:A:360:ARG:HE	2:A:395:PHE:HB3	1.78	0.48
6:3:352:SER:OG	6:3:409:ASP:OD2	2.32	0.48
7:2:647:VAL:HG13	7:2:649:LEU:H	1.78	0.47
5:7:396:ARG:HA	5:7:402:GLN:HG3	1.96	0.47
2:A:303:LYS:NZ	2:A:527:PHE:O	2.38	0.47
7:2:481:ILE:HD11	7:2:492:LYS:HA	1.97	0.47
3:4:770:LYS:O	3:4:774:THR:OG1	2.28	0.46
1:B:1599:GLU:HG2	1:B:1600:ILE:HG22	1.97	0.46
1:B:1740:LEU:HD13	1:B:1743:HIS:HB3	1.97	0.46
1:B:1730:ASP:O	1:B:1735:ALA:N	2.41	0.46
7:2:290:LEU:HA	19:Q:593:LYS:HD2	1.98	0.46
13:C:251:ARG:HD3	17:I:480:HIS:HB2	1.97	0.45
13:C:212:ASP:OD1	13:C:212:ASP:N	2.49	0.45
3:4:790:MET:SD	3:4:790:MET:N	2.88	0.45
8:5:383:PRO:O	8:5:385:THR:OG1	2.34	0.45
12:G:146:LEU:HA	12:G:149:MET:HG2	1.99	0.45
10:E:145:LEU:HB3	10:E:148:LEU:HD12	1.99	0.44
2:A:17:ARG:HG3	2:A:49:ILE:HG21	1.99	0.44
13:C:259:GLU:OE2	17:I:462:GLN:NE2	2.51	0.44
4:6:387:ARG:NH2	4:6:531:ASP:OD1	2.50	0.43
14:K:211:GLU:N	14:K:211:GLU:OE1	2.51	0.43
2:A:329:PRO:HA	2:A:334:GLN:HG2	1.99	0.43
17:I:730:TRP:NE1	17:J:563:GLN:O	2.47	0.43
1:B:2236:CYS:SG	1:B:2237:SER:N	2.91	0.43
2:A:354:ASP:N	2:A:354:ASP:OD1	2.51	0.43
4:6:325:ILE:HA	4:6:325:ILE:HD13	1.84	0.42
8:5:389:GLN:HG3	22:5:802:ANP:H2'	2.02	0.42
7:2:526:GLY:N	22:2:1003:ANP:HNB1	2.18	0.42
15:L:70:GLN:HA	15:L:73:ILE:HG12	2.02	0.42
6:3:369:THR:HG22	6:3:409:ASP:HB3	2.02	0.42
13:C:81:VAL:O	13:C:108:ASN:ND2	2.52	0.42
3:4:706:ALA:HB2	3:4:754:GLU:HA	2.02	0.41
7:2:307:ARG:NH1	7:2:413:GLU:OE2	2.46	0.41
4:6:323:GLU:OE1	4:6:324:SER:N	2.53	0.41
6:3:344:ILE:HD12	6:3:482:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:5:519:ILE:HG12	8:5:650:ASP:HB3	2.02	0.41
4:6:601:LEU:HD22	4:6:616:ILE:HG21	2.01	0.41
6:3:603:MET:N	6:3:603:MET:SD	2.93	0.41
4:6:444:ILE:HG23	4:6:489:VAL:HG21	2.01	0.41
3:4:264:ASN:HB2	3:4:284:THR:HG21	2.03	0.41
5:7:182:TYR:HB3	5:7:220:LEU:HB3	2.03	0.41
7:2:870:ARG:HD3	13:C:440:ILE:HG12	2.03	0.41
14:K:121:LYS:HD2	14:K:169:VAL:HG13	2.03	0.41
19:Q:602:GLN:HE21	19:Q:602:GLN:HB2	1.67	0.41
1:B:1562:LYS:NZ	1:B:1623:ASP:OD1	2.49	0.40
1:B:2132:LEU:HD13	7:2:833:LEU:HD21	2.03	0.40
7:2:291:VAL:O	19:Q:593:LYS:NZ	2.45	0.40
7:2:829:ASN:OD1	7:2:830:GLU:N	2.54	0.40
7:2:284:ARG:HD2	7:2:442:ASN:O	2.22	0.40
7:2:762:ILE:HD12	7:2:762:ILE:HA	1.98	0.40
14:K:428:GLU:HG2	14:K:431:SER:HB2	2.02	0.40
17:I:794:ASN:HA	17:I:797:ILE:HD12	2.03	0.40
4:6:463:ASP:OD2	4:6:464:LYS:NZ	2.50	0.40
7:2:312:VAL:HG22	7:2:378:ILE:HG22	2.03	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	B	731/2286 (32%)	683 (93%)	48 (7%)	0	100	100
2	A	525/527 (100%)	500 (95%)	25 (5%)	0	100	100
3	4	611/863 (71%)	588 (96%)	23 (4%)	0	100	100
4	6	624/821 (76%)	608 (97%)	15 (2%)	1 (0%)	47	79
5	7	585/719 (81%)	568 (97%)	17 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	3	614/808 (76%)	588 (96%)	26 (4%)	0	100	100
7	2	697/904 (77%)	666 (96%)	30 (4%)	1 (0%)	51	83
8	5	597/734 (81%)	580 (97%)	17 (3%)	0	100	100
9	D	193/196 (98%)	188 (97%)	5 (3%)	0	100	100
10	E	174/185 (94%)	170 (98%)	4 (2%)	0	100	100
11	F	190/216 (88%)	185 (97%)	5 (3%)	0	100	100
12	G	201/261 (77%)	198 (98%)	3 (2%)	0	100	100
13	C	530/572 (93%)	524 (99%)	6 (1%)	0	100	100
14	K	630/1208 (52%)	612 (97%)	18 (3%)	0	100	100
15	L	85/338 (25%)	80 (94%)	5 (6%)	0	100	100
17	H	400/1160 (34%)	388 (97%)	12 (3%)	0	100	100
17	I	400/1160 (34%)	393 (98%)	7 (2%)	0	100	100
17	J	401/1160 (35%)	392 (98%)	9 (2%)	0	100	100
19	Q	73/1403 (5%)	73 (100%)	0	0	100	100
All	All	8261/15521 (53%)	7984 (97%)	275 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	6	44	ILE
7	2	713	GLU

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	B	677/2012 (34%)	656 (97%)	21 (3%)	40	72
2	A	471/471 (100%)	465 (99%)	6 (1%)	69	87
3	4	549/753 (73%)	540 (98%)	9 (2%)	62	84
4	6	556/724 (77%)	546 (98%)	10 (2%)	59	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	7	515/619 (83%)	507 (98%)	8 (2%)	62	84
6	3	534/707 (76%)	527 (99%)	7 (1%)	69	87
7	2	618/781 (79%)	609 (98%)	9 (2%)	65	85
8	5	515/625 (82%)	511 (99%)	4 (1%)	81	93
9	D	173/174 (99%)	173 (100%)	0	100	100
10	E	160/169 (95%)	160 (100%)	0	100	100
11	F	167/186 (90%)	163 (98%)	4 (2%)	49	77
12	G	188/232 (81%)	188 (100%)	0	100	100
13	C	487/523 (93%)	484 (99%)	3 (1%)	86	94
14	K	561/1055 (53%)	554 (99%)	7 (1%)	71	88
15	L	78/300 (26%)	75 (96%)	3 (4%)	33	67
17	H	346/1017 (34%)	341 (99%)	5 (1%)	67	86
17	I	346/1017 (34%)	337 (97%)	9 (3%)	46	76
17	J	347/1017 (34%)	338 (97%)	9 (3%)	46	76
19	Q	72/1261 (6%)	67 (93%)	5 (7%)	15	49
All	All	7360/13643 (54%)	7241 (98%)	119 (2%)	64	84

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1382	ARG
1	B	1393	MET
1	B	1411	ILE
1	B	1453	ARG
1	B	1480	GLU
1	B	1639	LEU
1	B	1659	ASN
1	B	1665	SER
1	B	1709	ASP
1	B	1793	ARG
1	B	1858	ARG
1	B	1917	MET
1	B	1932	ARG
1	B	1959	ARG
1	B	2064	PHE
1	B	2082	GLU
1	B	2095	LEU

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Mol	Chain	Res	Type
1	B	2102	LEU
1	B	2125	LEU
1	B	2159	ARG
1	B	2190	CYS
2	A	132	GLU
2	A	165	LEU
2	A	199	ASP
2	A	208	LEU
2	A	307	MET
2	A	419	LEU
3	4	249	TYR
3	4	386	ASP
3	4	454	ARG
3	4	541	VAL
3	4	610	ARG
3	4	633	ASN
3	4	656	GLU
3	4	675	GLU
3	4	777	ARG
4	6	8	GLU
4	6	290	ARG
4	6	323	GLU
4	6	324	SER
4	6	329	MET
4	6	347	TYR
4	6	473	ILE
4	6	477	MET
4	6	512	ARG
4	6	577	LEU
5	7	345	TYR
5	7	358	LEU
5	7	370	LYS
5	7	379	LEU
5	7	391	LEU
5	7	396	ARG
5	7	407	ARG
5	7	566	CYS
6	3	13	ARG
6	3	76	PHE
6	3	271	ASP
6	3	289	LYS
6	3	303	LEU

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Mol	Chain	Res	Type
6	3	311	ASP
6	3	398	MET
7	2	178	LYS
7	2	290	LEU
7	2	481	ILE
7	2	658	ASP
7	2	738	MET
7	2	740	GLN
7	2	834	PHE
7	2	870	ARG
7	2	888	MET
8	5	287	VAL
8	5	297	LEU
8	5	391	LEU
8	5	641	LEU
11	F	68	LEU
11	F	70	LEU
11	F	84	LEU
11	F	169	ASP
13	C	170	ARG
13	C	499	MET
13	C	536	ARG
14	K	19	TYR
14	K	284	VAL
14	K	322	ARG
14	K	386	MET
14	K	434	ARG
14	K	480	GLU
14	K	725	ILE
15	L	70	GLN
15	L	140	LEU
15	L	142	ARG
17	H	445	ARG
17	H	506	GLU
17	H	654	LEU
17	H	669	LYS
17	H	682	GLU
17	I	525	TRP
17	I	617	ASP
17	I	674	HIS
17	I	682	GLU
17	I	703	ARG

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Mol	Chain	Res	Type
17	I	721	GLU
17	I	769	LEU
17	I	777	ARG
17	I	778	GLU
17	J	457	CYS
17	J	462	GLN
17	J	489	ILE
17	J	515	HIS
17	J	593	PHE
17	J	649	MET
17	J	673	ASP
17	J	725	MET
17	J	768	MET
19	Q	315	HIS
19	Q	525	ASN
19	Q	536	TRP
19	Q	593	LYS
19	Q	602	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 13 ligands modelled in this entry, 9 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	5	802	23	29,33,33	1.15	4 (13%)	31,52,52	1.01	2 (6%)
22	ANP	2	1003	23	29,33,33	1.06	3 (10%)	31,52,52	0.96	2 (6%)
22	ANP	3	1500	23	29,33,33	1.11	3 (10%)	31,52,52	0.96	2 (6%)
21	SO4	A	601	-	4,4,4	0.14	0	6,6,6	0.05	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	5	802	23	-	6/14/38/38	0/3/3/3
22	ANP	2	1003	23	-	3/14/38/38	0/3/3/3
22	ANP	3	1500	23	-	3/14/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	802	ANP	PB-O3A	-3.44	1.54	1.59
22	3	1500	ANP	PB-O3A	-3.12	1.55	1.59
22	2	1003	ANP	PB-O3A	-2.73	1.55	1.59
22	3	1500	ANP	PG-O1G	2.35	1.49	1.46
22	2	1003	ANP	PG-O1G	2.33	1.49	1.46
22	5	802	ANP	PG-O1G	2.27	1.49	1.46
22	5	802	ANP	PG-N3B	2.22	1.69	1.63
22	2	1003	ANP	PG-N3B	2.18	1.69	1.63
22	3	1500	ANP	PG-N3B	2.17	1.69	1.63
22	5	802	ANP	PB-O1B	2.07	1.49	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	802	ANP	PB-O3A-PA	-3.65	119.75	132.62
22	3	1500	ANP	PB-O3A-PA	-3.31	120.97	132.62
22	2	1003	ANP	PB-O3A-PA	-3.06	121.82	132.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	1500	ANP	C5-C6-N6	2.31	123.87	120.35
22	5	802	ANP	C5-C6-N6	2.29	123.83	120.35
22	2	1003	ANP	C5-C6-N6	2.25	123.77	120.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

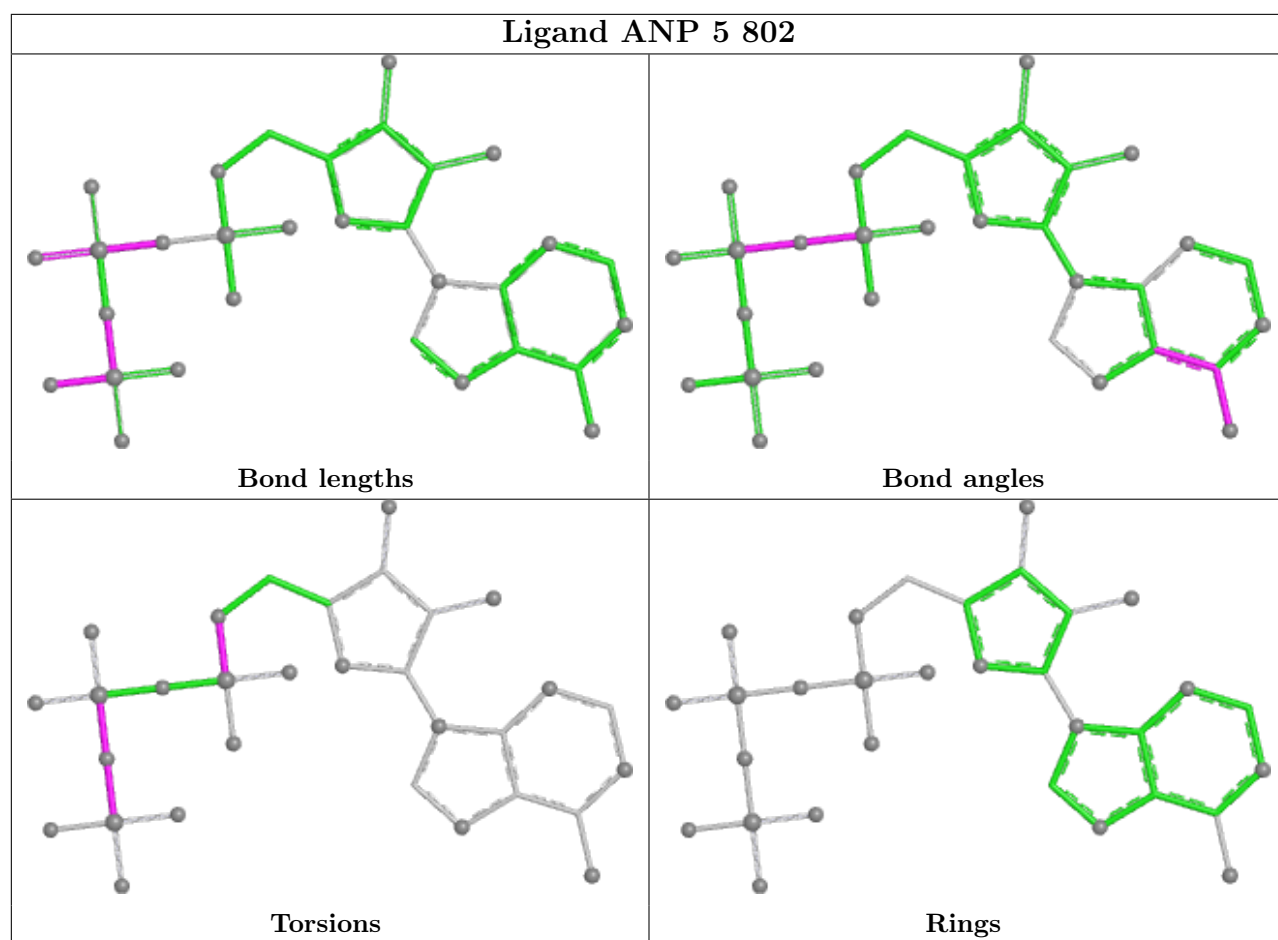
Mol	Chain	Res	Type	Atoms
22	3	1500	ANP	PB-N3B-PG-O1G
22	2	1003	ANP	PB-N3B-PG-O1G
22	2	1003	ANP	PA-O3A-PB-O1B
22	2	1003	ANP	PA-O3A-PB-O2B
22	5	802	ANP	PB-N3B-PG-O1G
22	5	802	ANP	PG-N3B-PB-O1B
22	5	802	ANP	PG-N3B-PB-O3A
22	5	802	ANP	C5'-O5'-PA-O1A
22	5	802	ANP	C5'-O5'-PA-O2A
22	3	1500	ANP	C5'-O5'-PA-O3A
22	5	802	ANP	C5'-O5'-PA-O3A
22	3	1500	ANP	C5'-O5'-PA-O1A

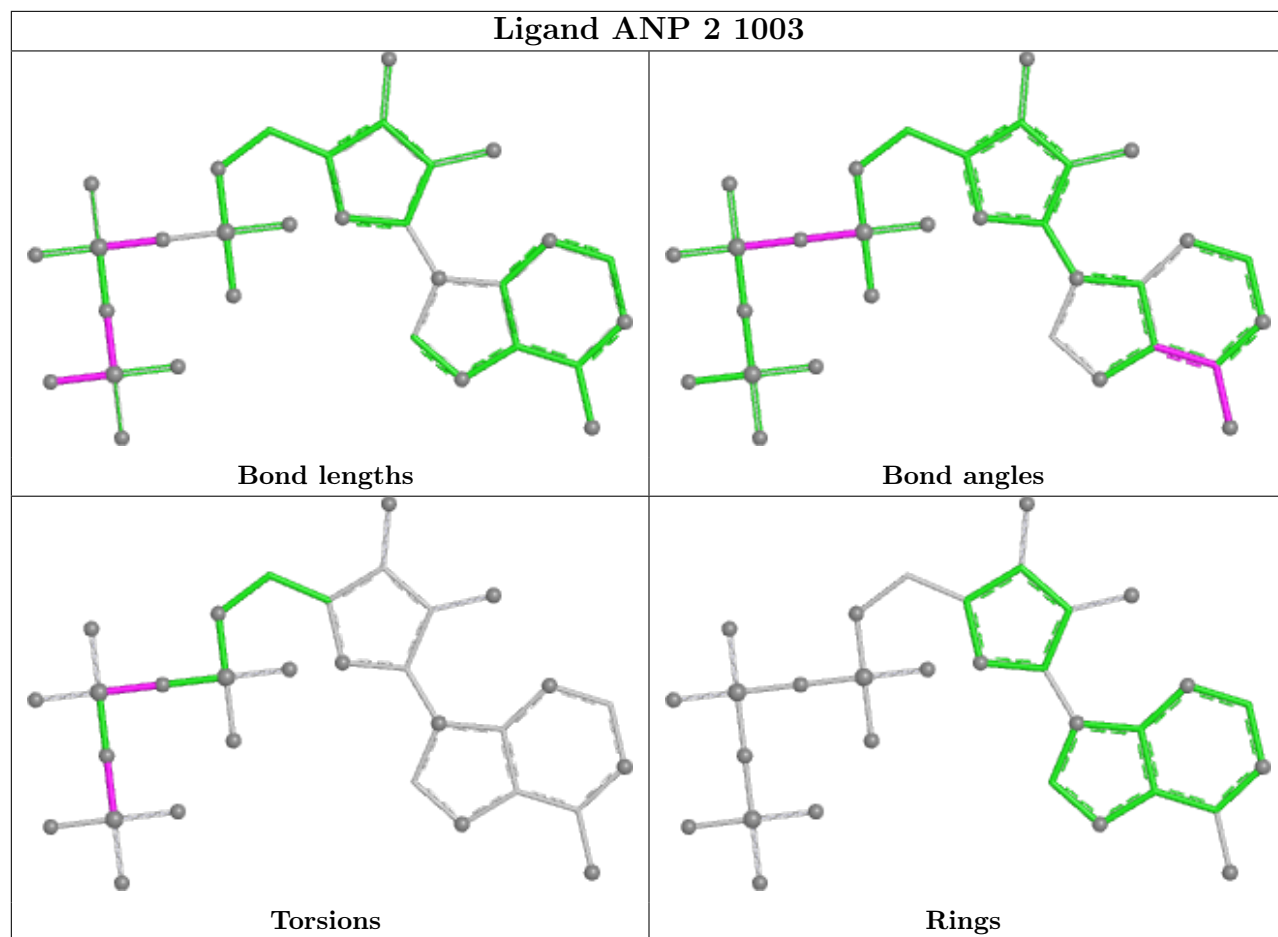
There are no ring outliers.

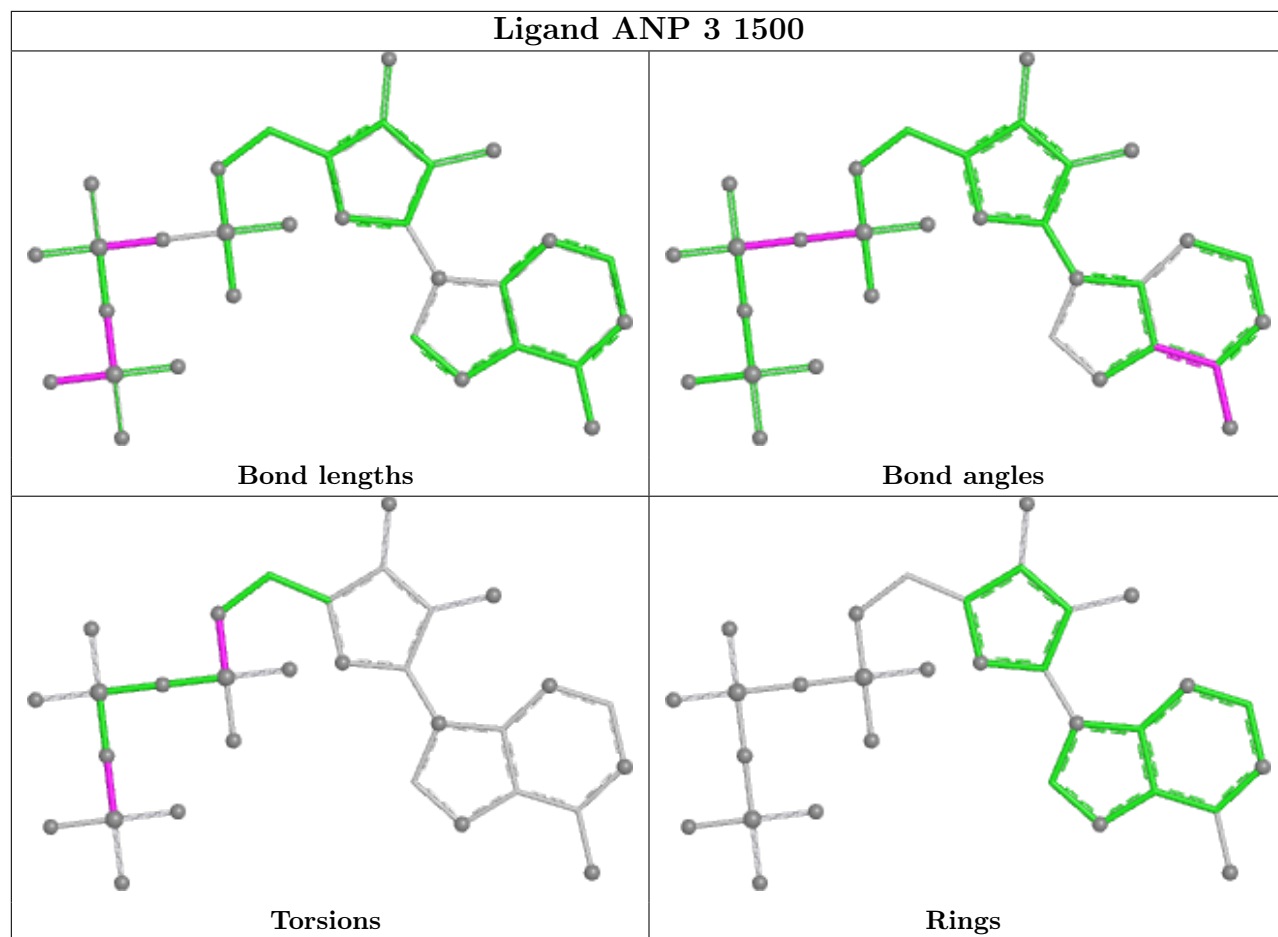
3 monomers are involved in 4 short contacts:

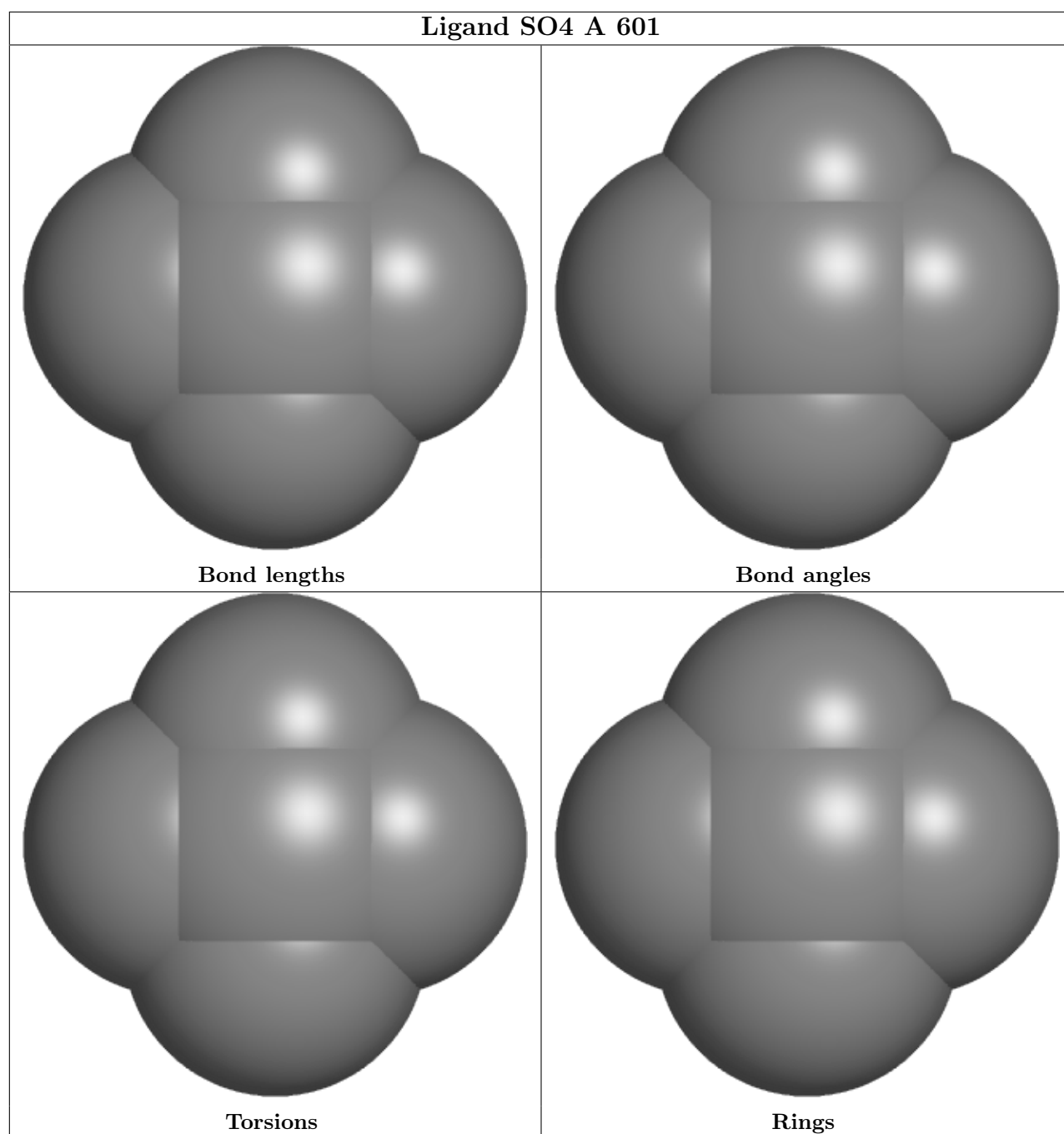
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	5	802	ANP	1	0
22	2	1003	ANP	2	0
22	3	1500	ANP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

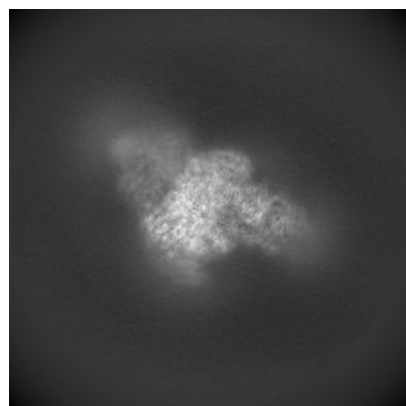
6 Map visualisation [i](#)

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

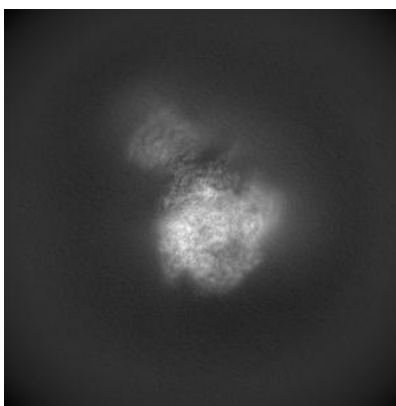
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

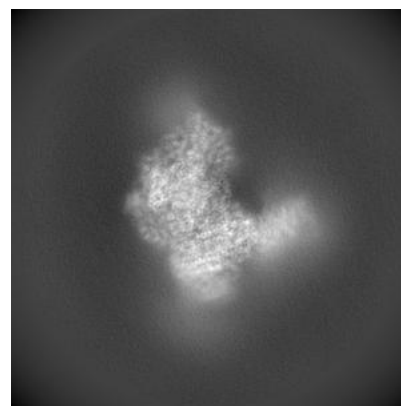
6.1.1 Primary map



X

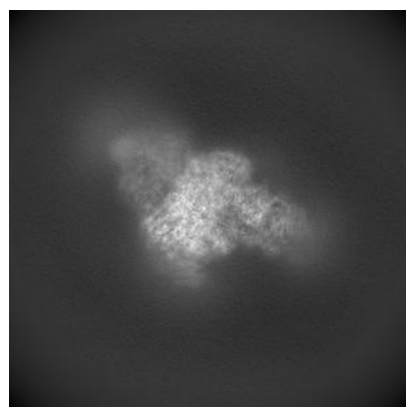


Y

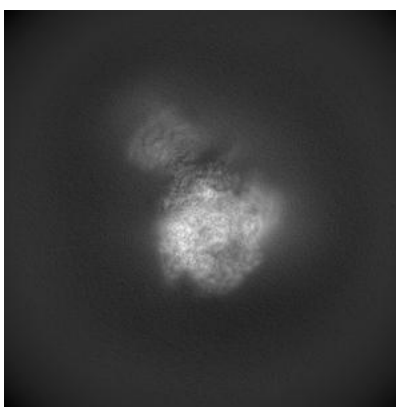


Z

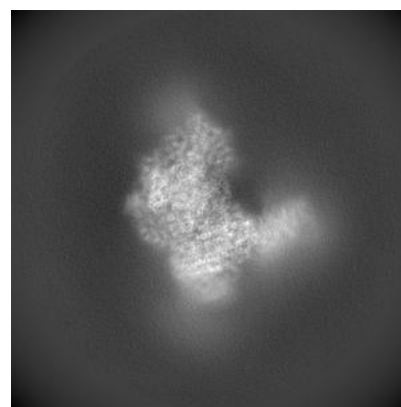
6.1.2 Raw map



X



Y

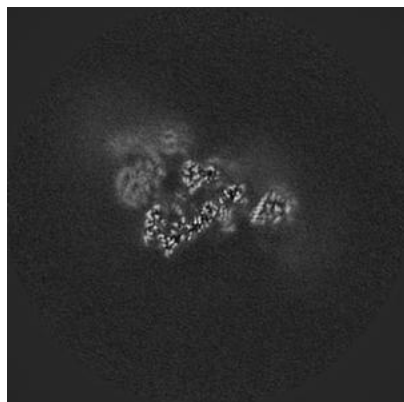


Z

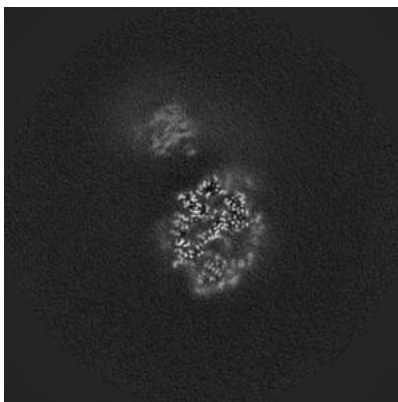
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

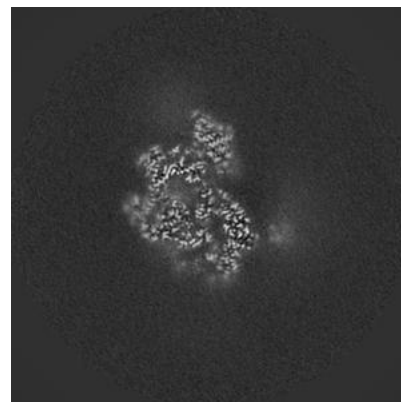
6.2.1 Primary map



X Index: 220

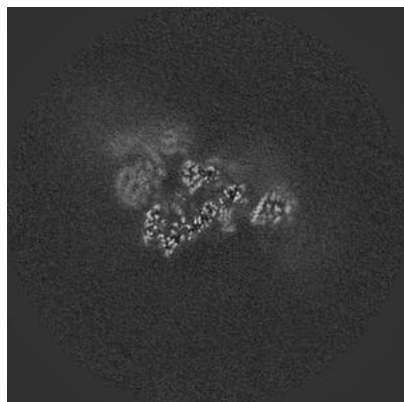


Y Index: 220

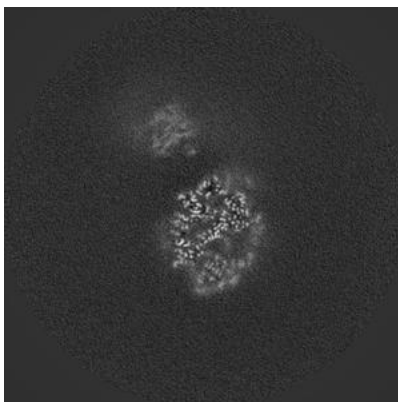


Z Index: 220

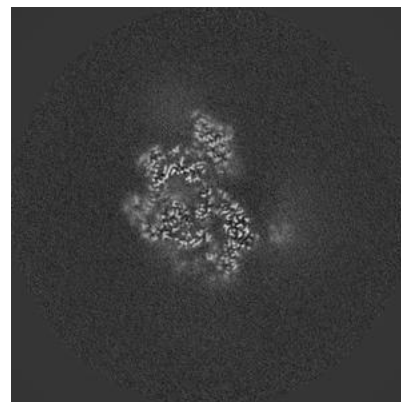
6.2.2 Raw map



X Index: 220



Y Index: 220

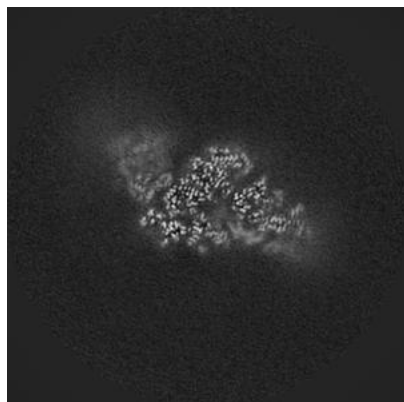


Z Index: 220

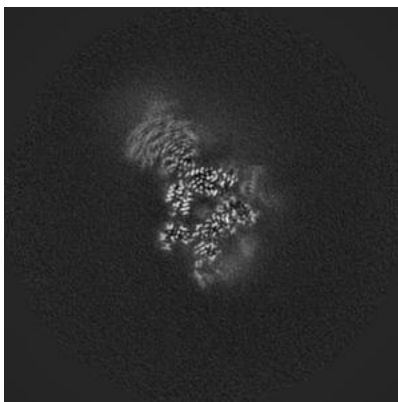
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

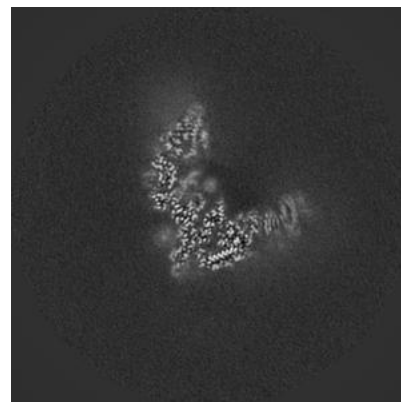
6.3.1 Primary map



X Index: 200

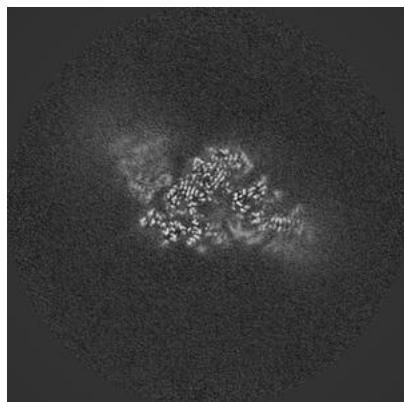


Y Index: 202

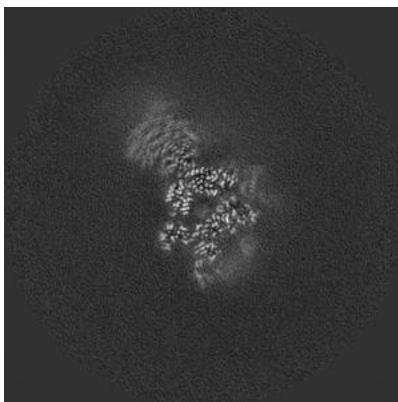


Z Index: 196

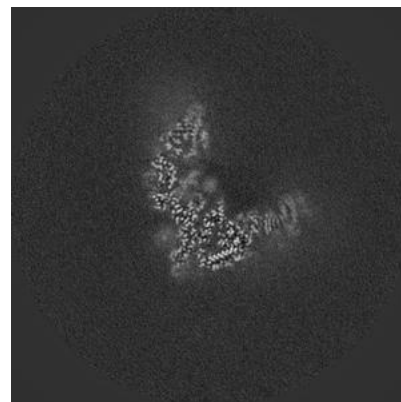
6.3.2 Raw map



X Index: 199



Y Index: 202

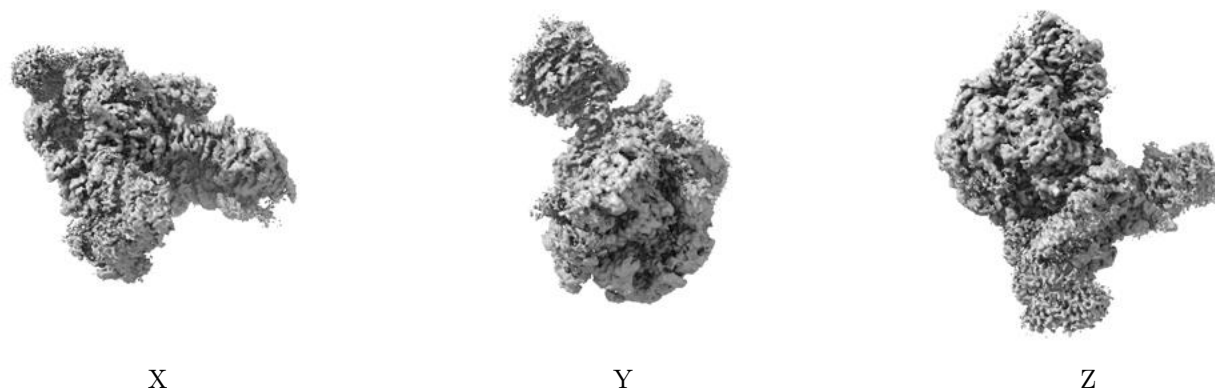


Z Index: 196

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

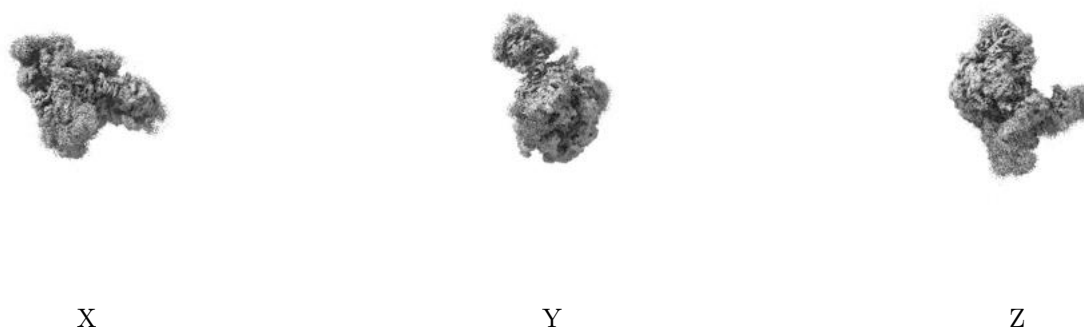
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0113. 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.

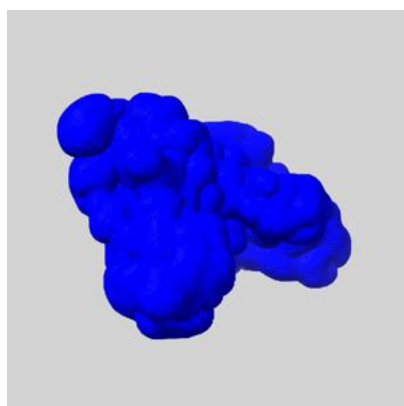
6.5 Mask visualisation [i](#)

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

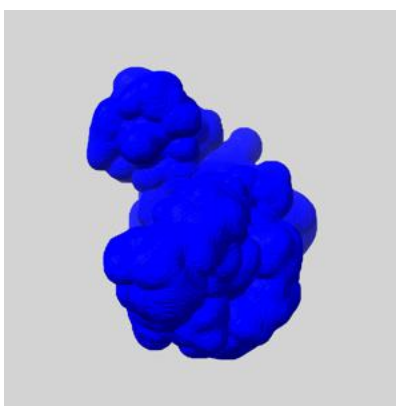
A mask typically either:

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

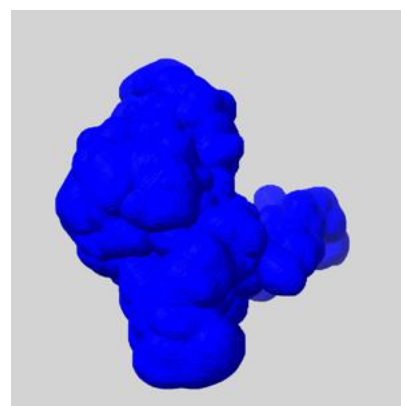
6.5.1 emd_13375_msk_1.map [i](#)



X



Y

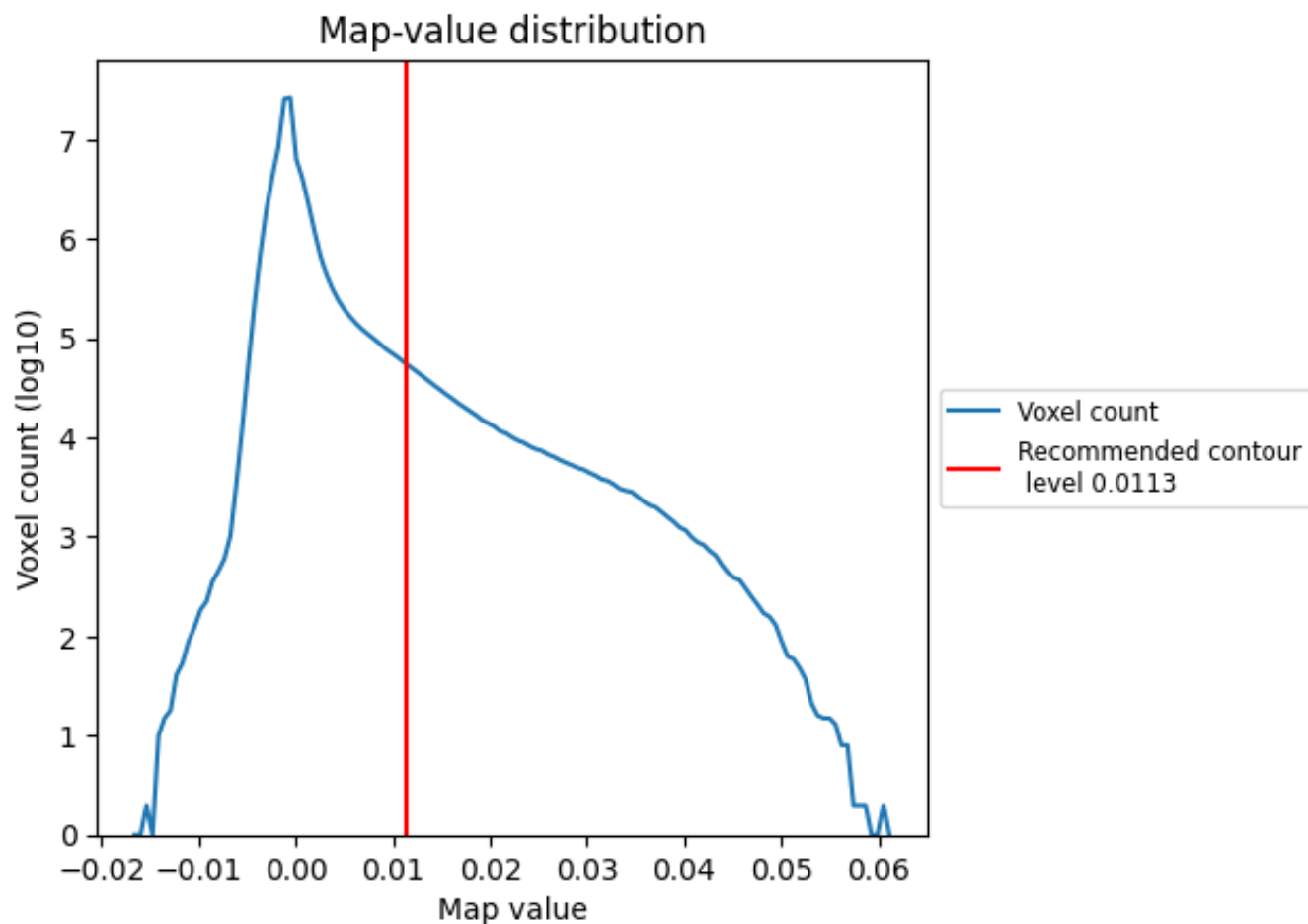


Z

7 Map analysis [i](#)

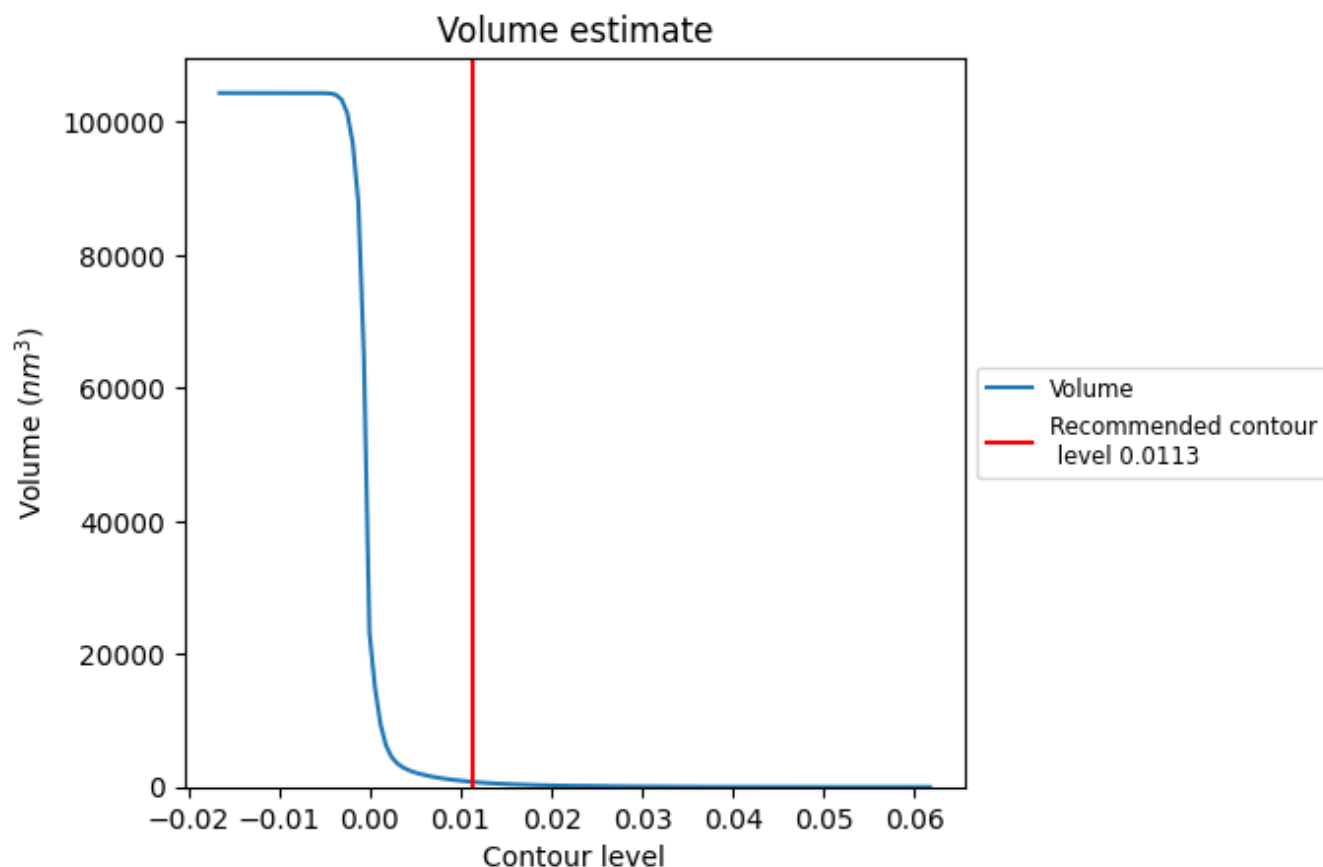
This section contains the results of statistical analysis of the map.

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.

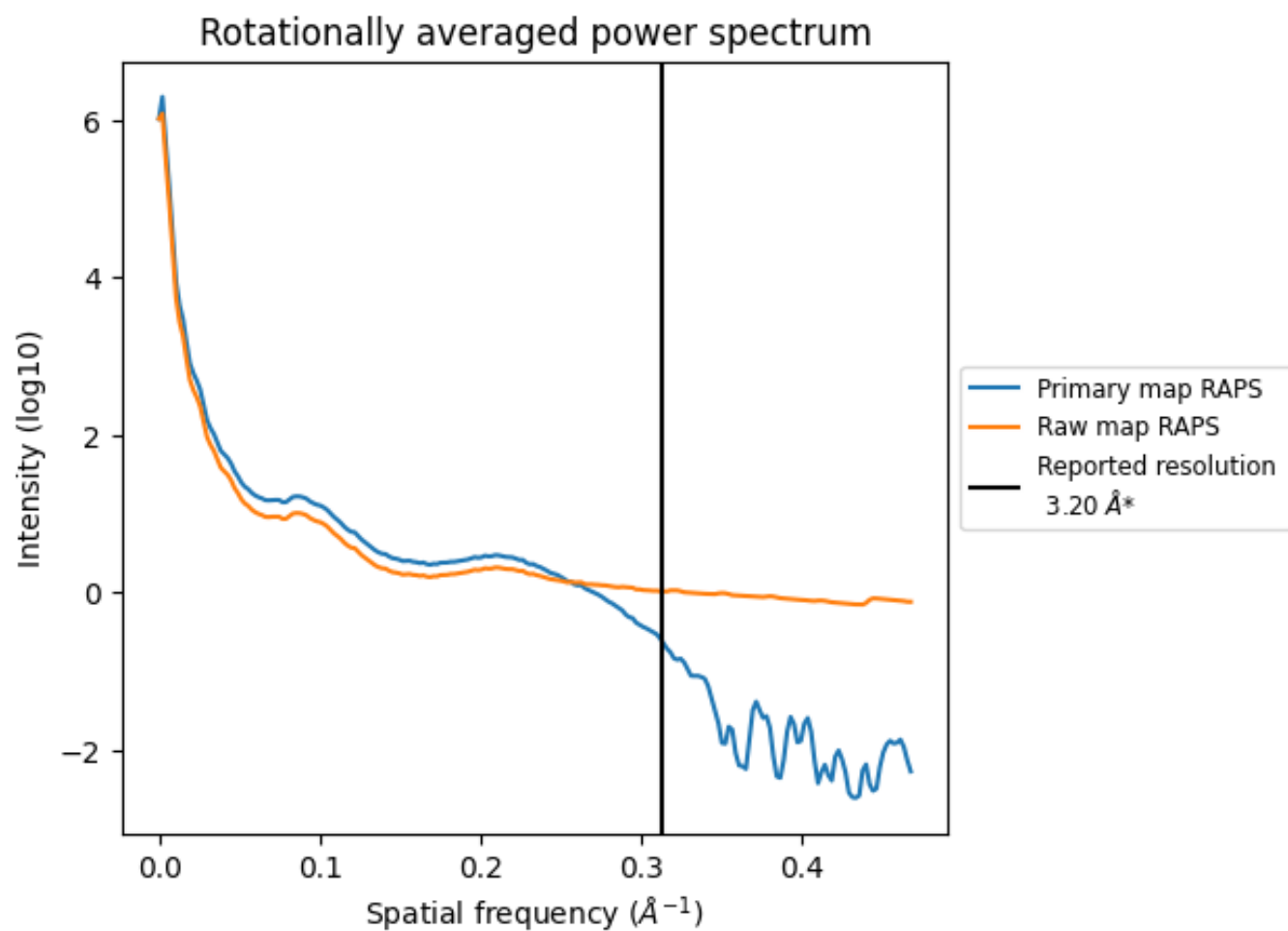
7.2 Volume estimate [i](#)



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 ⓘ

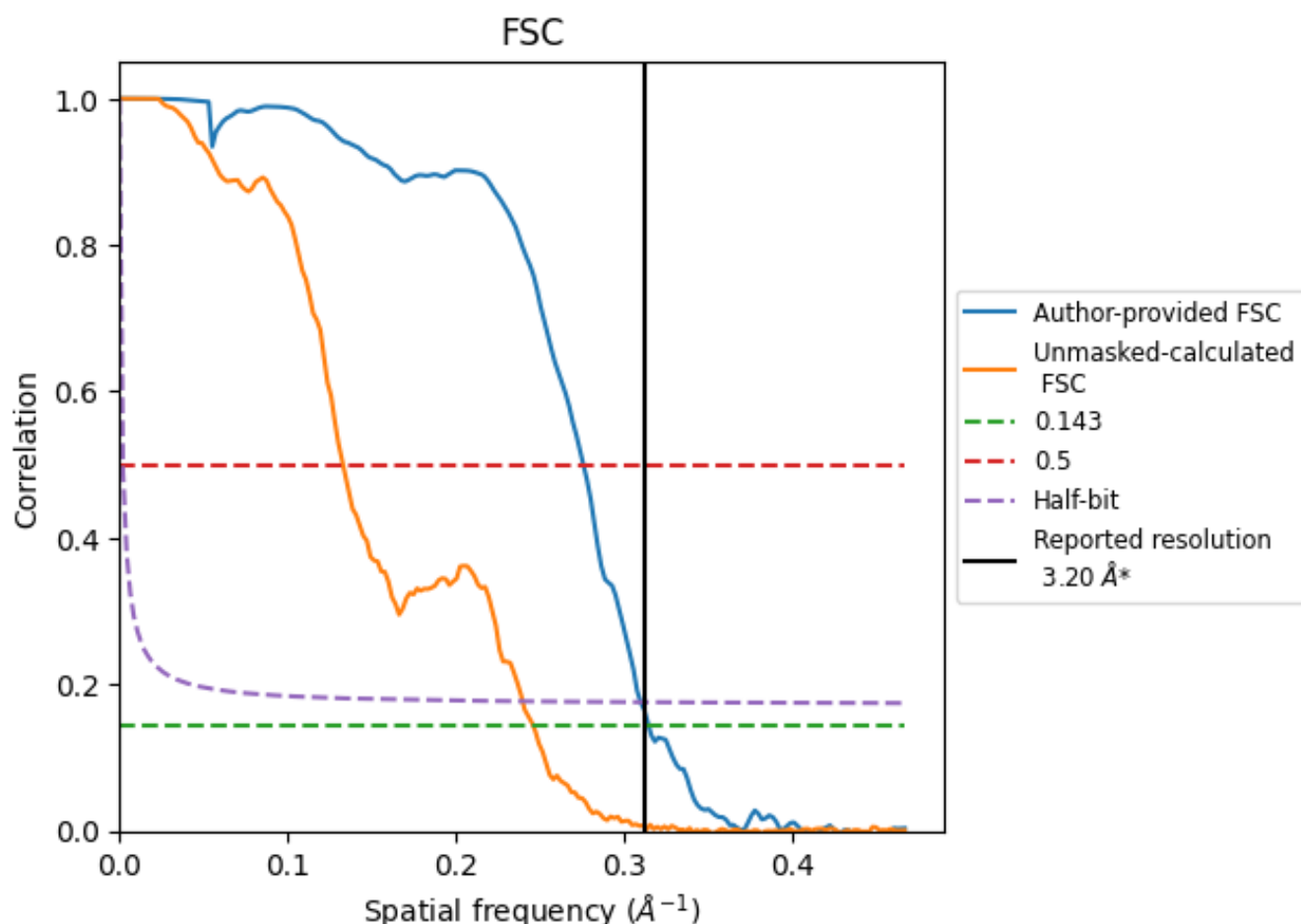


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

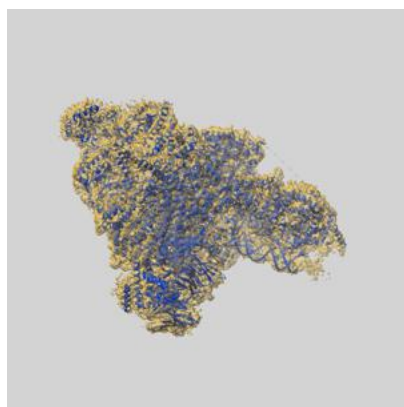
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.62	3.22
Unmasked-calculated*	4.06	7.52	4.17

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

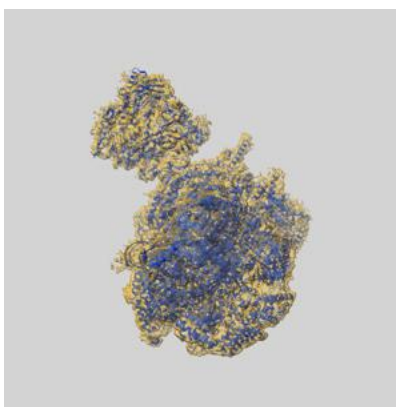
9 Map-model fit [i](#)

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 15.

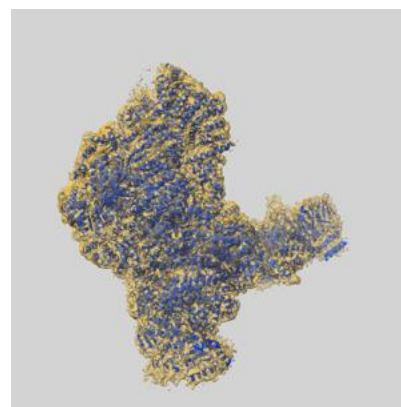
9.1 Map-model overlay [i](#)



X



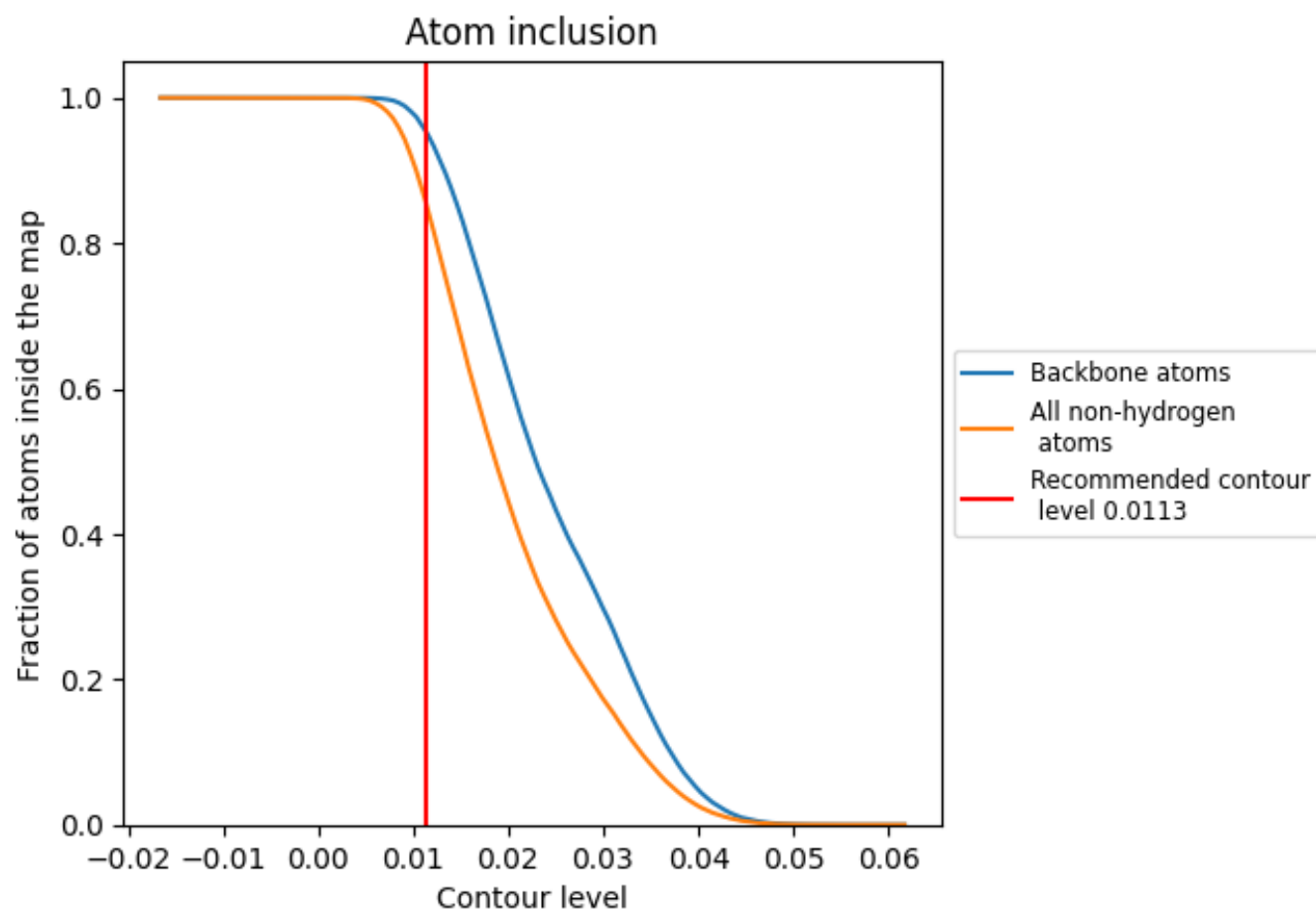
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0113 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 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.