Full wwPDB EM Validation Report ⓘ

Nov 5, 2026 – 03:24 pm GMT

PDB ID	:	30AR / pdb_000030ar
EMDB ID	:	EMD-57512
Title	:	Cryo-EM structure of human PRIMPOL bound to the CMG helicase
Authors	:	Roske, J.J.; Polo Rivera, C.; Yeeles, J.T.P.
Deposited on	:	2026-04-17
Resolution	:	3.30 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:

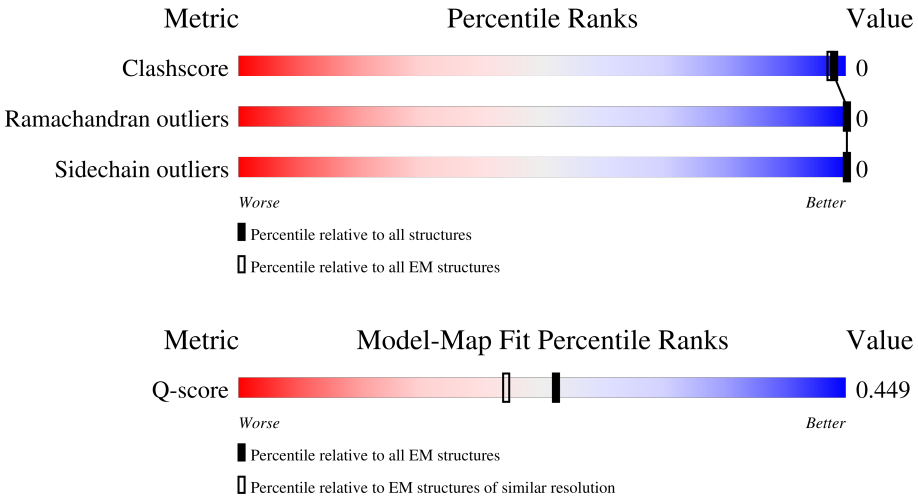
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



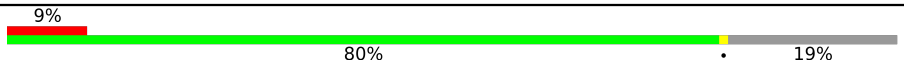
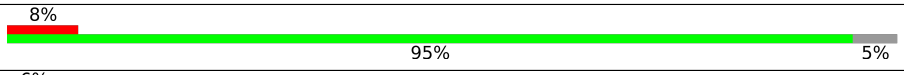
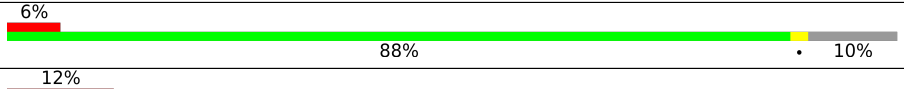
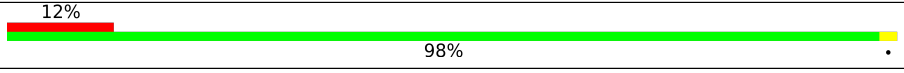
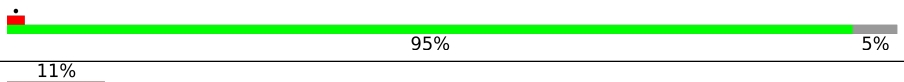
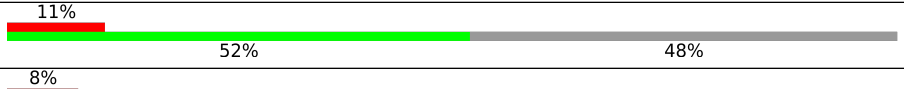
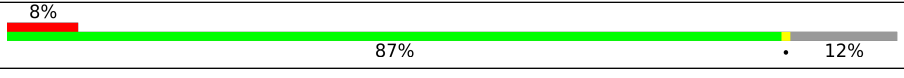
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	904	7% 76% · 23%
2	3	808	6% 77% · 22%
3	4	863	· 67% · 32%
4	5	734	7% 76% 23%

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Mol	Chain	Length	Quality of chain
5	6	821	
6	7	719	
7	C	566	
8	G	223	
9	I	196	
10	N	185	
11	P	560	
12	S	216	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 42847 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	693	5525	3482	987	1024	32	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	633	4970	3108	876	960	26	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	583	4675	2950	824	876	25	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	564	4422	2779	784	825	34	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	667	5395	3401	952	1015	27	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	588	4675	2936	830	880	29	0	0

- Molecule 7 is a protein called Cell division control protein 45 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	538	Total	C	N	O	S	0	0
			4380	2785	750	814	31		

- Molecule 8 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	200	Total	C	N	O	S	0	0
			1654	1050	283	311	10		

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

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

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

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

- Molecule 11 is a protein called DNA-directed primase/polymerase protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	291	Total	C	N	O	S	0	0
			2402	1545	412	436	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	191	Total	C	N	O	S	0	0
			1525	964	265	290	6		

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

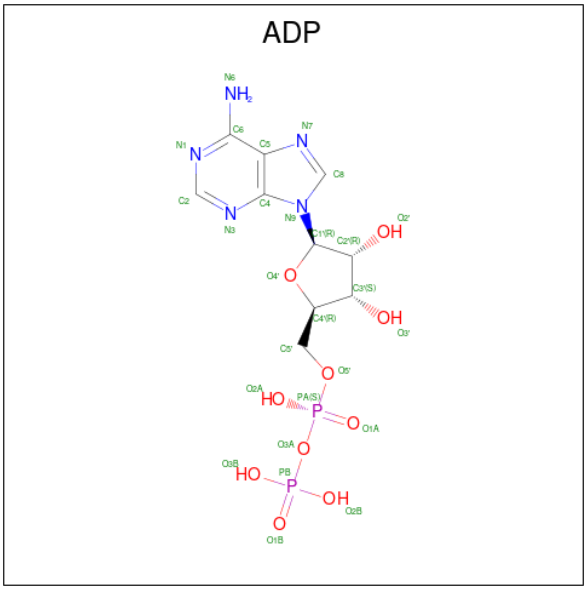
Mol	Chain	Residues	Atoms		AltConf
13	2	1	Total	Zn	0
			1	1	
13	4	1	Total	Zn	0
			1	1	

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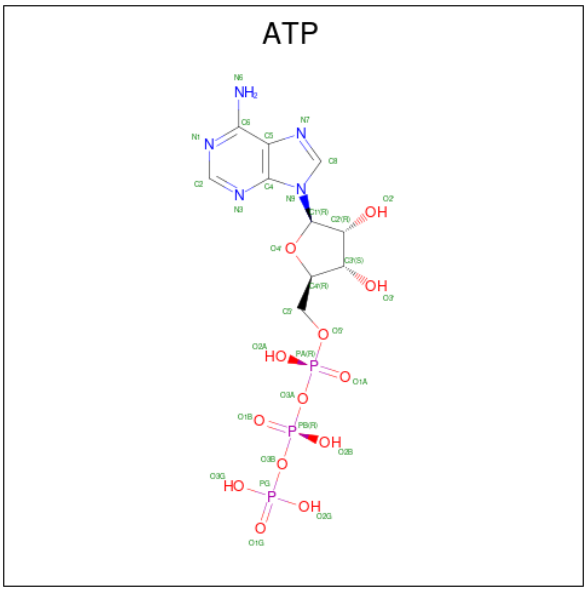
Mol	Chain	Residues	Atoms	AltConf
13	5	1	Total Zn 1 1	0
13	6	1	Total Zn 1 1	0
13	7	1	Total Zn 1 1	0

- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms	AltConf
14	2	1	Total C N O P 27 10 5 10 2	0
14	3	1	Total C N O P 27 10 5 10 2	0
14	7	1	Total C N O P 27 10 5 10 2	0

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
15	4	1	Total	C	N	O	P	0
			31	10	5	13	3	
15	5	1	Total	C	N	O	P	0
			31	10	5	13	3	
15	6	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
16	6	1	Total	Mg	0
			1	1	

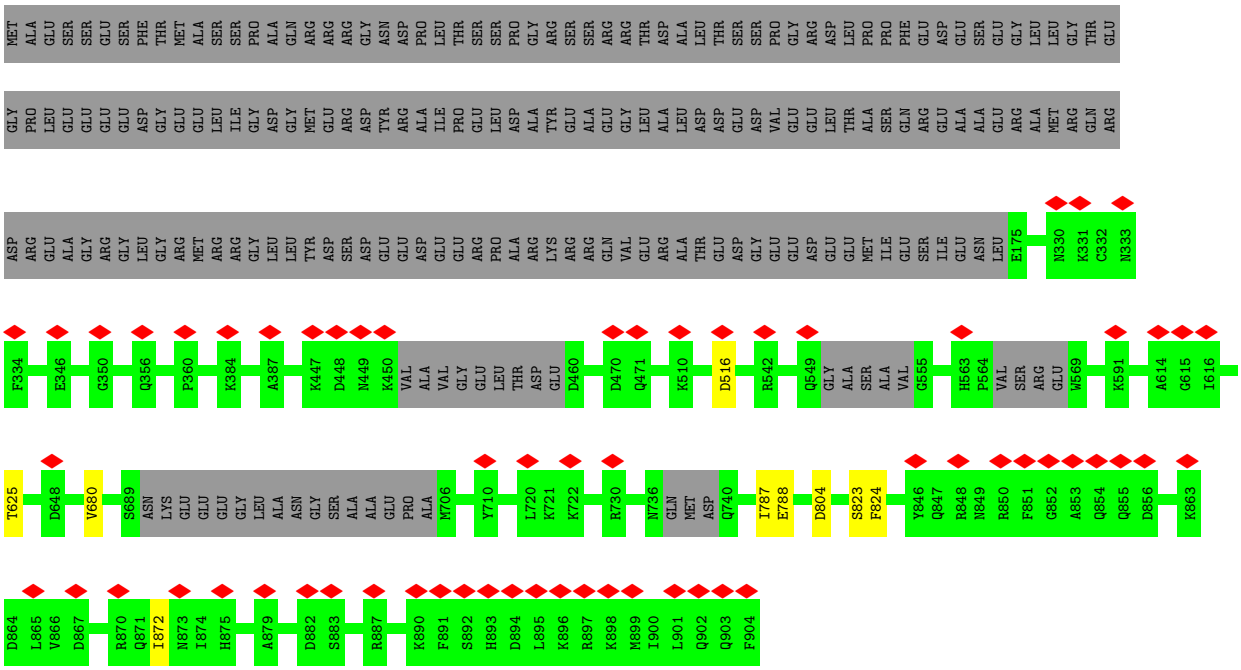
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA replication licensing factor MCM2

Chain 2:

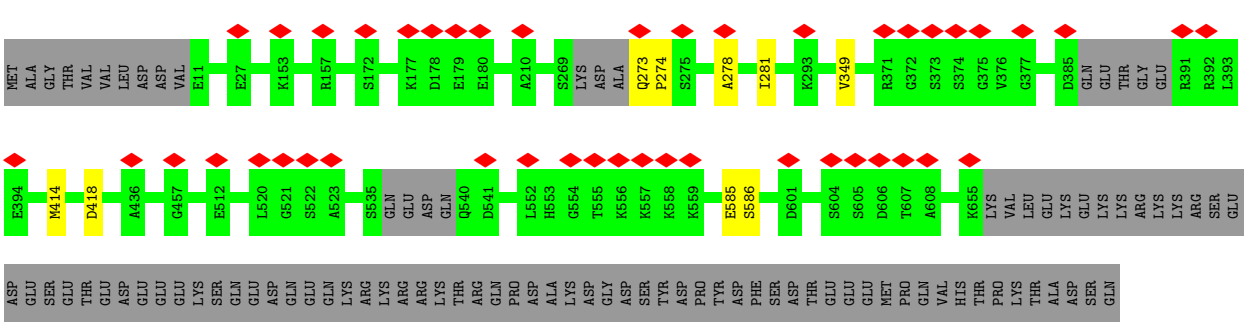


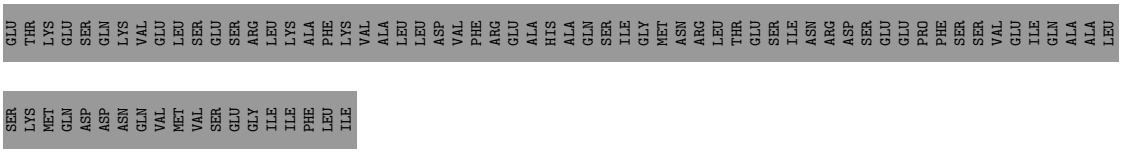


• Molecule 2: DNA replication licensing factor MCM3

Chain 3:

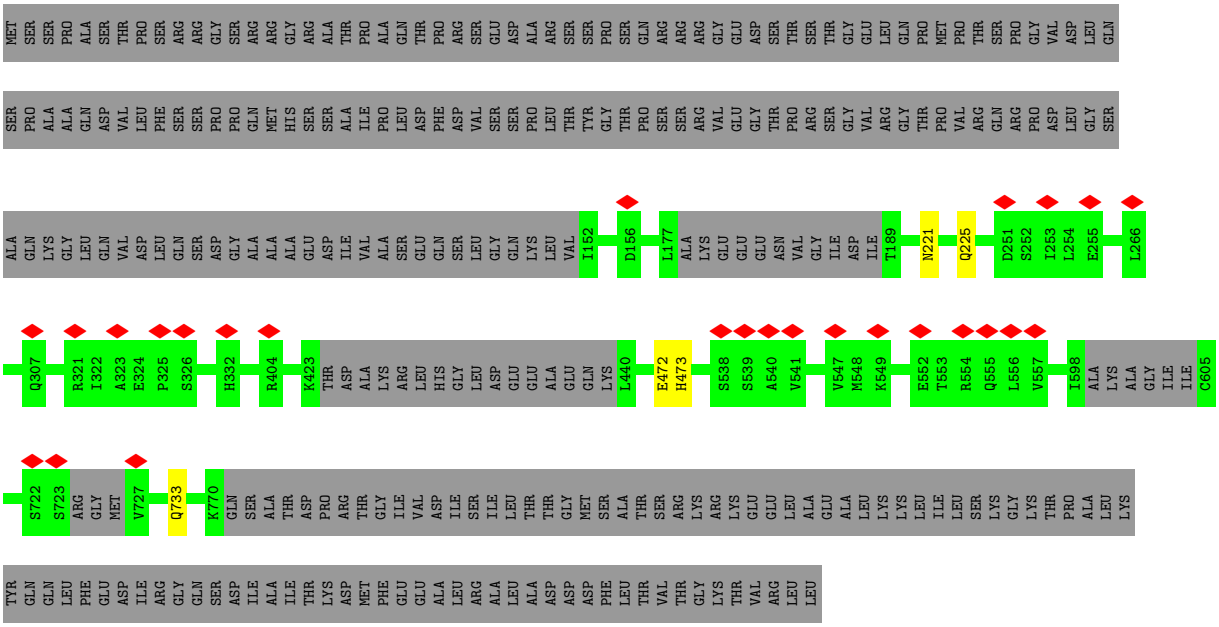






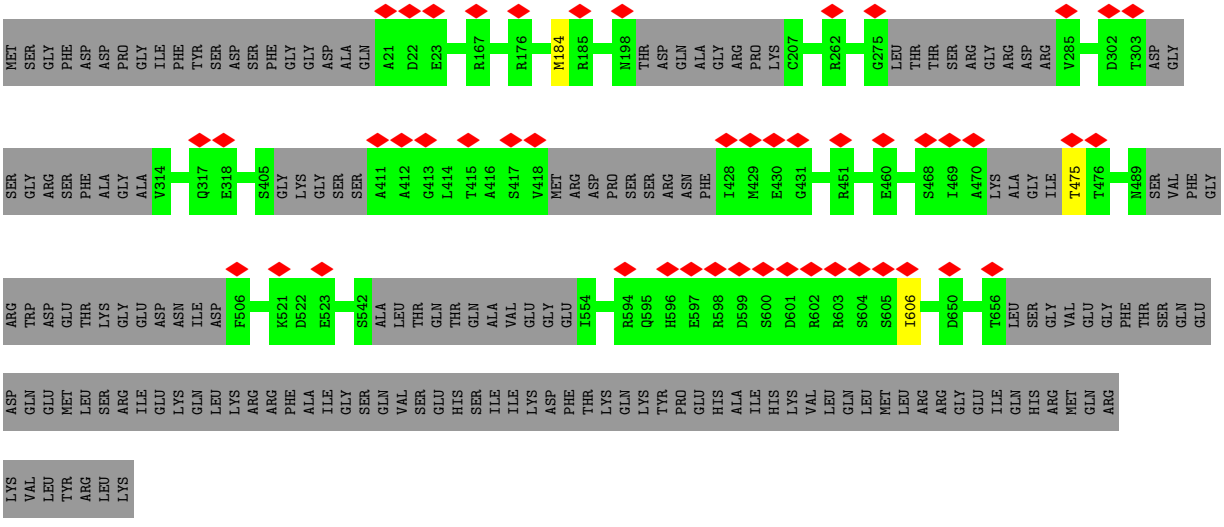
• Molecule 3: DNA replication licensing factor MCM4





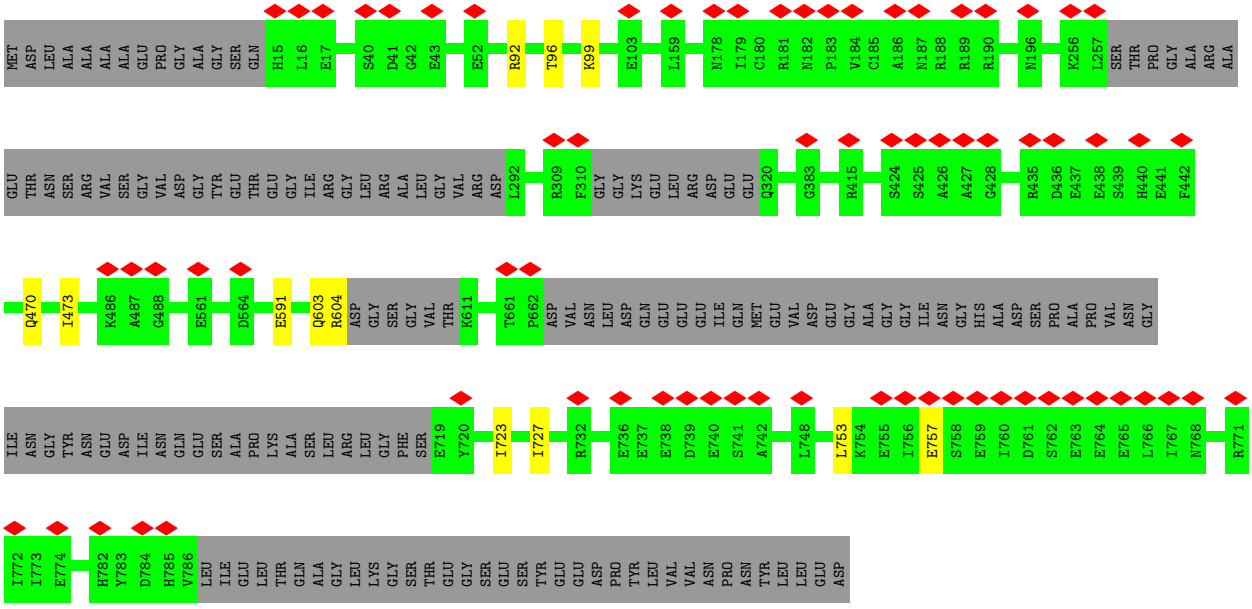
• Molecule 4: DNA replication licensing factor MCM5





• Molecule 5: DNA replication licensing factor MCM6

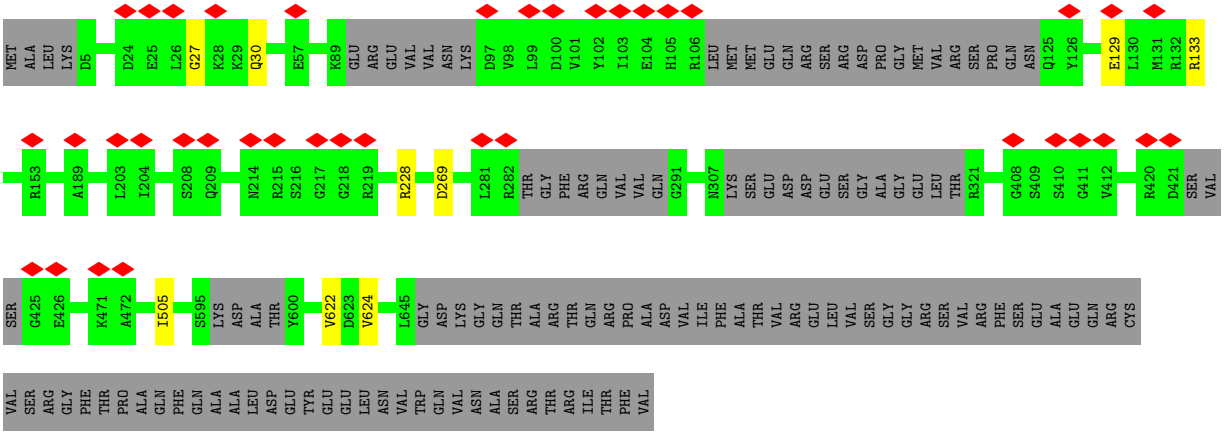




• Molecule 6: DNA replication licensing factor MCM7

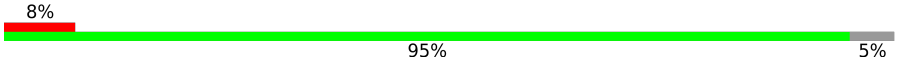
Chain 7:

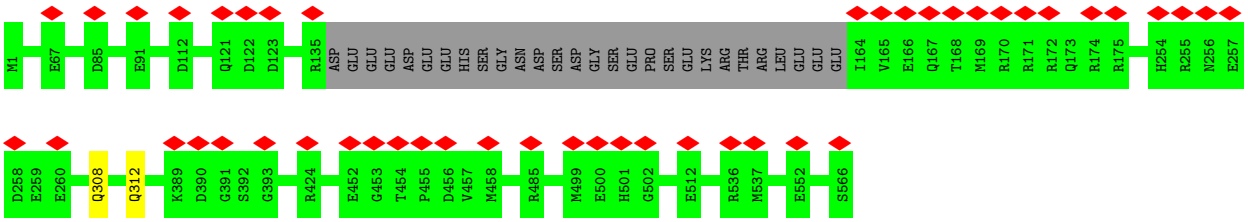




• Molecule 7: Cell division control protein 45 homolog

Chain C:

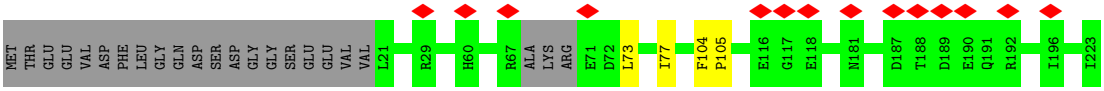




• Molecule 8: DNA replication complex GINS protein SLD5

Chain G:

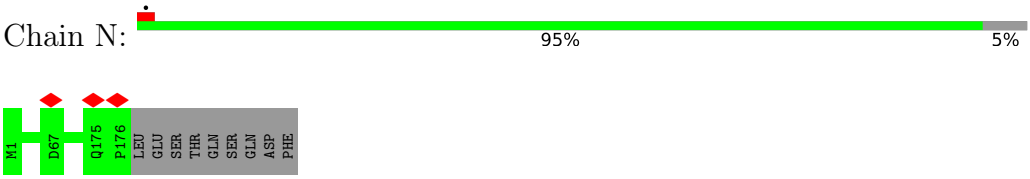




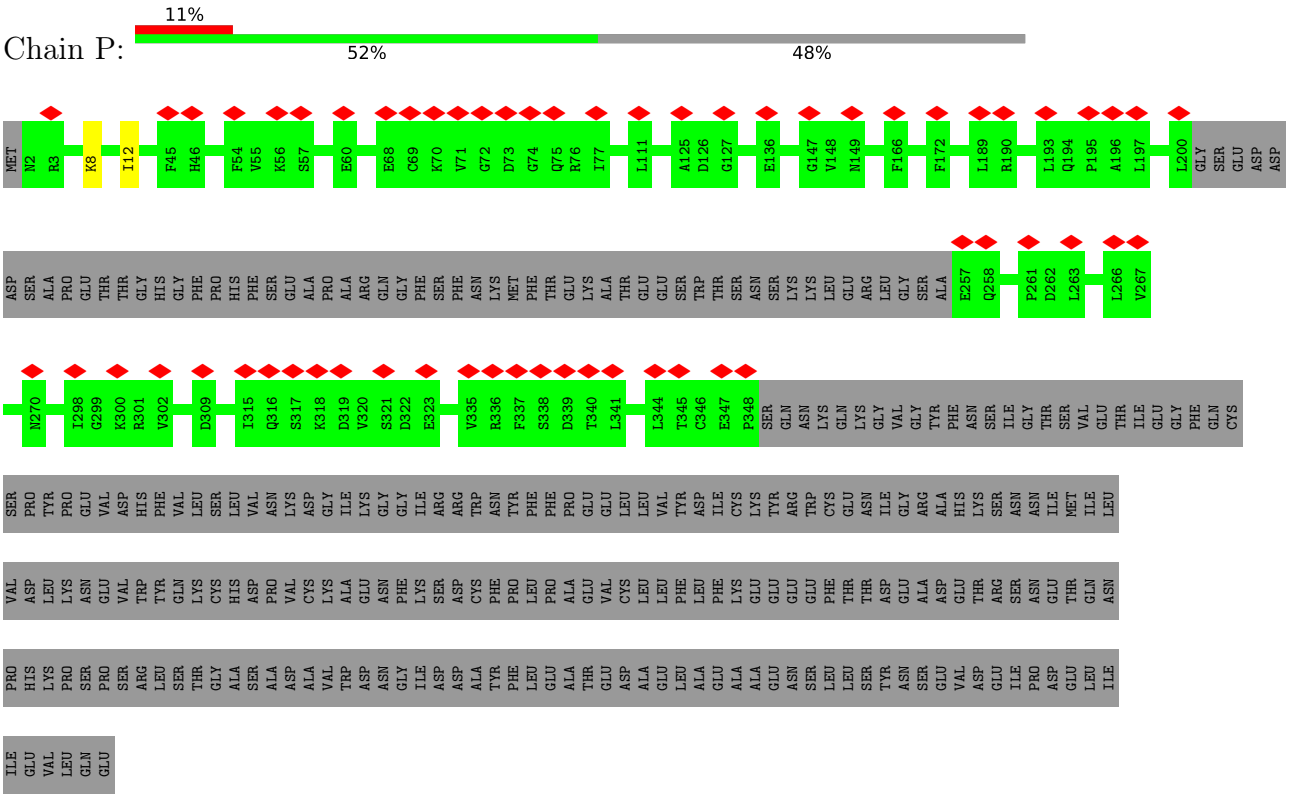
• Molecule 9: DNA replication complex GINS protein PSF1



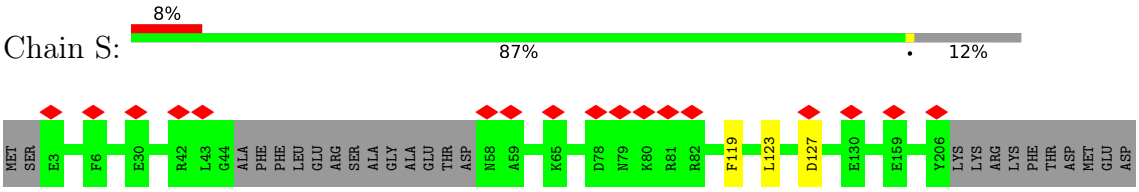
• Molecule 10: DNA replication complex GINS protein PSF2



• Molecule 11: DNA-directed primase/polymerase protein



• Molecule 12: DNA replication complex GINS protein PSF3



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39.1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	32.275	Depositor
Minimum map value	-12.565	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.795	Depositor
Recommended contour level	5	Depositor
Map size (Å)	369.59998, 369.59998, 369.59998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.13	0/5628	0.37	0/7593
2	3	0.13	0/5047	0.37	0/6811
3	4	0.13	0/4760	0.36	0/6435
4	5	0.14	0/4484	0.41	0/6027
5	6	0.13	0/5484	0.40	0/7395
6	7	0.15	0/4747	0.39	0/6405
7	C	0.13	0/4472	0.36	0/6037
8	G	0.13	0/1685	0.36	0/2270
9	I	0.14	0/1645	0.38	0/2210
10	N	0.15	0/1462	0.37	0/1981
11	P	0.12	0/2459	0.35	0/3318
12	S	0.14	0/1558	0.38	0/2104
All	All	0.13	0/43431	0.38	0/58586

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	5525	0	5533	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3	4970	0	4996	5	0
3	4	4675	0	4690	3	0
4	5	4422	0	4503	3	0
5	6	5395	0	5429	7	0
6	7	4675	0	4711	7	0
7	C	4380	0	4330	1	0
8	G	1654	0	1668	2	0
9	I	1613	0	1606	2	0
10	N	1431	0	1456	0	0
11	P	2402	0	2388	1	0
12	S	1525	0	1481	2	0
13	2	1	0	0	0	0
13	4	1	0	0	0	0
13	5	1	0	0	0	0
13	6	1	0	0	0	0
13	7	1	0	0	0	0
14	2	27	0	12	0	0
14	3	27	0	12	0	0
14	7	27	0	12	0	0
15	4	31	0	12	0	0
15	5	31	0	12	0	0
15	6	31	0	12	0	0
16	6	1	0	0	0	0
All	All	42847	0	42863	38	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 (38) 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)
6:7:622:VAL:HG12	6:7:624:VAL:H	1.73	0.53
2:3:273:GLN:N	2:3:274:PRO:CD	2.73	0.51
6:7:133:ARG:H	6:7:228:ARG:HH12	1.59	0.50
5:6:470:GLN:HA	5:6:473:ILE:HG22	1.94	0.50
3:4:472:GLU:HG3	3:4:473:HIS:H	1.77	0.50
6:7:129:GLU:O	6:7:228:ARG:NH1	2.45	0.49
8:G:73:LEU:O	8:G:77:ILE:HG12	2.14	0.47
6:7:133:ARG:H	6:7:228:ARG:NH1	2.13	0.46
11:P:8:LYS:O	11:P:12:ILE:HG12	2.17	0.45
5:6:92:ARG:O	5:6:96:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:S:119:PHE:CE1	12:S:123:LEU:HD11	2.53	0.44
2:3:414:MET:CG	2:3:418:ASP:HB2	2.47	0.44
7:C:308:GLN:O	7:C:312:GLN:HG2	2.19	0.43
1:2:787:ILE:HG22	1:2:788:GLU:N	2.32	0.43
4:5:184:MET:HA	4:5:184:MET:HE2	2.00	0.43
1:2:804:ASP:OD1	1:2:804:ASP:C	2.62	0.43
12:S:127:ASP:C	12:S:127:ASP:OD1	2.61	0.43
2:3:349:VAL:HG12	2:3:349:VAL:O	2.19	0.43
4:5:475:THR:O	4:5:475:THR:HG23	2.18	0.43
5:6:753:LEU:O	5:6:757:GLU:HG2	2.19	0.42
5:6:603:GLN:O	5:6:604:ARG:C	2.62	0.42
4:5:606:ILE:HG23	4:5:606:ILE:O	2.19	0.42
8:G:104:PHE:CG	8:G:105:PRO:HD3	2.54	0.42
5:6:96:THR:O	5:6:99:LYS:HG2	2.18	0.42
3:4:733:GLN:HA	3:4:733:GLN:OE1	2.19	0.42
1:2:680:VAL:HG11	5:6:591:GLU:HG3	2.01	0.41
6:7:27:GLY:HA3	6:7:30:GLN:HG2	2.01	0.41
1:2:872:ILE:HG22	1:2:872:ILE:O	2.20	0.41
9:I:79:TYR:CZ	9:I:83:ARG:HD2	2.56	0.41
1:2:516:ASP:HB3	1:2:625:THR:HG22	2.01	0.41
1:2:823:SER:O	1:2:824:PHE:C	2.63	0.41
9:I:72:ASN:O	9:I:76:THR:HG22	2.21	0.41
2:3:585:GLU:HG3	2:3:586:SER:N	2.36	0.41
2:3:278:ALA:HA	2:3:281:ILE:HG22	2.03	0.40
5:6:723:ILE:O	5:6:727:ILE:HG12	2.21	0.40
6:7:505:ILE:O	6:7:505:ILE:CG2	2.70	0.40
3:4:221:ASN:O	3:4:225:GLN:HG2	2.22	0.40
6:7:269:ASP:OD1	6:7:269:ASP:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	681/904 (75%)	669 (98%)	12 (2%)	0	100	100
2	3	625/808 (77%)	602 (96%)	23 (4%)	0	100	100
3	4	573/863 (66%)	557 (97%)	16 (3%)	0	100	100
4	5	546/734 (74%)	539 (99%)	7 (1%)	0	100	100
5	6	657/821 (80%)	644 (98%)	13 (2%)	0	100	100
6	7	574/719 (80%)	562 (98%)	12 (2%)	0	100	100
7	C	534/566 (94%)	523 (98%)	11 (2%)	0	100	100
8	G	196/223 (88%)	194 (99%)	2 (1%)	0	100	100
9	I	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
10	N	174/185 (94%)	172 (99%)	2 (1%)	0	100	100
11	P	287/560 (51%)	278 (97%)	9 (3%)	0	100	100
12	S	187/216 (87%)	180 (96%)	7 (4%)	0	100	100
All	All	5228/6795 (77%)	5109 (98%)	119 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	611/781 (78%)	611 (100%)	0	100	100
2	3	547/707 (77%)	547 (100%)	0	100	100
3	4	521/753 (69%)	521 (100%)	0	100	100
4	5	483/625 (77%)	483 (100%)	0	100	100
5	6	606/724 (84%)	606 (100%)	0	100	100
6	7	508/619 (82%)	508 (100%)	0	100	100
7	C	491/517 (95%)	491 (100%)	0	100	100
8	G	186/205 (91%)	186 (100%)	0	100	100
9	I	174/174 (100%)	174 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	N	160/169 (95%)	160 (100%)	0	100	100
11	P	267/503 (53%)	267 (100%)	0	100	100
12	S	165/186 (89%)	165 (100%)	0	100	100
All	All	4719/5963 (79%)	4719 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	287	HIS
1	2	303	ASN
1	2	321	GLN
1	2	343	GLN
1	2	371	GLN
1	2	443	HIS
1	2	561	GLN
1	2	847	GLN
1	2	849	ASN
1	2	855	GLN
1	2	903	GLN
2	3	443	ASN
3	4	214	HIS
3	4	407	ASN
3	4	580	ASN
4	5	535	HIS
4	5	596	HIS
5	6	342	GLN
5	6	348	HIS
5	6	359	HIS
5	6	504	ASN
5	6	644	HIS
5	6	730	HIS
5	6	750	ASN
6	7	270	HIS
6	7	439	GLN
6	7	542	GLN
7	C	292	ASN
7	C	306	HIS
7	C	369	HIS
7	C	414	HIS

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Mol	Chain	Res	Type
8	G	32	GLN
9	I	66	HIS
10	N	106	ASN
10	N	142	HIS
10	N	154	ASN
11	P	11	GLN
11	P	63	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	ADP	3	1001	-	27,29,29	1.36	4 (14%)	42,45,45	2.10	10 (23%)
15	ATP	5	1001	-	29,33,33	0.31	0	44,52,52	0.55	1 (2%)
15	ATP	6	1001	16	29,33,33	0.32	0	44,52,52	0.55	0
14	ADP	2	1001	-	27,29,29	1.36	4 (14%)	42,45,45	2.20	11 (26%)
14	ADP	7	1001	-	27,29,29	1.33	4 (14%)	42,45,45	2.05	11 (26%)
15	ATP	4	1001	-	29,33,33	0.34	0	44,52,52	0.67	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
14	ADP	3	1001	-	-	2/16/32/32	0/3/3/3
15	ATP	5	1001	-	-	8/22/38/38	0/3/3/3
15	ATP	6	1001	16	-	2/22/38/38	0/3/3/3
14	ADP	2	1001	-	-	3/16/32/32	0/3/3/3
14	ADP	7	1001	-	-	2/16/32/32	0/3/3/3
15	ATP	4	1001	-	-	1/22/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	1001	ADP	C5-C4	4.52	1.47	1.39
14	3	1001	ADP	C5-C4	4.41	1.47	1.39
14	7	1001	ADP	C5-C4	4.24	1.46	1.39
14	2	1001	ADP	C5-C6	2.69	1.48	1.41
14	3	1001	ADP	C5-C6	2.66	1.48	1.41
14	7	1001	ADP	C5-C6	2.54	1.48	1.41
14	2	1001	ADP	C5-N7	-2.43	1.34	1.39
14	7	1001	ADP	C8-N7	2.39	1.36	1.31
14	3	1001	ADP	C5-N7	-2.35	1.34	1.39
14	3	1001	ADP	C8-N7	2.29	1.35	1.31
14	2	1001	ADP	C8-N7	2.24	1.35	1.31
14	7	1001	ADP	C5-N7	-2.23	1.34	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	1001	ADP	C5-C4-N3	-7.47	117.01	126.75
14	3	1001	ADP	C5-C4-N3	-6.99	117.63	126.75
14	7	1001	ADP	C5-C4-N3	-6.16	118.72	126.75
14	2	1001	ADP	N3-C4-N9	5.73	136.51	127.08
14	3	1001	ADP	N3-C4-N9	5.42	136.02	127.08
14	7	1001	ADP	PA-O3A-PB	-4.85	116.19	132.83
14	7	1001	ADP	N3-C4-N9	4.78	134.96	127.08
14	2	1001	ADP	C2-N3-C4	4.57	122.55	111.75
14	3	1001	ADP	PA-O3A-PB	-4.42	117.66	132.83
14	3	1001	ADP	C2-N3-C4	4.38	122.09	111.75
14	7	1001	ADP	C2-N3-C4	4.00	121.19	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	1001	ADP	PA-O3A-PB	-3.91	119.41	132.83
14	3	1001	ADP	N3-C2-N1	-3.55	123.05	128.60
14	2	1001	ADP	C4-C5-N7	-3.55	106.30	110.62
14	2	1001	ADP	N3-C2-N1	-3.53	123.08	128.60
14	7	1001	ADP	N3-C2-N1	-3.44	123.22	128.60
14	7	1001	ADP	C4-C5-N7	-3.36	106.52	110.62
14	3	1001	ADP	C4-C5-N7	-3.33	106.57	110.62
14	2	1001	ADP	C5-N7-C8	3.20	108.06	103.51
14	3	1001	ADP	C5-N7-C8	2.97	107.72	103.51
14	7	1001	ADP	C5-N7-C8	2.95	107.70	103.51
14	7	1001	ADP	C4-N9-C8	2.84	108.81	105.73
14	7	1001	ADP	N9-C8-N7	-2.38	110.65	113.91
14	3	1001	ADP	C4-N9-C8	2.35	108.27	105.73
14	2	1001	ADP	O4'-C1'-C2'	-2.31	101.61	106.64
14	7	1001	ADP	C6-C5-N7	2.23	136.17	132.02
14	2	1001	ADP	C1'-N9-C8	-2.22	122.11	127.14
14	2	1001	ADP	C4-N9-C8	2.09	107.99	105.73
14	3	1001	ADP	N9-C8-N7	-2.06	111.10	113.91
15	5	1001	ATP	PB-O3B-PG	2.02	139.74	132.83
14	3	1001	ADP	C6-C5-N7	2.01	135.77	132.02
14	7	1001	ADP	O3B-PB-O2B	2.01	115.31	107.64
14	2	1001	ADP	N9-C8-N7	-2.00	111.18	113.91

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	7	1001	ADP	C5'-O5'-PA-O2A
14	7	1001	ADP	C5'-O5'-PA-O3A
15	5	1001	ATP	C5'-O5'-PA-O1A
15	5	1001	ATP	C5'-O5'-PA-O2A
15	5	1001	ATP	C5'-O5'-PA-O3A
15	5	1001	ATP	O4'-C4'-C5'-O5'
15	5	1001	ATP	C3'-C4'-C5'-O5'
15	6	1001	ATP	O4'-C4'-C5'-O5'
15	6	1001	ATP	C3'-C4'-C5'-O5'
14	3	1001	ADP	PA-O3A-PB-O1B
15	5	1001	ATP	PB-O3B-PG-O1G
14	2	1001	ADP	C2'-C1'-N9-C4
14	2	1001	ADP	C2'-C1'-N9-C8
15	5	1001	ATP	PB-O3B-PG-O2G
15	4	1001	ATP	PB-O3A-PA-O2A

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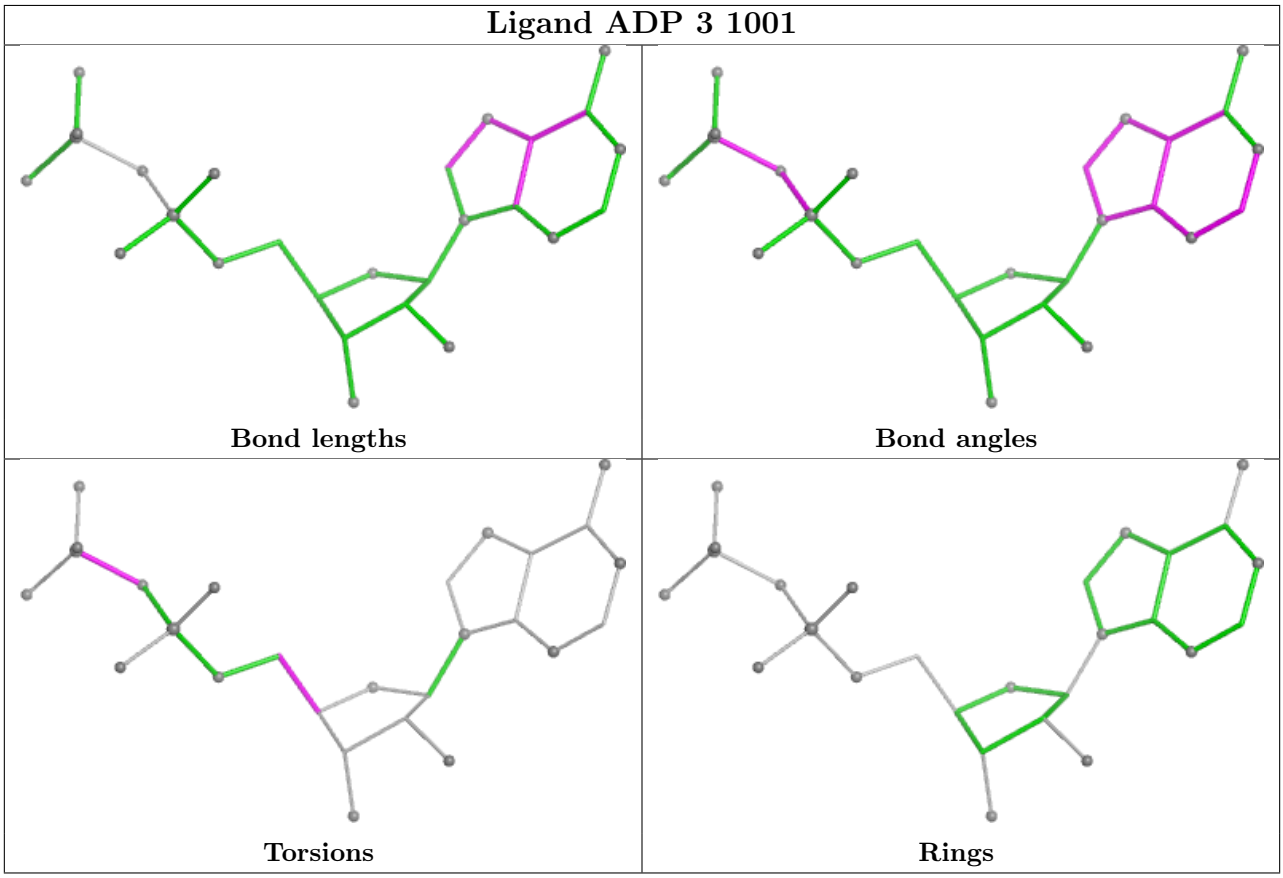
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Mol	Chain	Res	Type	Atoms
15	5	1001	ATP	C4'-C5'-O5'-PA
14	2	1001	ADP	C3'-C4'-C5'-O5'
14	3	1001	ADP	O4'-C4'-C5'-O5'

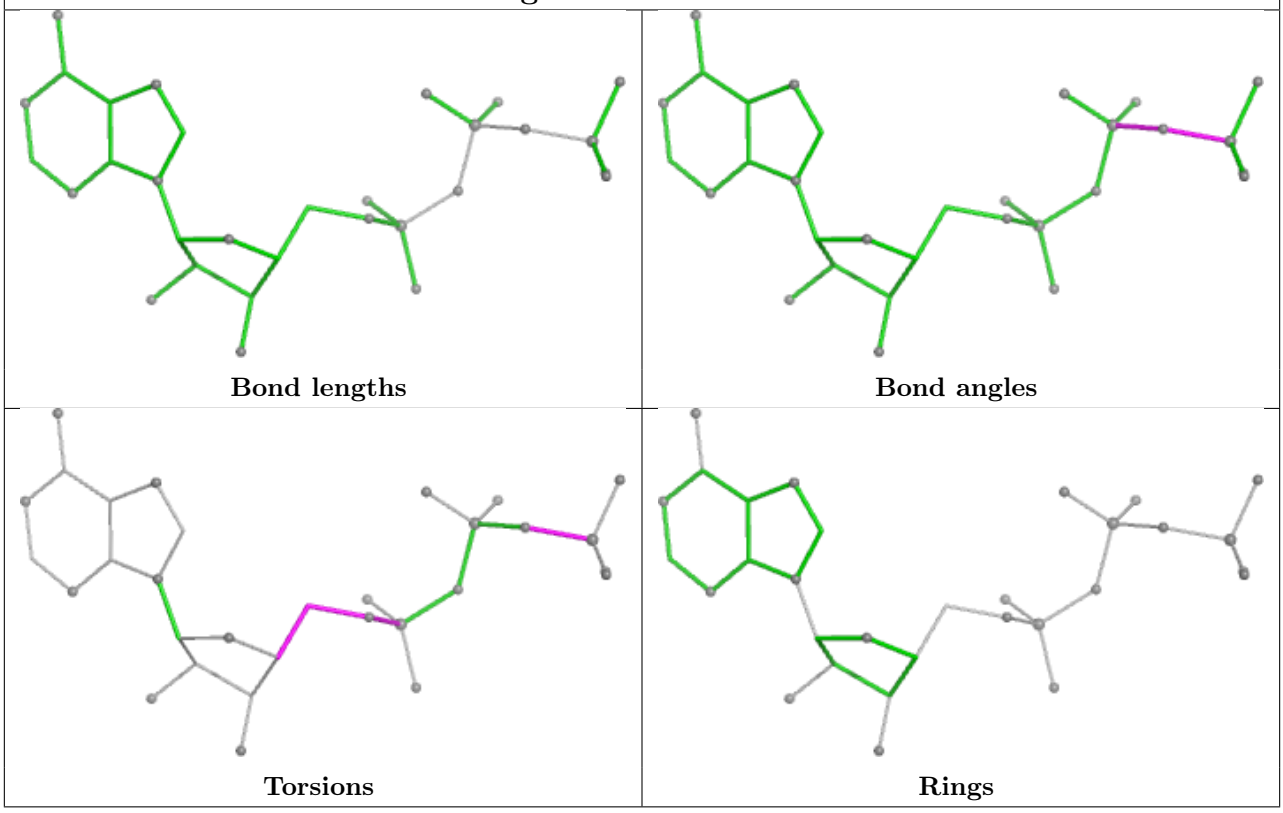
There are no ring outliers.

No monomer is involved in short contacts.

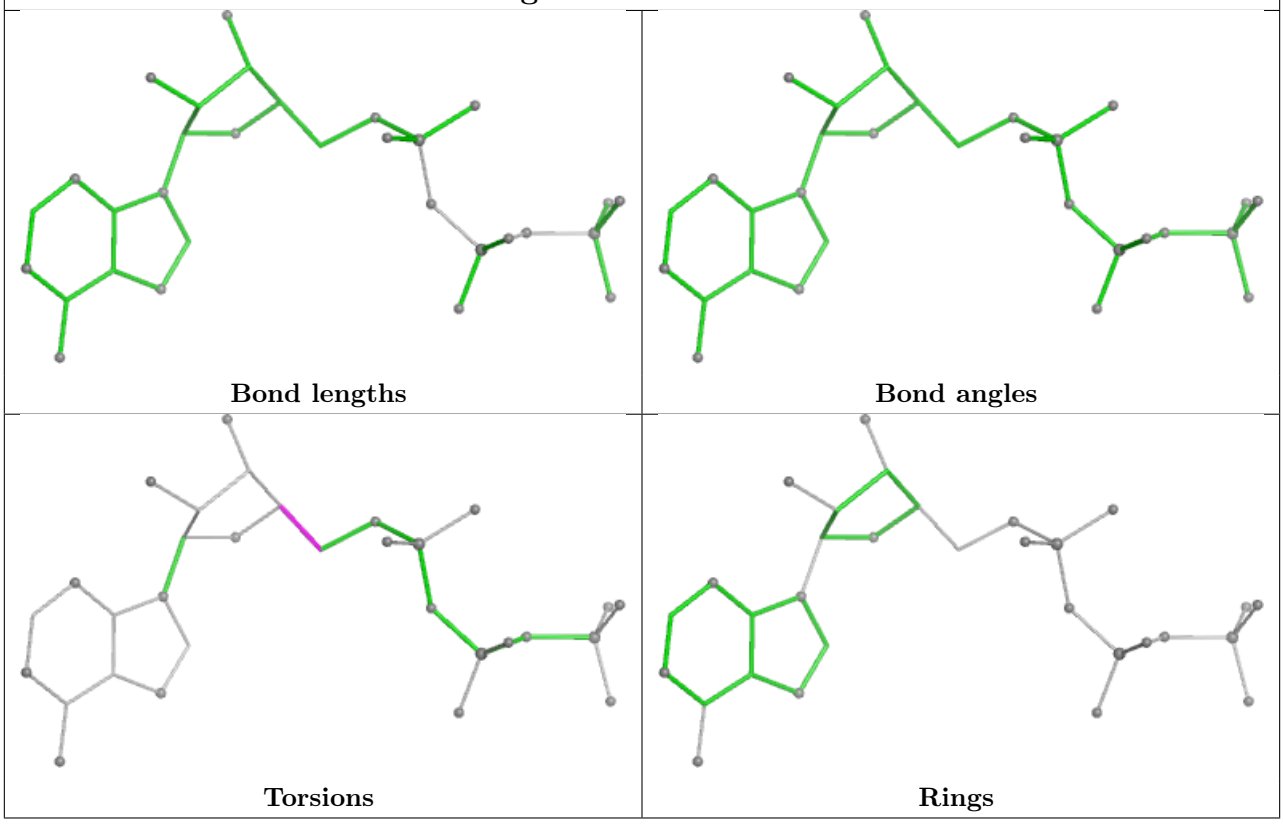
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



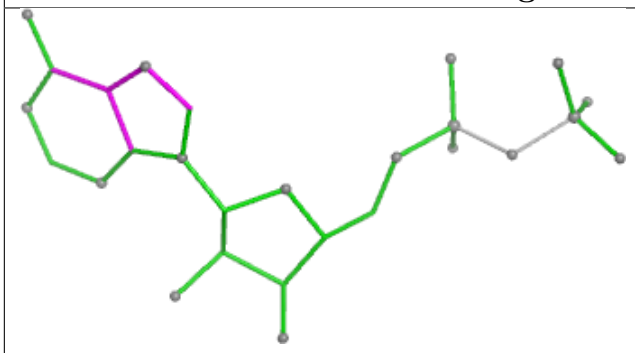
Ligand ATP 5 1001



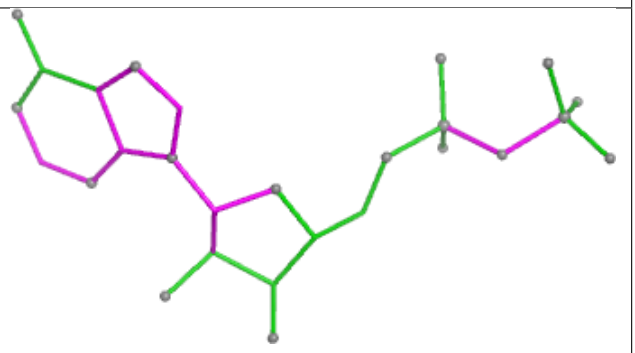
Ligand ATP 6 1001



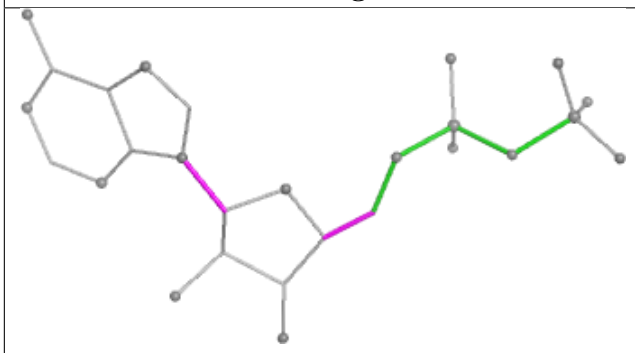
Ligand ADP 2 1001



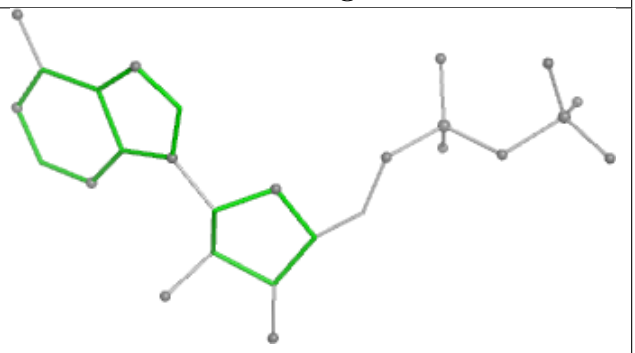
Bond lengths



Bond angles

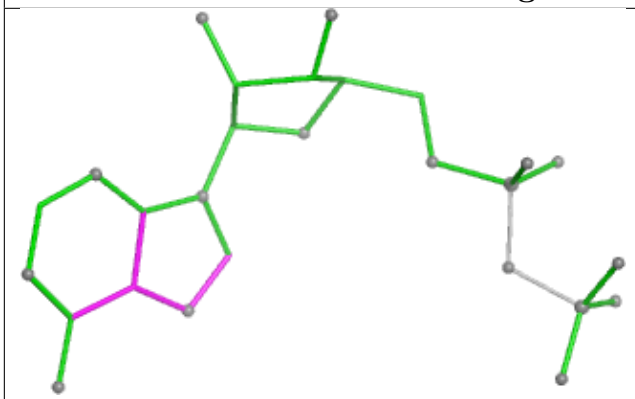


Torsions

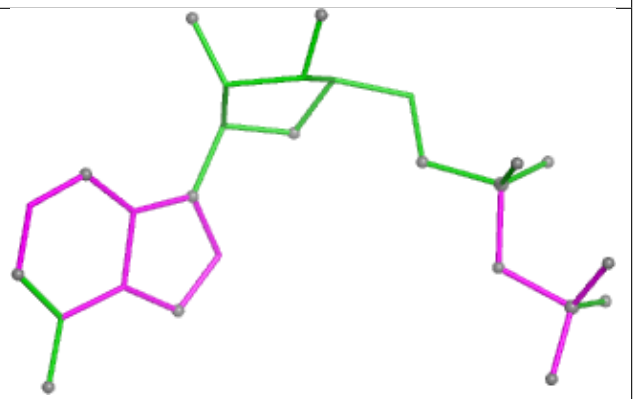


Rings

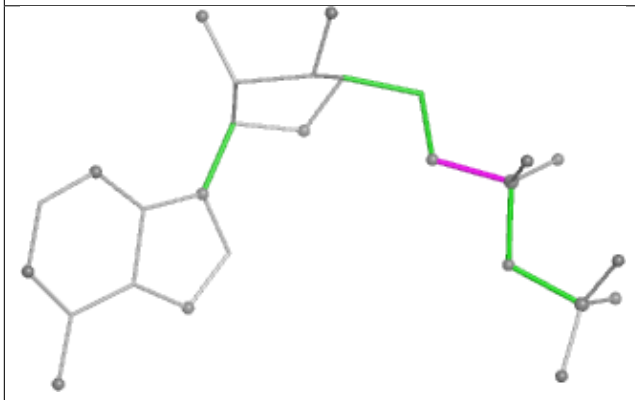
Ligand ADP 7 1001



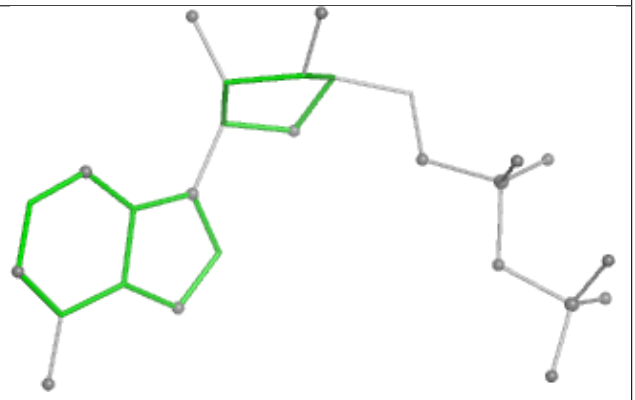
Bond lengths



Bond angles

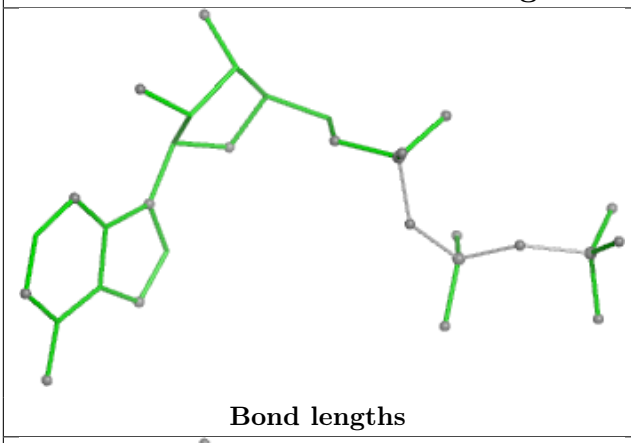


Torsions

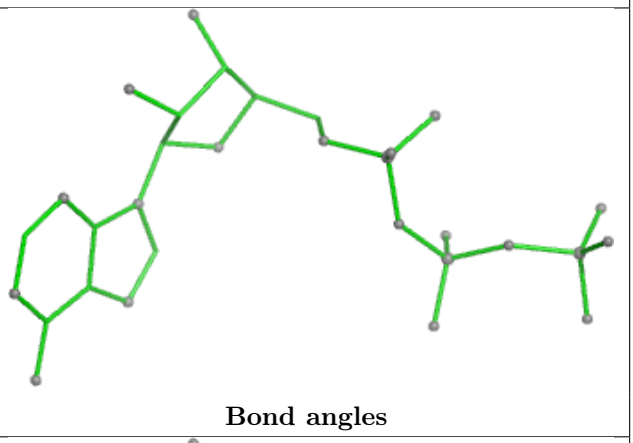


Rings

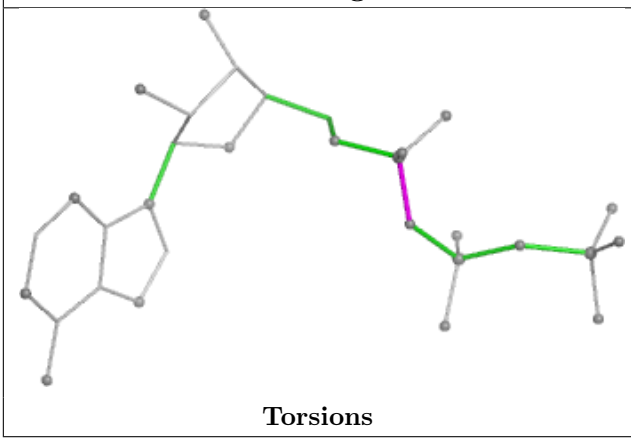
Ligand ATP 4 1001



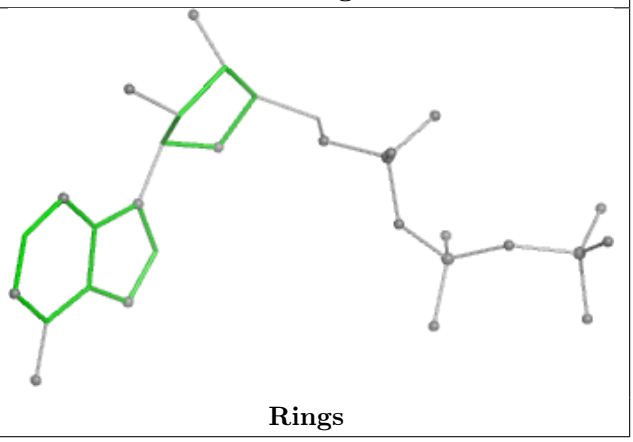
Bond lengths



Bond angles



Torsions



Rings

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.

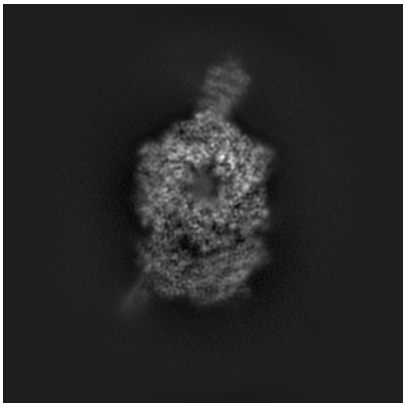
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-57512. These allow visual inspection of the internal detail of the map and identification of artifacts.

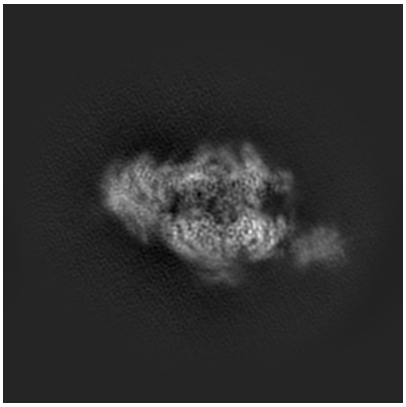
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

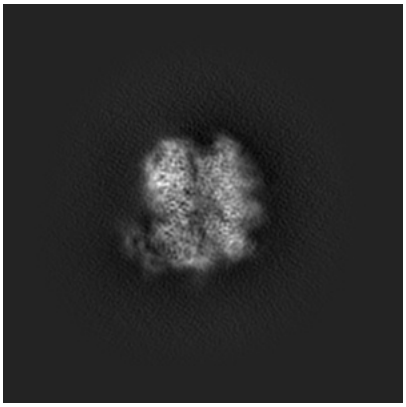
6.1.1 Primary map



X



Y

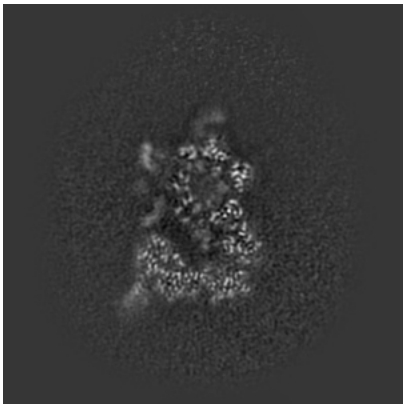


Z

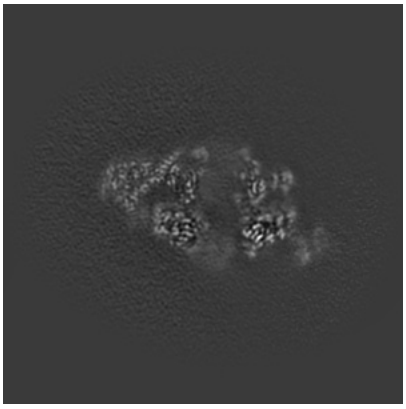
The images above show the map projected in three orthogonal directions.

6.2 Central slices

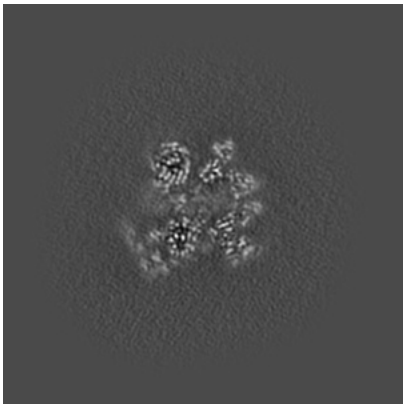
6.2.1 Primary map



X Index: 220



Y Index: 220

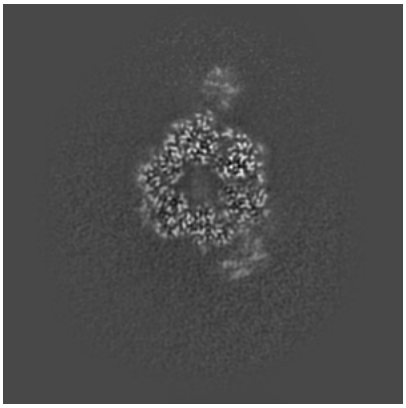


Z Index: 220

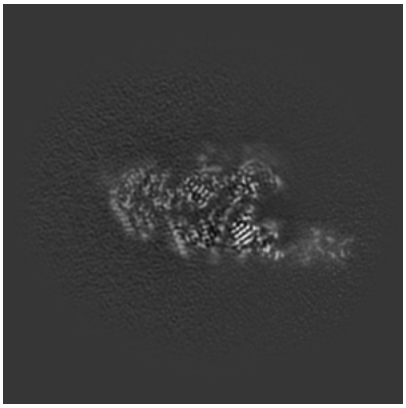
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

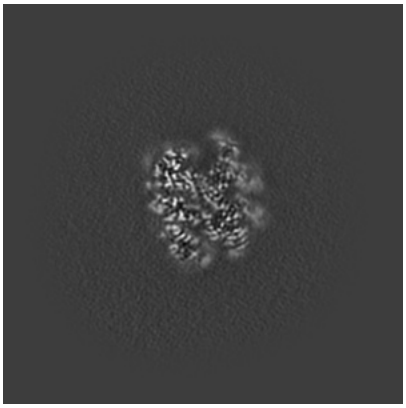
6.3.1 Primary map



X Index: 187



Y Index: 251

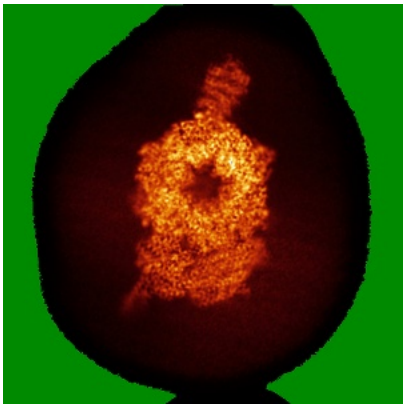


Z Index: 271

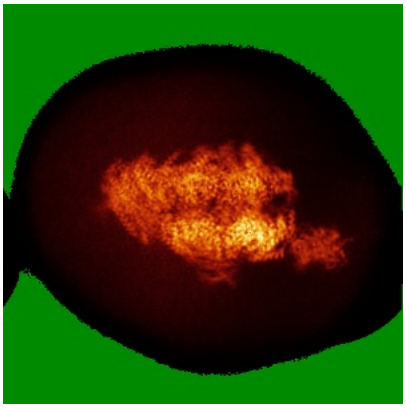
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

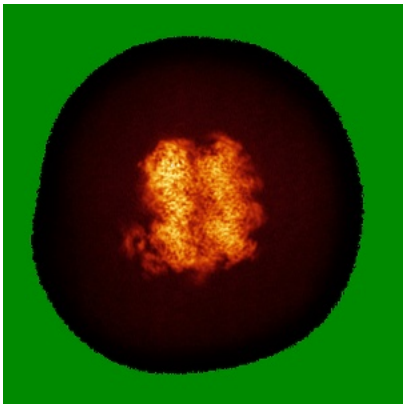
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

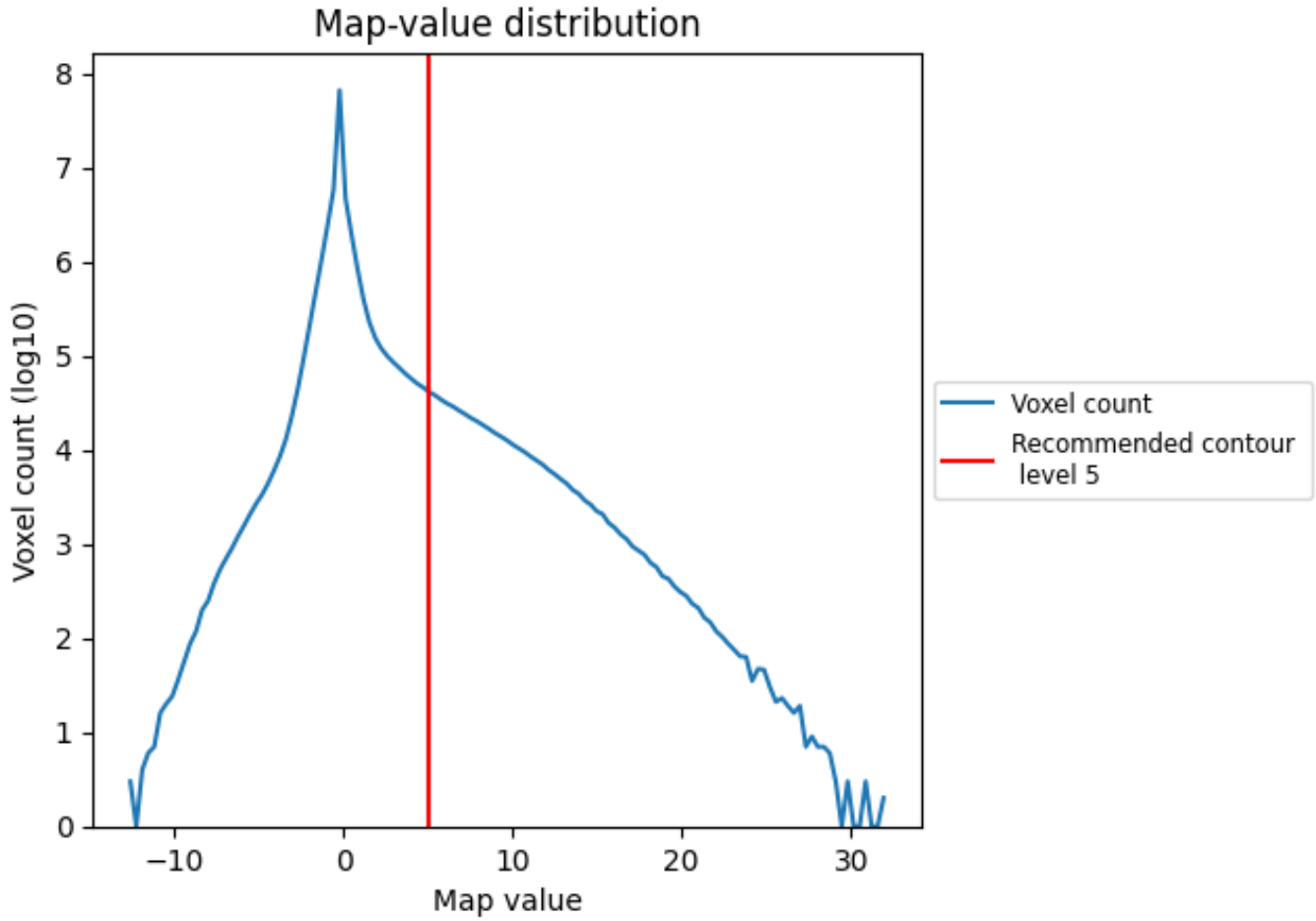
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

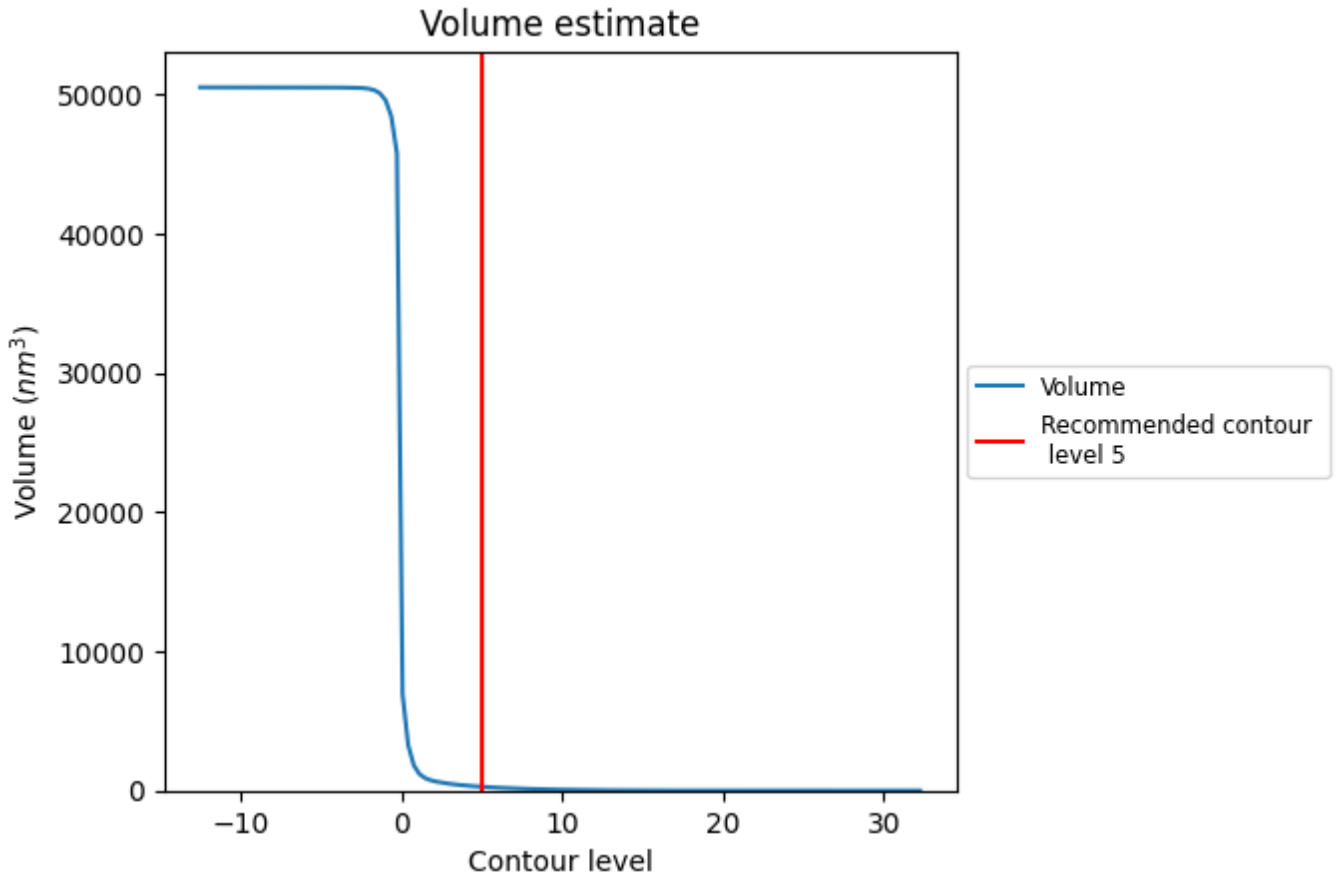
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

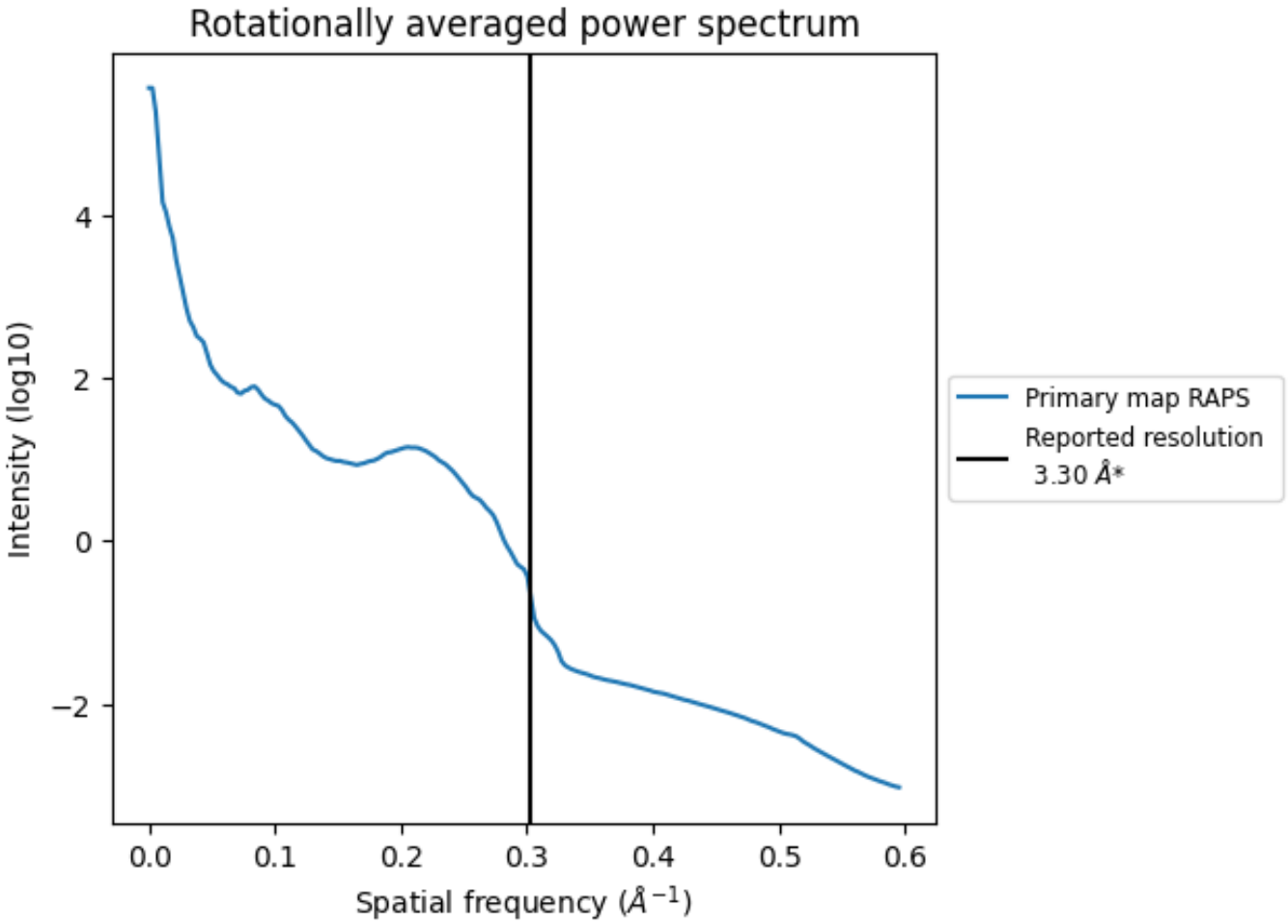
7.2 Volume estimate (i)



The volume at the recommended contour level is 270 nm^3; this corresponds to an approximate mass of 244 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

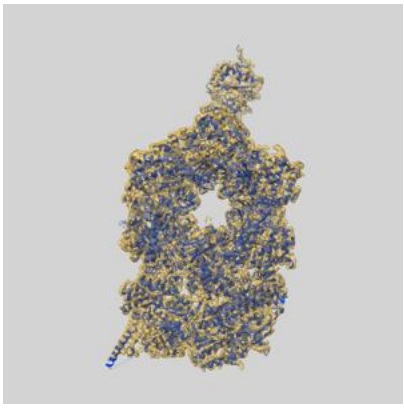
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

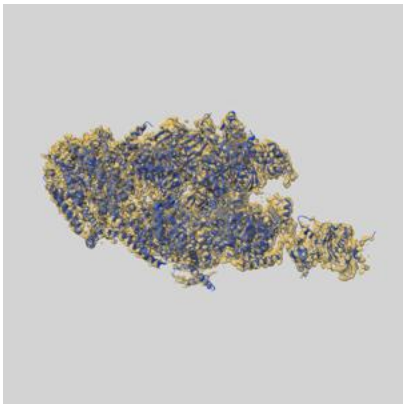
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-57512 and PDB model 30AR. Per-residue inclusion information can be found in section 3 on page 8.

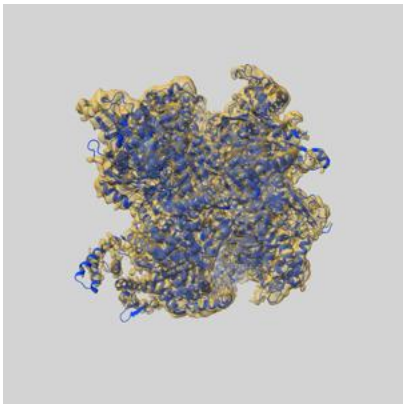
9.1 Map-model overlay



X



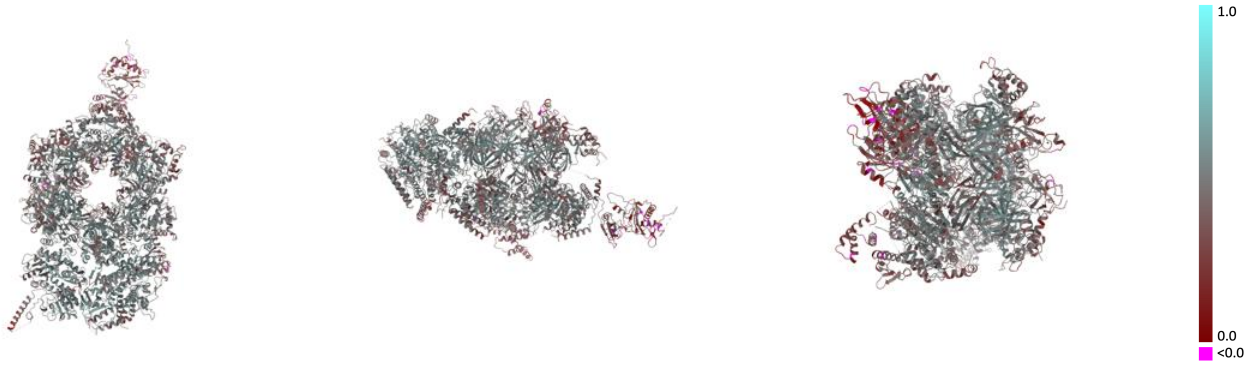
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

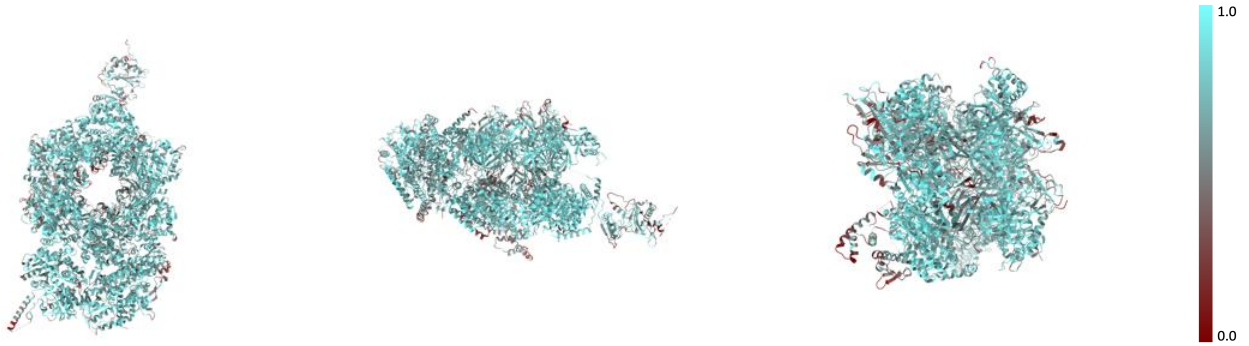
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

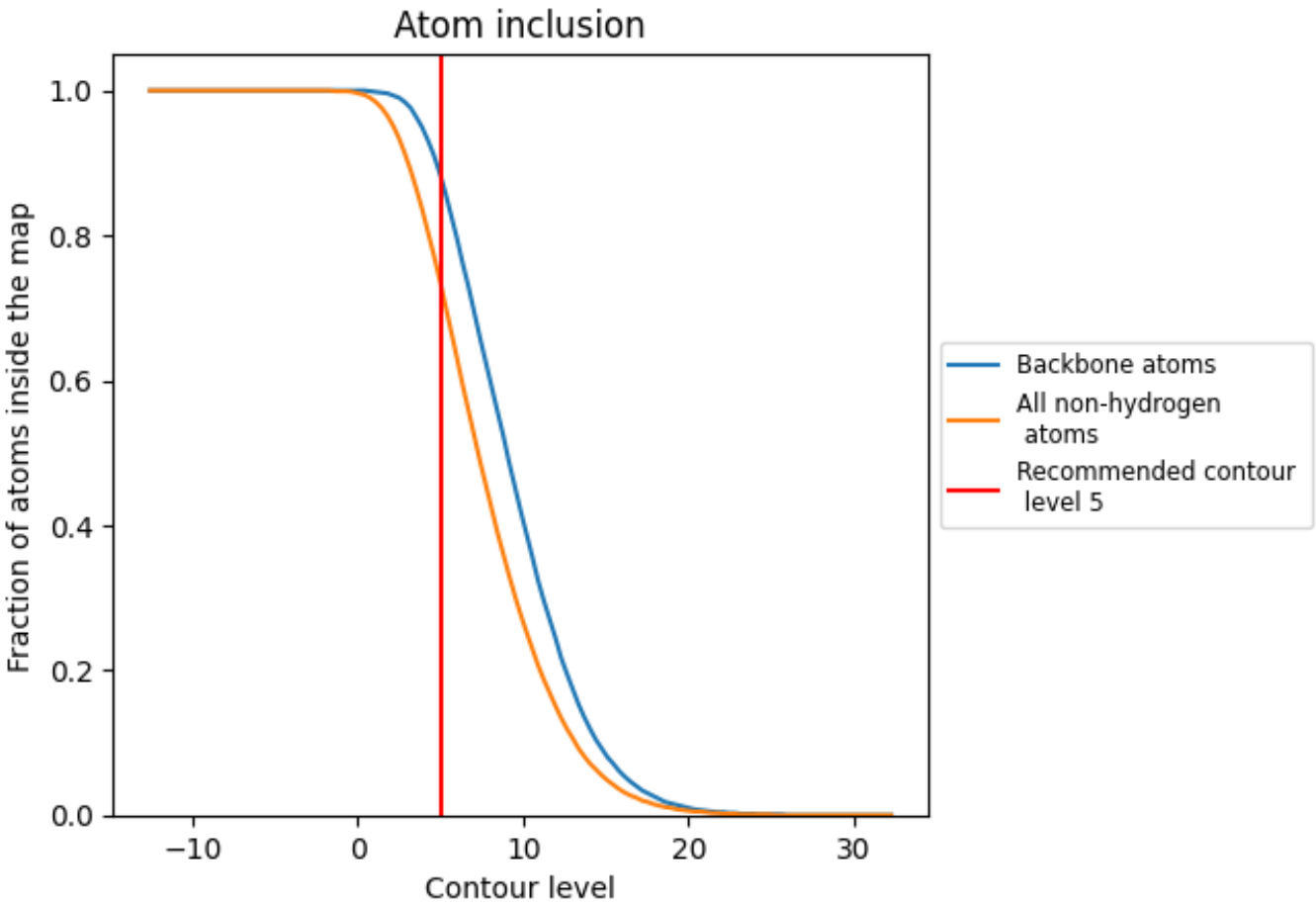
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7350	0.4490
2	0.7320	0.4520
3	0.7340	0.4620
4	0.7930	0.4490
5	0.7370	0.4810
6	0.7100	0.4210
7	0.7780	0.4530
C	0.7370	0.4750
G	0.7260	0.4710
I	0.6720	0.4520
N	0.7990	0.5210
P	0.6190	0.2920
S	0.7250	0.4800

