wwPDB EM Validation Summary Report ⓘ

Jul 8, 2024 – 12:27 am BST

PDB ID	:	7QHS
EMDB ID	:	EMD-13978
Title	:	S. cerevisiae CMGE nucleating origin DNA melting
Authors	:	Lewis, J.S.; Sousa, J.S.; Costa, A.
Deposited on	:	2021-12-14
Resolution	:	3.30 Å(reported)
Based on initial models	:	6SKL, 6HV9

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

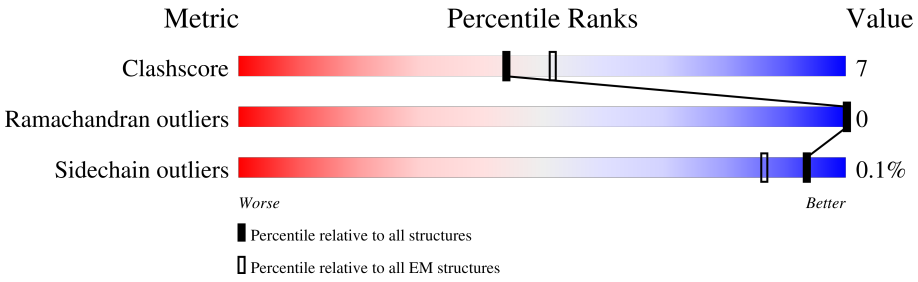
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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

Mol	Chain	Length	Quality of chain
1	2	868	66% 10% 24%
2	3	1006	56% 7% 37%
3	4	933	48% 17% 35%
4	6	1017	52% 10% 38%
5	7	845	60% 18% 22%
6	H	208	75% 25%
7	I	213	75% 14% 11%
8	C	229	67% 9% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	D	294	
10	E	657	
11	F	689	
12	G	2222	
13	A	26	
14	B	26	
15	5	775	

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 53670 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	660	Total	C	N	O	S	0	0
			5231	3284	937	991	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	633	Total	C	N	O	S	0	0
			4958	3119	882	944	13		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-34	MET	-	initiating methionine	UNP P24279
3	-33	LYS	-	expression tag	UNP P24279
3	-32	ARG	-	expression tag	UNP P24279
3	-31	ARG	-	expression tag	UNP P24279
3	-30	TRP	-	expression tag	UNP P24279
3	-29	LYS	-	expression tag	UNP P24279
3	-28	LYS	-	expression tag	UNP P24279
3	-27	ASN	-	expression tag	UNP P24279
3	-26	PHE	-	expression tag	UNP P24279
3	-25	ILE	-	expression tag	UNP P24279
3	-24	ALA	-	expression tag	UNP P24279
3	-23	VAL	-	expression tag	UNP P24279
3	-22	SER	-	expression tag	UNP P24279
3	-21	ALA	-	expression tag	UNP P24279
3	-20	ALA	-	expression tag	UNP P24279
3	-19	ASN	-	expression tag	UNP P24279
3	-18	ARG	-	expression tag	UNP P24279
3	-17	PHE	-	expression tag	UNP P24279
3	-16	LYS	-	expression tag	UNP P24279
3	-15	LYS	-	expression tag	UNP P24279
3	-14	ILE	-	expression tag	UNP P24279

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
3	-13	SER	-	expression tag	UNP P24279
3	-12	SER	-	expression tag	UNP P24279
3	-11	SER	-	expression tag	UNP P24279
3	-10	GLY	-	expression tag	UNP P24279
3	-9	ALA	-	expression tag	UNP P24279
3	-8	LEU	-	expression tag	UNP P24279
3	-7	GLU	-	expression tag	UNP P24279
3	-6	ASN	-	expression tag	UNP P24279
3	-5	LEU	-	expression tag	UNP P24279
3	-4	TYR	-	expression tag	UNP P24279
3	-3	PHE	-	expression tag	UNP P24279
3	-2	GLN	-	expression tag	UNP P24279
3	-1	GLY	-	expression tag	UNP P24279
3	0	GLU	-	expression tag	UNP P24279

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	609	Total	C	N	O	S	0	0
			4850	3055	838	930	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	629	Total	C	N	O	S	0	0
			4972	3134	867	946	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	658	Total	C	N	O	S	0	0
			5181	3268	897	987	29		

- Molecule 6 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	208	Total	C	N	O	S	0	0
			1697	1065	290	332	10		

- Molecule 7 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	189	Total	C	N	O	S	0	0
			1581	1018	277	282	4		

- Molecule 8 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	173	Total	C	N	O	S	0	0
			1398	911	224	256	7		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-34	TRP	-	expression tag	UNP Q12146
C	-33	SER	-	expression tag	UNP Q12146
C	-32	HIS	-	expression tag	UNP Q12146
C	-31	PRO	-	expression tag	UNP Q12146
C	-30	GLN	-	expression tag	UNP Q12146
C	-29	PHE	-	expression tag	UNP Q12146
C	-28	GLU	-	expression tag	UNP Q12146
C	-27	LYS	-	expression tag	UNP Q12146
C	-26	GLY	-	expression tag	UNP Q12146
C	-25	GLY	-	expression tag	UNP Q12146
C	-24	GLY	-	expression tag	UNP Q12146
C	-23	SER	-	expression tag	UNP Q12146
C	-22	GLY	-	expression tag	UNP Q12146
C	-21	GLY	-	expression tag	UNP Q12146
C	-20	GLY	-	expression tag	UNP Q12146
C	-19	SER	-	expression tag	UNP Q12146
C	-18	GLY	-	expression tag	UNP Q12146
C	-17	GLY	-	expression tag	UNP Q12146
C	-16	GLY	-	expression tag	UNP Q12146
C	-15	SER	-	expression tag	UNP Q12146
C	-14	TRP	-	expression tag	UNP Q12146
C	-13	SER	-	expression tag	UNP Q12146
C	-12	HIS	-	expression tag	UNP Q12146
C	-11	PRO	-	expression tag	UNP Q12146
C	-10	GLN	-	expression tag	UNP Q12146
C	-9	PHE	-	expression tag	UNP Q12146
C	-8	GLU	-	expression tag	UNP Q12146
C	-7	LYS	-	expression tag	UNP Q12146
C	-6	GLU	-	expression tag	UNP Q12146
C	-5	ASN	-	expression tag	UNP Q12146
C	-4	LEU	-	expression tag	UNP Q12146

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	TYR	-	expression tag	UNP Q12146
C	-2	PHE	-	expression tag	UNP Q12146
C	-1	GLN	-	expression tag	UNP Q12146
C	0	SER	-	expression tag	UNP Q12146

- Molecule 9 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	242	Total	C	N	O	S	0	0
			1990	1267	328	381	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	566	Total	C	N	O	S	0	0
			4599	2937	778	870	14		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	167G	TYR	GLU	conflict	UNP Q08032
E	167H	LYS	GLU	conflict	UNP Q08032
E	167J	ASP	GLU	conflict	UNP Q08032
E	167L	GLY	-	insertion	UNP Q08032
E	167M	ASP	-	insertion	UNP Q08032
E	167N	TYR	-	insertion	UNP Q08032
E	167O	LYS	-	insertion	UNP Q08032
E	167P	ASP	-	insertion	UNP Q08032
E	167Q	ASP	-	insertion	UNP Q08032
E	167R	ASP	-	insertion	UNP Q08032

- Molecule 11 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	551	Total	C	N	O	S	0	0
			4396	2819	755	804	18		

- Molecule 12 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	756	Total	C	N	O	S	0	0
			6113	3956	1006	1114	37		

- Molecule 13 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	26	Total	C	N	O	P	0	0
			546	260	130	130	26		

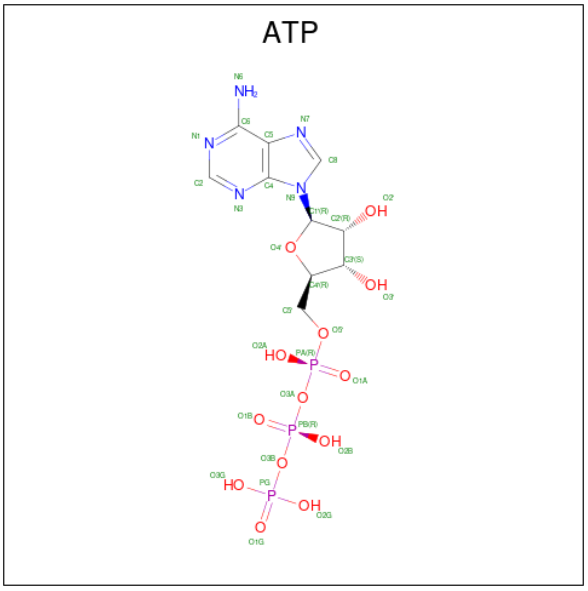
- Molecule 14 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	26	Total	C	N	O	P	0	0
			520	260	52	182	26		

- Molecule 15 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	690	Total	C	N	O	S	0	0
			5450	3423	948	1055	24		

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	2	1	Total	C	N	O	P	0
			31	10	5	13	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
16	3	1	Total	C	N	O	P	0
			31	10	5	13	3	
16	7	1	Total	C	N	O	P	0
			31	10	5	13	3	
16	5	1	Total	C	N	O	P	0
			31	10	5	13	3	

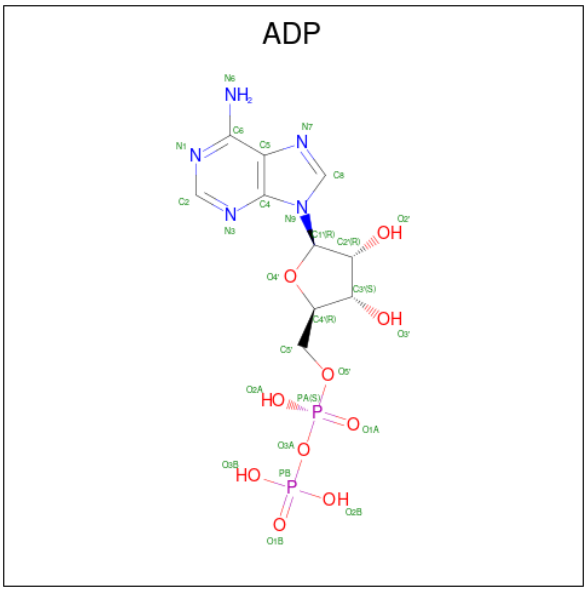
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	2	1	Total	Zn	0
			1	1	
17	4	1	Total	Zn	0
			1	1	
17	6	1	Total	Zn	0
			1	1	
17	7	1	Total	Zn	0
			1	1	
17	G	2	Total	Zn	0
			2	2	
17	5	1	Total	Zn	0
			1	1	

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	3	1	Total	Mg	0
			1	1	
18	7	1	Total	Mg	0
			1	1	
18	5	1	Total	Mg	0
			1	1	

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



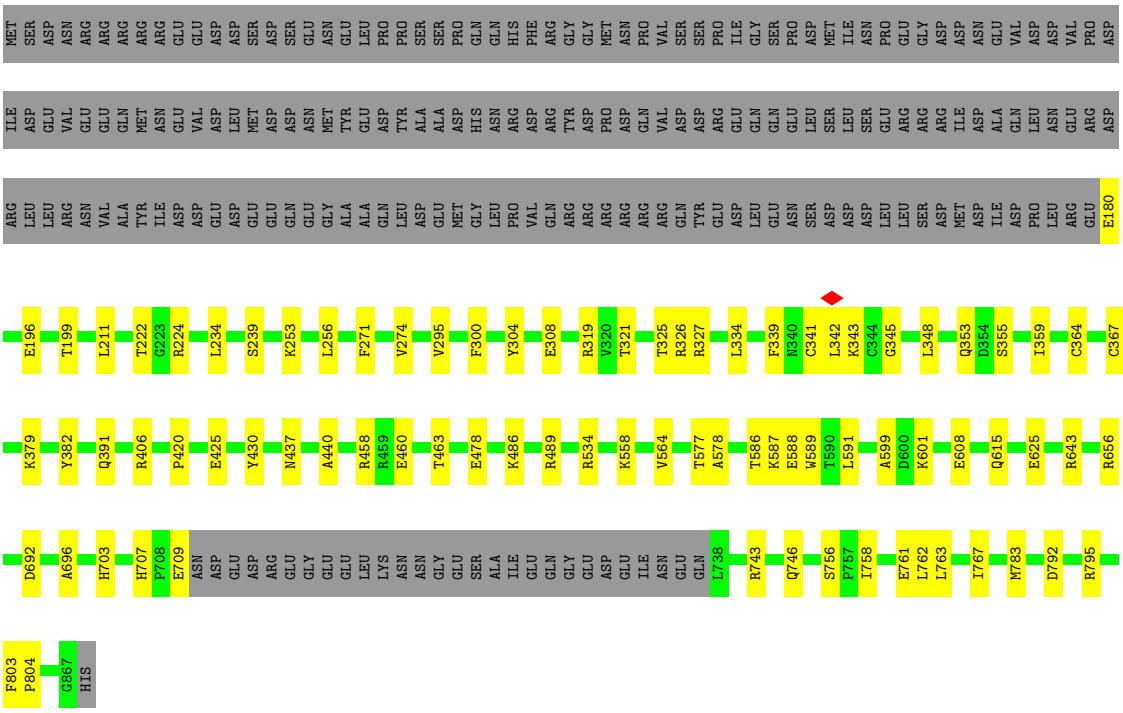
Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	6	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

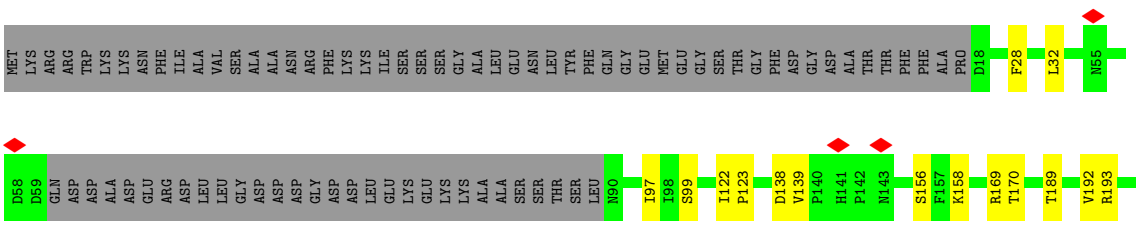
• Molecule 1: DNA replication licensing factor MCM2

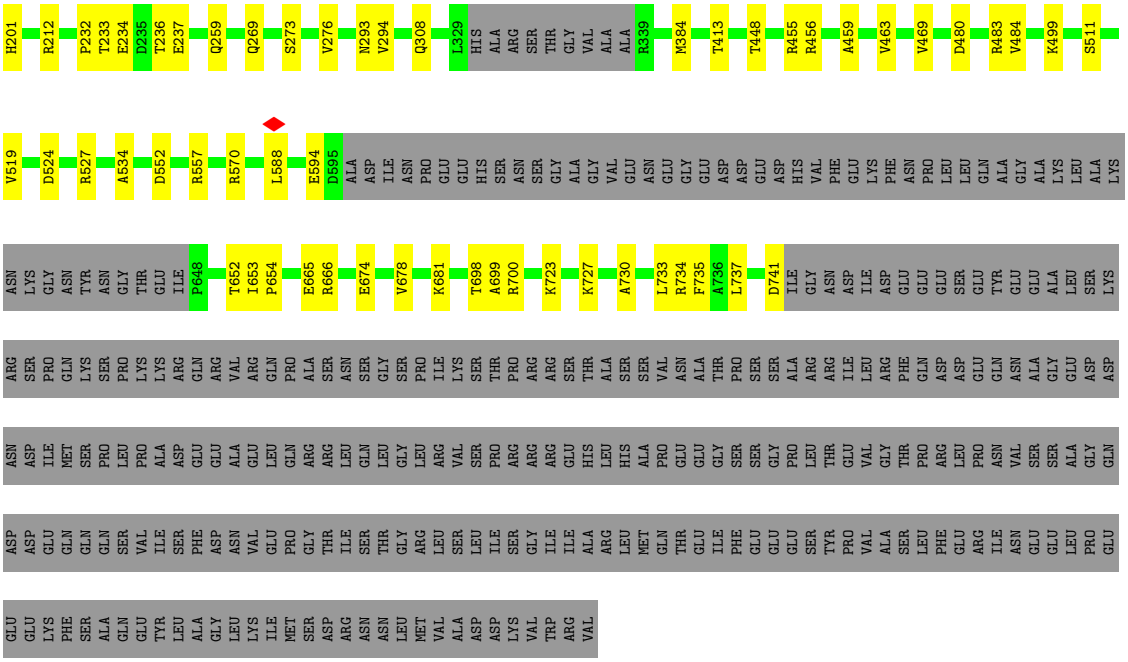
Chain 2:



• Molecule 2: DNA replication licensing factor MCM3

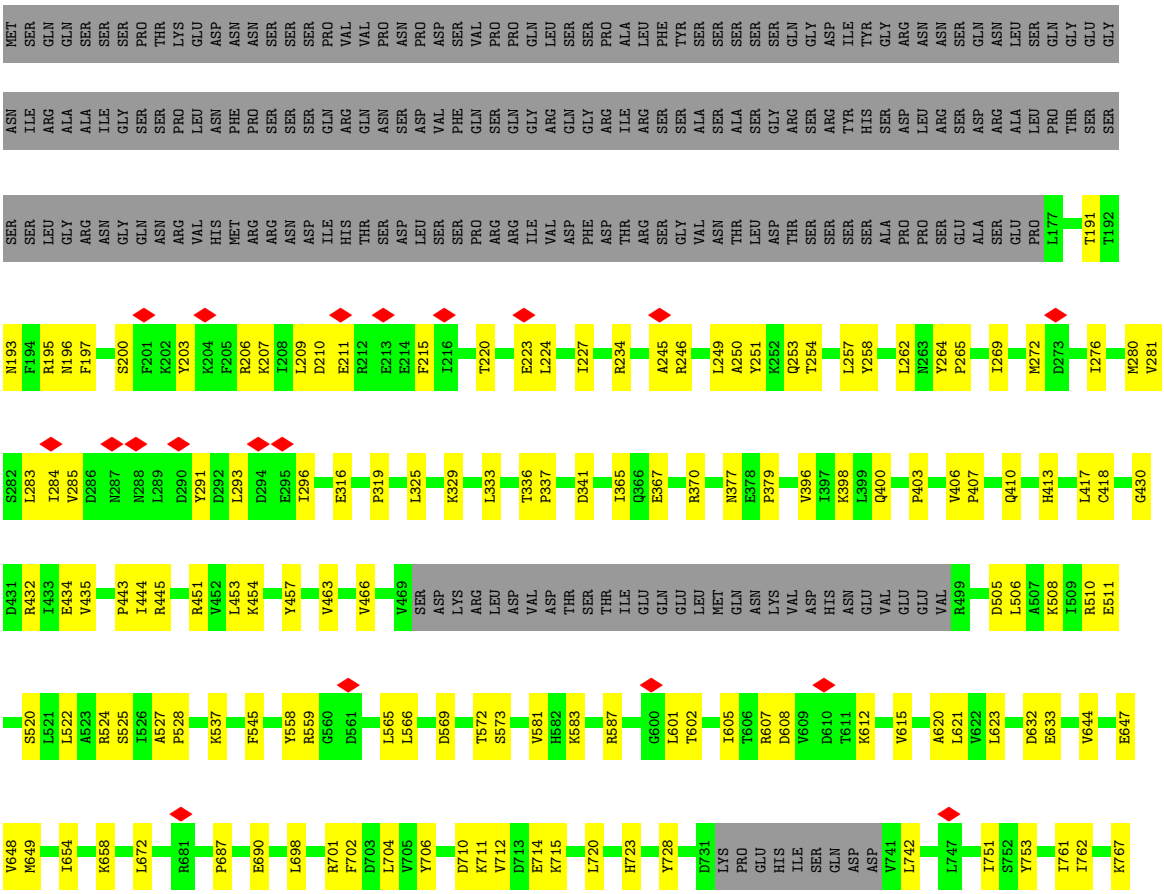
Chain 3:

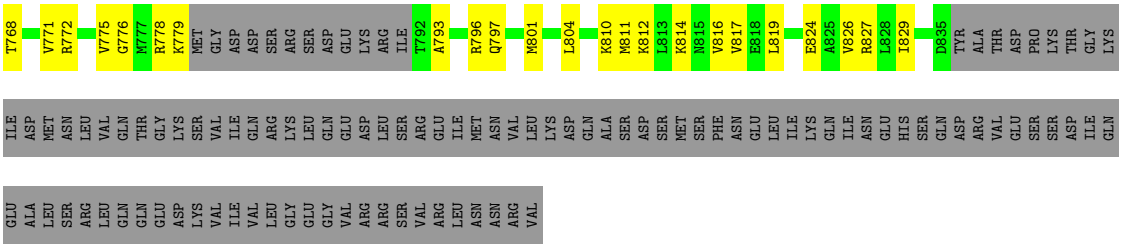




• Molecule 3: DNA replication licensing factor MCM4

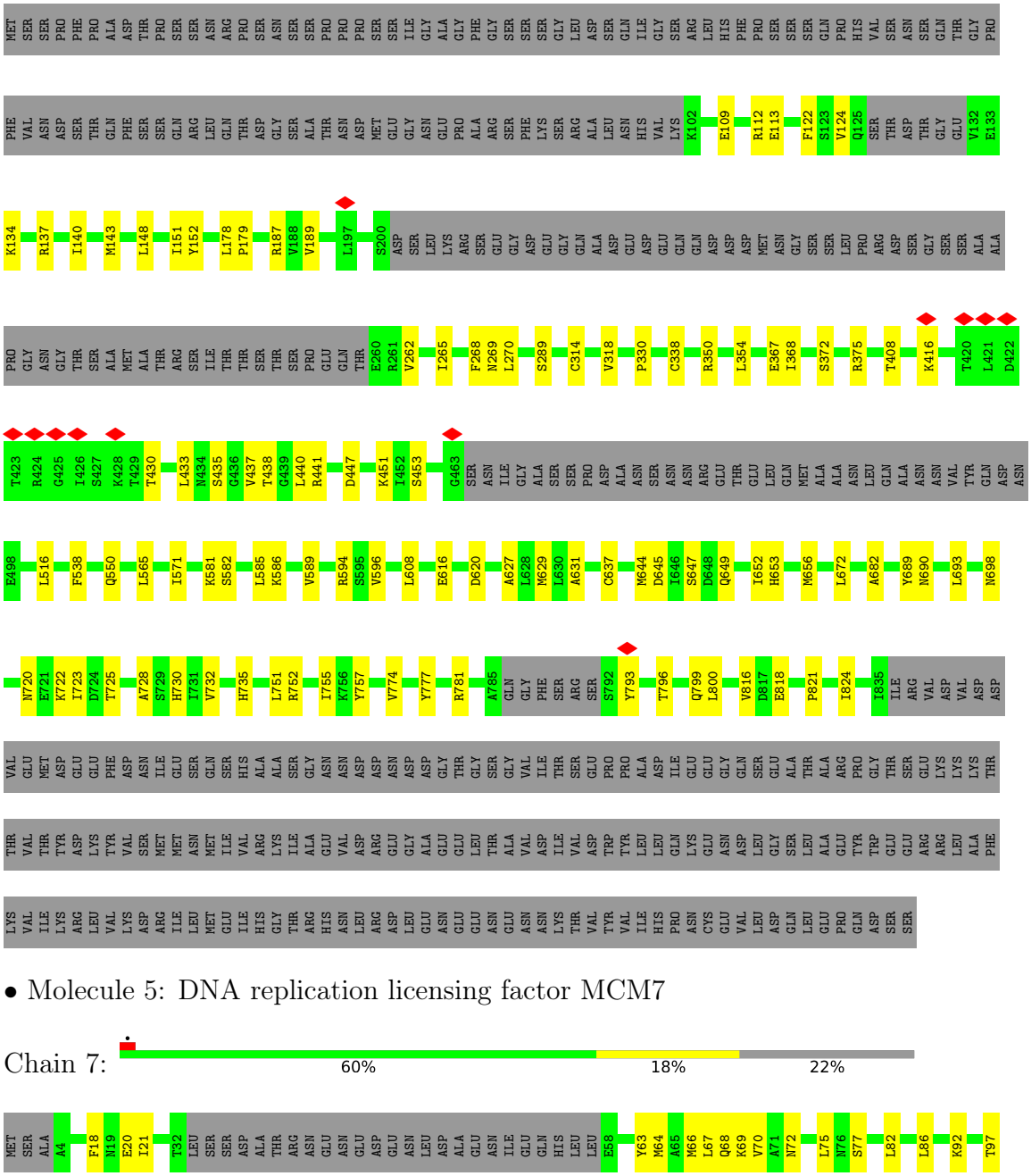
Chain 4:





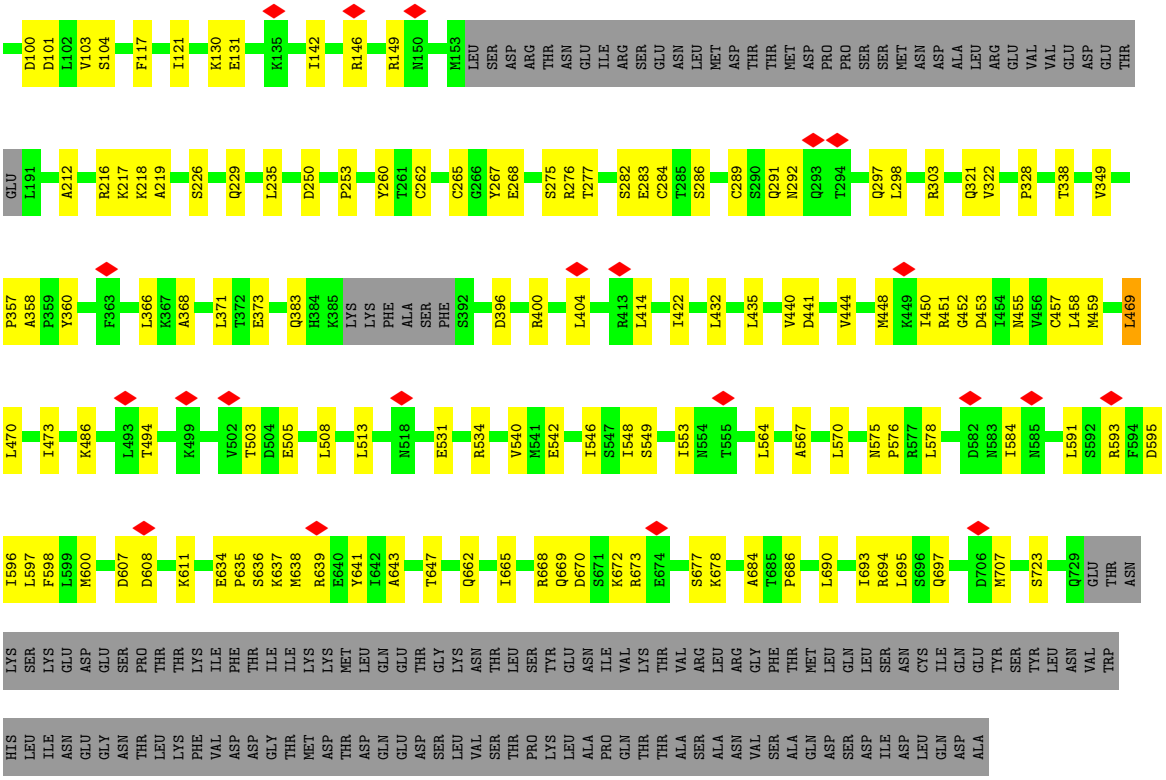
• Molecule 4: DNA replication licensing factor MCM6

Chain 6:



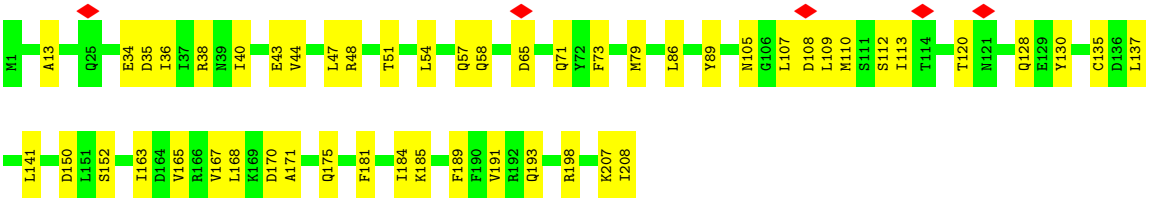
• Molecule 5: DNA replication licensing factor MCM7

Chain 7:



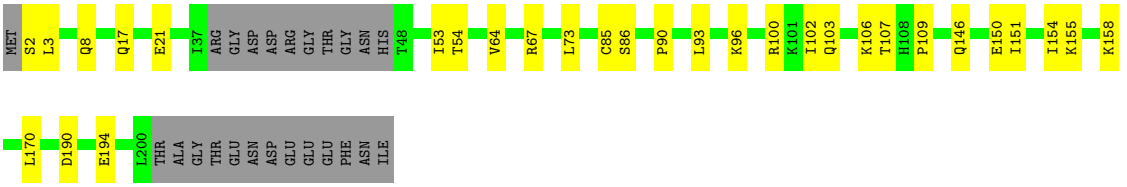
• Molecule 6: DNA replication complex GINS protein PSF1

Chain H:



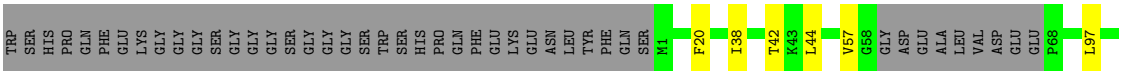
• Molecule 7: DNA replication complex GINS protein PSF2

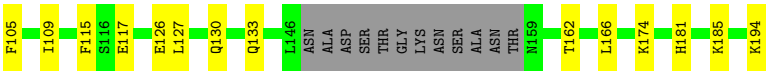
Chain I:



• Molecule 8: DNA replication complex GINS protein PSF3

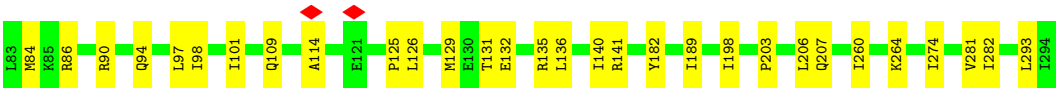
Chain C:





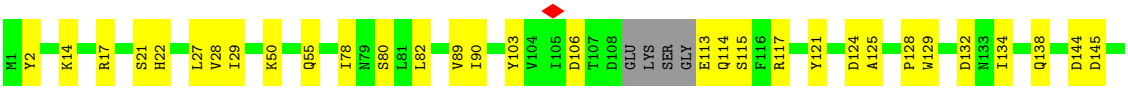
• Molecule 9: DNA replication complex GINS protein SLD5

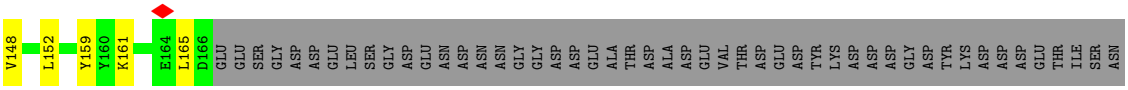
Chain D:

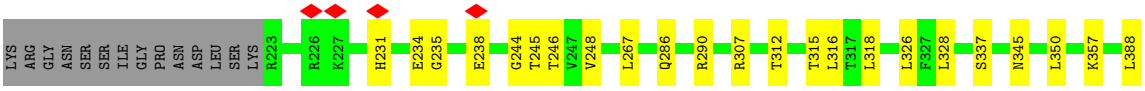


• Molecule 10: Cell division control protein 45

Chain E:

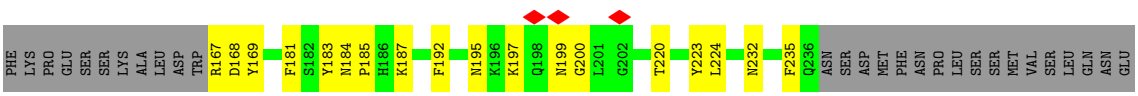


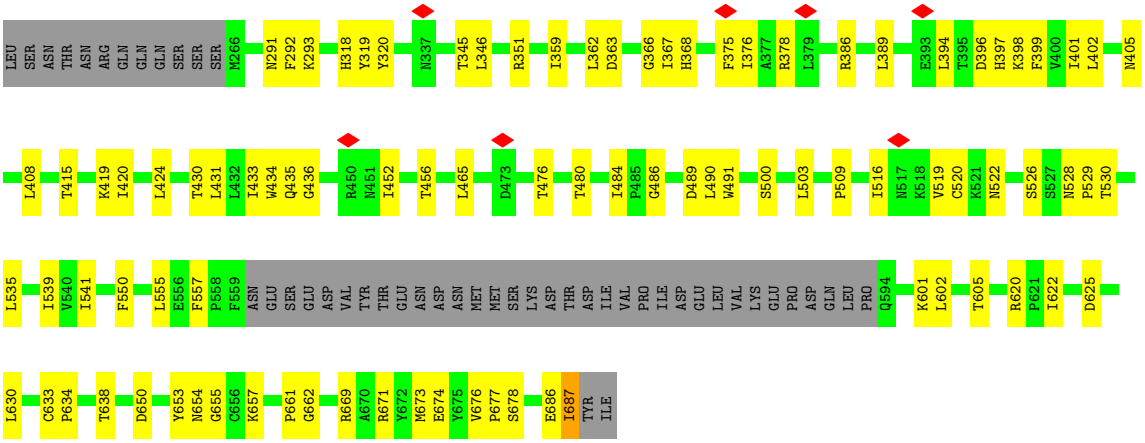




• Molecule 11: DNA polymerase epsilon subunit B

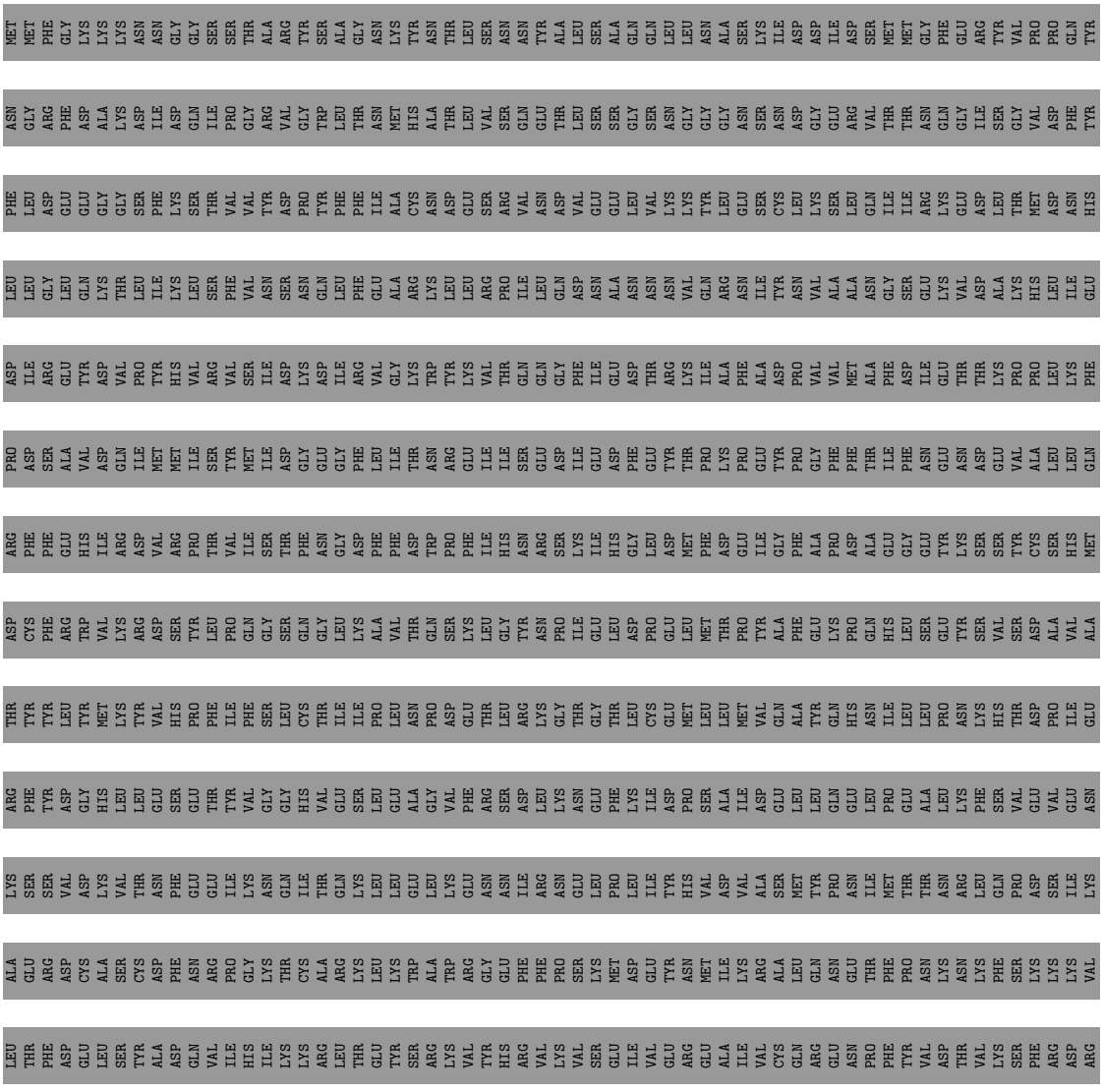
Chain F:

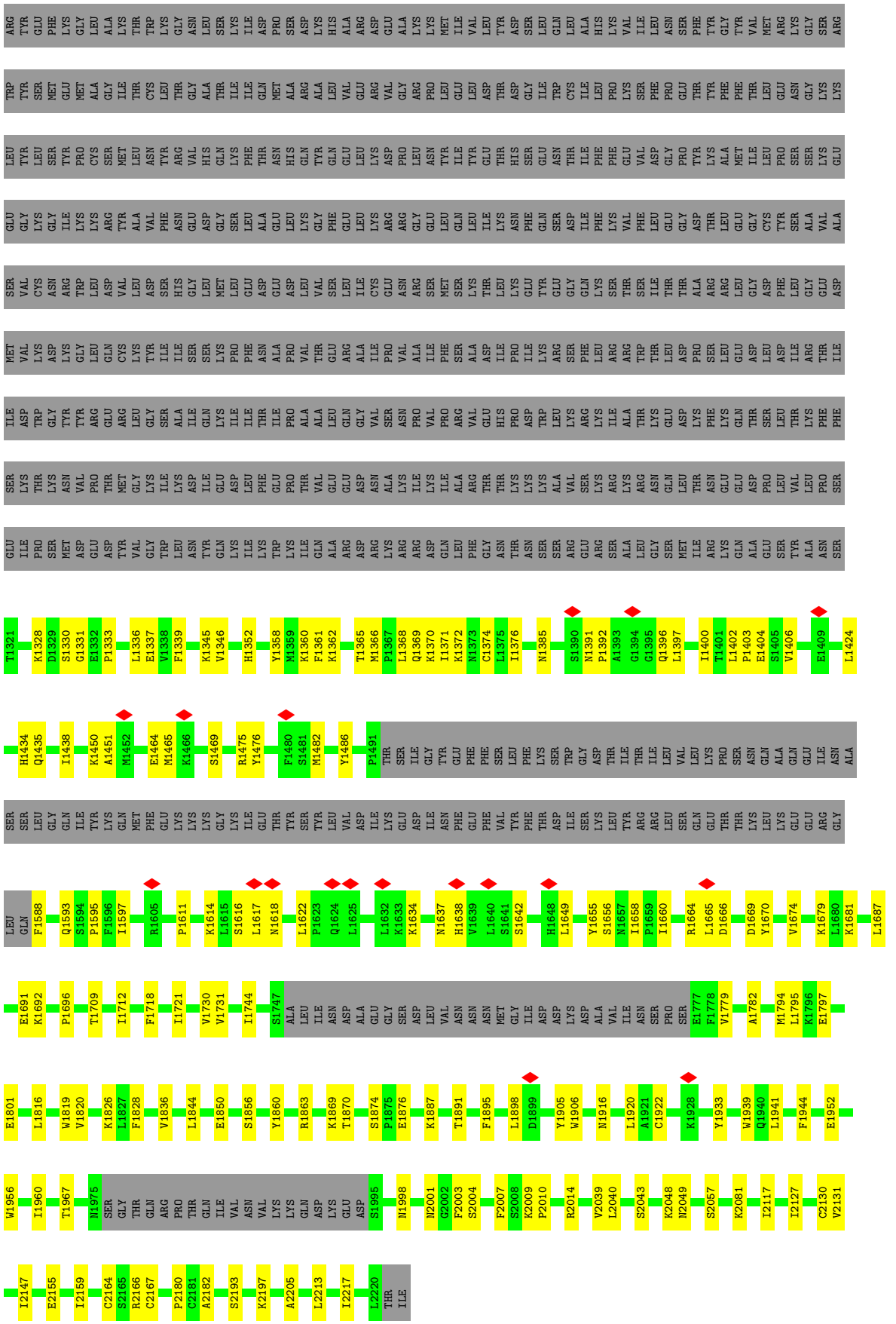




• Molecule 12: DNA polymerase epsilon catalytic subunit A

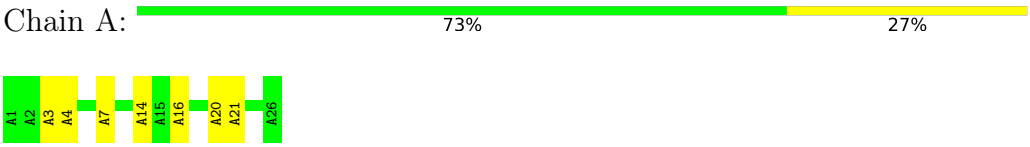
Chain G:





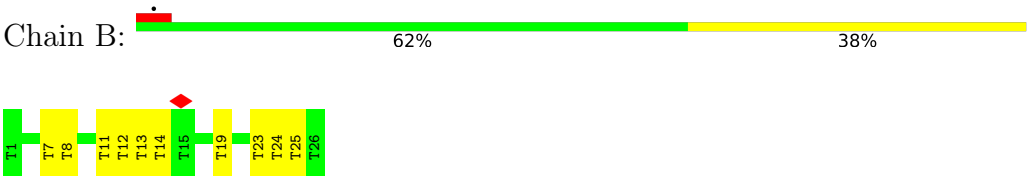
• Molecule 13: DNA (26-MER)

Chain A:



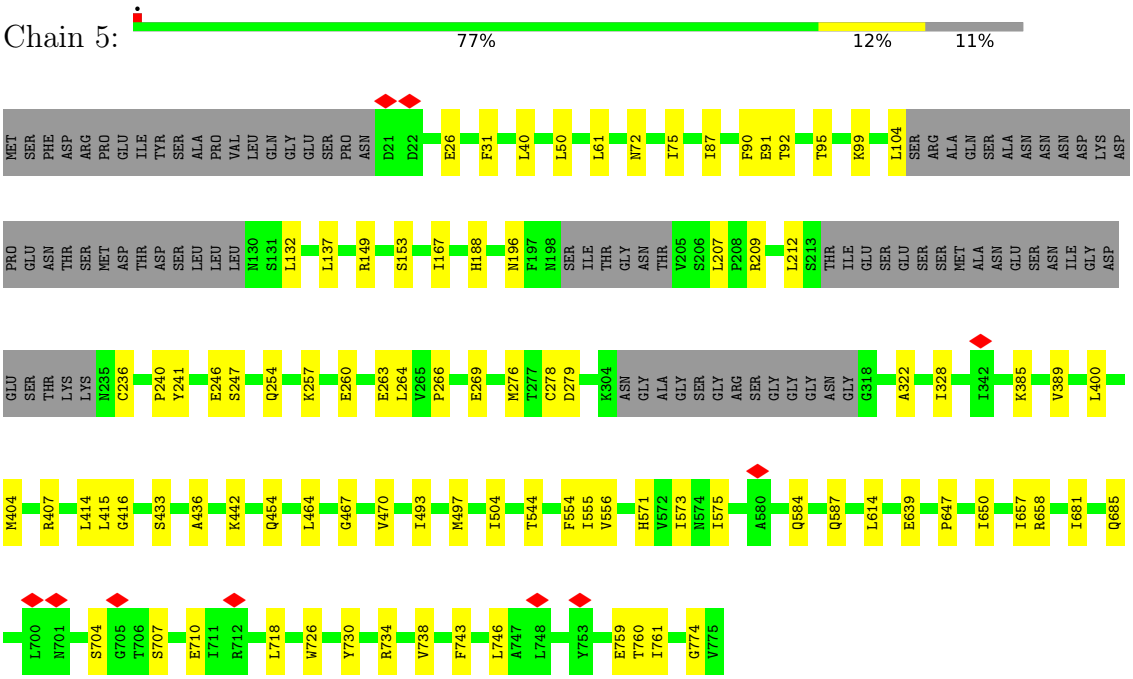
• Molecule 14: DNA (26-MER)

Chain B:



• Molecule 15: DNA replication licensing factor MCM5

Chain 5:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	71348	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 ($e^-/Å^2$)	1.60	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.913	Depositor
Minimum map value	-0.926	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	221.40001, 209.52, 179.28001	wwPDB
Map dimensions	166, 194, 205	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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, MG, ZN, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	2	0.25	0/5319	0.52	0/7182
2	3	0.24	0/5044	0.50	0/6842
3	4	0.25	0/4921	0.52	0/6651
4	6	0.25	0/5051	0.50	0/6813
5	7	0.27	0/5261	0.51	0/7110
6	H	0.26	0/1719	0.52	0/2314
7	I	0.23	0/1613	0.49	0/2182
8	C	0.24	0/1431	0.41	0/1933
9	D	0.26	0/2032	0.48	0/2750
10	E	0.25	0/4685	0.48	0/6341
11	F	0.27	0/4492	0.51	0/6078
12	G	0.25	0/6250	0.46	0/8458
13	A	0.52	0/623	0.69	0/958
14	B	0.51	0/571	1.28	0/880
15	5	0.25	0/5530	0.50	0/7471
All	All	0.26	0/54542	0.52	0/73963

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	5231	0	5280	58	0
2	3	4958	0	5005	43	0
3	4	4850	0	4926	113	0
4	6	4972	0	5007	68	0
5	7	5181	0	5258	103	0
6	H	1697	0	1698	38	0
7	I	1581	0	1635	21	0
8	C	1398	0	1418	12	0
9	D	1990	0	1985	27	0
10	E	4599	0	4603	52	0
11	F	4396	0	4442	102	0
12	G	6113	0	6177	95	0
13	A	546	0	287	5	0
14	B	520	0	313	8	0
15	5	5450	0	5510	59	0
16	2	31	0	12	0	0
16	3	31	0	12	0	0
16	5	31	0	12	0	0
16	7	31	0	12	1	0
17	2	1	0	0	0	0
17	4	1	0	0	0	0
17	5	1	0	0	0	0
17	6	1	0	0	0	0
17	7	1	0	0	0	0
17	G	2	0	0	0	0
18	3	1	0	0	0	0
18	5	1	0	0	0	0
18	7	1	0	0	0	0
19	4	27	0	12	0	0
19	6	27	0	12	4	0
All	All	53670	0	53616	740	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 7.

The worst 5 of 740 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)
11:F:526:SER:HB2	11:F:530:THR:HG21	1.48	0.91
12:G:1438:ILE:HD11	12:G:1658:ILE:HG23	1.56	0.87
2:3:652:THR:HG22	2:3:654:PRO:HD2	1.59	0.85
12:G:1649:LEU:HB3	12:G:1660:ILE:HD11	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:169:TYR:OH	11:F:368:HIS:ND1	2.20	0.75

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	656/868 (76%)	641 (98%)	15 (2%)	0	100	100
2	3	625/1006 (62%)	609 (97%)	16 (3%)	0	100	100
3	4	601/933 (64%)	579 (96%)	22 (4%)	0	100	100
4	6	619/1017 (61%)	599 (97%)	20 (3%)	0	100	100
5	7	650/845 (77%)	615 (95%)	35 (5%)	0	100	100
6	H	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
7	I	185/213 (87%)	174 (94%)	11 (6%)	0	100	100
8	C	167/229 (73%)	164 (98%)	3 (2%)	0	100	100
9	D	240/294 (82%)	231 (96%)	9 (4%)	0	100	100
10	E	558/657 (85%)	546 (98%)	12 (2%)	0	100	100
11	F	543/689 (79%)	510 (94%)	33 (6%)	0	100	100
12	G	748/2222 (34%)	716 (96%)	32 (4%)	0	100	100
15	5	680/775 (88%)	653 (96%)	27 (4%)	0	100	100
All	All	6478/9956 (65%)	6232 (96%)	246 (4%)	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	578/770 (75%)	578 (100%)	0	100 100
2	3	549/864 (64%)	549 (100%)	0	100 100
3	4	551/848 (65%)	551 (100%)	0	100 100
4	6	549/886 (62%)	548 (100%)	1 (0%)	93 97
5	7	580/753 (77%)	577 (100%)	3 (0%)	88 93
6	H	193/193 (100%)	192 (100%)	1 (0%)	88 93
7	I	179/198 (90%)	179 (100%)	0	100 100
8	C	157/199 (79%)	157 (100%)	0	100 100
9	D	232/279 (83%)	232 (100%)	0	100 100
10	E	512/592 (86%)	511 (100%)	1 (0%)	93 97
11	F	494/629 (78%)	492 (100%)	2 (0%)	91 95
12	G	694/2014 (34%)	694 (100%)	0	100 100
15	5	618/688 (90%)	618 (100%)	0	100 100
All	All	5886/8913 (66%)	5878 (100%)	8 (0%)	93 97

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	F	687	ILE
11	F	167	ARG
6	H	57	GLN
5	7	639	ARG
10	E	307	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	6	698	ASN
15	5	196	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	5	499	GLN
2	3	417	GLN
2	3	201	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 10 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	$\#\|Z\| > 2$
16	ATP	7	901	18	26,33,33	0.62	0	31,52,52	0.78	2 (6%)
19	ADP	4	1001	-	24,29,29	0.95	1 (4%)	29,45,45	1.44	4 (13%)
19	ADP	6	1201	-	24,29,29	0.93	1 (4%)	29,45,45	1.45	4 (13%)
16	ATP	5	1701	18	26,33,33	0.61	0	31,52,52	0.76	1 (3%)
16	ATP	2	901	-	26,33,33	0.61	0	31,52,52	0.78	2 (6%)
16	ATP	3	1101	18	26,33,33	0.62	0	31,52,52	0.76	1 (3%)

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
16	ATP	7	901	18	-	6/18/38/38	0/3/3/3
19	ADP	4	1001	-	-	5/12/32/32	0/3/3/3
19	ADP	6	1201	-	-	3/12/32/32	0/3/3/3
16	ATP	5	1701	18	-	1/18/38/38	0/3/3/3
16	ATP	2	901	-	-	3/18/38/38	0/3/3/3
16	ATP	3	1101	18	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1001	ADP	C5-C4	2.50	1.47	1.40
19	6	1201	ADP	C5-C4	2.44	1.47	1.40

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	1001	ADP	C3'-C2'-C1'	3.63	106.44	100.98
19	6	1201	ADP	PA-O3A-PB	-3.61	120.44	132.83
19	6	1201	ADP	N3-C2-N1	-3.26	123.58	128.68
19	4	1001	ADP	N3-C2-N1	-3.14	123.78	128.68
19	6	1201	ADP	C3'-C2'-C1'	3.11	105.67	100.98

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	7	901	ATP	PB-O3B-PG-O2G
16	7	901	ATP	C5'-O5'-PA-O3A
16	7	901	ATP	C4'-C5'-O5'-PA
19	4	1001	ADP	C5'-O5'-PA-O1A
19	4	1001	ADP	C5'-O5'-PA-O2A

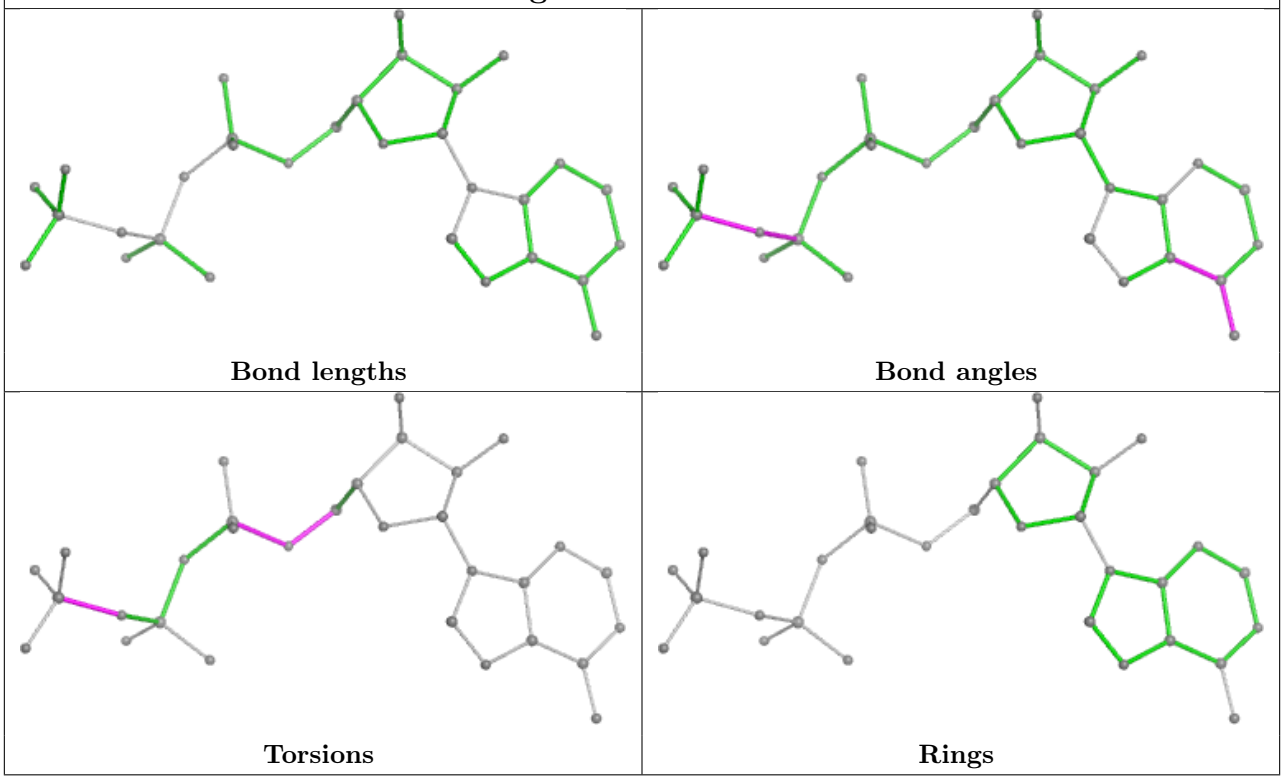
There are no ring outliers.

2 monomers are involved in 5 short contacts:

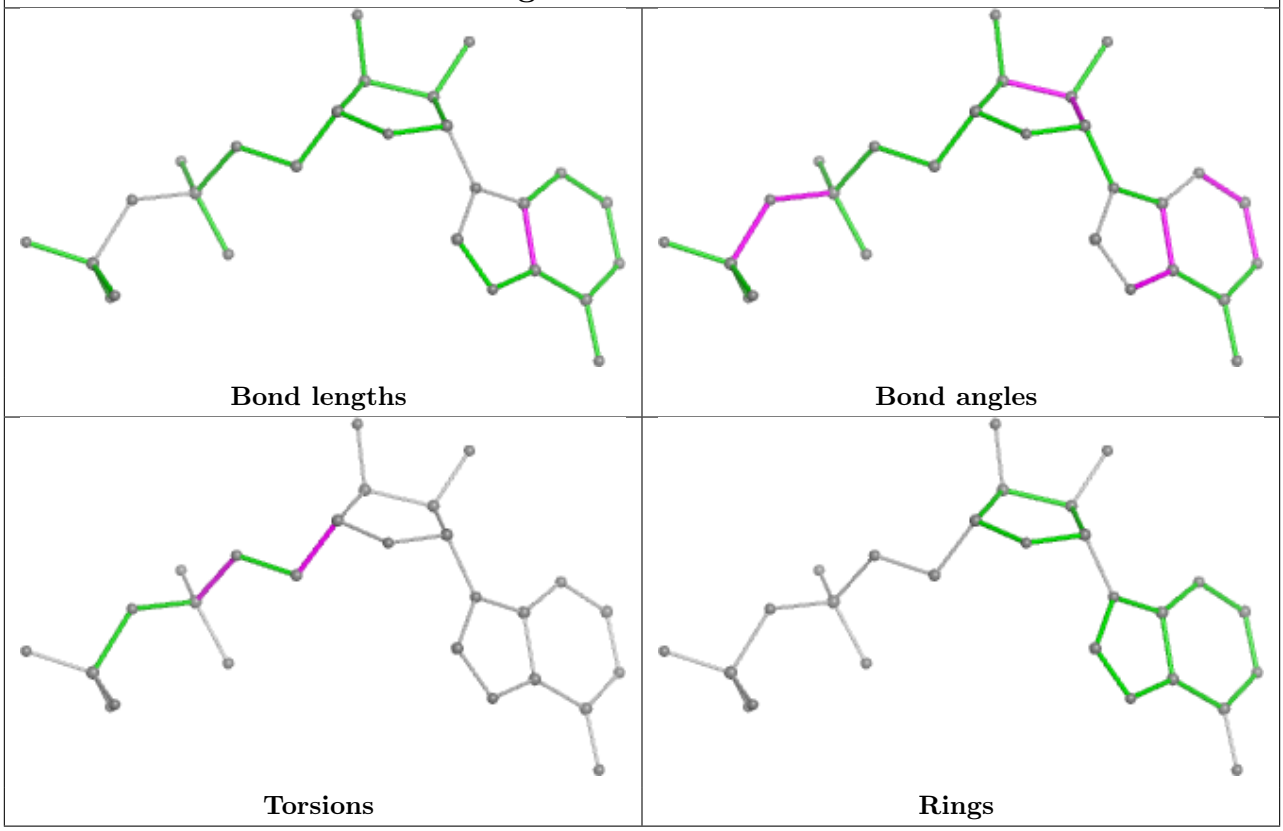
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	7	901	ATP	1	0
19	6	1201	ADP	4	0

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 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.

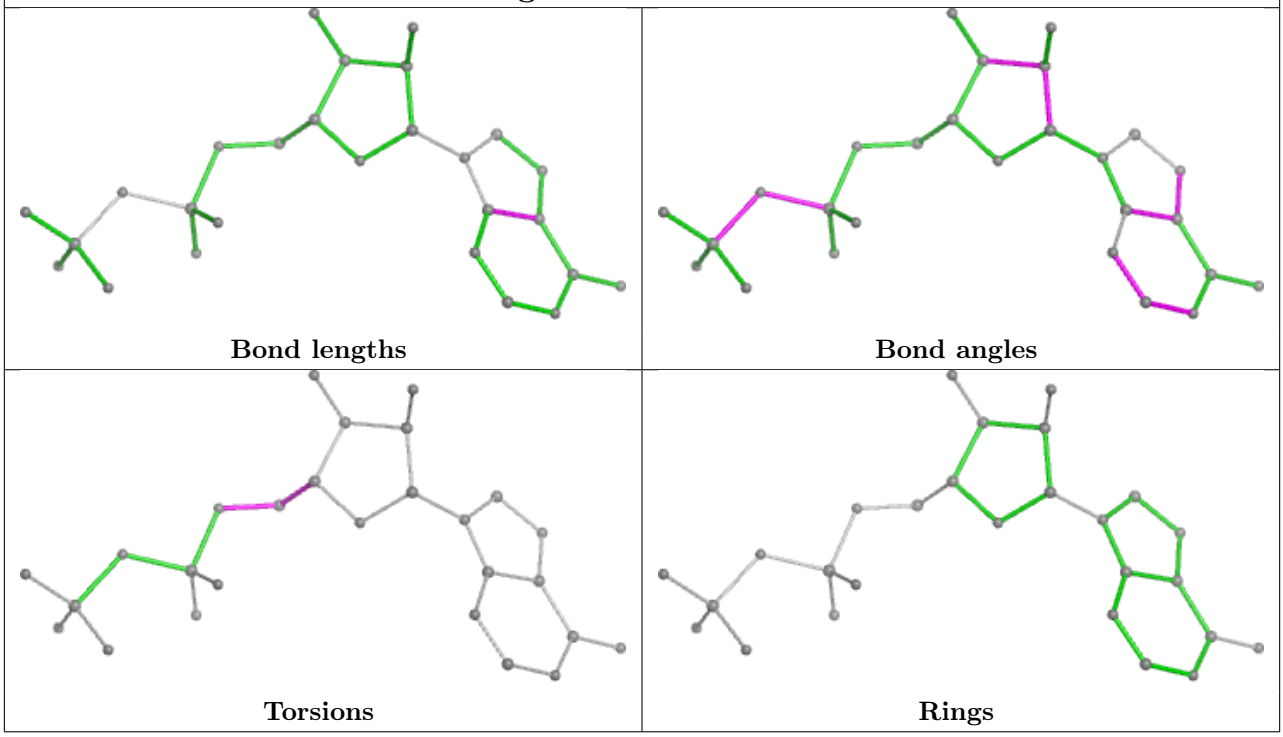
Ligand ATP 7 901



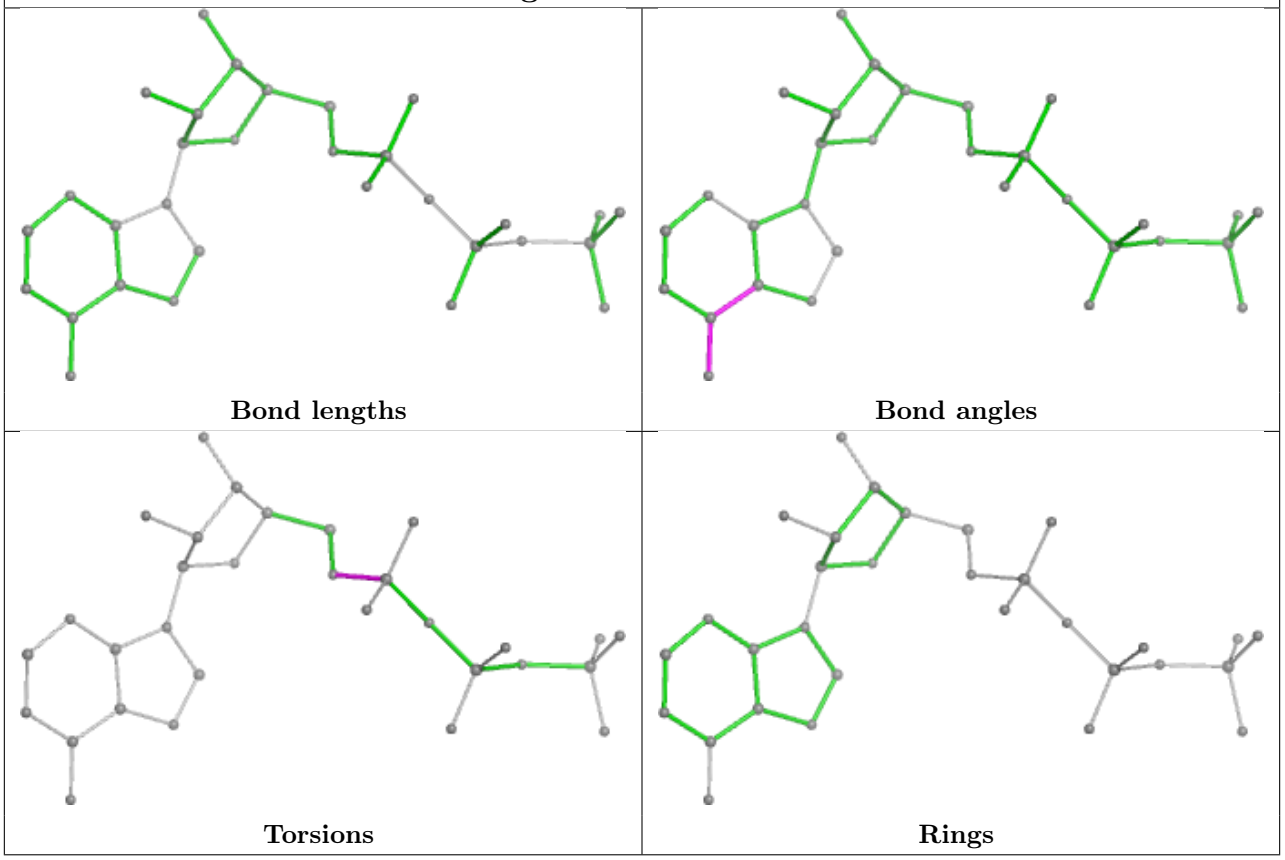
Ligand ADP 4 1001



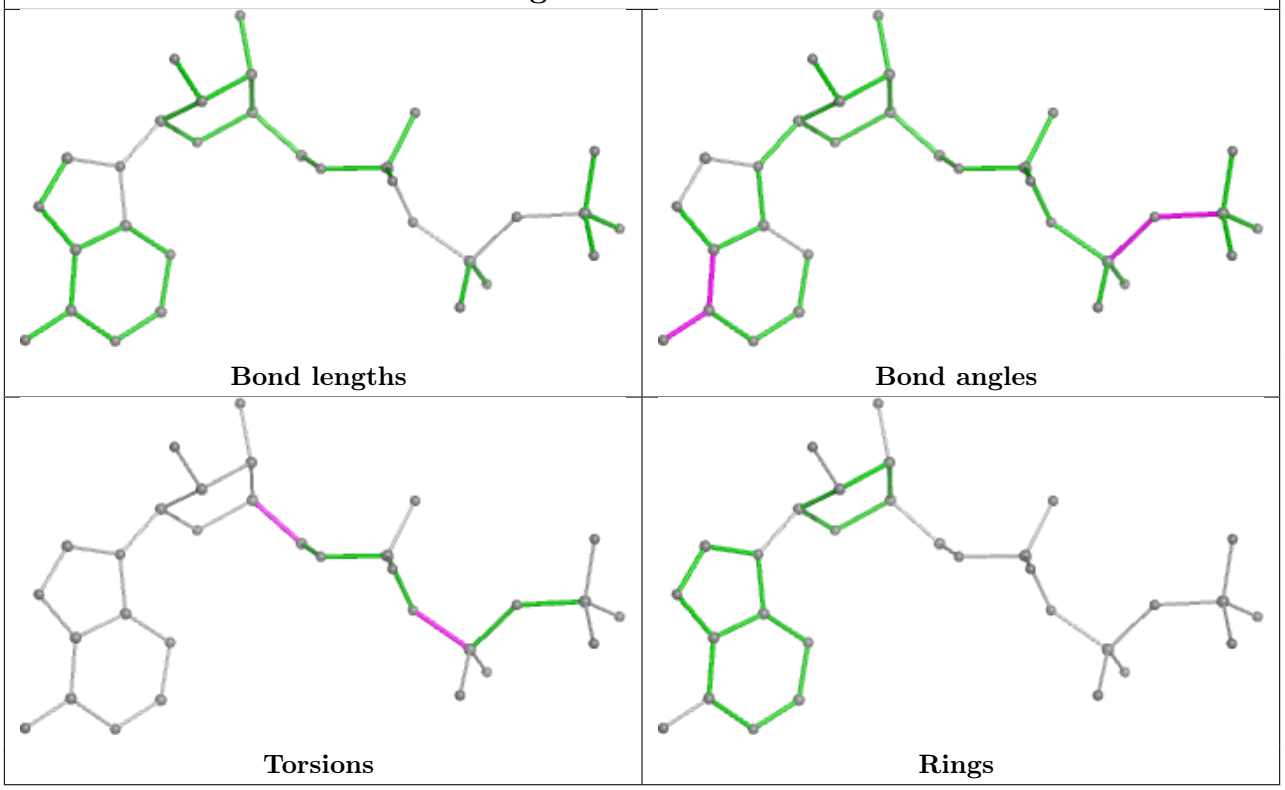
Ligand ADP 6 1201



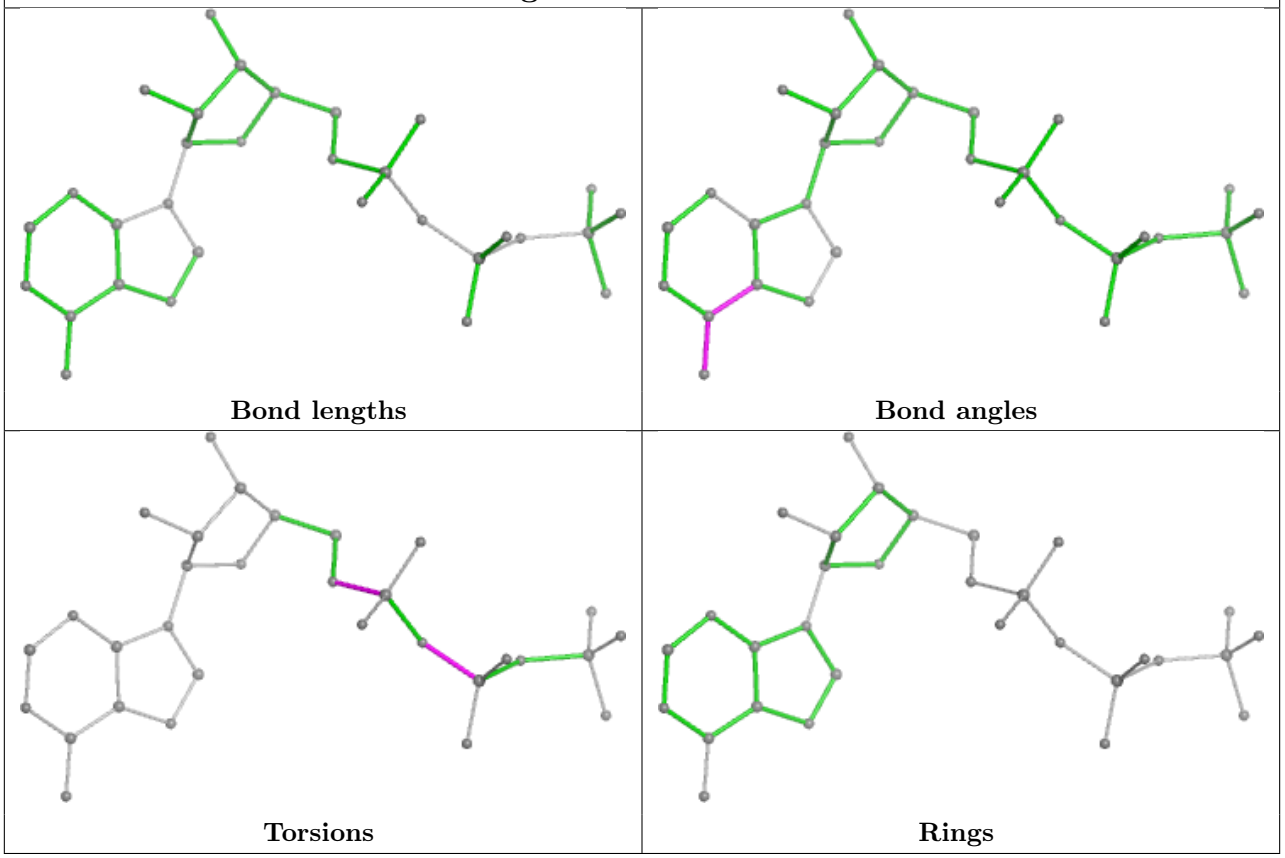
Ligand ATP 5 1701



Ligand ATP 2 901



Ligand ATP 3 1101



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.

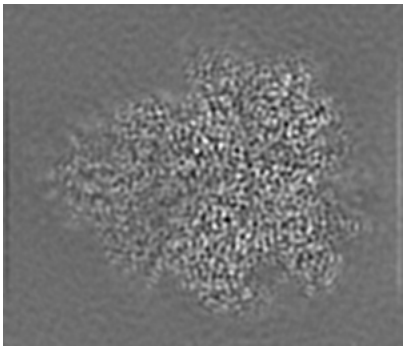
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13978. These allow visual inspection of the internal detail of the map and identification of artifacts.

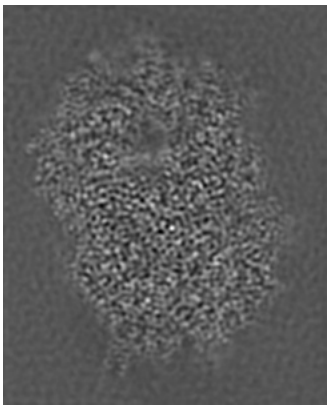
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

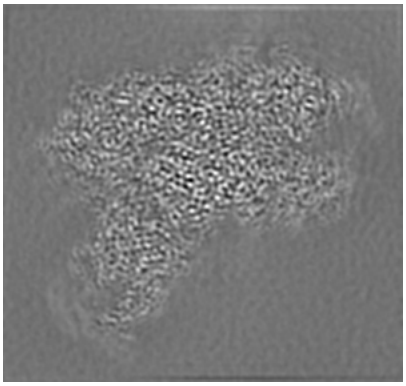
6.1.1 Primary map



X

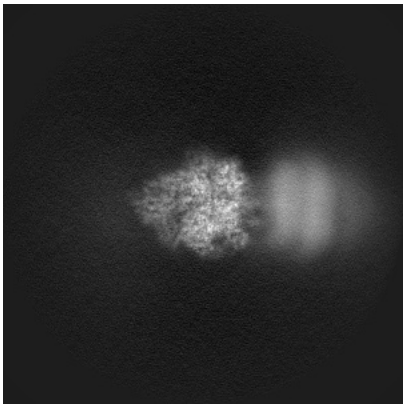


Y

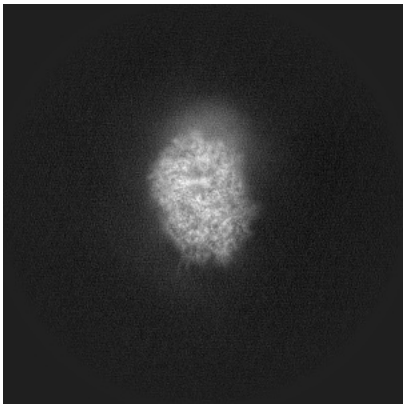


Z

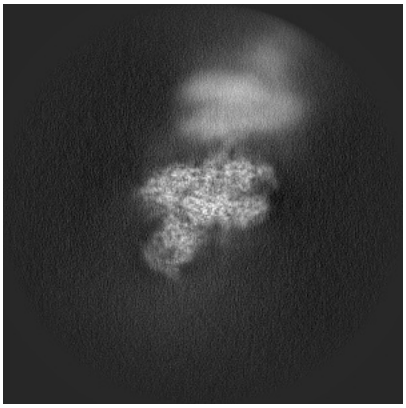
6.1.2 Raw map



X



Y

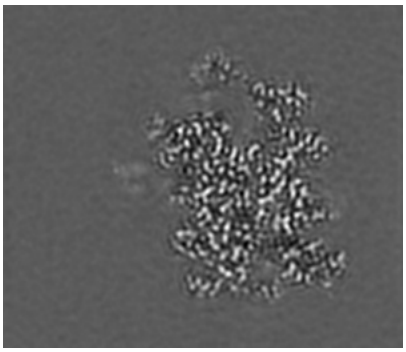


Z

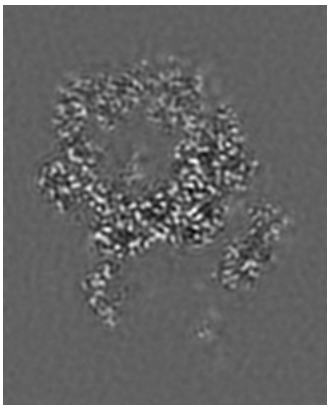
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

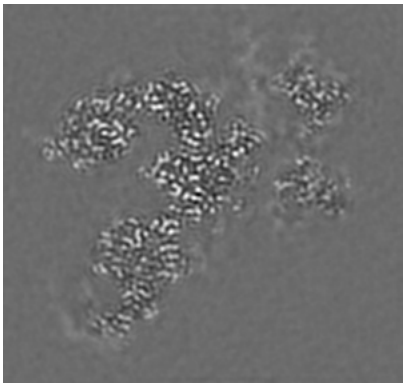
6.2.1 Primary map



X Index: 102

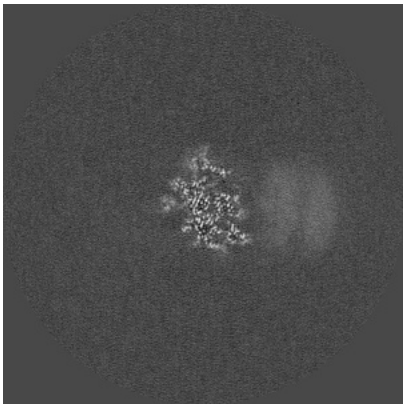


Y Index: 97

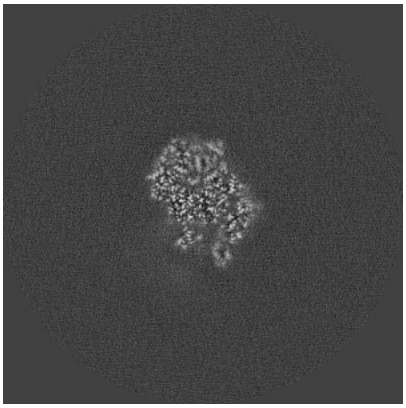


Z Index: 83

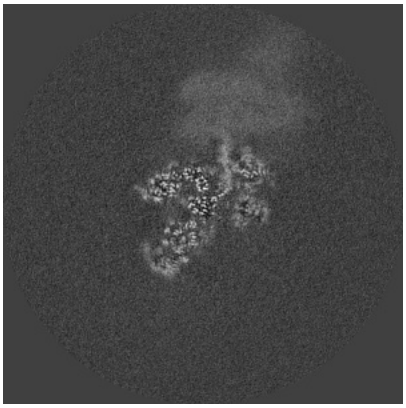
6.2.2 Raw map



X Index: 256



Y Index: 256

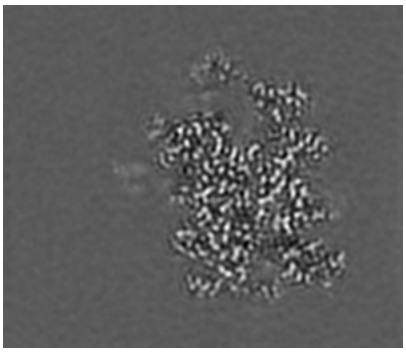


Z Index: 256

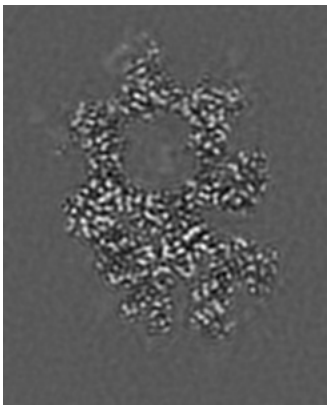
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

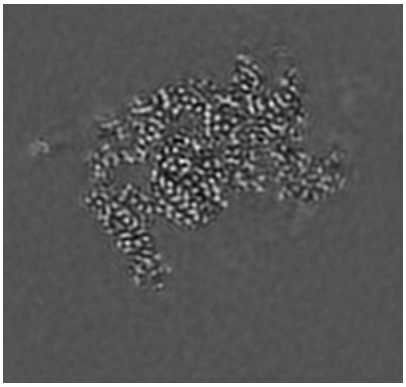
6.3.1 Primary map



X Index: 102

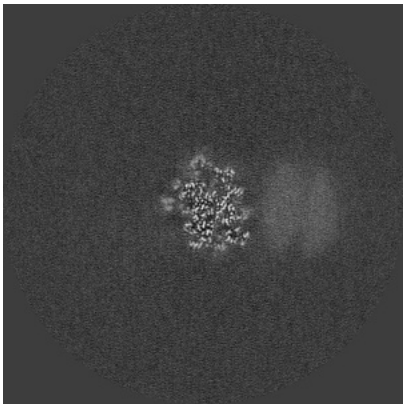


Y Index: 141

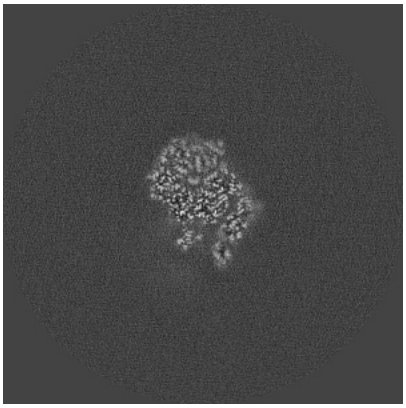


Z Index: 51

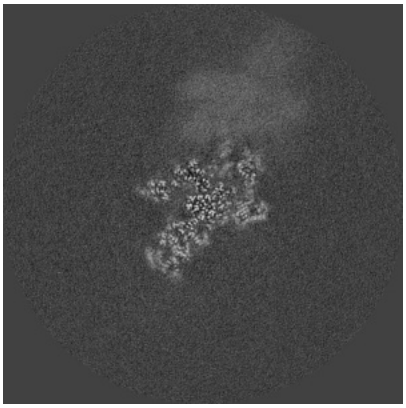
6.3.2 Raw map



X Index: 260



Y Index: 255

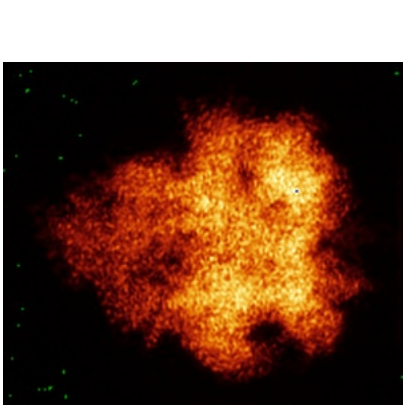


Z Index: 261

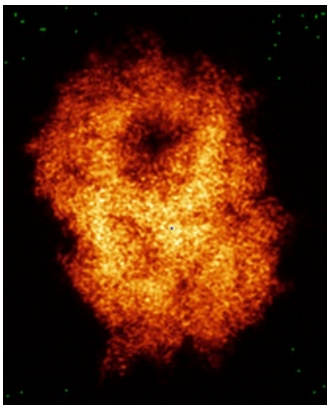
The images above show the largest variance slices of the map in three orthogonal directions.

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

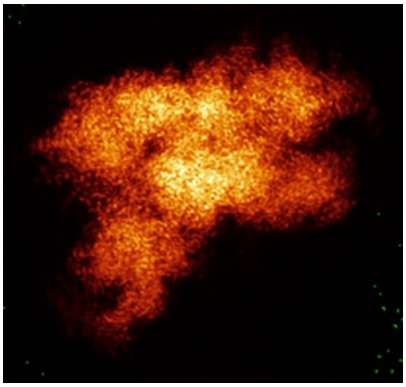
6.4.1 Primary map



X

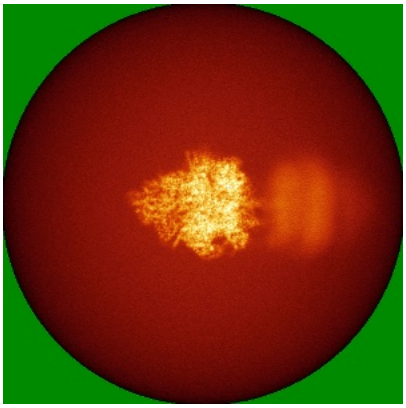


Y

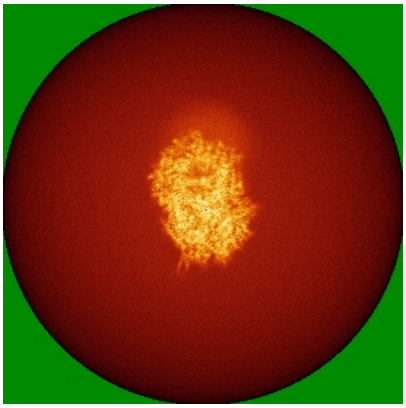


Z

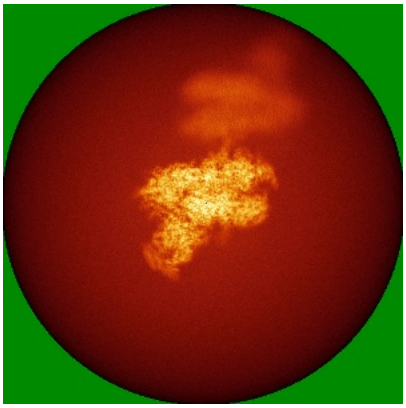
6.4.2 Raw map



X



Y

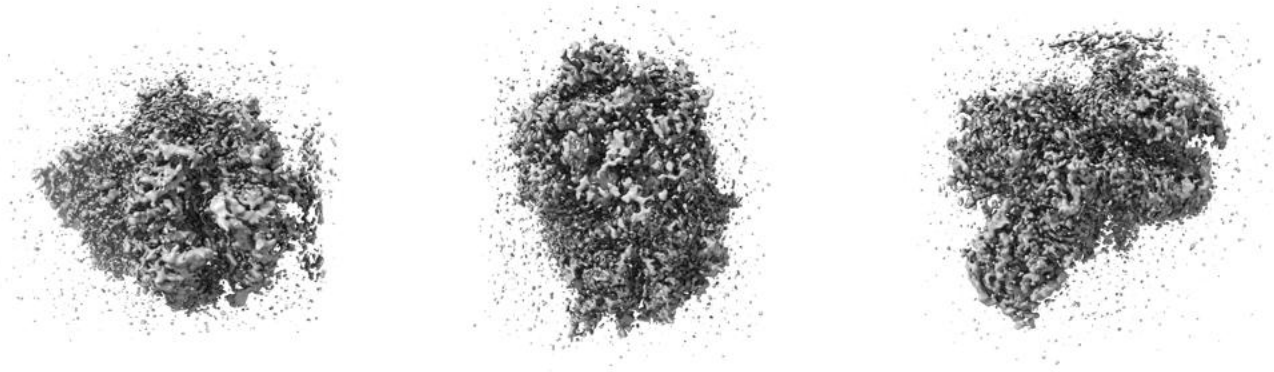


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

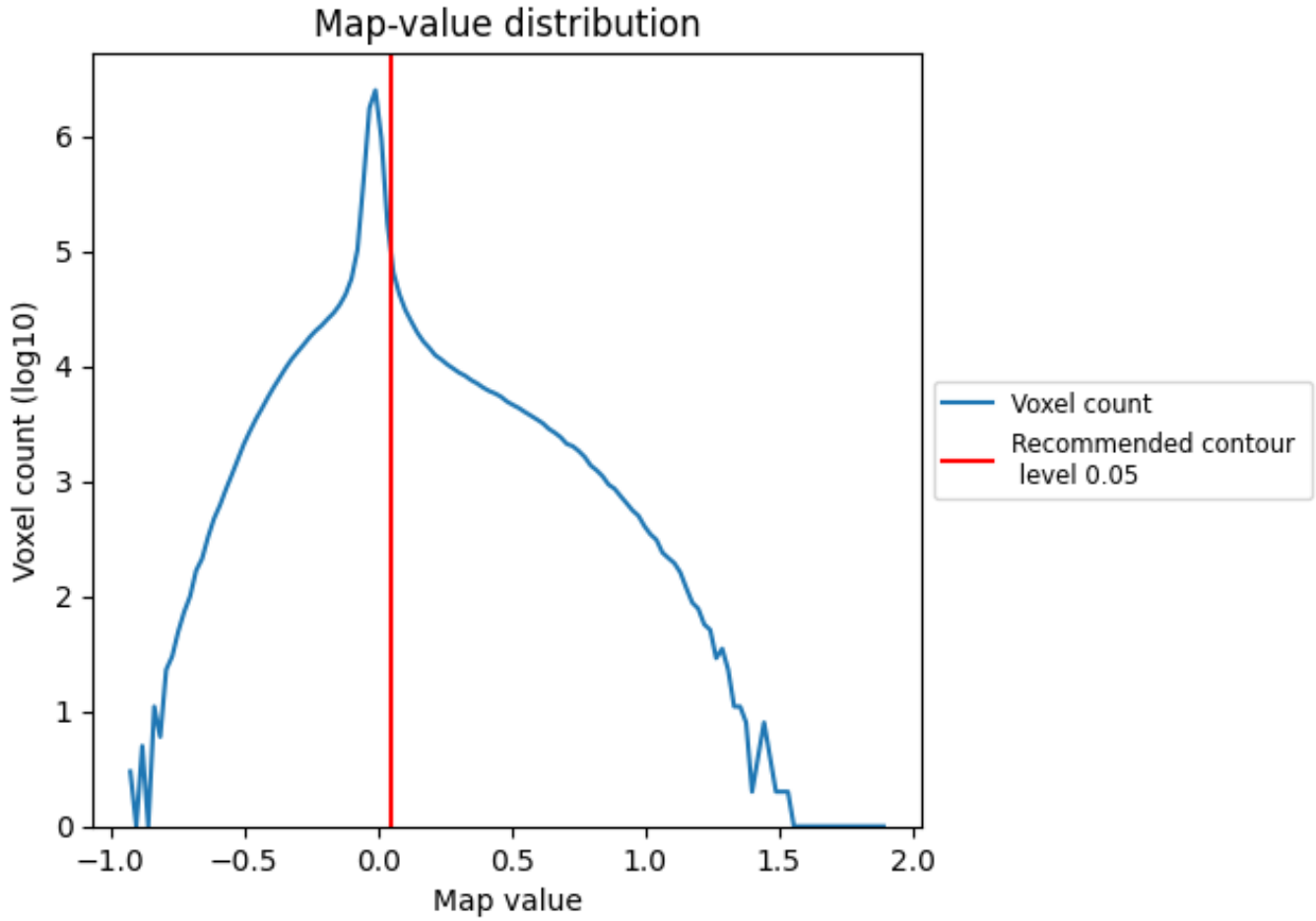
6.6 Mask visualisation (i)

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

7 Map analysis

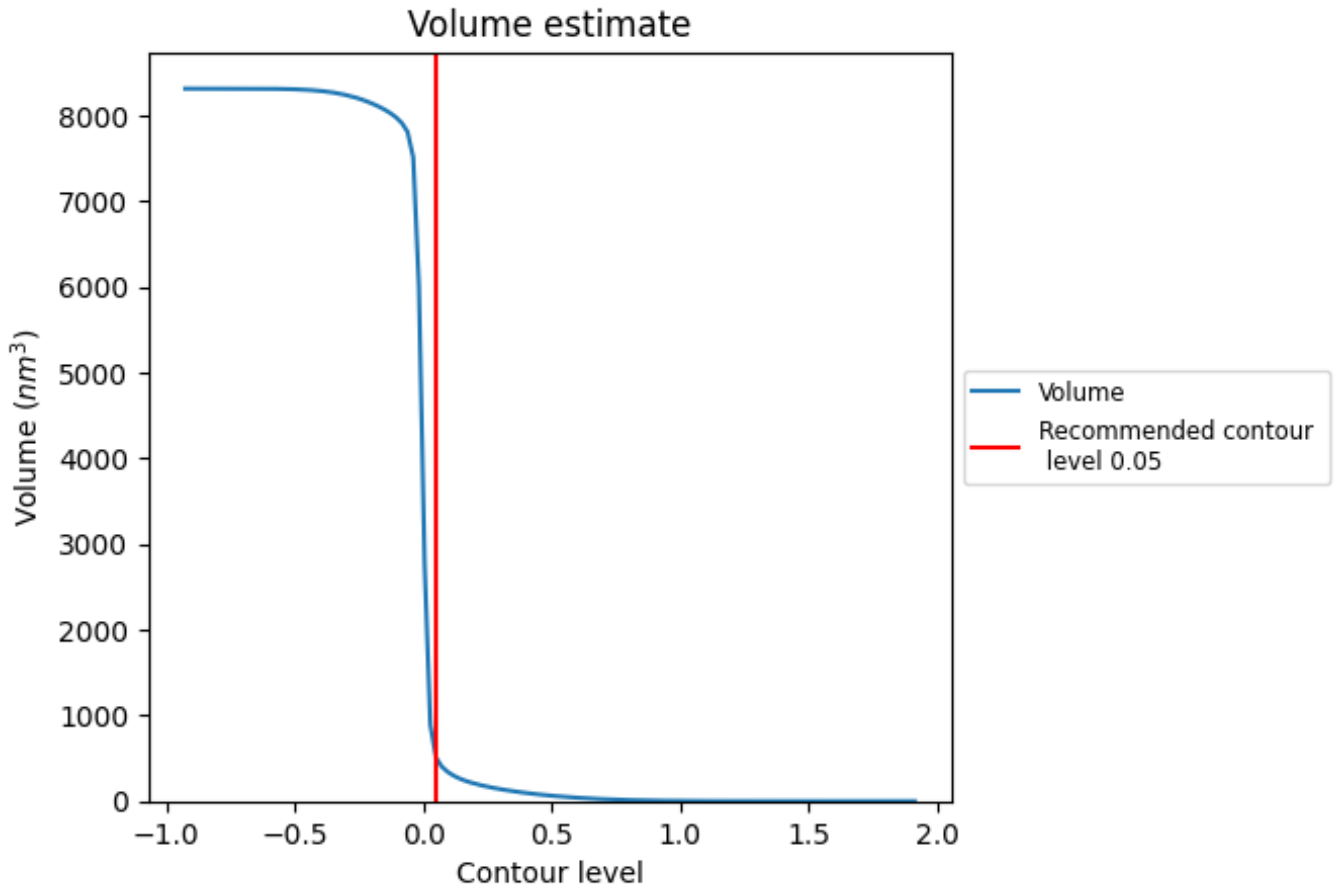
This section contains the results of statistical analysis of the map.

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 507 nm^3; this corresponds to an approximate mass of 458 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.

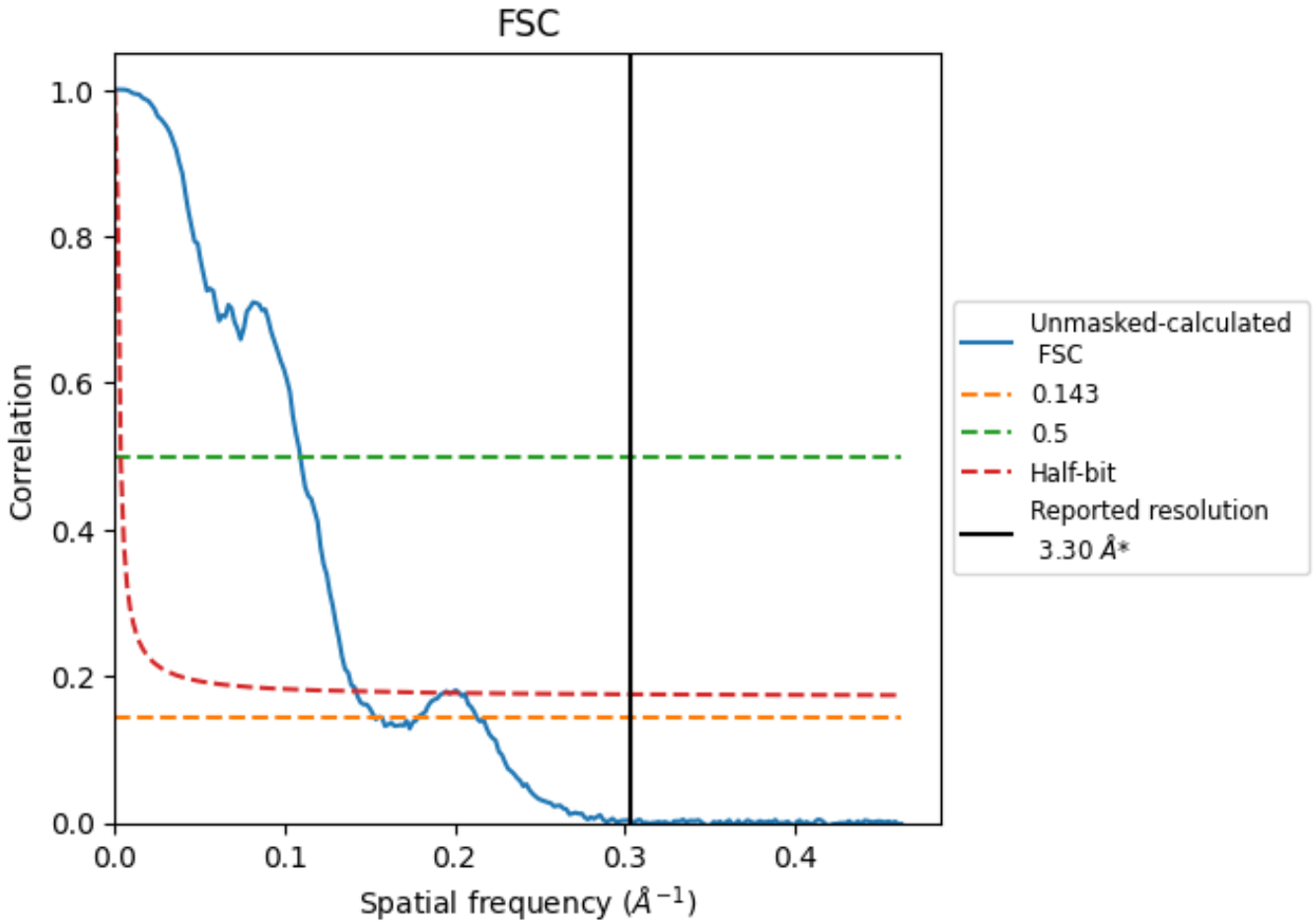
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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



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

8.2 Resolution estimates (i)

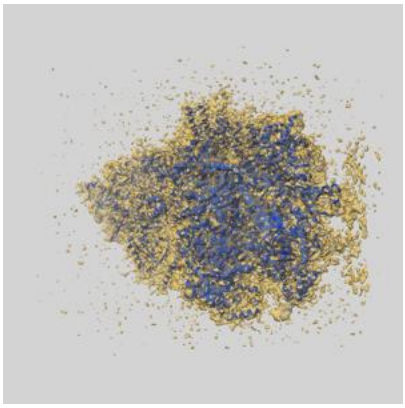
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.53	9.16	7.05

*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 6.53 differs from the reported value 3.3 by more than 10 %

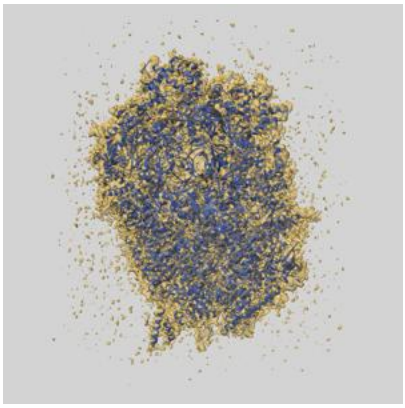
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13978 and PDB model 7QHS. Per-residue inclusion information can be found in section 3 on page 11.

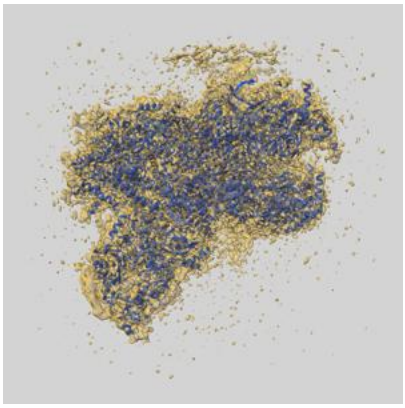
9.1 Map-model overlay



X



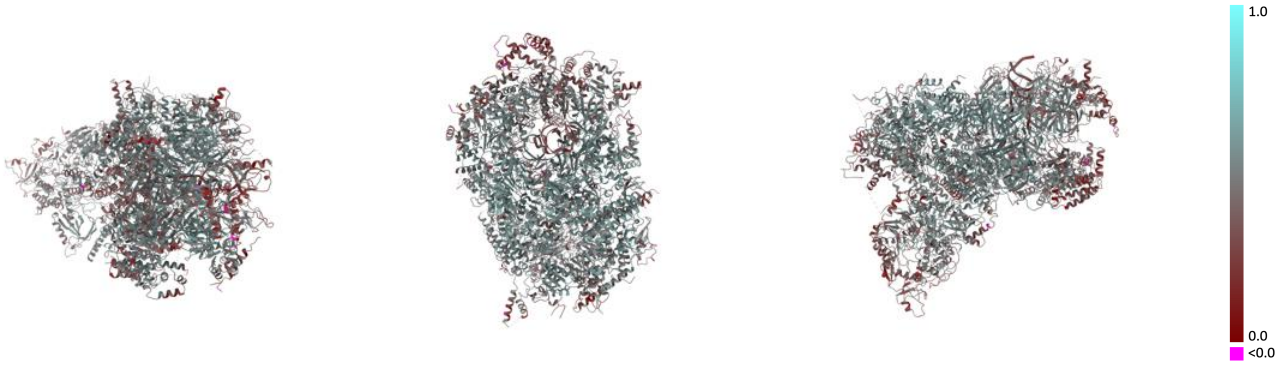
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

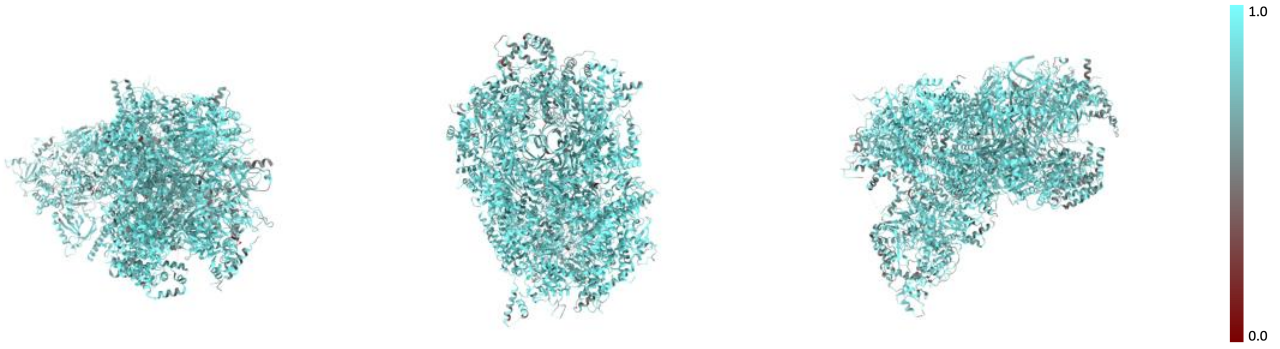
9.2 Q-score mapped to coordinate model



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.

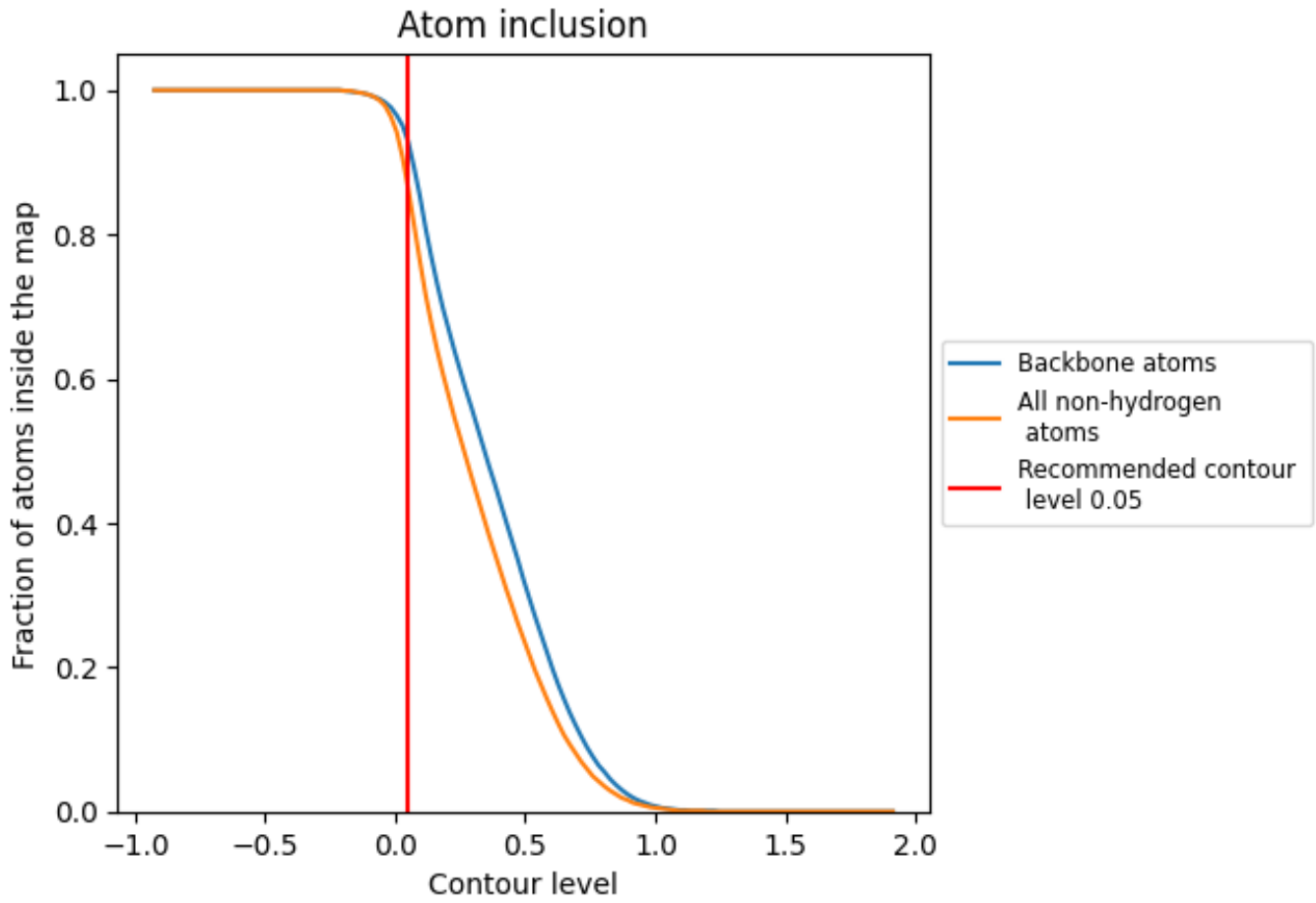
9.3 Atom inclusion mapped to coordinate model



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8630	0.4730
2	0.9180	0.5340
3	0.9110	0.5200
4	0.8040	0.4010
5	0.9040	0.5270
6	0.8700	0.4810
7	0.7980	0.4020
A	0.8430	0.3860
B	0.7600	0.3370
C	0.8950	0.5100
D	0.8650	0.4760
E	0.8970	0.5040
F	0.8310	0.4380
G	0.8310	0.4480
H	0.8400	0.4550
I	0.9140	0.5240