



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 10:52 AM UTC

PDB ID : 8KG6 / pdb_00008kg6
EMDB ID : EMD-37211
Title : Yeast replisome in state I
Authors : Dang, S.; Zhai, Y.; Feng, J.; Yu, D.; Xu, Z.
Deposited on : 2023-08-17
Resolution : 3.07 Å(reported)
Based on initial model : 6XKL

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

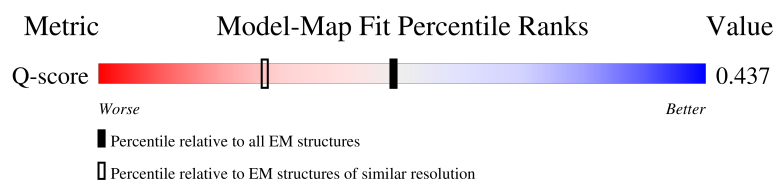
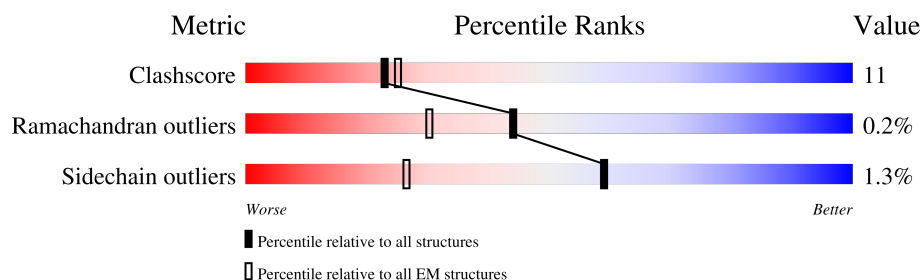
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.07 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	13977 (2.57 - 3.57)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	868	60% 16% • 24%
2	3	971	53% 13% • 34%
3	4	933	50% 23% • 25%
4	5	775	67% 19% • 13%

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Mol	Chain	Length	Quality of chain
5	6	1017	
6	7	845	
7	A	208	
8	B	213	
9	C	194	
10	D	294	
11	E	650	
12	F	927	
12	G	927	
12	H	927	
13	I	71	
14	J	61	
15	K	1238	
16	L	317	
17	M	2222	
18	N	689	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 70613 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	662	Total	C	N	O	S	0	0
			5245	3292	942	992	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	645	Total	C	N	O	S	0	0
			5005	3148	888	956	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	696	Total	C	N	O	S	0	0
			5494	3447	949	1067	31		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	677	Total	C	N	O	S	0	0
			5334	3345	928	1037	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	619	Total	C	N	O	S	0	0
			4880	3085	854	916	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	647	Total	C	N	O	S	0	0
			5023	3169	877	950	27		

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	200	Total	C	N	O	S	0	0
			1625	1021	280	316	8		

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	195	Total	C	N	O	S	0	0
			1630	1046	289	290	5		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	173	Total	C	N	O	S	0	0
			1394	907	224	256	7		

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	243	Total	C	N	O	S	0	0
			2004	1276	327	389	12		

- Molecule 11 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	568	Total	C	N	O	S	0	0
			4591	2930	774	873	14		

- Molecule 12 is a protein called DNA polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	433	Total	C	N	O	S	0	0
			3467	2223	577	651	16		
12	G	421	Total	C	N	O	S	0	0
			3362	2162	555	629	16		
12	H	421	Total	C	N	O	S	0	0
			3358	2159	553	631	15		

- Molecule 13 is a DNA chain called DNA (71-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	35	Total	C	N	O	P	0	0
			722	350	112	225	35		

- Molecule 14 is a DNA chain called DNA (61-mer).

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

- Molecule 15 is a protein called Topoisomerase 1-associated factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	660	Total	C	N	O	S	0	0
			5350	3466	904	961	19		

- Molecule 16 is a protein called Chromosome segregation in meiosis protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	94	Total	C	N	O	S	0	0
			788	507	144	133	4		

- Molecule 17 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	813	Total	C	N	O	S	0	0
			6490	4202	1060	1193	35		

- Molecule 18 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	536	Total	C	N	O	S	0	0
			4254	2726	725	786	17		

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

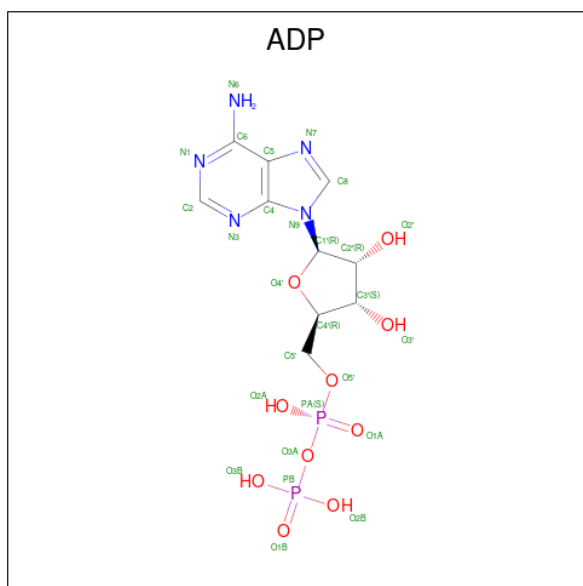
Mol	Chain	Residues	Atoms		AltConf
19	2	1	Total	Zn	0
			1	1	
19	4	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
19	5	1	Total	Zn	0
			1	1	
19	6	1	Total	Zn	0
			1	1	
19	7	1	Total	Zn	0
			1	1	
19	M	2	Total	Zn	0
			2	2	

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	3	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

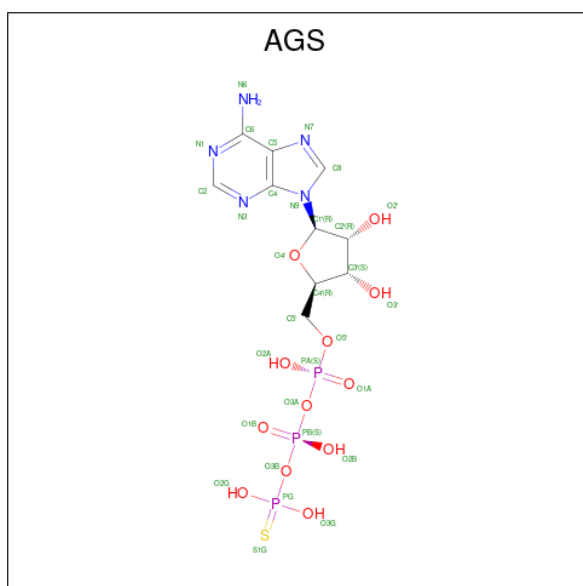
Mol	Chain	Residues	Atoms		AltConf
21	2	1	Total	Mg	0
			1	1	
21	3	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
21	5	1	Total	Mg	0
			1	1	
21	6	1	Total	Mg	0
			1	1	
21	7	1	Total	Mg	0
			1	1	

- Molecule 22 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).

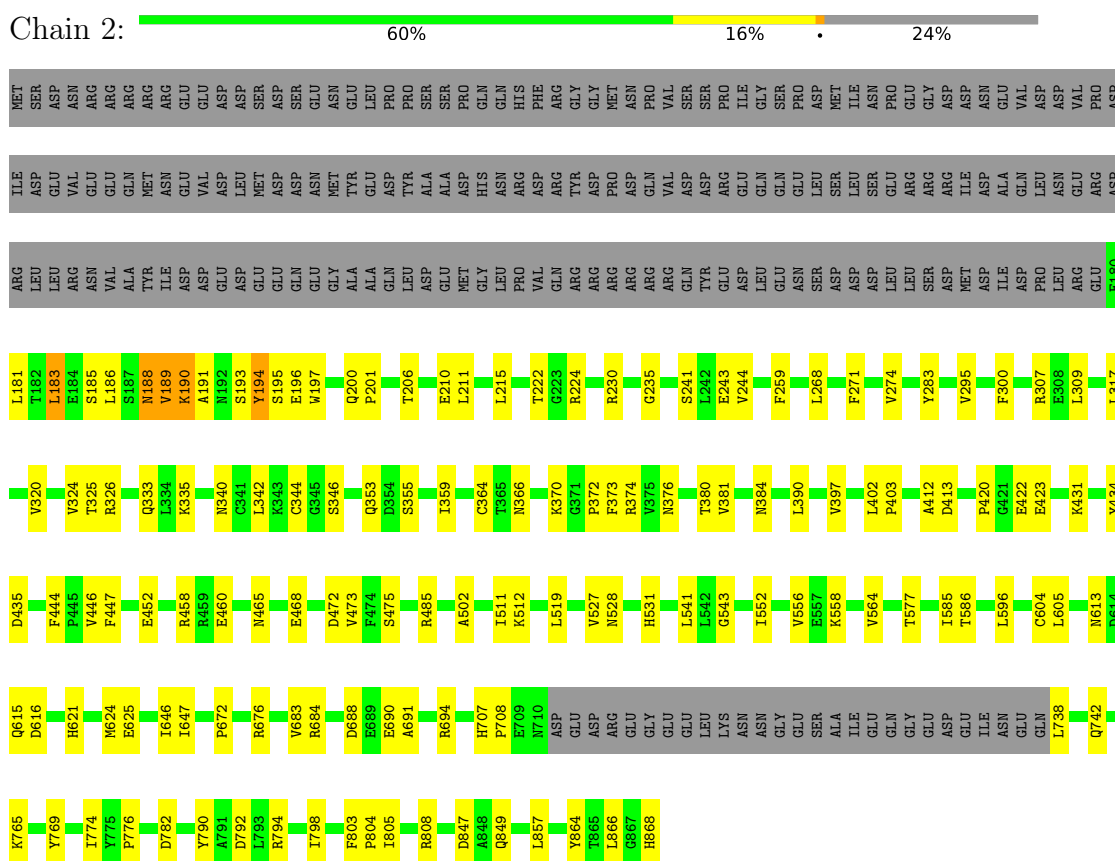


Mol	Chain	Residues	Atoms						AltConf
22	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
22	6	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
22	7	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

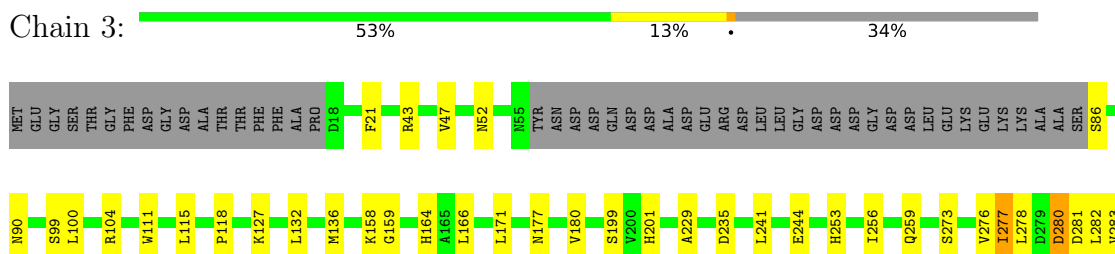
3 Residue-property plots

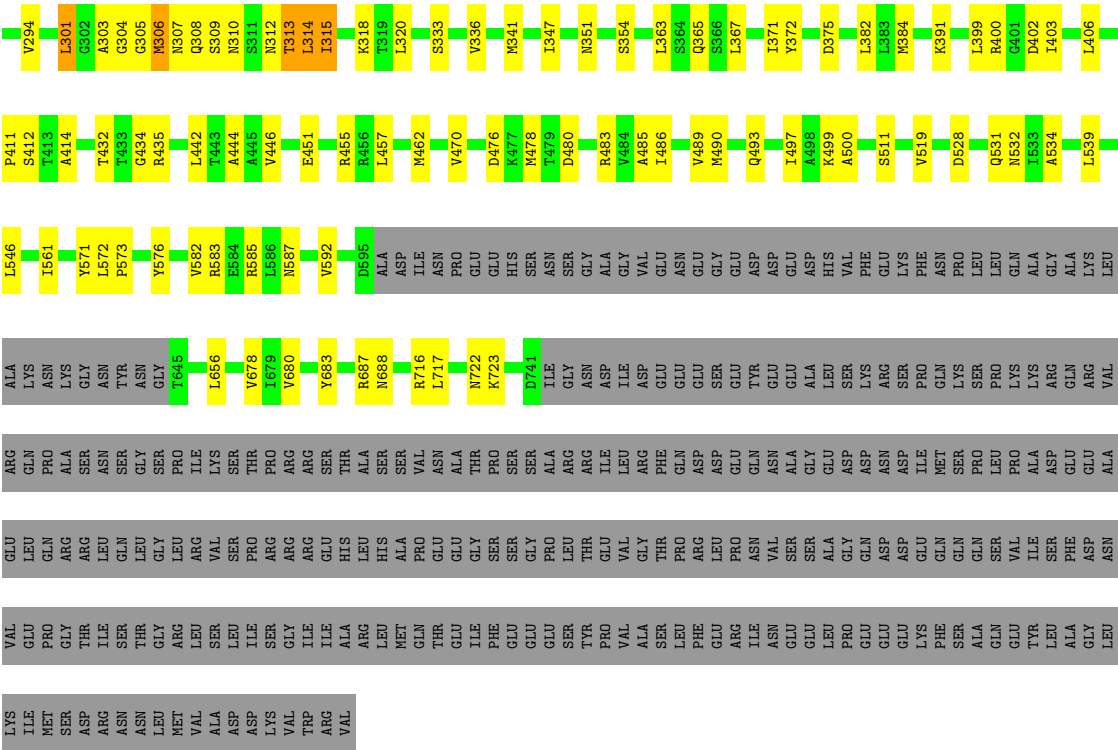
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

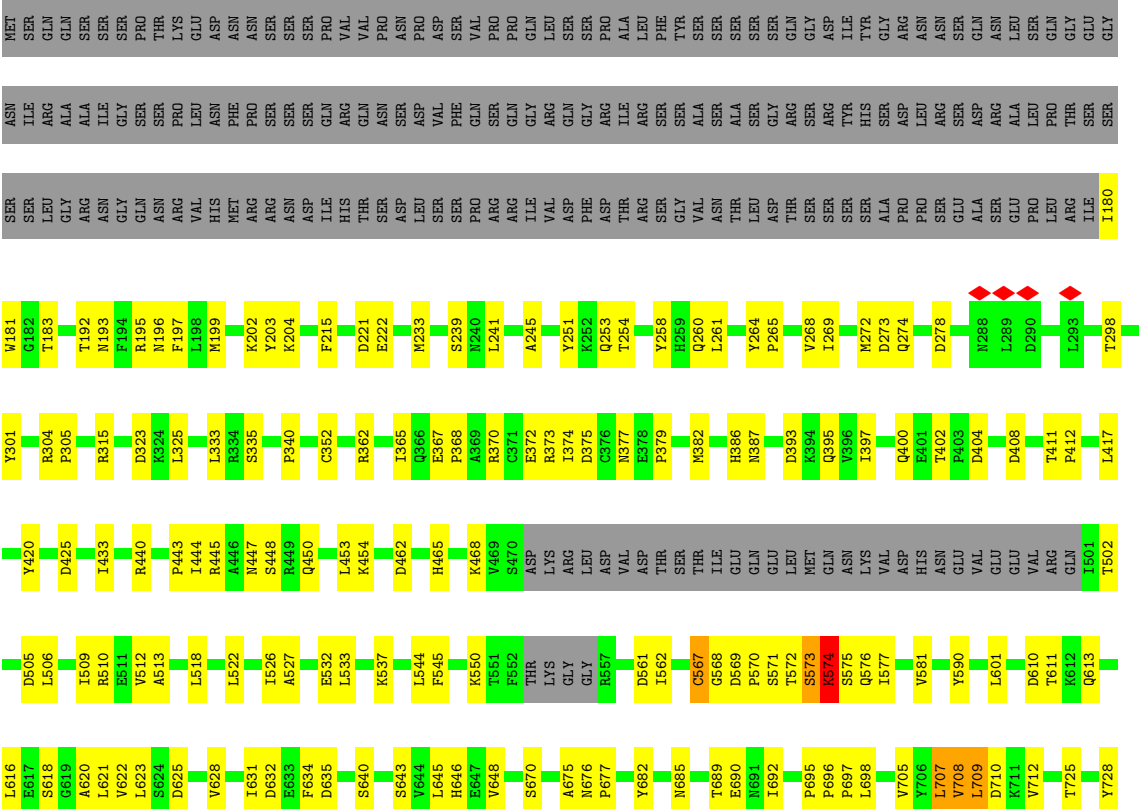


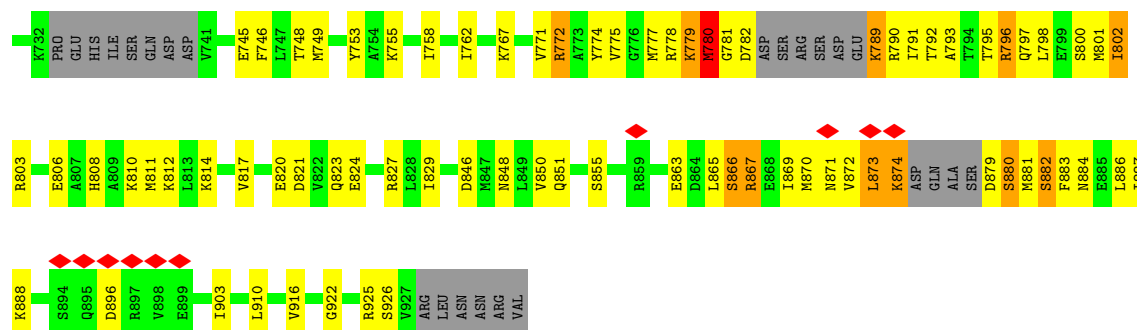
• Molecule 2: DNA replication licensing factor MCM3





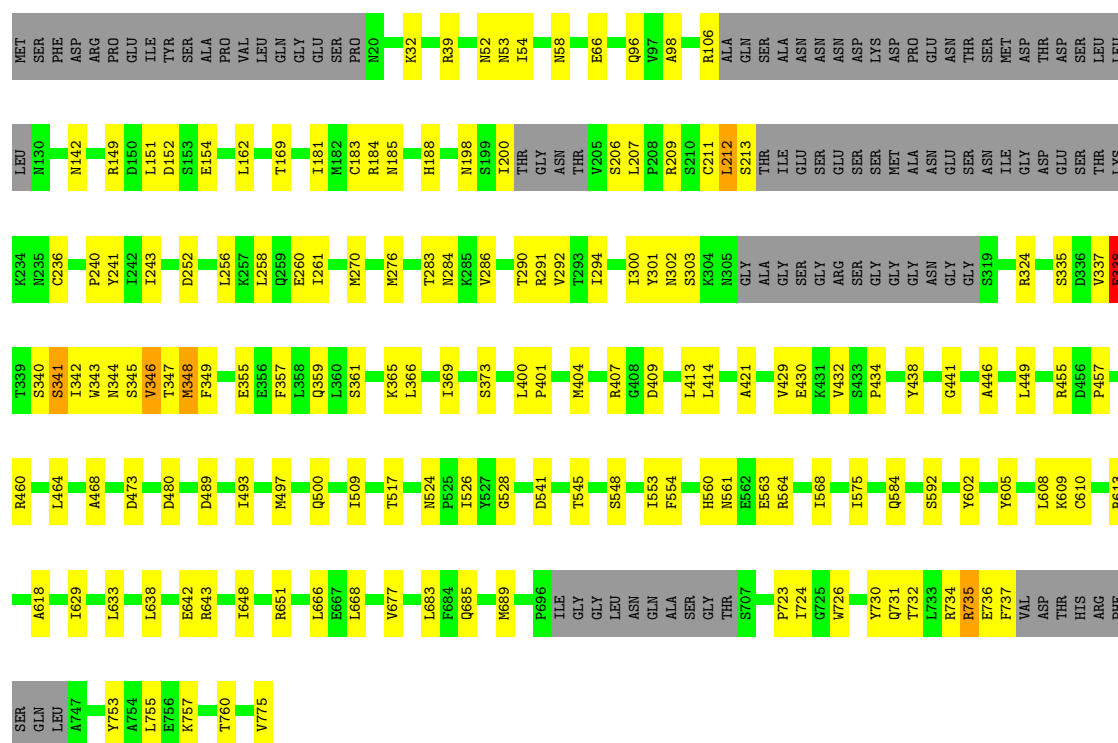
● Molecule 3: DNA replication licensing factor MCM4





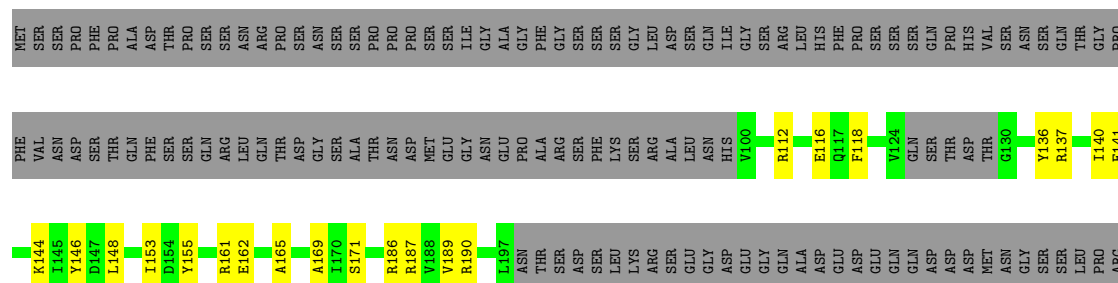
• Molecule 4: Minichromosome maintenance protein 5

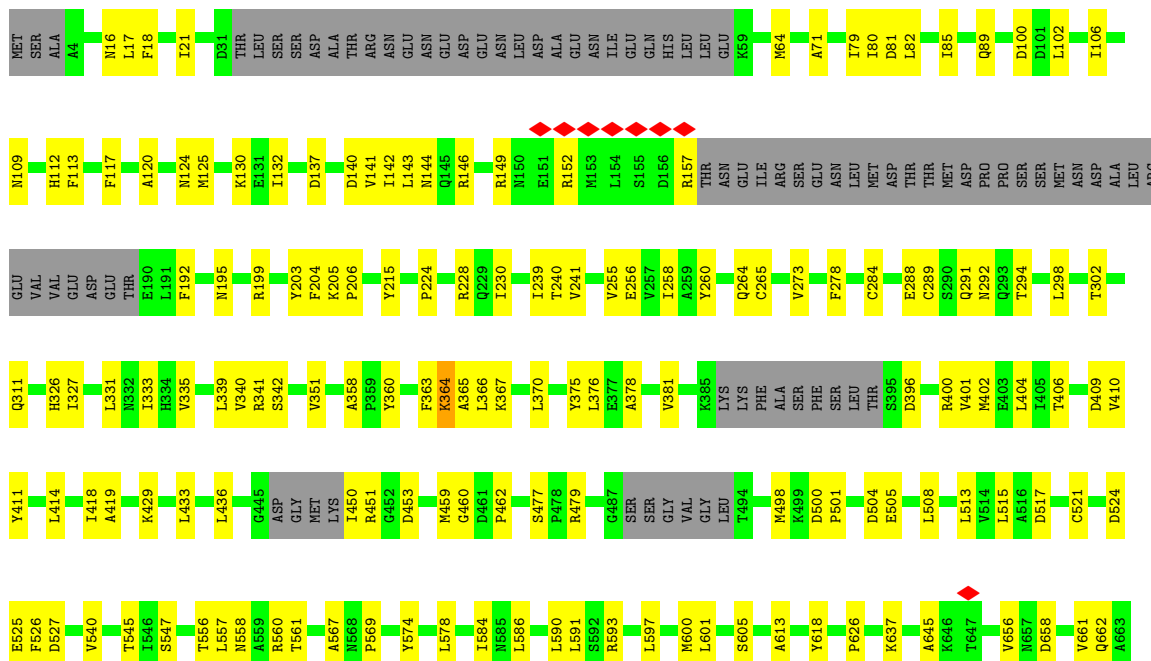
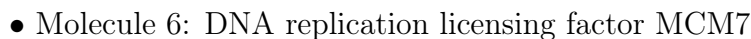
Chain 5: 67% 19% 13%

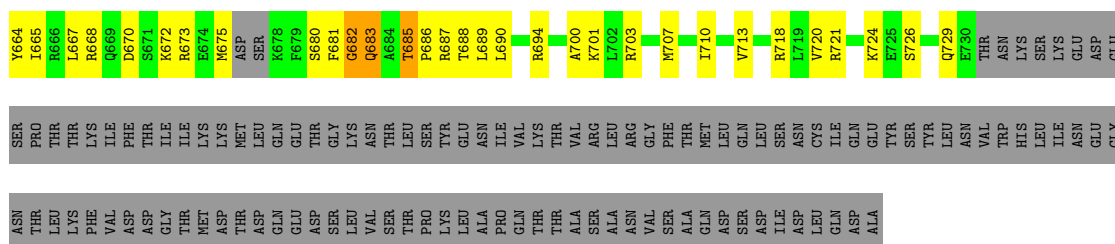


• Molecule 5: DNA replication licensing factor MCM6

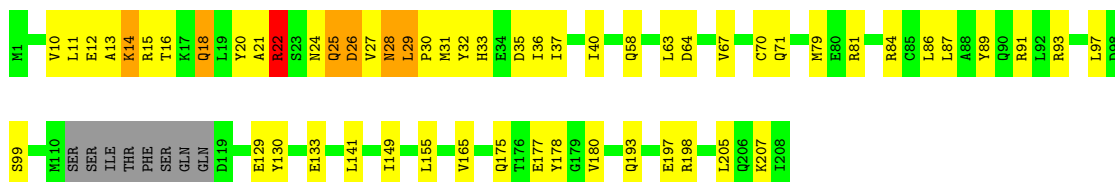
Chain 6: 46% 15% 39%



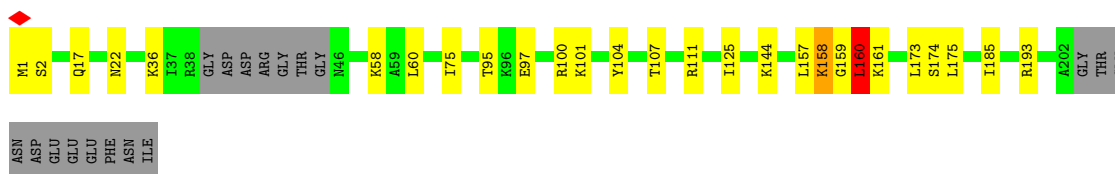




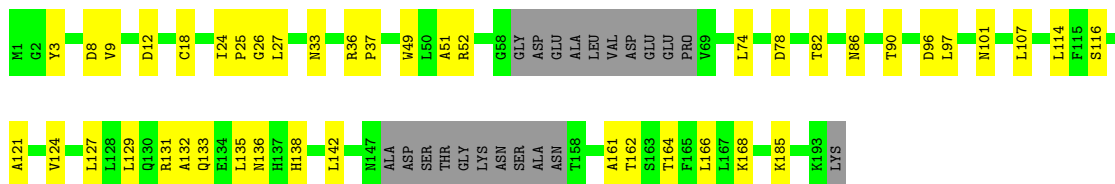
- Molecule 7: DNA replication complex GINS protein PSF1



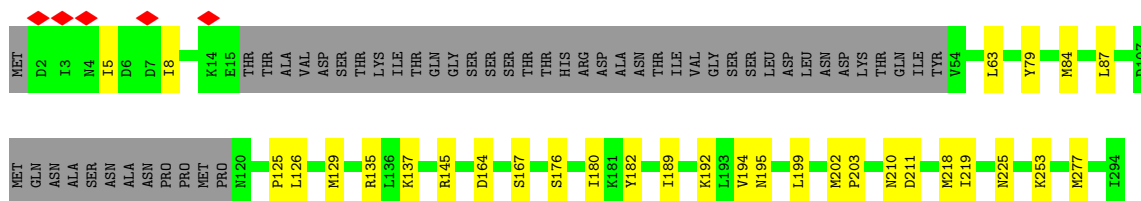
- Molecule 8: DNA replication complex GINS protein PSF2



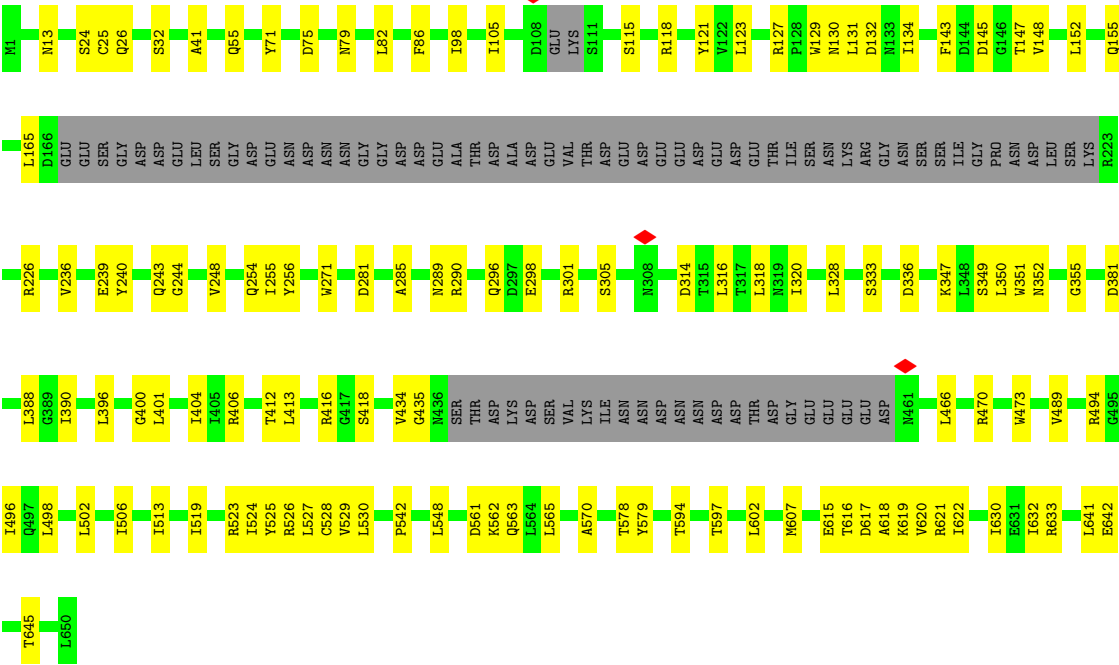
- Molecule 9: DNA replication complex GINS protein PSF3



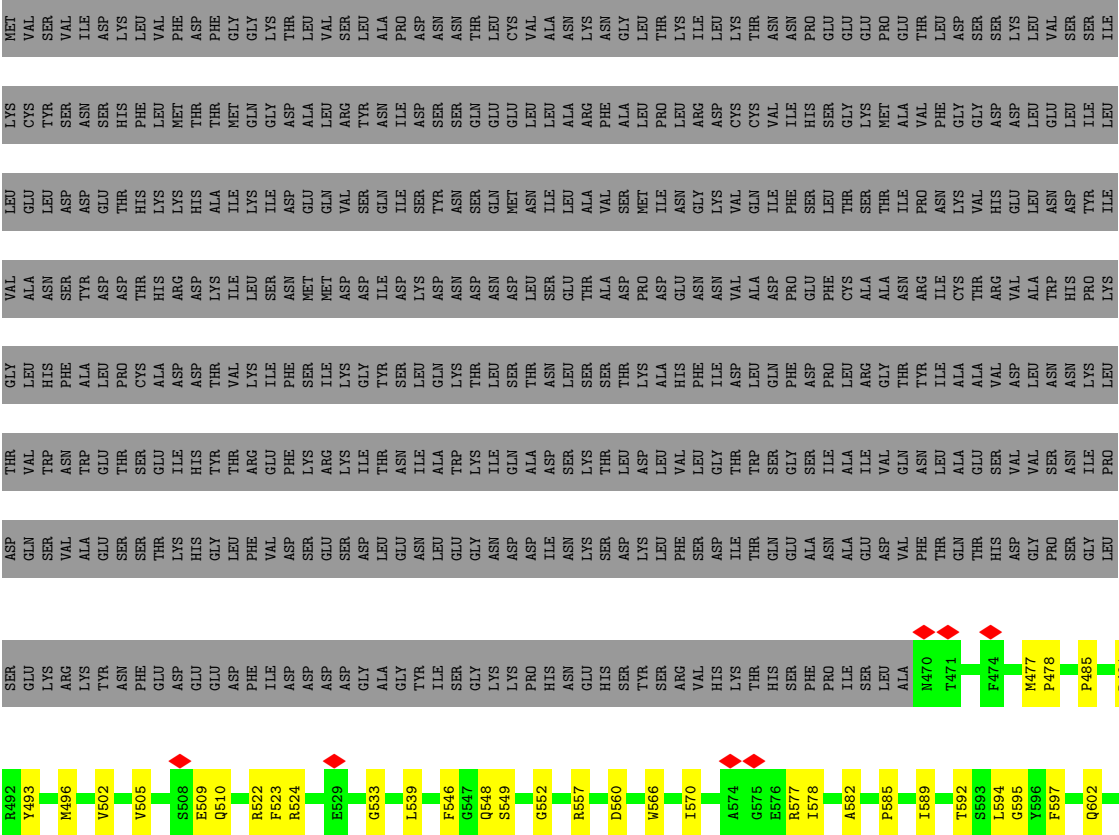
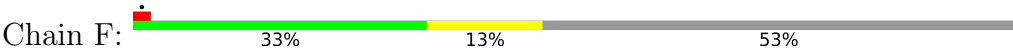
- Molecule 10: DNA replication complex GINS protein SLD5

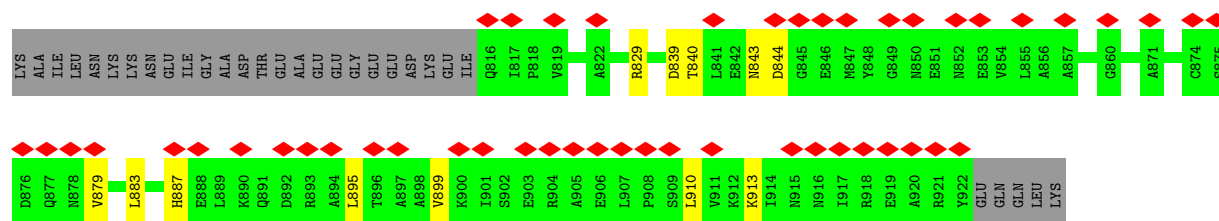


- Molecule 11: Cell division control protein 45

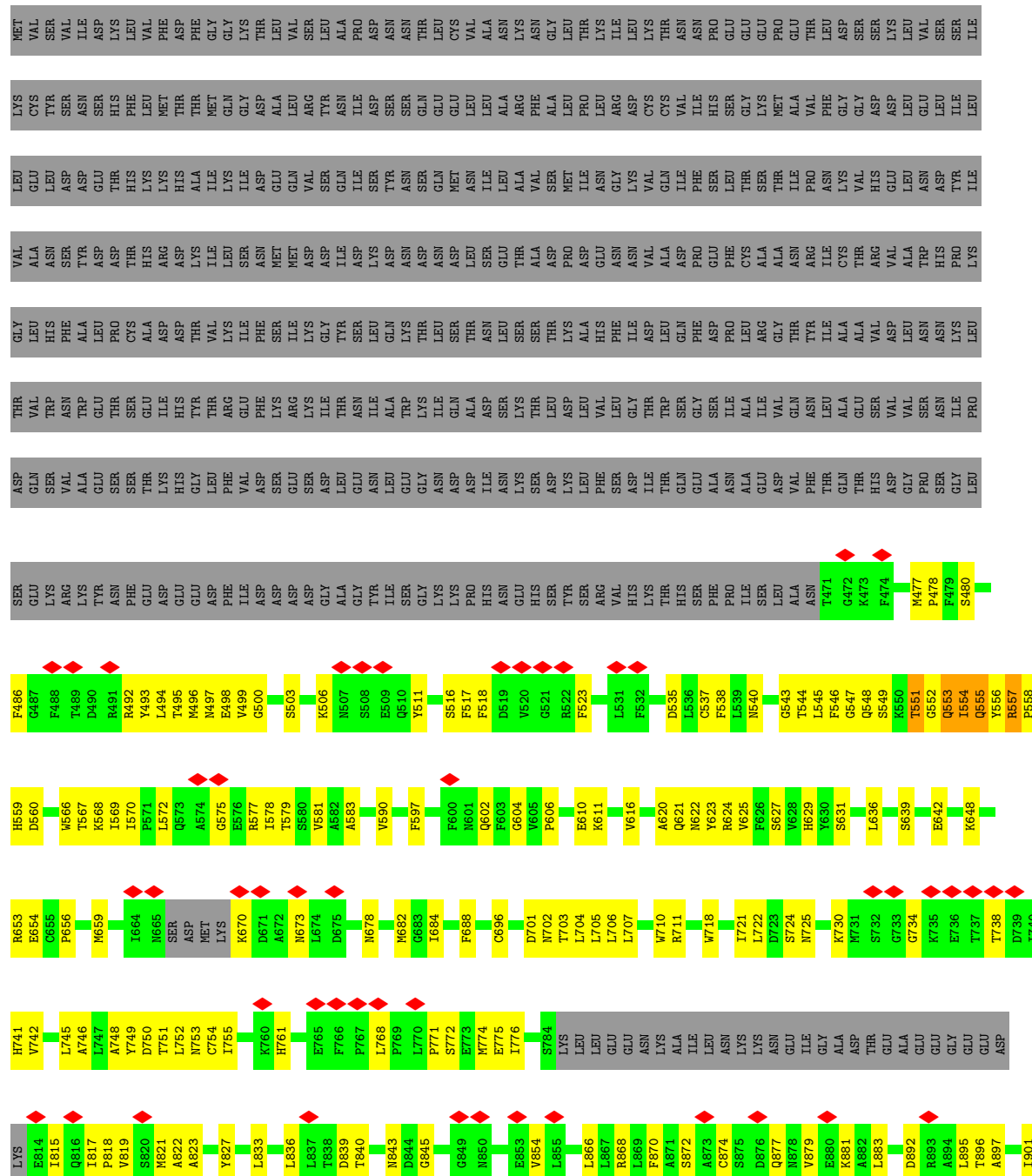
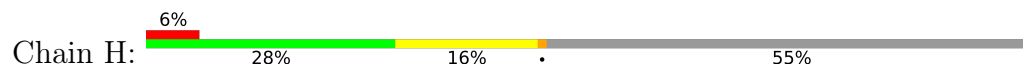


• Molecule 12: DNA polymerase alpha-binding protein

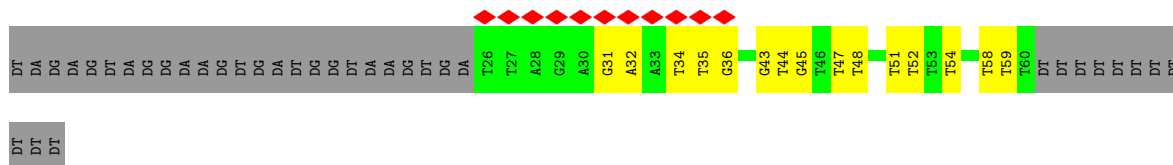
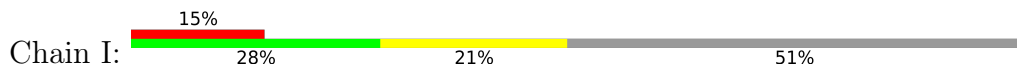




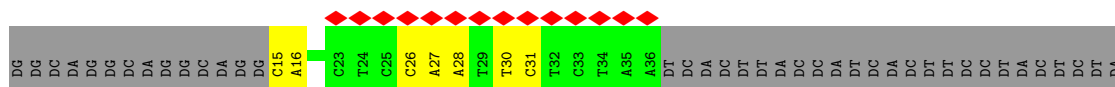
• Molecule 12: DNA polymerase alpha-binding protein



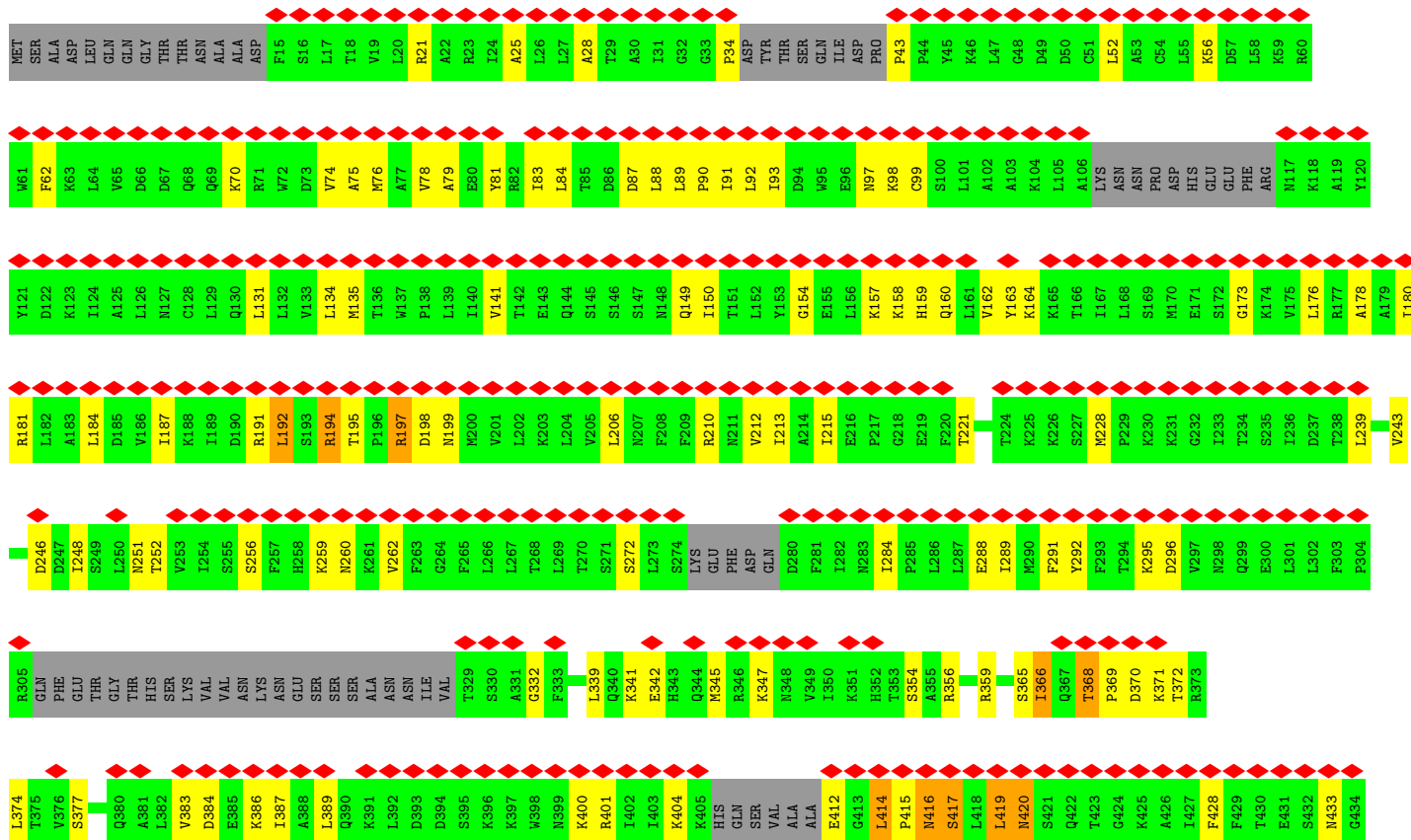
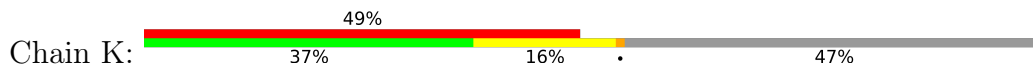
- Molecule 13: DNA (71-mer)

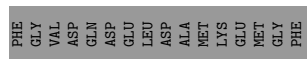


- Molecule 14: DNA (61-mer)



- Molecule 15: Topoisomerase 1-associated factor 1

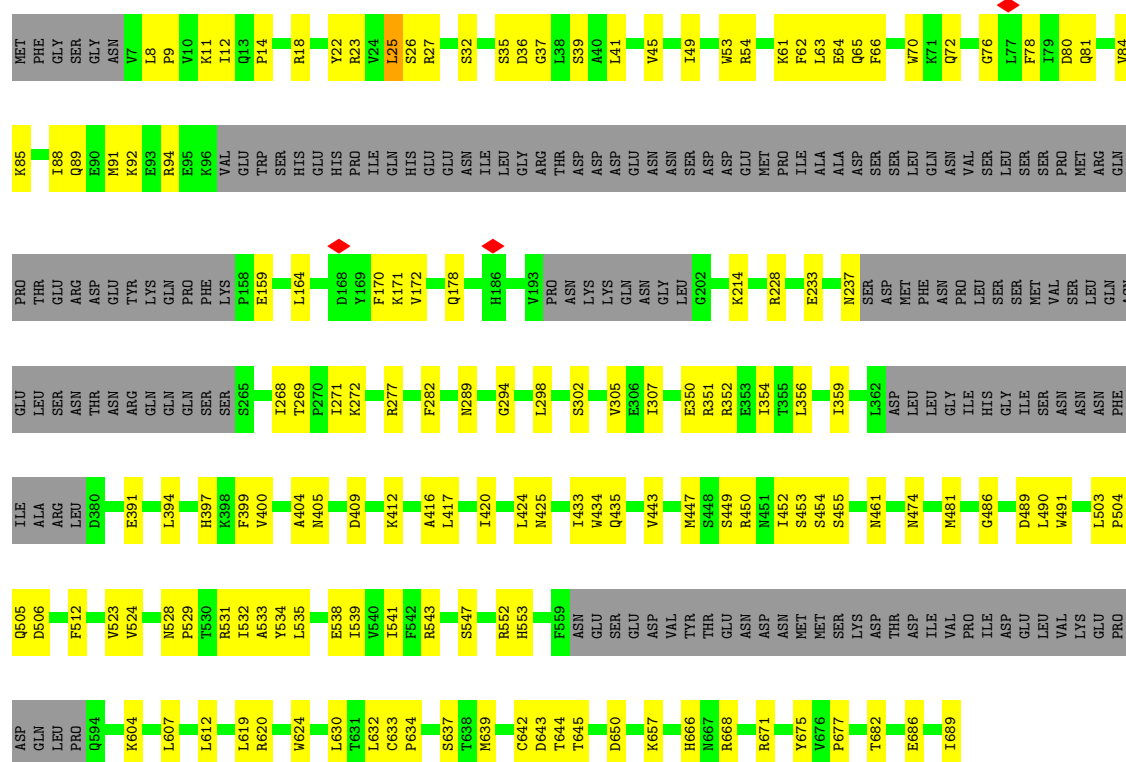




Chain M: 27% 9% 63%



Chain N: 56% 21% 22%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	384519	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.382	Depositor
Minimum map value	-1.647	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	572.39996, 572.39996, 572.39996	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0/5334	0.34	0/7203
2	3	0.26	0/5091	0.36	0/6914
3	4	0.29	1/5566 (0.0%)	0.46	1/7519 (0.0%)
4	5	0.30	0/5407	0.41	0/7302
5	6	0.20	0/4957	0.31	0/6684
6	7	0.21	0/5097	0.37	1/6896 (0.0%)
7	A	0.34	0/1645	0.48	0/2215
8	B	0.26	0/1663	0.41	1/2249 (0.0%)
9	C	0.20	0/1426	0.28	0/1929
10	D	0.19	0/2040	0.31	0/2755
11	E	0.19	0/4677	0.28	0/6335
12	F	0.13	0/3553	0.28	0/4811
12	G	0.09	0/3448	0.27	0/4675
12	H	0.21	0/3443	0.33	0/4668
13	I	0.20	0/805	0.39	0/1244
14	J	0.14	0/488	0.29	0/747
15	K	0.21	0/5449	0.36	0/7340
16	L	0.09	0/804	0.22	0/1074
17	M	0.26	0/6632	0.42	2/8976 (0.0%)
18	N	0.17	0/4345	0.32	0/5884
All	All	0.23	1/71870 (0.0%)	0.36	5/97420 (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
3	4	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	567	CYS	N-CA	5.08	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	160	LEU	N-CA-C	-7.40	104.38	113.19
6	7	364	LYS	N-CA-C	-6.42	105.17	112.87
17	M	1810	ASP	CA-C-N	-5.69	112.86	120.54
17	M	1810	ASP	C-N-CA	-5.69	112.86	120.54
3	4	567	CYS	CB-CA-C	-5.41	109.28	117.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	4	790	ARG	Sidechain

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	5245	0	5289	107	0
2	3	5005	0	5043	94	0
3	4	5494	0	5531	197	0
4	5	5334	0	5383	113	0
5	6	4880	0	4914	126	0
6	7	5023	0	5042	140	0
7	A	1625	0	1621	53	0
8	B	1630	0	1685	20	0
9	C	1394	0	1405	34	0
10	D	2004	0	2001	29	0
11	E	4591	0	4567	80	0
12	F	3467	0	3410	91	0
12	G	3362	0	3299	74	0
12	H	3358	0	3283	115	0
13	I	722	0	407	16	0
14	J	438	0	249	10	0
15	K	5350	0	5519	155	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	L	788	0	827	16	0
17	M	6490	0	6446	159	0
18	N	4254	0	4256	106	0
19	2	1	0	0	0	0
19	4	1	0	0	0	0
19	5	1	0	0	0	0
19	6	1	0	0	0	0
19	7	1	0	0	0	0
19	M	2	0	0	0	0
20	2	27	0	12	2	0
20	3	27	0	12	1	0
21	2	1	0	0	0	0
21	3	1	0	0	0	0
21	5	1	0	0	0	0
21	6	1	0	0	0	0
21	7	1	0	0	0	0
22	5	31	0	12	3	0
22	6	31	0	12	2	0
22	7	31	0	12	1	0
All	All	70613	0	70237	1578	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 11.

The worst 5 of 1578 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)
5:6:536:ALA:HA	5:6:742:ILE:CD1	1.68	1.22
5:6:535:PRO:HB2	5:6:742:ILE:HG21	1.28	1.14
3:4:775:VAL:HB	3:4:779:LYS:HZ2	1.24	1.03
3:4:762:ILE:HG23	5:6:736:MET:HG3	1.37	1.01
3:4:775:VAL:HB	3:4:779:LYS:NZ	1.81	0.94

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	658/868 (76%)	632 (96%)	26 (4%)	0	100	100
2	3	639/971 (66%)	605 (95%)	33 (5%)	1 (0%)	43	71
3	4	684/933 (73%)	646 (94%)	35 (5%)	3 (0%)	30	58
4	5	663/775 (86%)	632 (95%)	29 (4%)	2 (0%)	36	64
5	6	605/1017 (60%)	579 (96%)	26 (4%)	0	100	100
6	7	633/845 (75%)	584 (92%)	47 (7%)	2 (0%)	36	64
7	A	196/208 (94%)	181 (92%)	14 (7%)	1 (0%)	24	54
8	B	191/213 (90%)	182 (95%)	9 (5%)	0	100	100
9	C	167/194 (86%)	160 (96%)	7 (4%)	0	100	100
10	D	237/294 (81%)	229 (97%)	8 (3%)	0	100	100
11	E	560/650 (86%)	544 (97%)	16 (3%)	0	100	100
12	F	429/927 (46%)	407 (95%)	22 (5%)	0	100	100
12	G	417/927 (45%)	393 (94%)	24 (6%)	0	100	100
12	H	415/927 (45%)	385 (93%)	30 (7%)	0	100	100
15	K	644/1238 (52%)	620 (96%)	21 (3%)	3 (0%)	24	54
16	L	92/317 (29%)	89 (97%)	3 (3%)	0	100	100
17	M	799/2222 (36%)	745 (93%)	52 (6%)	2 (0%)	36	64
18	N	524/689 (76%)	491 (94%)	33 (6%)	0	100	100
All	All	8553/14215 (60%)	8104 (95%)	435 (5%)	14 (0%)	44	71

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	5	346	VAL
15	K	417	SER
3	4	780	MET
7	A	22	ARG

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Mol	Chain	Res	Type
17	M	1406	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	579/770 (75%)	572 (99%)	7 (1%)	63	75
2	3	551/835 (66%)	541 (98%)	10 (2%)	51	70
3	4	621/848 (73%)	596 (96%)	25 (4%)	28	56
4	5	605/688 (88%)	598 (99%)	7 (1%)	63	75
5	6	535/886 (60%)	532 (99%)	3 (1%)	78	81
6	7	550/753 (73%)	549 (100%)	1 (0%)	87	87
7	A	182/193 (94%)	174 (96%)	8 (4%)	25	54
8	B	184/198 (93%)	182 (99%)	2 (1%)	65	76
9	C	156/173 (90%)	156 (100%)	0	100	100
10	D	234/279 (84%)	234 (100%)	0	100	100
11	E	509/586 (87%)	509 (100%)	0	100	100
12	F	382/825 (46%)	382 (100%)	0	100	100
12	G	370/825 (45%)	370 (100%)	0	100	100
12	H	368/825 (45%)	361 (98%)	7 (2%)	50	70
15	K	600/1125 (53%)	591 (98%)	9 (2%)	57	73
16	L	87/285 (30%)	87 (100%)	0	100	100
17	M	720/2014 (36%)	701 (97%)	19 (3%)	40	65
18	N	474/629 (75%)	472 (100%)	2 (0%)	84	84
All	All	7707/12737 (60%)	7607 (99%)	100 (1%)	59	74

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A	25	GLN

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Mol	Chain	Res	Type
15	K	192	LEU
18	N	26	SER
7	A	28	ASN
12	H	554	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
12	F	916	ASN
17	M	1587	GLN
12	G	725	ASN
15	K	159	HIS
17	M	1865	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 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
20	ADP	3	1001	21	28,29,29	1.37	5 (17%)	43,45,45	1.81	8 (18%)
22	AGS	7	903	21	32,33,33	0.54	1 (3%)	45,52,52	0.65	1 (2%)
22	AGS	6	1103	21	32,33,33	0.59	1 (3%)	45,52,52	0.75	1 (2%)
20	ADP	2	902	21	28,29,29	1.37	5 (17%)	43,45,45	1.74	7 (16%)
22	AGS	5	802	21	32,33,33	0.73	1 (3%)	45,52,52	0.77	1 (2%)

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
20	ADP	3	1001	21	-	2/16/32/32	0/3/3/3
22	AGS	7	903	21	-	5/21/38/38	0/3/3/3
22	AGS	6	1103	21	-	4/21/38/38	0/3/3/3
20	ADP	2	902	21	-	2/16/32/32	0/3/3/3
22	AGS	5	802	21	-	7/21/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	1001	ADP	C5-C4	4.29	1.46	1.39
20	2	902	ADP	C5-C4	4.29	1.46	1.39
20	2	902	ADP	C5-N7	-2.65	1.34	1.39
20	3	1001	ADP	C5-N7	-2.61	1.34	1.39
20	2	902	ADP	C5-C6	2.37	1.47	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	1001	ADP	C5-C4-N3	-5.80	118.73	126.72
20	2	902	ADP	C5-C4-N3	-5.51	119.13	126.72
20	3	1001	ADP	N3-C4-N9	4.69	135.14	127.17
22	5	802	AGS	PB-O3B-PG	-4.47	116.81	133.17
20	2	902	ADP	N3-C4-N9	4.39	134.64	127.17

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

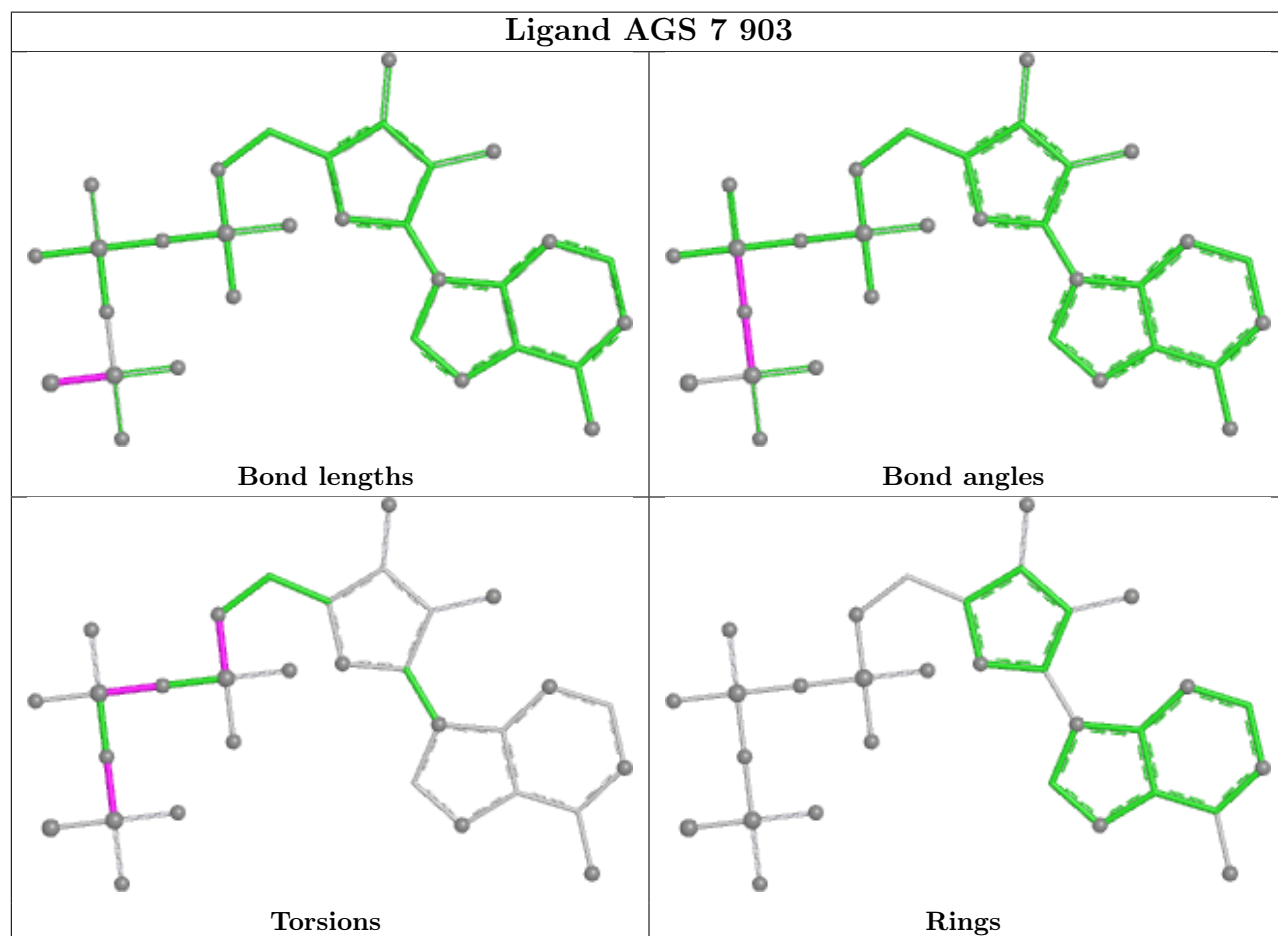
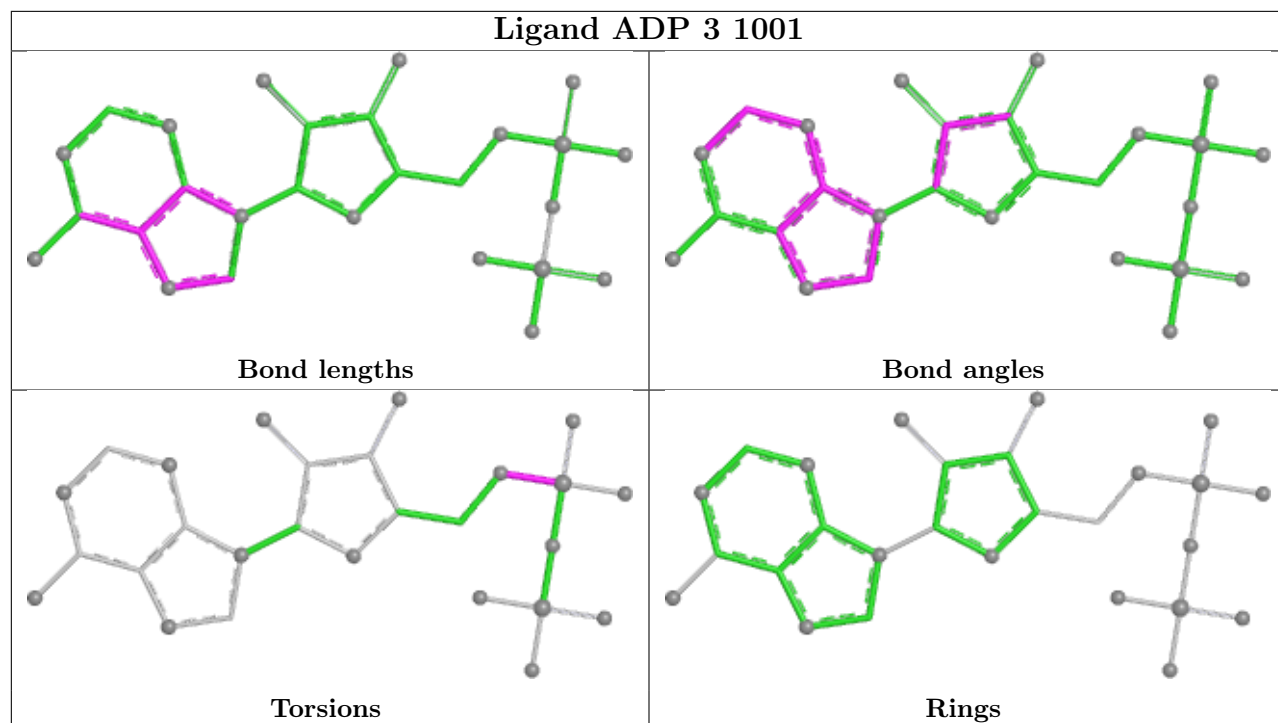
Mol	Chain	Res	Type	Atoms
20	2	902	ADP	C5'-O5'-PA-O3A
20	3	1001	ADP	C5'-O5'-PA-O2A
20	3	1001	ADP	C5'-O5'-PA-O3A
22	5	802	AGS	PB-O3B-PG-O2G
22	5	802	AGS	PB-O3B-PG-O3G

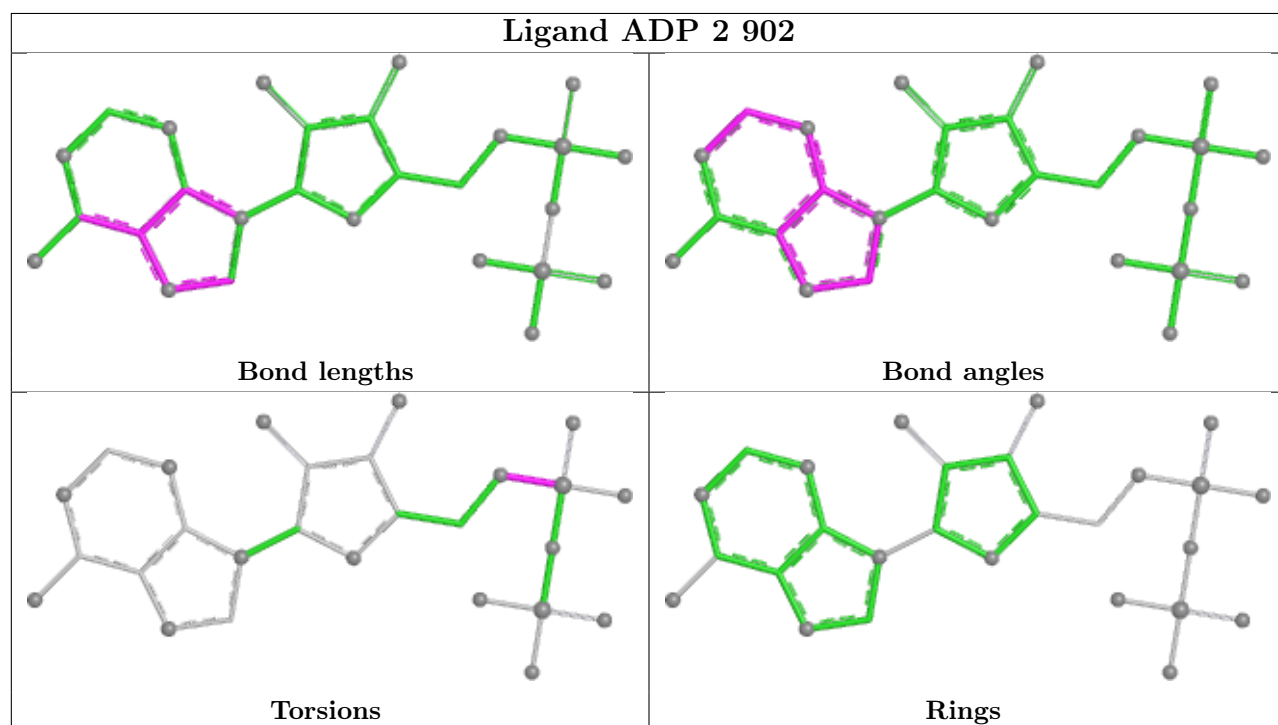
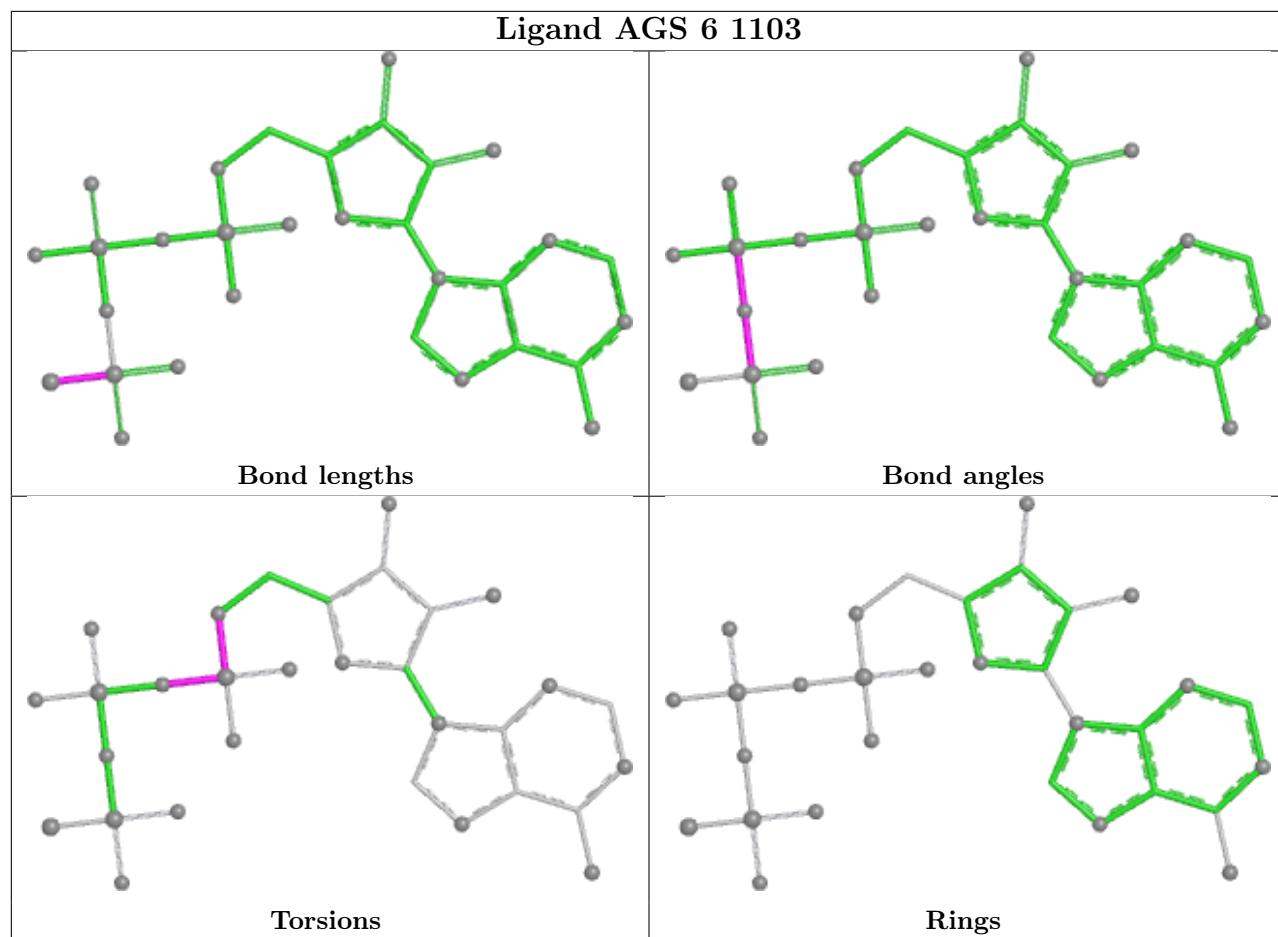
There are no ring outliers.

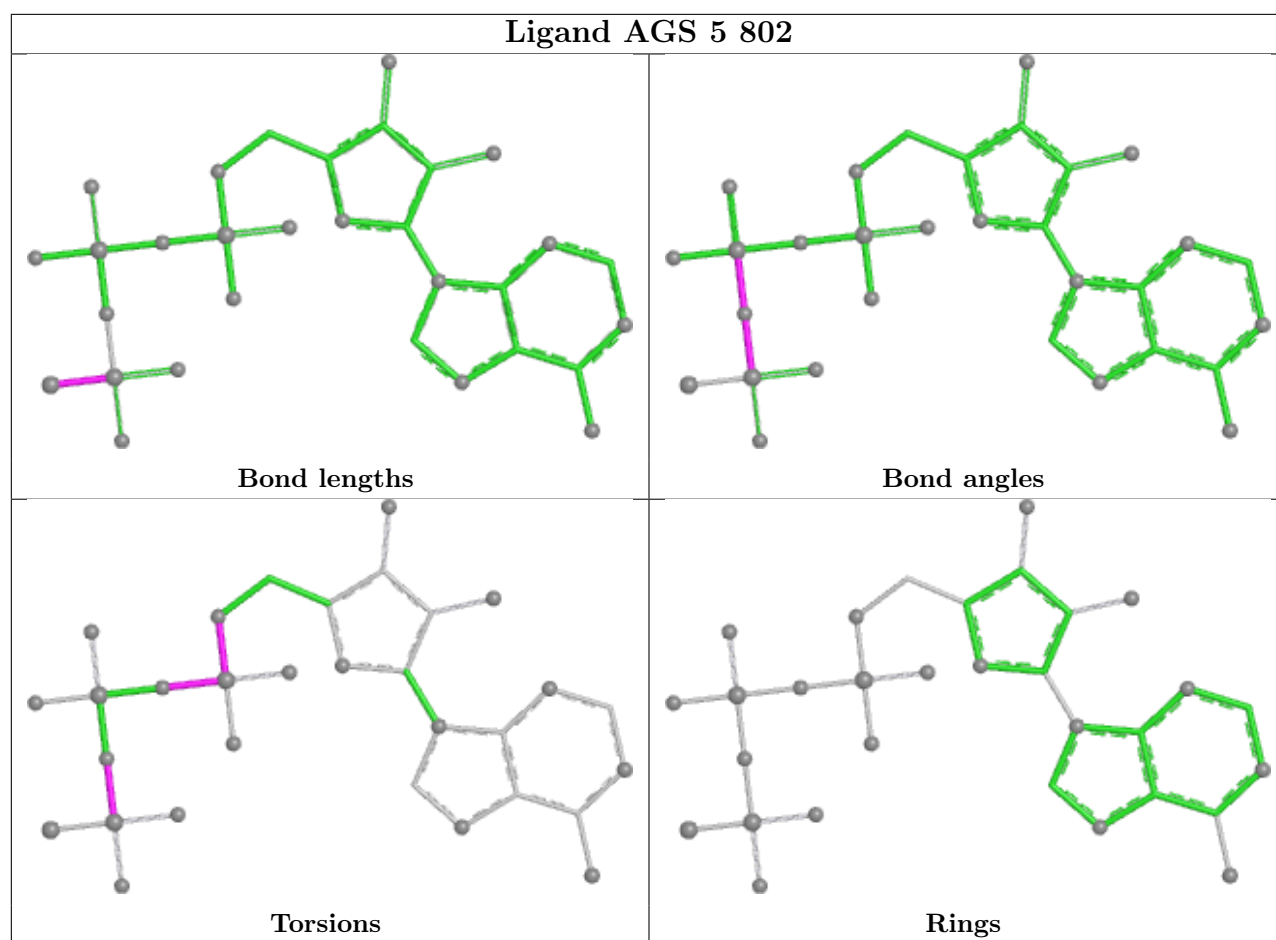
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	1001	ADP	1	0
22	7	903	AGS	1	0
22	6	1103	AGS	2	0
20	2	902	ADP	2	0
22	5	802	AGS	3	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.

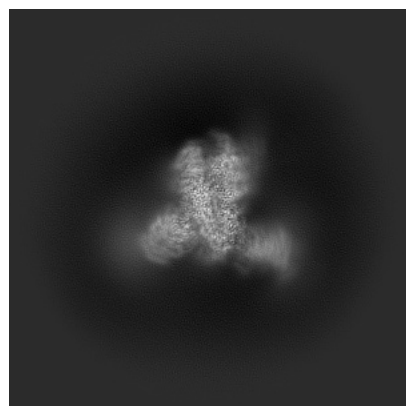
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37211. These allow visual inspection of the internal detail of the map and identification of artifacts.

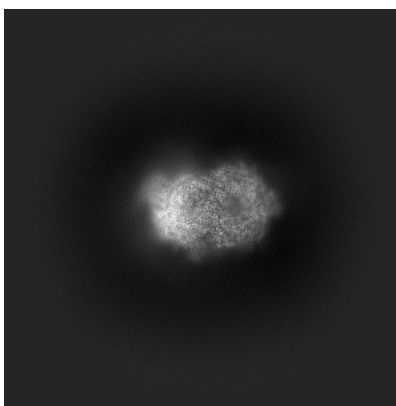
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

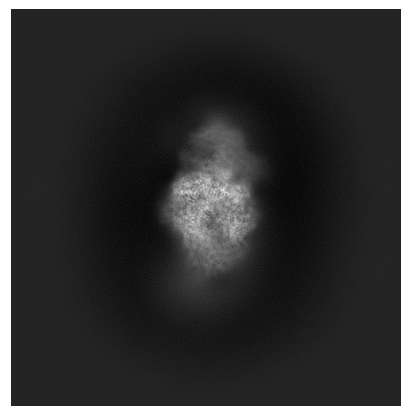
6.1.1 Primary map



X

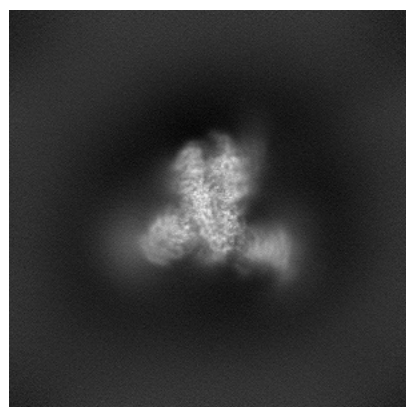


Y

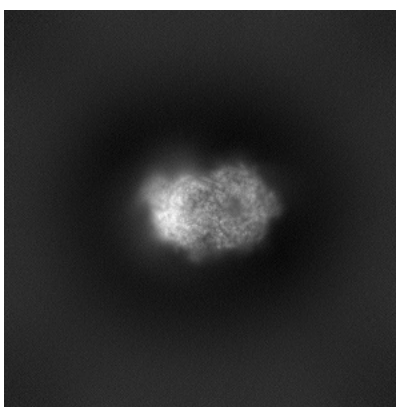


Z

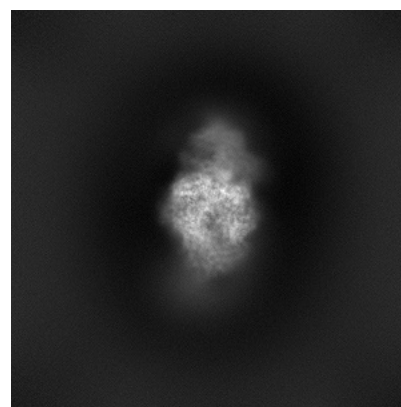
6.1.2 Raw map



X



Y

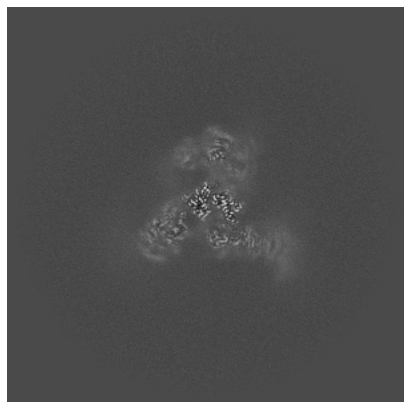


Z

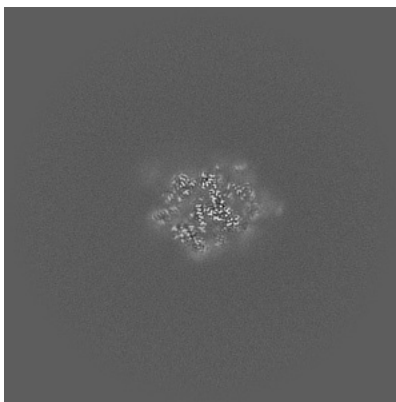
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

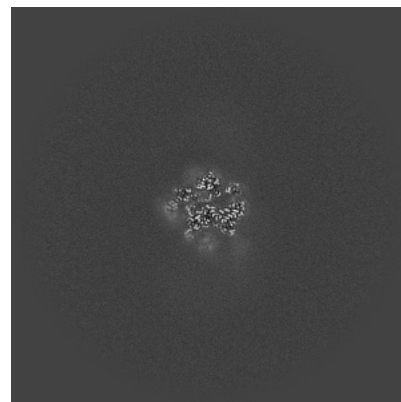
6.2.1 Primary map



X Index: 270

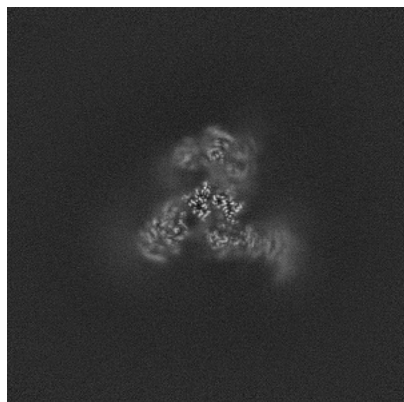


Y Index: 270

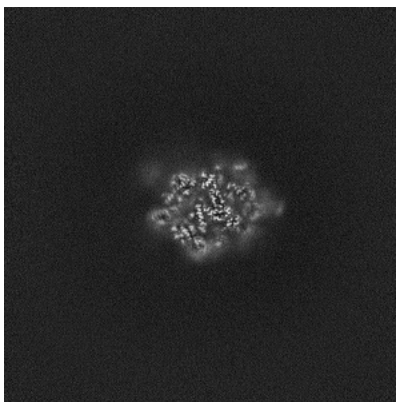


Z Index: 270

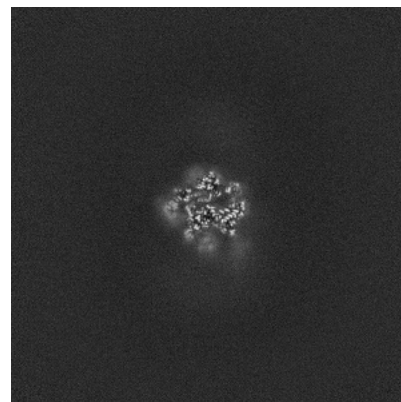
6.2.2 Raw map



X Index: 270



Y Index: 270

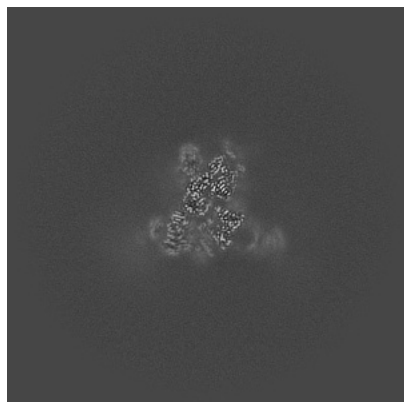


Z Index: 270

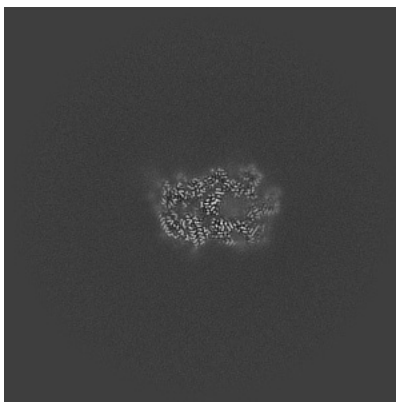
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

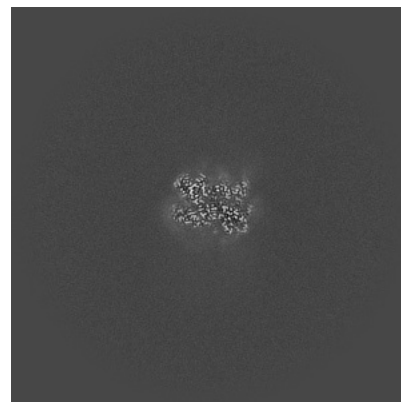
6.3.1 Primary map



X Index: 247

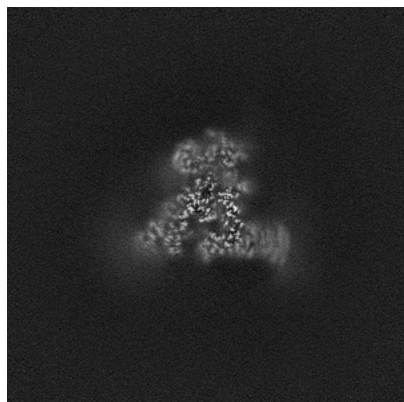


Y Index: 292

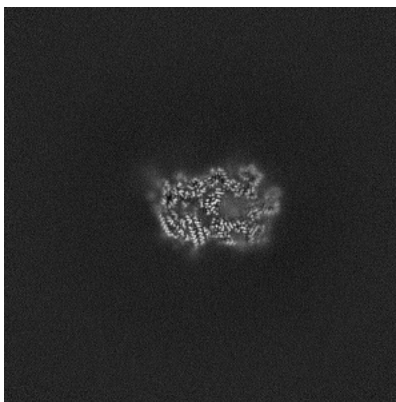


Z Index: 287

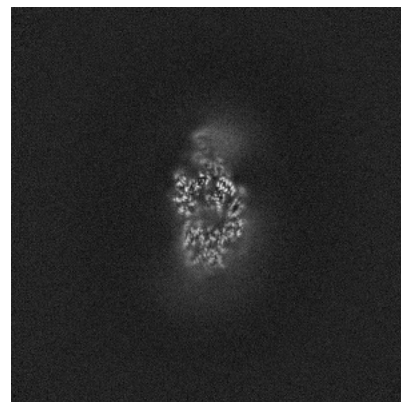
6.3.2 Raw map



X Index: 260



Y Index: 292

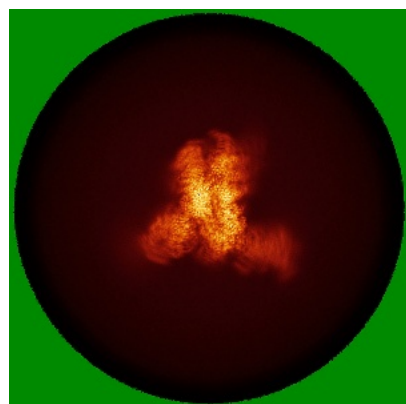


Z Index: 237

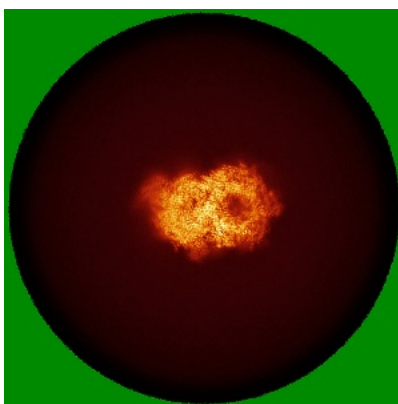
The images above show the largest variance slices of the map in three orthogonal directions.

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

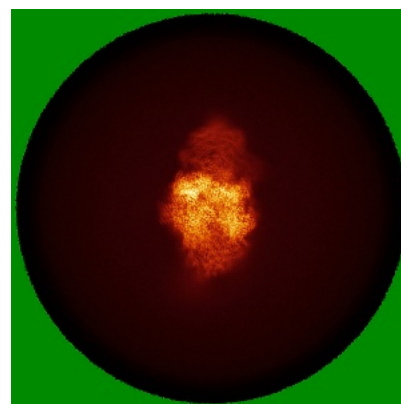
6.4.1 Primary map



X

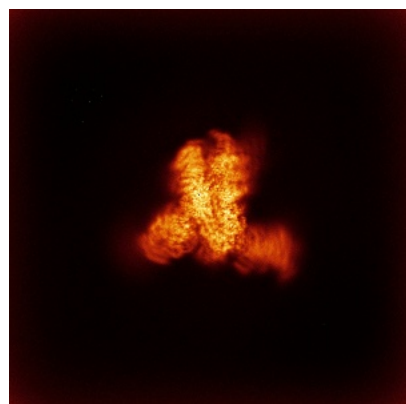


Y

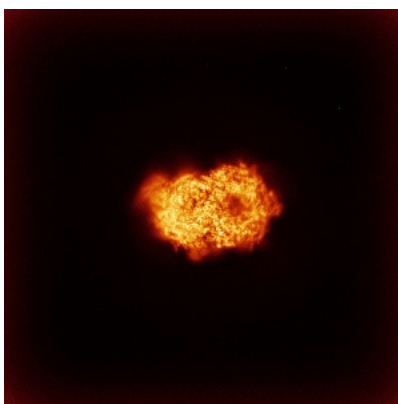


Z

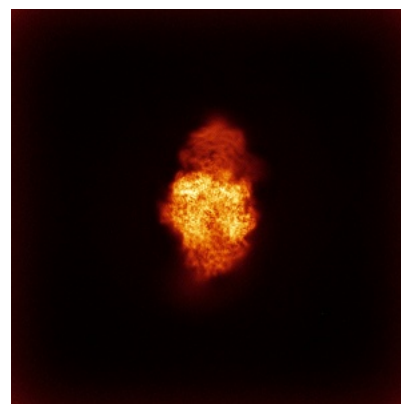
6.4.2 Raw map



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 0.35. 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.

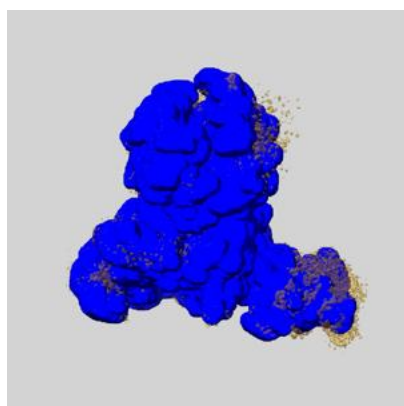
6.6 Mask visualisation [i](#)

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

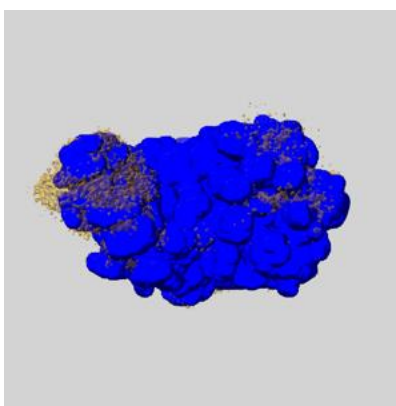
A mask typically either:

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

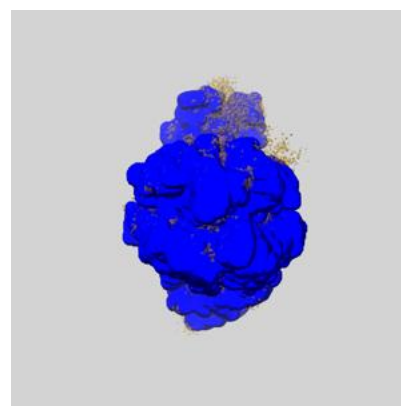
6.6.1 emd_37211_msk_1.map [i](#)



X



Y

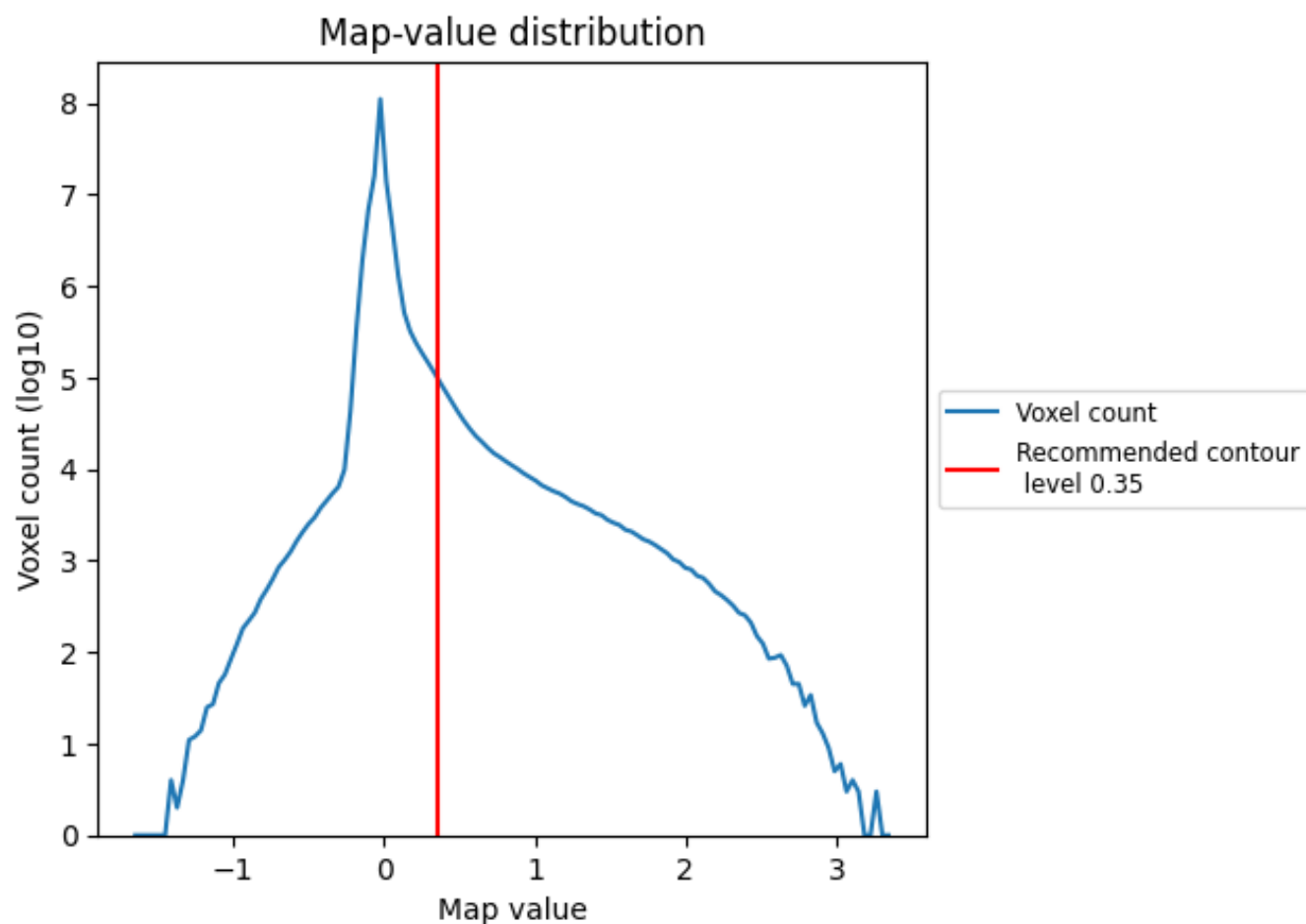


Z

7 Map analysis [i](#)

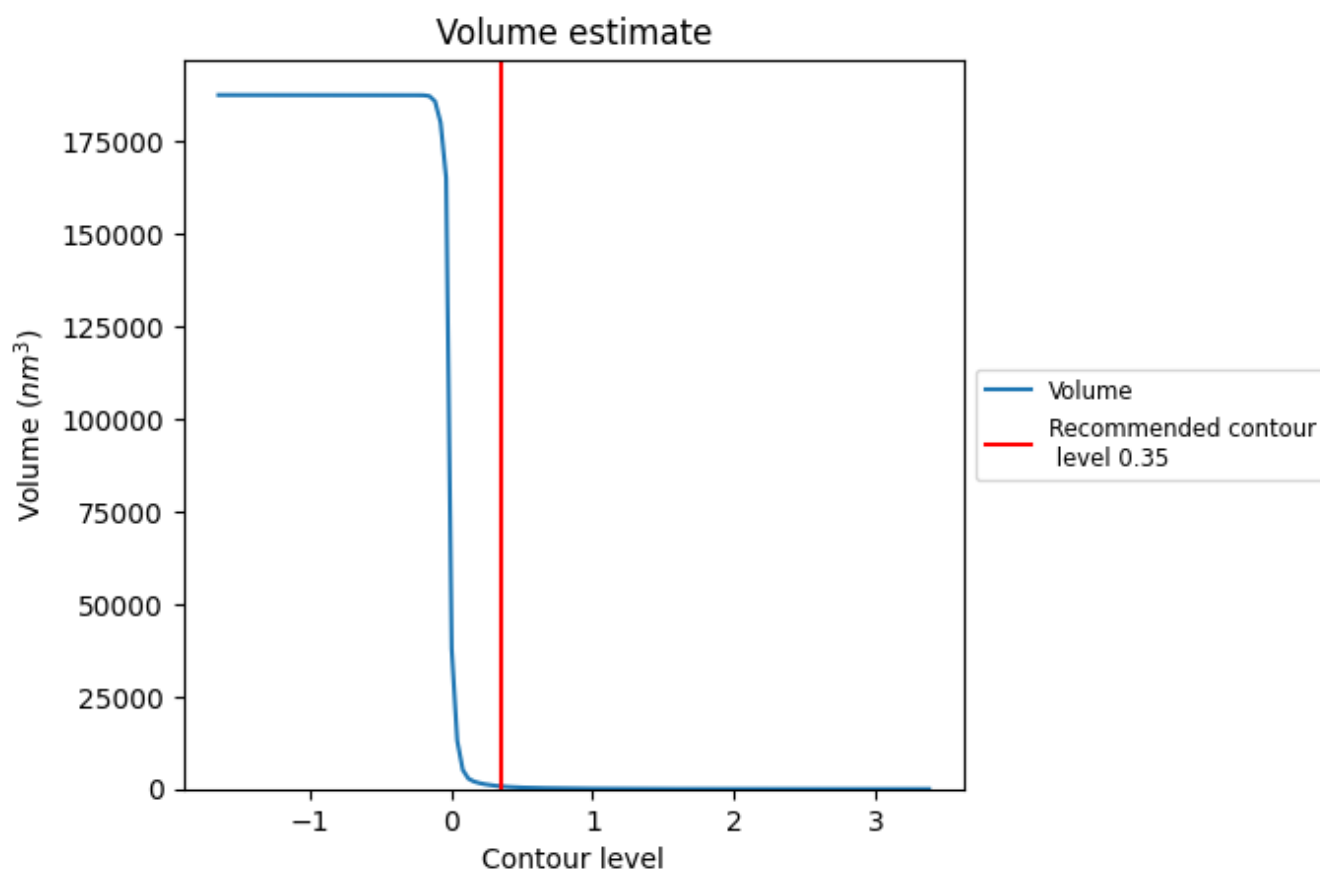
This section contains the results of statistical analysis of the map.

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.

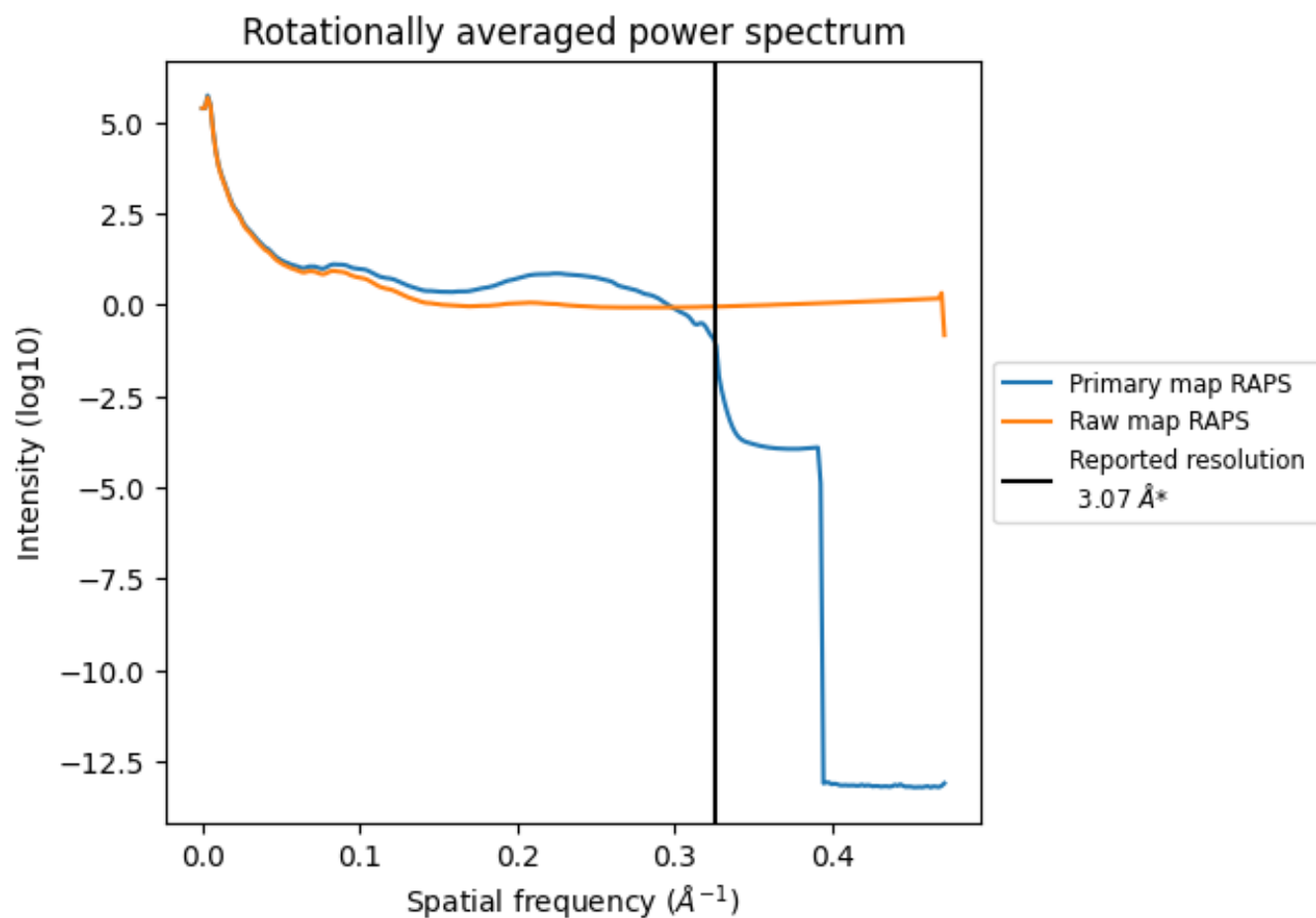
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 720 nm^3 ; this corresponds to an approximate mass of 651 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 ⓘ

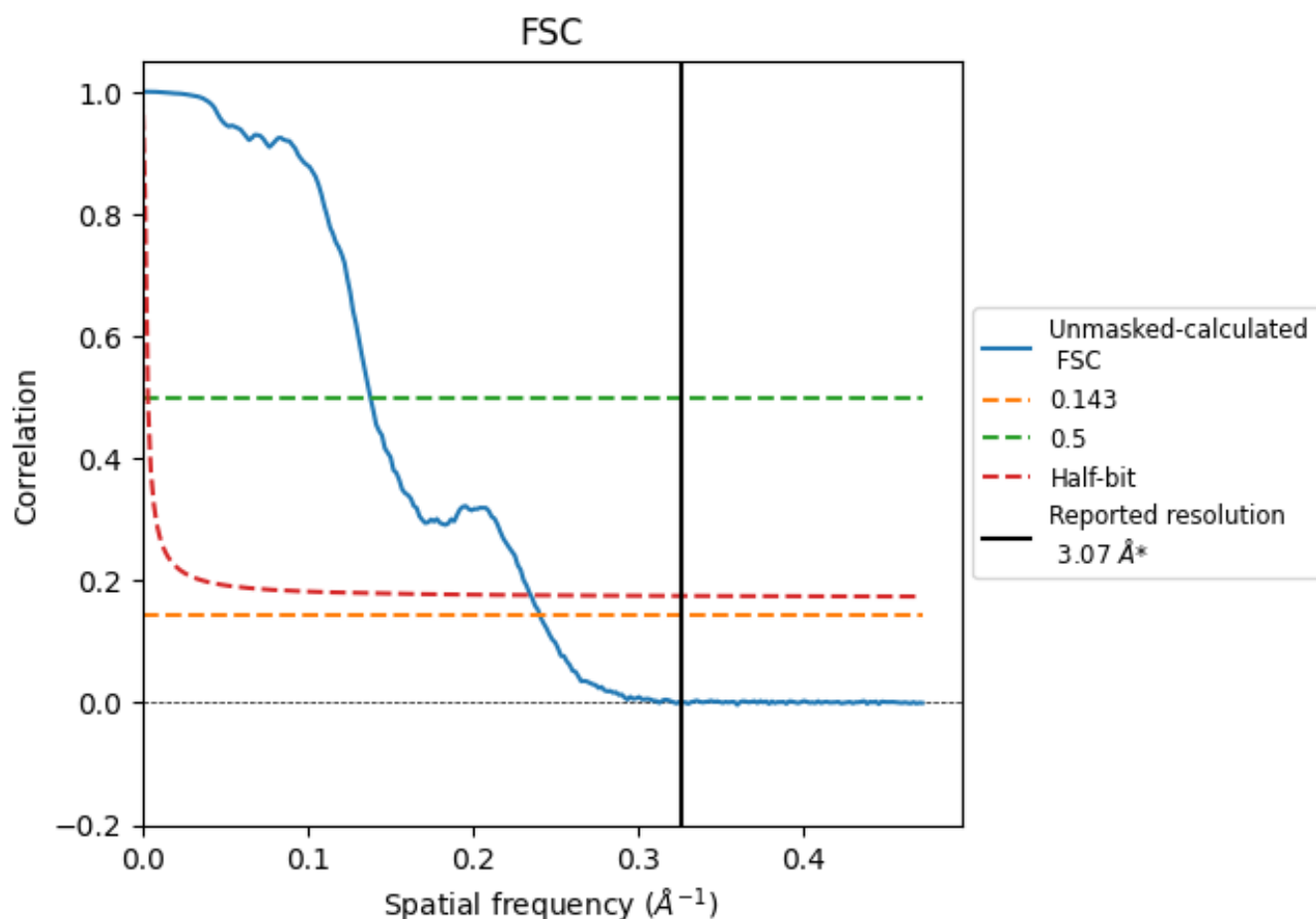


*Reported resolution corresponds to spatial frequency of 0.326 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.326 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

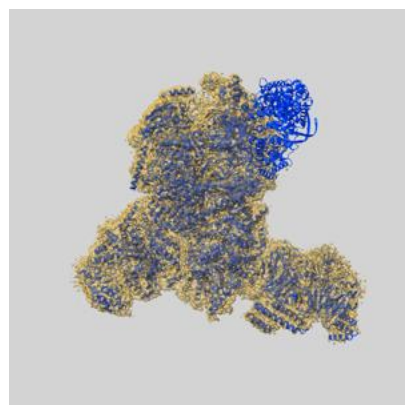
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	7.25	4.26

*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 4.16 differs from the reported value 3.07 by more than 10 %

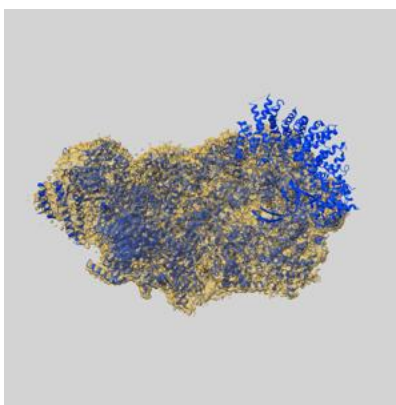
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37211 and PDB model 8KG6. Per-residue inclusion information can be found in section [3](#) on page [9](#).

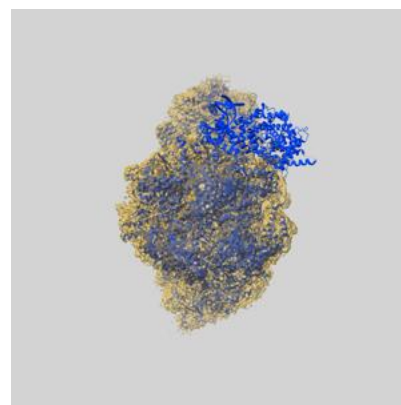
9.1 Map-model overlay [i](#)



X



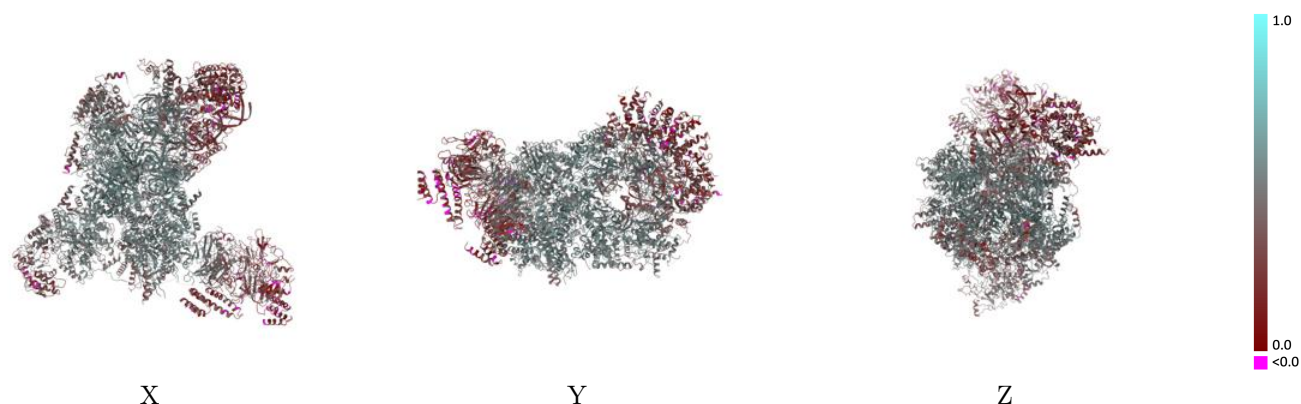
Y



Z

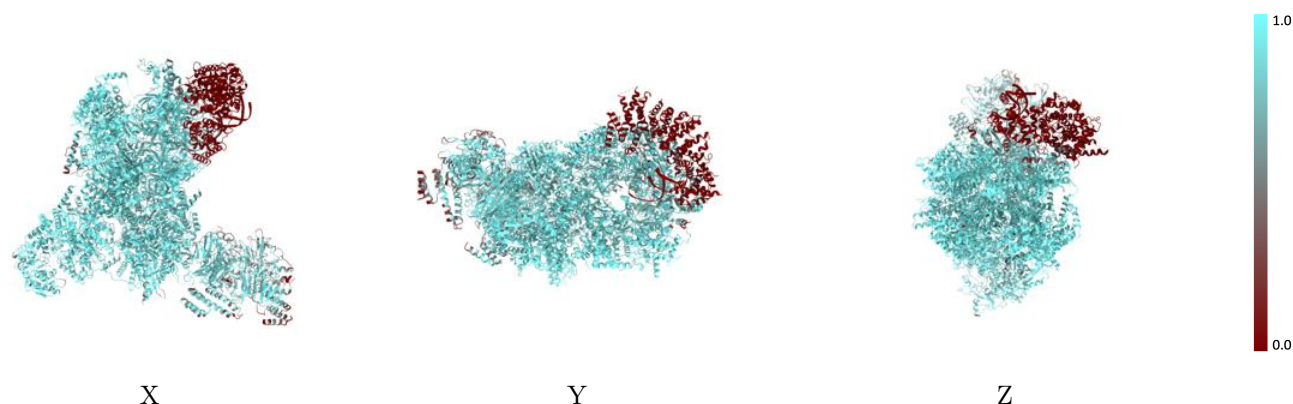
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



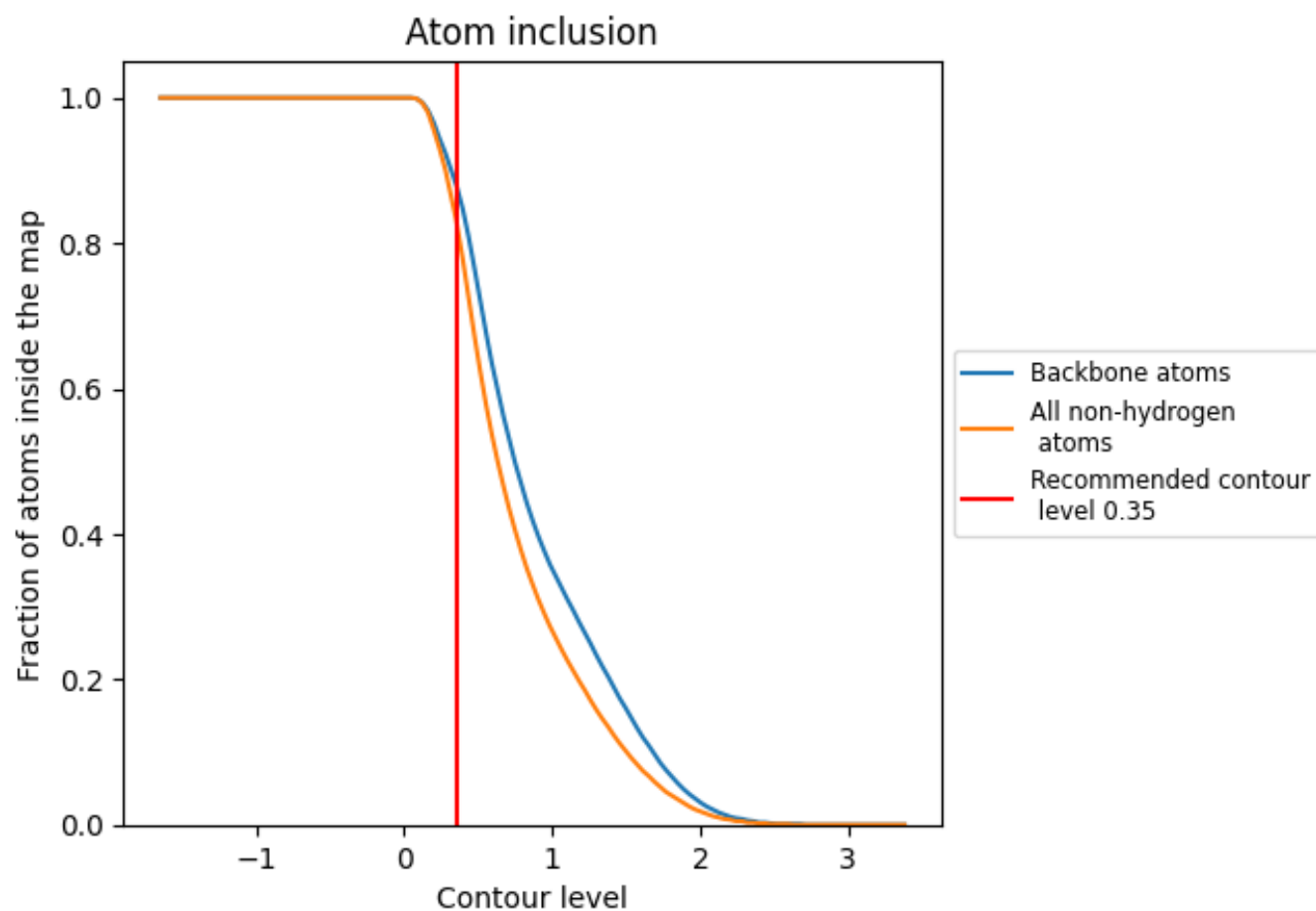
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8330	 0.4370
2	 0.9600	 0.5330
3	 0.9710	 0.5320
4	 0.8990	 0.4220
5	 0.9520	 0.5310
6	 0.9560	 0.4970
7	 0.9270	 0.4400
A	 0.9430	 0.4760
B	 0.9780	 0.5500
C	 0.9720	 0.5130
D	 0.9390	 0.5040
E	 0.9510	 0.5140
F	 0.8350	 0.4000
G	 0.6860	 0.2220
H	 0.7200	 0.2670
I	 0.5890	 0.3550
J	 0.3650	 0.3120
K	 0.0790	 0.2590
L	 0.0250	 0.2590
M	 0.9310	 0.4300
N	 0.9420	 0.4680

