



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:36 AM UTC

PDB ID : 9BCX / pdb_00009bcx
EMDB ID : EMD-44441
Title : Cryo-EM structure of the *S. cerevisiae* ORC-Cdc6-Mcm2-7-DNA complex with a fully closed Mcm2-Mcm5 DNA entry gate
Authors : Yuan, Z.; Bai, L.; Li, H.; Speck, C.
Deposited on : 2024-04-10
Resolution : 6.10 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:

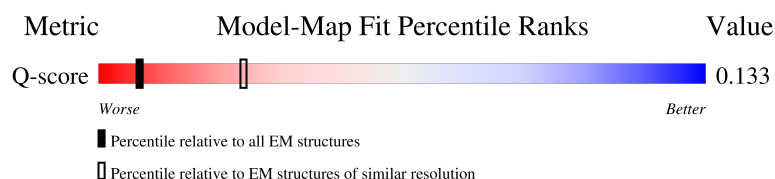
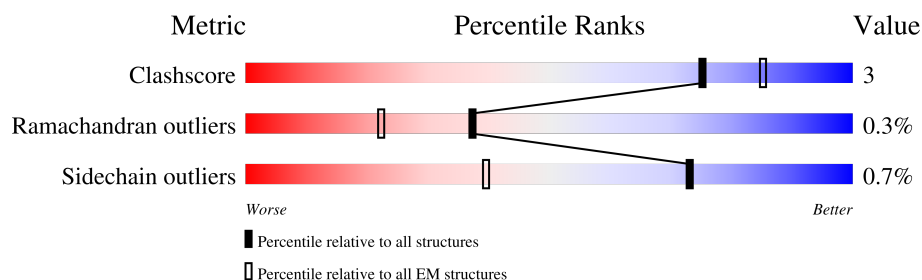
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 6.10 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.



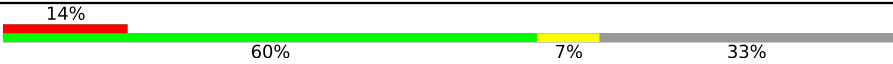
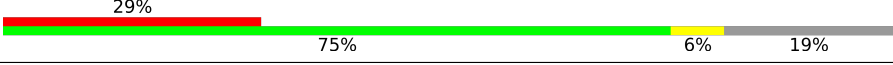
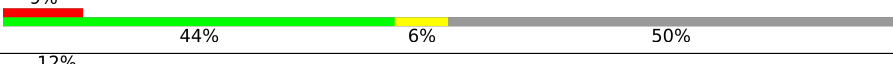
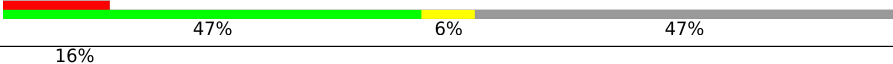
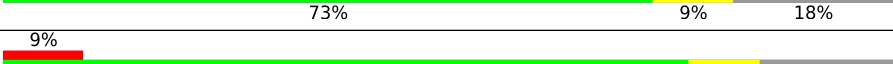
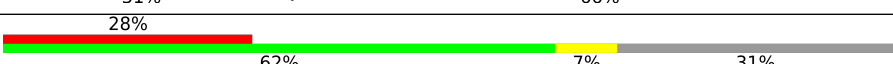
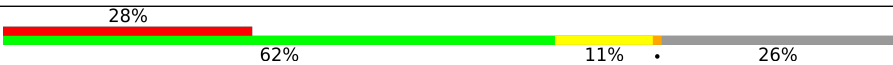
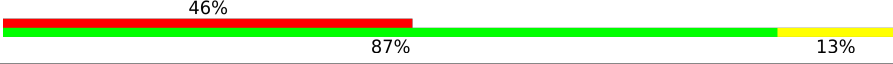
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	531 (5.60 - 6.60)

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	24% 68% 28%
2	3	971	25% 61% 5% 34%
3	5	775	33% 78% 5% 18%
4	4	933	15% 66% 7% 27%

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Mol	Chain	Length	Quality of chain
5	6	1017	
6	7	845	
7	B	914	
8	C	620	
9	D	616	
10	E	529	
11	F	479	
12	G	435	
13	I	513	
14	8	604	
15	O	39	
16	P	39	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 57494 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	627	Total	C	N	O	S	0	0
			4813	3025	849	921	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	640	Total	C	N	O	S	0	0
			4857	3061	856	932	8		

- Molecule 3 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	639	Total	C	N	O	S	0	0
			4974	3136	853	964	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	682	Total	C	N	O	S	0	0
			5305	3331	909	1036	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	686	Total	C	N	O	S	0	0
			5348	3373	917	1029	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	688	Total	C	N	O	S	0	0
			5386	3388	925	1042	31		

- Molecule 7 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	457	Total	C	N	O	S	0	0
			3618	2307	619	675	17		

- Molecule 8 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	330	Total	C	N	O	S	0	0
			2698	1750	445	489	14		

- Molecule 9 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	542	Total	C	N	O	S	0	0
			4410	2848	723	823	16		

- Molecule 10 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	434	Total	C	N	O	S	0	0
			3514	2253	594	655	12		

- Molecule 11 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	409	Total	C	N	O	S	0	0
			3336	2183	529	611	13		

- Molecule 12 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	150	Total	C	N	O	S	0	0
			1224	789	205	219	11		

- Molecule 13 is a protein called Cell division control protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	356	Total	C	N	O	S	0	0
			2788	1798	461	513	16		

- Molecule 14 is a protein called TAH11 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	8	447	Total	C	N	O	S	0	0
			3527	2241	614	659	13		

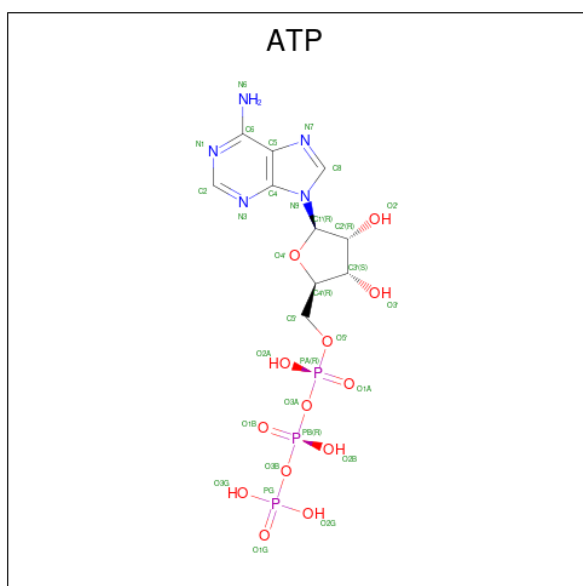
- Molecule 15 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	39	Total	C	N	O	P	0	0
			795	383	127	246	39		

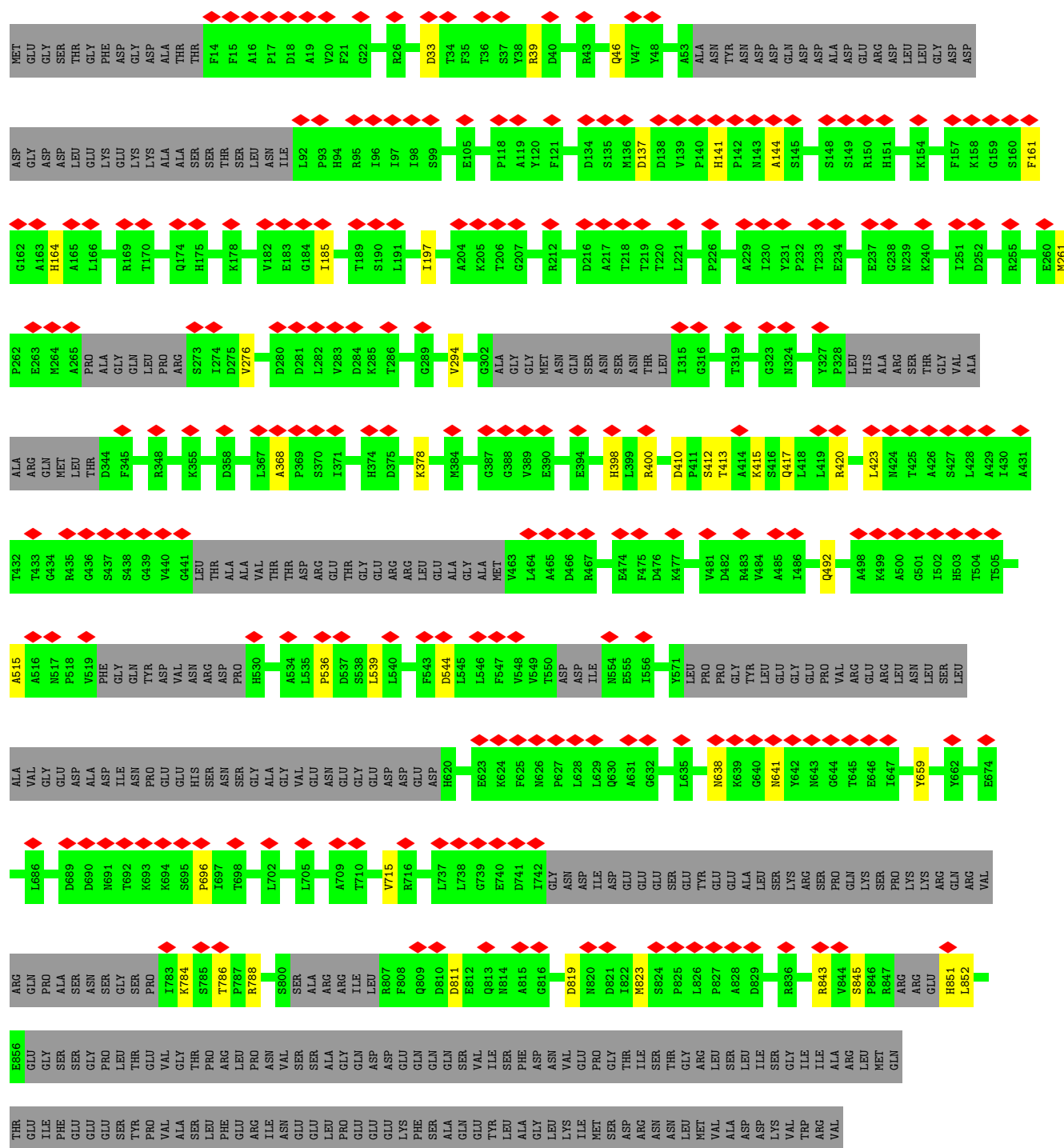
- Molecule 16 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	39	Total	C	N	O	P	0	0
			804	382	161	222	39		

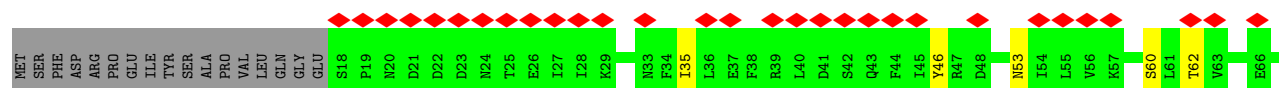
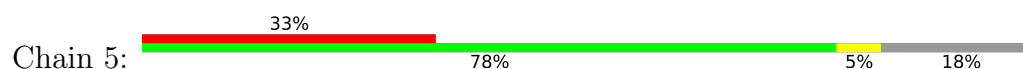
- Molecule 17 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

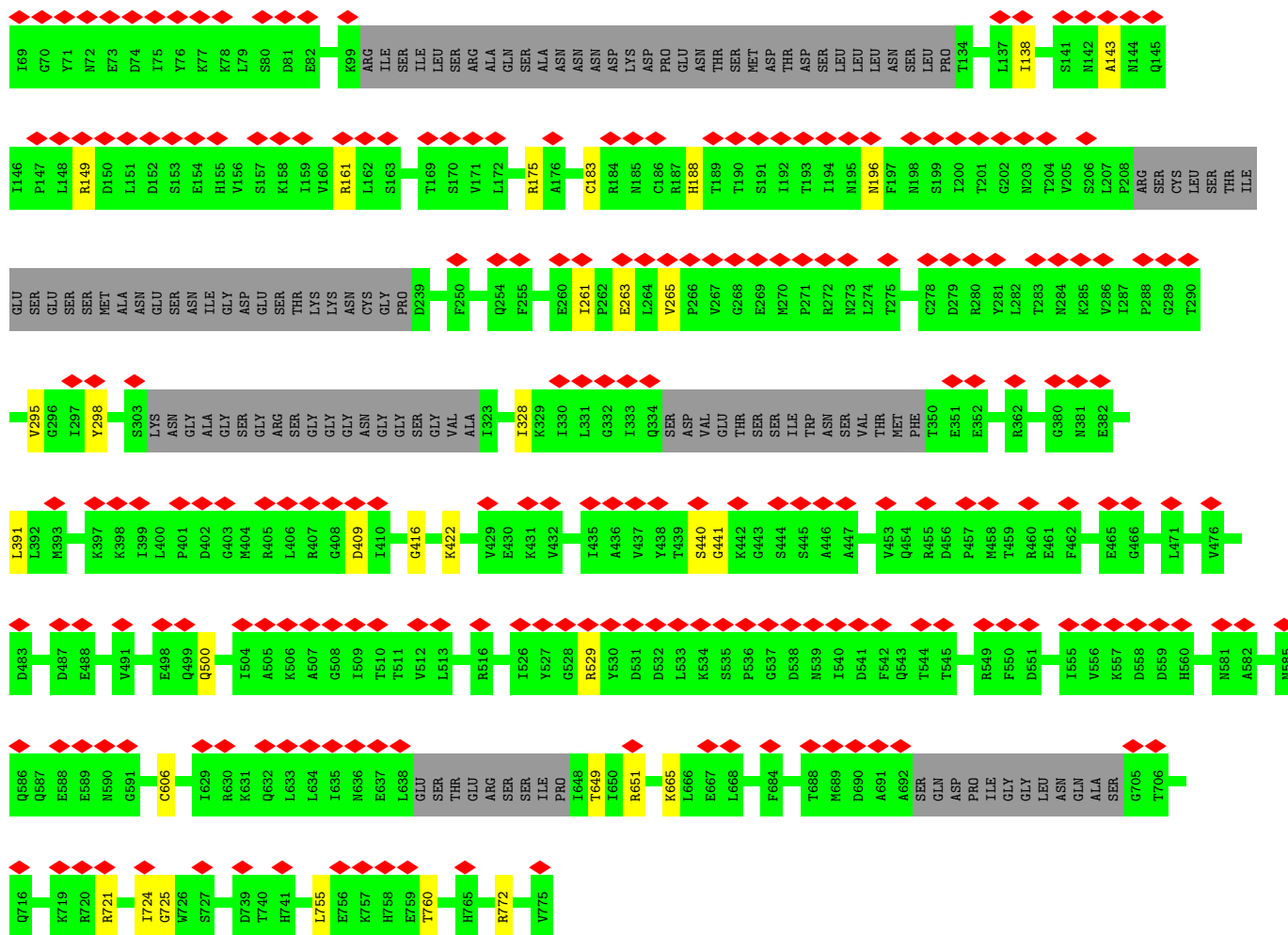


Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total 1	Mg 1	0
18	E	1	Total 1	Mg 1	0
18	F	1	Total 1	Mg 1	0
18	I	1	Total 1	Mg 1	0

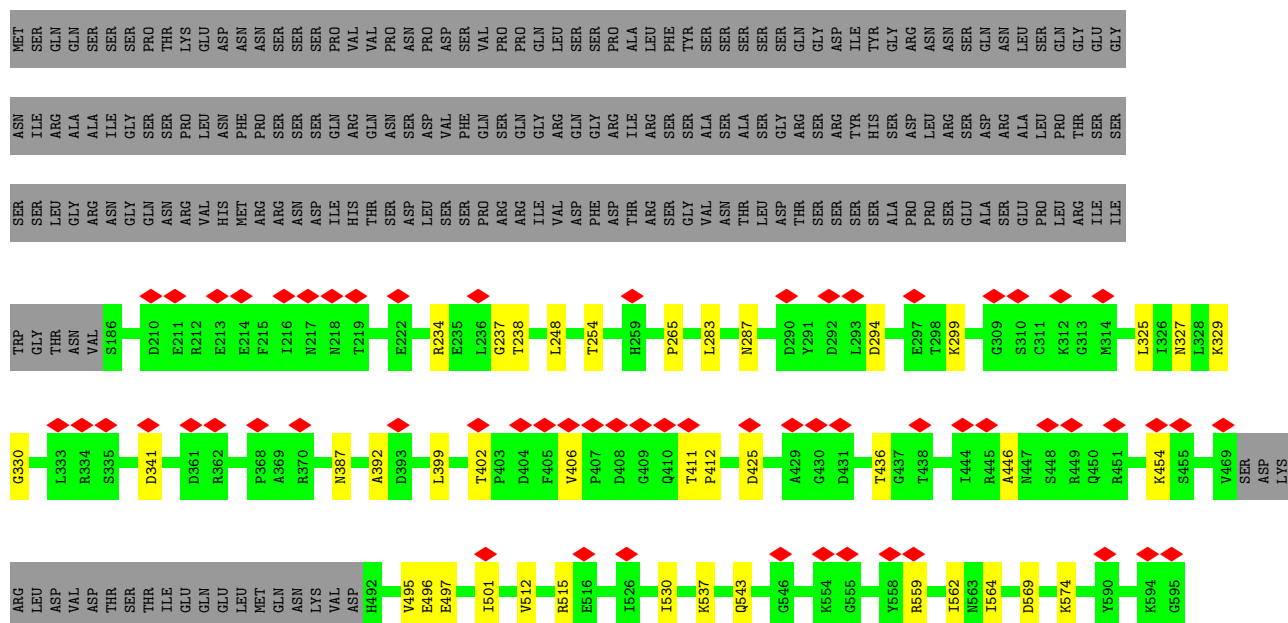


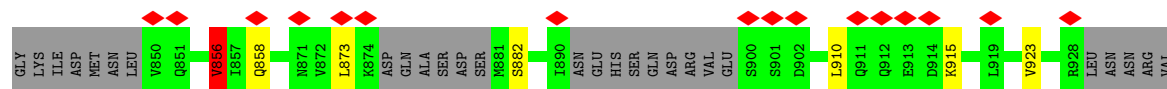
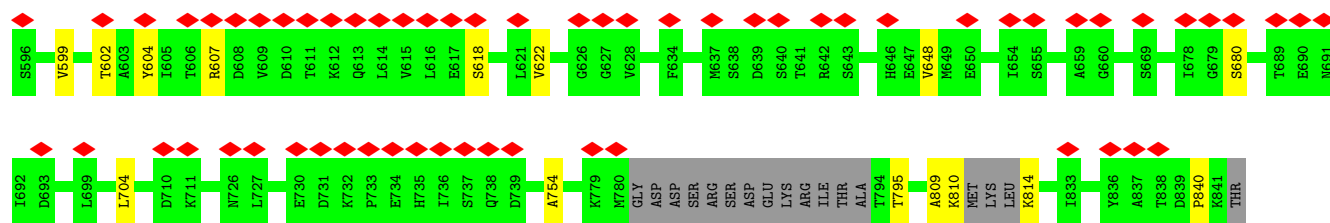
• Molecule 3: DNA replication licensing factor MCM5



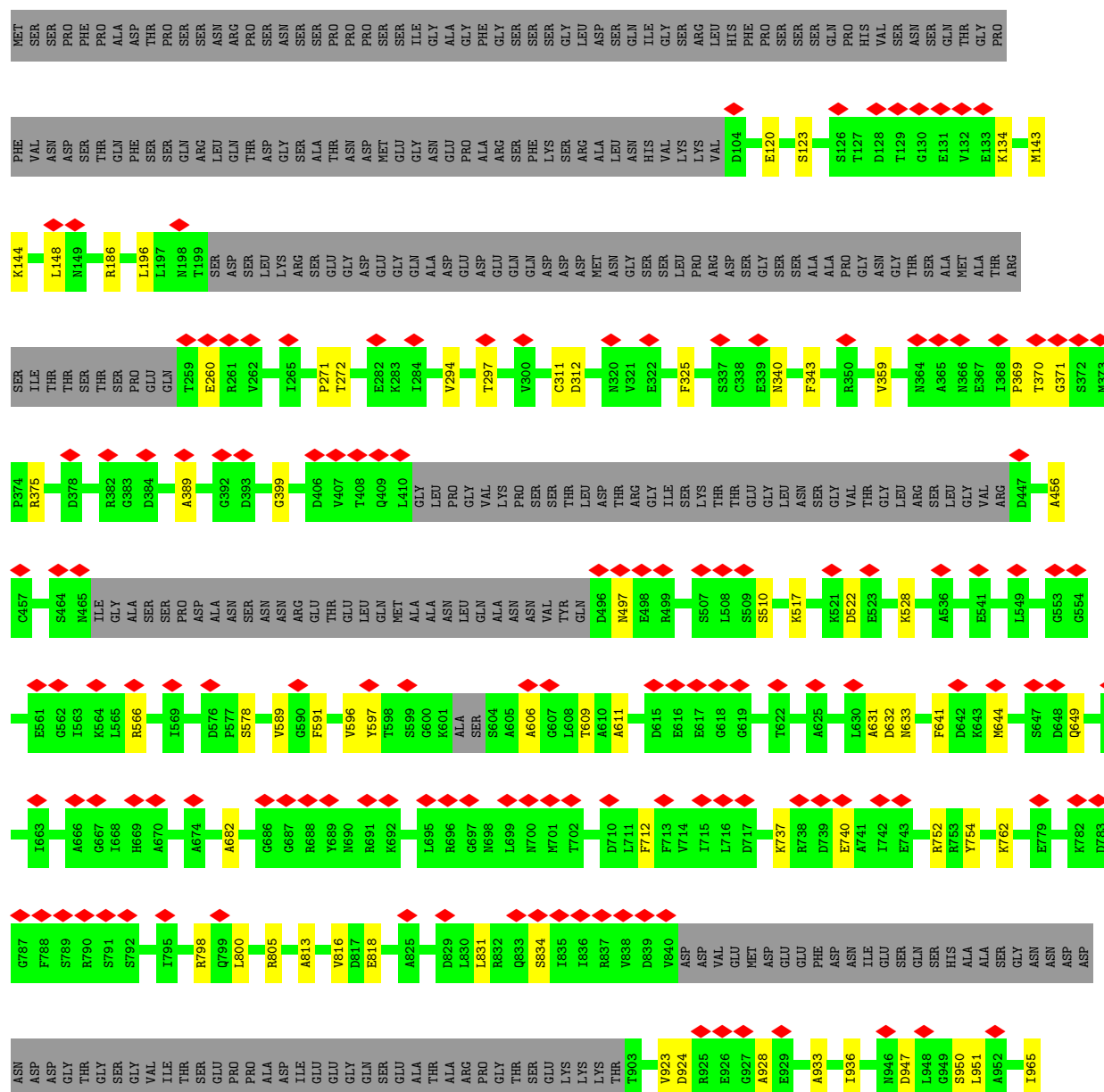


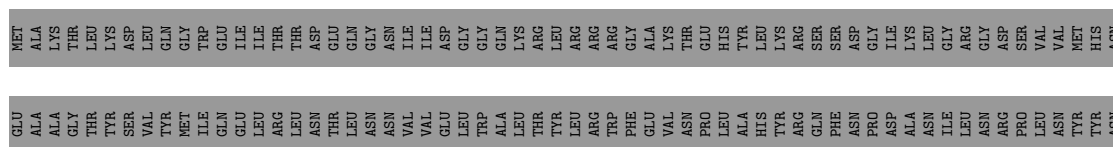
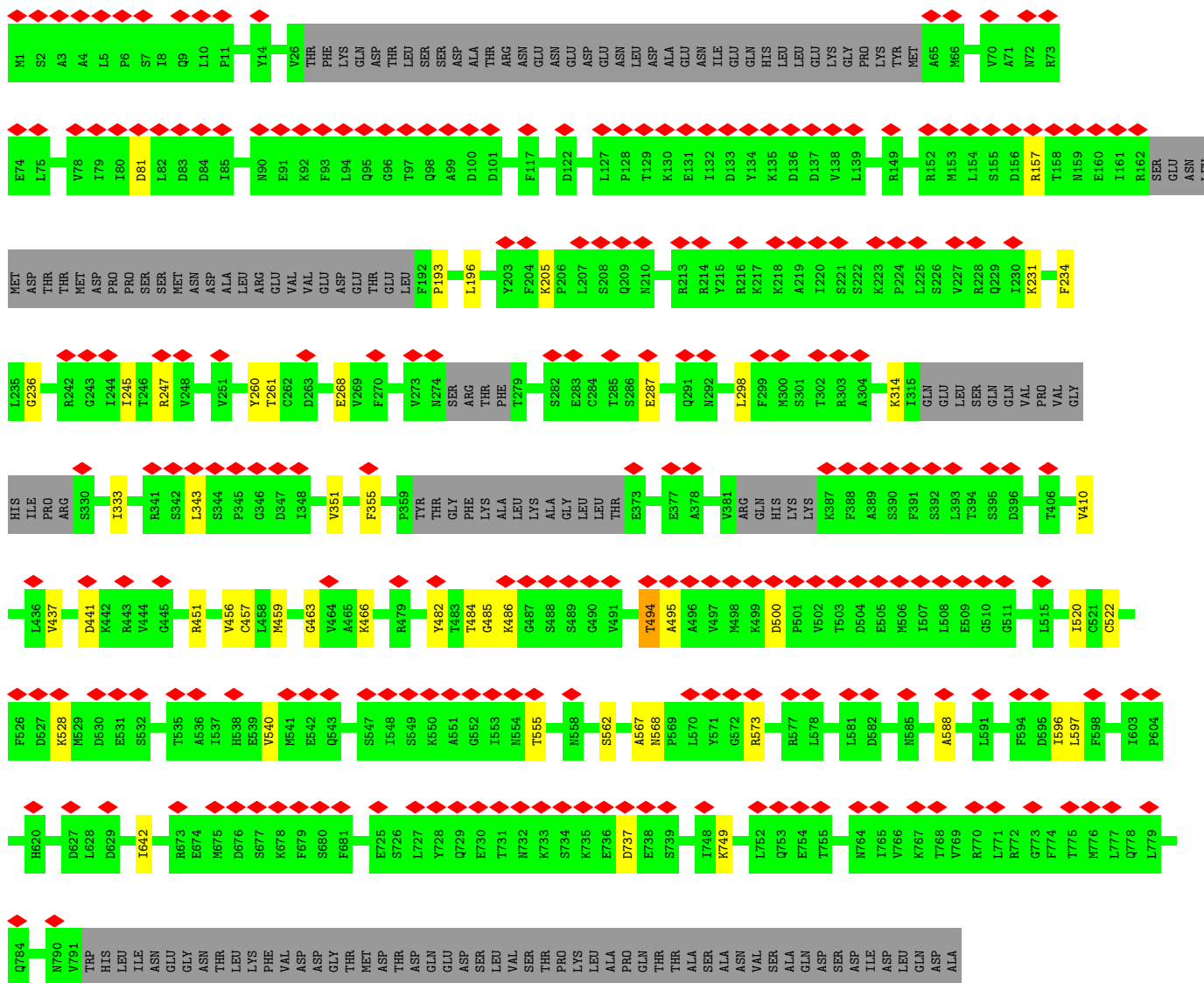
• Molecule 4: DNA replication licensing factor MCM4

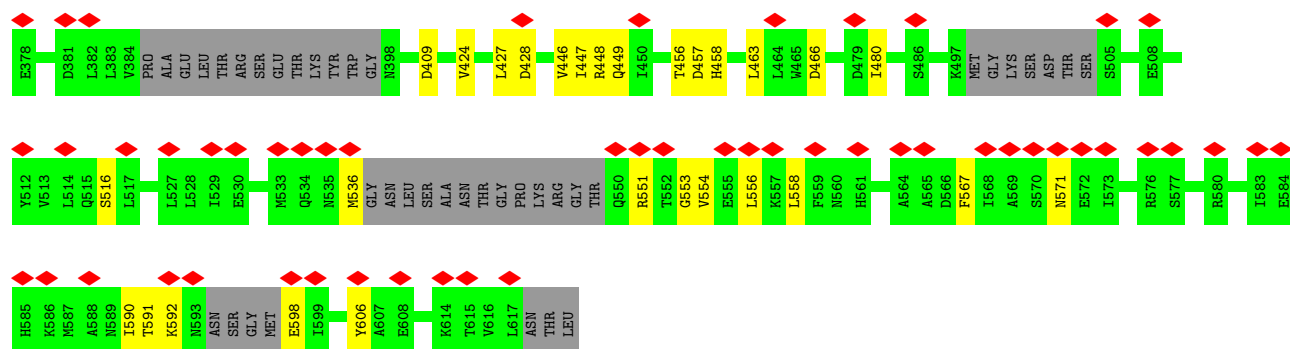




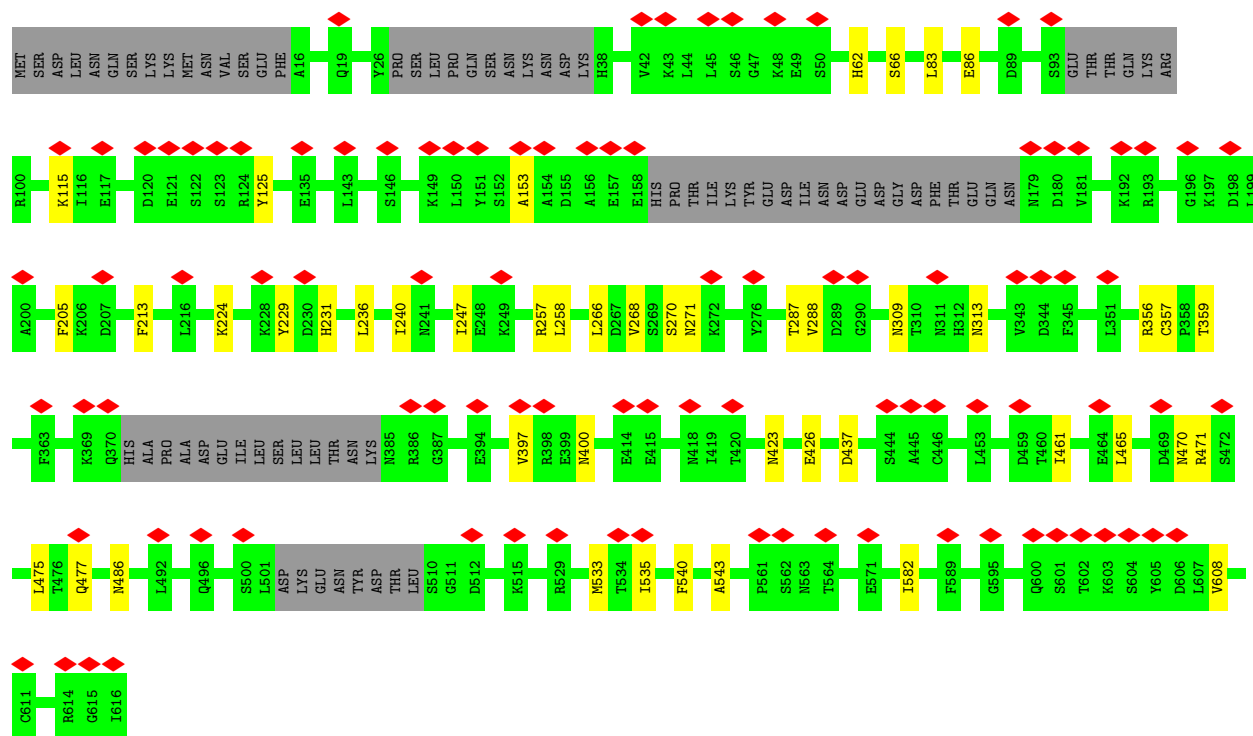
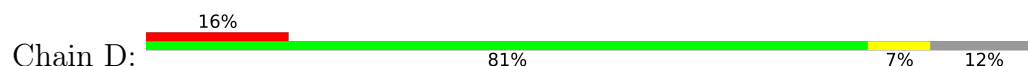
• Molecule 5: DNA replication licensing factor MCM6



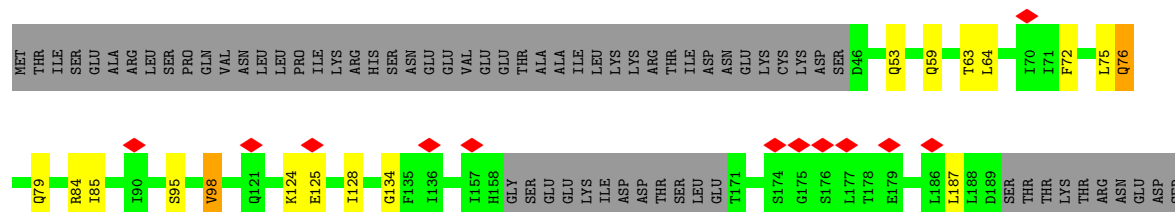


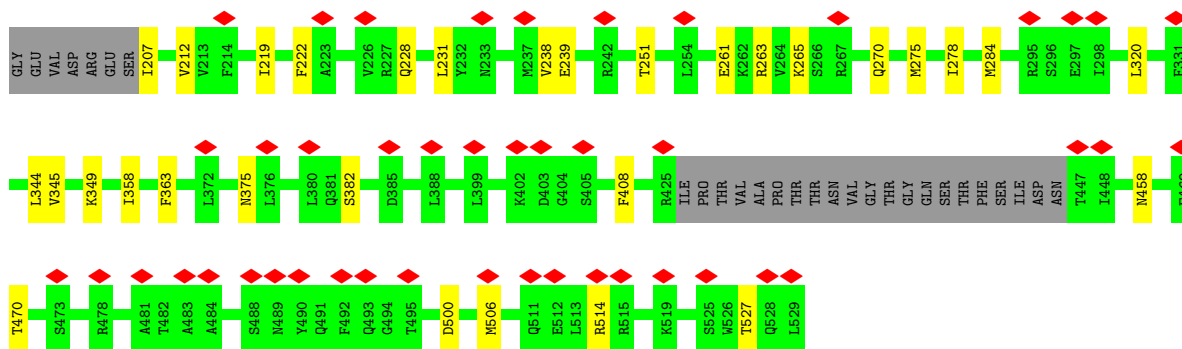


• Molecule 9: Origin recognition complex subunit 3

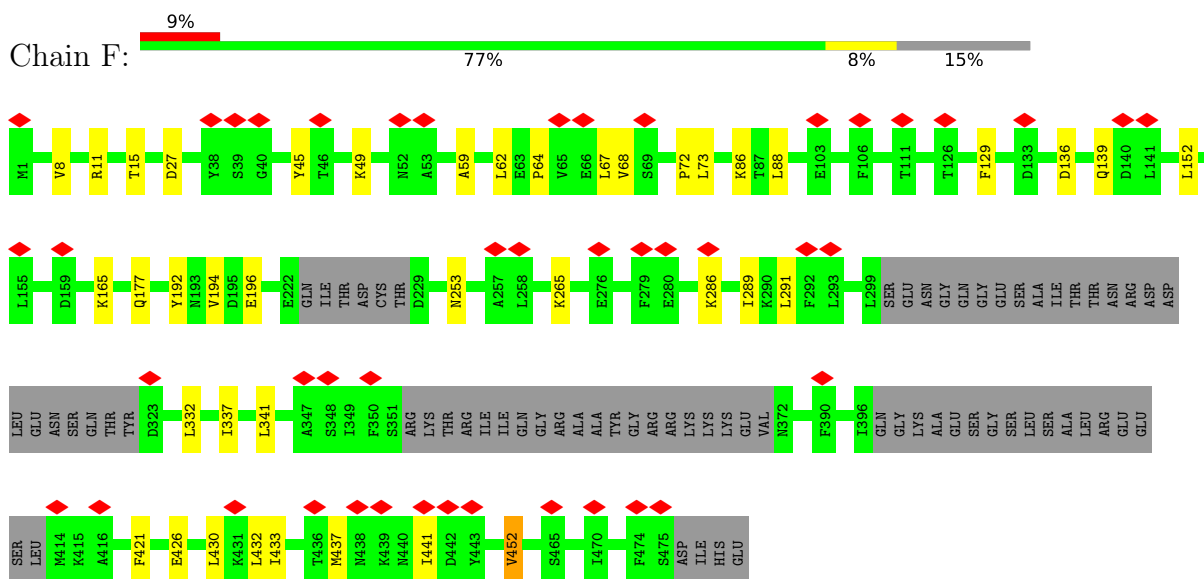


• Molecule 10: Origin recognition complex subunit 4

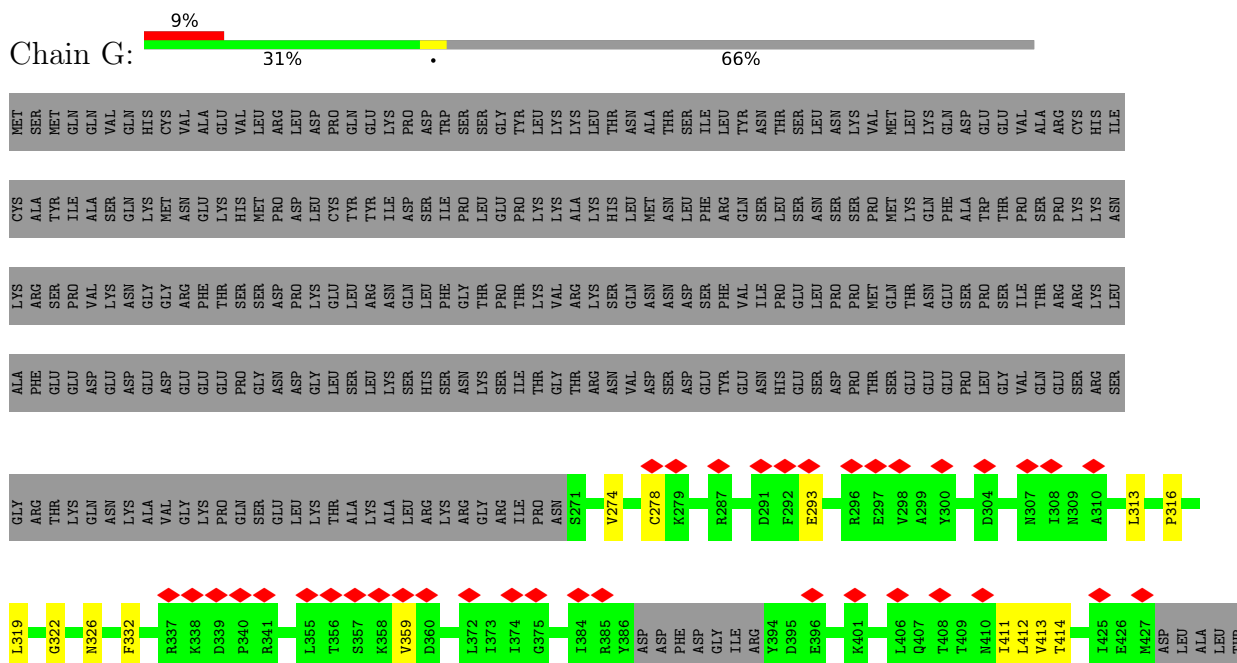




• Molecule 11: Origin recognition complex subunit 5

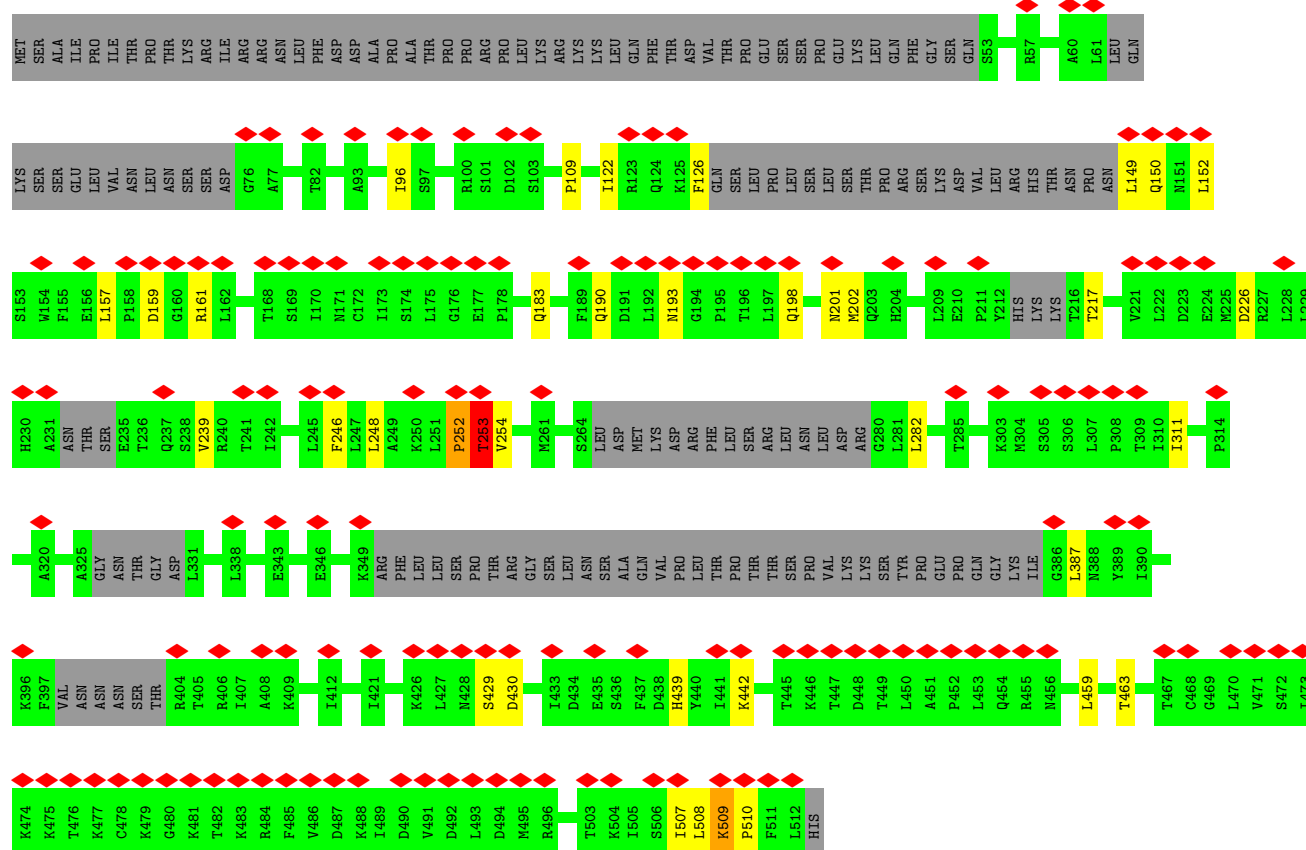


• Molecule 12: Origin recognition complex subunit 6

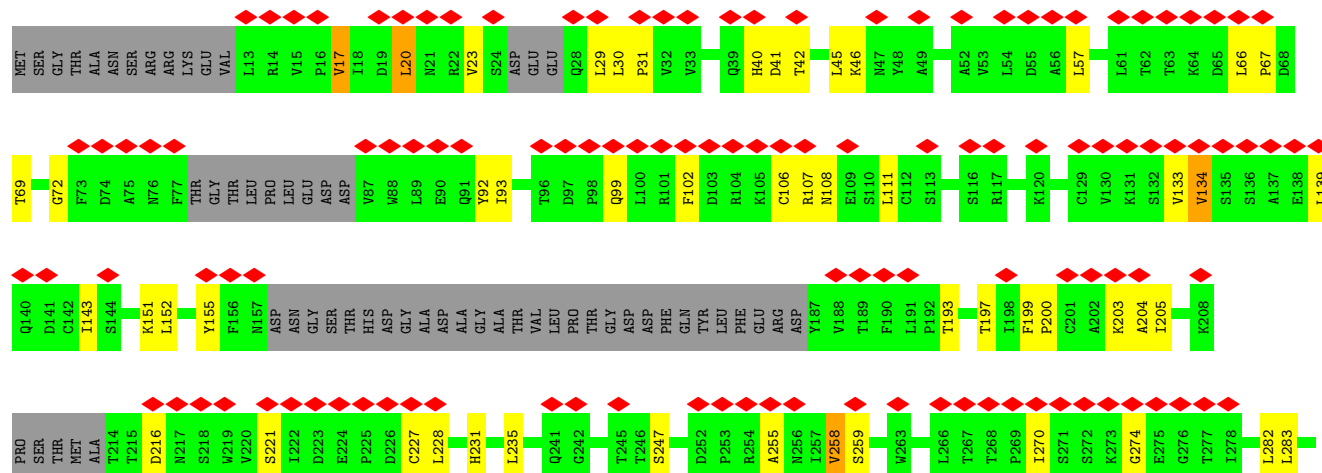


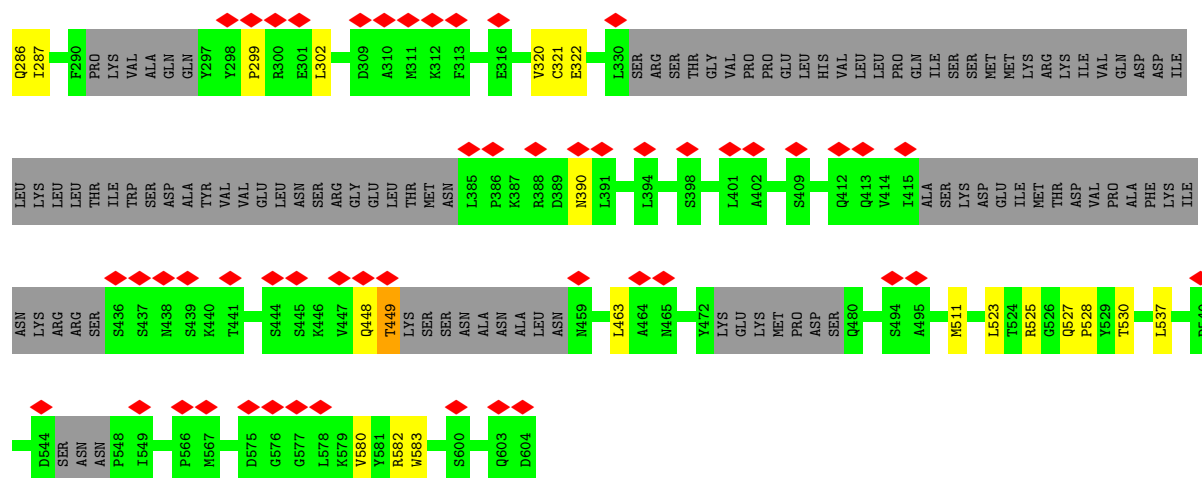
GLU
PRO
LEU

• Molecule 13: Cell division control protein 6

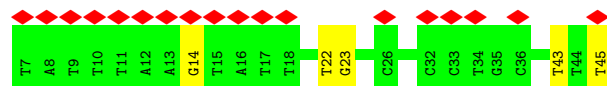
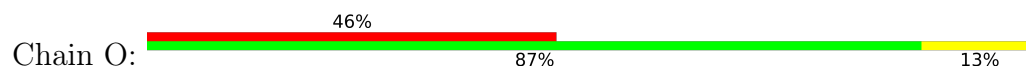


• Molecule 14: TAH11 isoform 1

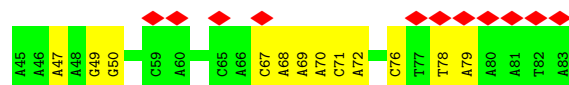




• Molecule 15: DNA (39-MER)



• Molecule 16: DNA (39-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53903	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size ($\text{\AA}$)	258.56, 258.56, 258.56	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.01, 1.01, 1.01	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.07	0/4887	0.21	0/6613
2	3	0.07	0/4935	0.19	0/6701
3	5	0.05	0/5042	0.17	0/6818
4	4	0.07	0/5374	0.20	0/7269
5	6	0.06	0/5430	0.18	0/7342
6	7	0.07	0/5460	0.20	0/7377
7	B	0.06	0/3670	0.19	0/4938
8	C	0.08	0/2754	0.21	0/3714
9	D	0.06	0/4499	0.18	0/6075
10	E	0.07	0/3575	0.19	0/4834
11	F	0.07	0/3416	0.19	0/4643
12	G	0.07	0/1242	0.17	0/1676
13	I	0.07	0/2827	0.23	0/3809
14	8	0.14	0/3584	0.26	0/4848
15	O	0.13	0/886	0.32	0/1366
16	P	0.12	0/906	0.23	0/1395
All	All	0.07	0/58487	0.20	0/79418

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	4813	0	4730	21	0
2	3	4857	0	4768	24	0
3	5	4974	0	4976	21	0
4	4	5305	0	5271	33	0
5	6	5348	0	5247	41	0
6	7	5386	0	5430	28	0
7	B	3618	0	3692	33	0
8	C	2698	0	2691	25	0
9	D	4410	0	4320	30	0
10	E	3514	0	3554	29	0
11	F	3336	0	3346	28	0
12	G	1224	0	1249	8	0
13	I	2788	0	2847	21	0
14	8	3527	0	3522	42	0
15	O	795	0	448	5	0
16	P	804	0	436	9	0
17	B	31	0	12	3	0
17	E	31	0	12	0	0
17	F	31	0	12	1	0
18	B	1	0	0	0	0
18	E	1	0	0	0	0
18	F	1	0	0	0	0
18	I	1	0	0	0	0
All	All	57494	0	56563	354	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 3.

All (354) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:496:GLU:HG2	4:4:497:GLU:HG3	1.71	0.70
8:C:242:THR:HG23	8:C:244:GLU:H	1.57	0.69
9:D:477:GLN:HE22	9:D:486:ASN:HD21	1.41	0.68
14:8:17:VAL:CG1	14:8:46:LYS:HE3	2.25	0.67
14:8:525:ARG:HA	14:8:583:TRP:NE1	2.10	0.65
5:6:272:THR:HG21	14:8:523:LEU:HD22	1.79	0.65
10:E:265:LYS:HG2	10:E:270:GLN:HE22	1.63	0.62
1:2:545:PRO:HB2	5:6:798:ARG:HH22	1.64	0.62
10:E:95:SER:HB3	10:E:238:VAL:HG13	1.82	0.61
5:6:924:ASP:OD1	11:F:286:LYS:HE2	2.01	0.60
5:6:370:THR:OG1	5:6:371:GLY:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:157:LEU:HD12	13:I:161:ARG:HB2	1.84	0.60
5:6:311:CYS:SG	5:6:340:ASN:ND2	2.75	0.60
9:D:271:ASN:ND2	9:D:313:ASN:OD1	2.36	0.59
5:6:399:GLY:HA3	5:6:456:ALA:HA	1.85	0.58
5:6:737:LYS:HB3	5:6:740:GLU:HB2	1.85	0.58
9:D:266:LEU:HD23	9:D:268:VAL:HG23	1.85	0.58
14:8:151:LYS:O	14:8:259:SER:OG	2.21	0.58
4:4:809:ALA:HB1	4:4:814:LYS:HB2	1.86	0.58
6:7:247:ARG:HD2	6:7:314:LYS:HD2	1.86	0.58
7:B:704:ARG:NH2	17:B:1001:ATP:O2G	2.33	0.57
13:I:509:LYS:H	13:I:510:PRO:HD2	1.69	0.57
2:3:819:ASP:HA	2:3:823:MET:HB2	1.86	0.57
14:8:17:VAL:HG12	14:8:46:LYS:HE3	1.86	0.57
8:C:447:ILE:HG22	8:C:449:GLN:H	1.69	0.57
10:E:59:GLN:HG2	10:E:64:LEU:HD11	1.85	0.57
10:E:320:LEU:HD11	10:E:358:ILE:HG13	1.86	0.56
1:2:519:LEU:O	1:2:771:ARG:NH1	2.38	0.56
2:3:811:ASP:HB2	2:3:852:LEU:HB3	1.86	0.56
7:B:822:LEU:HD12	7:B:890:CYS:HB3	1.87	0.56
8:C:466:ASP:HB2	11:F:426:GLU:HG2	1.87	0.56
7:B:686:ALA:HA	7:B:689:ILE:HD12	1.88	0.56
14:8:270:ILE:HB	14:8:274:GLY:HA3	1.88	0.56
14:8:203:LYS:O	14:8:205:ILE:N	2.39	0.55
14:8:299:PRO:HG2	14:8:302:LEU:HD12	1.88	0.55
2:3:161:PHE:HB3	2:3:164:HIS:HB2	1.88	0.55
10:E:219:ILE:HG22	10:E:251:THR:HB	1.89	0.55
14:8:200:PRO:HD2	14:8:258:VAL:HG13	1.89	0.55
16:P:49:DG:H2"	16:P:50:DG:H5"	1.87	0.55
3:5:261:ILE:HG22	3:5:263:GLU:H	1.72	0.55
5:6:517:LYS:HG2	14:8:463:LEU:HD21	1.88	0.54
14:8:133:VAL:HG12	14:8:134:VAL:HG23	1.88	0.54
3:5:161:ARG:HG3	3:5:295:VAL:HG22	1.88	0.54
10:E:408:PHE:HB3	10:E:500:ASP:HA	1.90	0.54
9:D:257:ARG:NH1	10:E:458:ASN:OD1	2.39	0.54
10:E:85:ILE:HD13	10:E:98:VAL:HG11	1.90	0.54
15:O:14:DG:N2	16:P:76:DC:O2	2.39	0.54
2:3:412:SER:HB2	3:5:649:THR:HB	1.89	0.54
7:B:871:ASN:ND2	11:F:177:GLN:O	2.40	0.54
13:I:159:ASP:OD1	13:I:159:ASP:N	2.40	0.54
1:2:324:VAL:HG21	1:2:418:SER:HB2	1.90	0.54
1:2:609:PHE:HB3	1:2:650:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:8:525:ARG:HA	14:8:583:TRP:HE1	1.71	0.54
1:2:696:ALA:HB2	5:6:800:LEU:HD21	1.89	0.53
14:8:106:CYS:SG	14:8:107:ARG:N	2.81	0.53
7:B:489:VAL:HG11	7:B:564:LEU:HD13	1.89	0.53
11:F:265:LYS:HG2	11:F:291:LEU:HD22	1.90	0.53
13:I:430:ASP:N	13:I:430:ASP:OD1	2.39	0.53
5:6:186:ARG:NH1	5:6:260:GLU:OE1	2.41	0.53
8:C:428:ASP:HB2	8:C:458:HIS:HB2	1.91	0.53
7:B:809:LEU:HD13	7:B:902:LYS:HG3	1.91	0.53
3:5:606:CYS:HB3	3:5:665:LYS:HG2	1.92	0.53
5:6:924:ASP:OD2	11:F:286:LYS:HD2	2.08	0.53
7:B:567:GLU:OE1	10:E:263:ARG:NH1	2.42	0.52
2:3:696:PRO:HA	6:7:573:ARG:HH21	1.74	0.52
11:F:67:LEU:HB3	11:F:72:PRO:HB2	1.92	0.52
12:G:322:GLY:O	12:G:326:ASN:ND2	2.43	0.52
3:5:721:ARG:HA	9:D:543:ALA:HA	1.91	0.52
9:D:357:CYS:SG	9:D:359:THR:OG1	2.65	0.52
14:8:46:LYS:HG2	14:8:227:CYS:SG	2.49	0.52
1:2:604:CYS:HB3	1:2:646:ILE:HA	1.90	0.52
4:4:569:ASP:O	4:4:574:LYS:NZ	2.43	0.52
4:4:680:SER:HB2	6:7:588:ALA:HB3	1.92	0.52
4:4:882:SER:HA	4:4:923:VAL:HA	1.92	0.52
5:6:606:ALA:HB1	5:6:611:ALA:HB2	1.90	0.52
5:6:644:MET:HB2	5:6:649:GLN:HE21	1.74	0.52
14:8:199:PHE:HE1	14:8:231:HIS:HB2	1.73	0.52
3:5:725:GLY:H	3:5:772:ARG:HB3	1.73	0.52
2:3:33:ASP:OD1	2:3:39:ARG:NH1	2.42	0.52
11:F:64:PRO:HA	11:F:67:LEU:HD12	1.91	0.52
1:2:544:ASP:OD1	1:2:657:TYR:N	2.43	0.52
13:I:507:ILE:HG13	13:I:508:LEU:HG	1.91	0.52
9:D:470:ASN:HB2	9:D:475:LEU:HD12	1.91	0.51
3:5:175:ARG:NH2	3:5:196:ASN:O	2.44	0.51
5:6:712:PHE:H	5:6:834:SER:HB2	1.75	0.51
6:7:486:LYS:HE3	6:7:528:LYS:HB3	1.93	0.51
14:8:321:CYS:SG	14:8:322:GLU:N	2.82	0.51
4:4:387:ASN:HD21	5:6:325:PHE:HE2	1.58	0.51
5:6:950:SER:OG	5:6:951:LEU:N	2.36	0.51
14:8:108:ASN:HD22	14:8:111:LEU:HD23	1.74	0.51
1:2:421:GLY:HA2	1:2:562:ARG:HH22	1.75	0.51
5:6:311:CYS:SG	5:6:312:ASP:N	2.83	0.51
6:7:441:ASP:OD1	6:7:441:ASP:N	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:298:TYR:HA	3:5:328:ILE:HG12	1.92	0.51
5:6:510:SER:OG	14:8:511:MET:SD	2.64	0.51
7:B:475:ILE:HD12	7:B:596:ILE:HG12	1.93	0.51
8:C:592:LYS:HB2	8:C:598:GLU:HG3	1.93	0.51
7:B:576:GLN:HE22	7:B:609:LEU:HA	1.75	0.51
5:6:340:ASN:ND2	5:6:343:PHE:O	2.42	0.50
10:E:134:GLY:HA2	10:E:222:PHE:HE1	1.76	0.50
14:8:46:LYS:HA	14:8:227:CYS:HA	1.93	0.50
4:4:238:THR:HG22	14:8:528:PRO:HG3	1.94	0.50
4:4:559:ARG:NH1	4:4:648:VAL:O	2.43	0.50
14:8:193:THR:HG21	14:8:287:ILE:HD12	1.93	0.50
1:2:364:CYS:SG	1:2:365:THR:N	2.84	0.50
7:B:860:GLN:OE1	10:E:375:ASN:ND2	2.45	0.50
13:I:459:LEU:O	13:I:463:THR:OG1	2.30	0.50
14:8:40:HIS:O	14:8:42:THR:N	2.44	0.50
2:3:851:HIS:N	8:C:567:PHE:O	2.45	0.50
5:6:123:SER:HB3	5:6:134:LYS:HG2	1.92	0.50
10:E:53:GLN:NE2	10:E:345:VAL:O	2.41	0.50
10:E:344:LEU:HD12	10:E:363:PHE:HB3	1.93	0.50
4:4:265:PRO:HG3	4:4:325:LEU:HB2	1.94	0.50
4:4:754:ALA:HB1	4:4:810:LYS:HG2	1.94	0.50
4:4:856:VAL:O	4:4:858:GLN:N	2.45	0.50
1:2:306:LEU:HD11	1:2:390:LEU:HD23	1.94	0.49
10:E:382:SER:O	11:F:253:ASN:ND2	2.43	0.49
10:E:514:ARG:NH1	10:E:527:THR:OG1	2.45	0.49
15:O:23:DG:N2	16:P:67:DC:O2	2.36	0.49
2:3:398:HIS:NE2	2:3:492:GLN:O	2.44	0.49
2:3:412:SER:OG	3:5:651:ARG:NH1	2.45	0.49
4:4:795:THR:OG1	5:6:578:SER:O	2.30	0.49
14:8:155:TYR:HB2	14:8:255:ALA:HB1	1.94	0.49
3:5:149:ARG:HH21	3:5:265:VAL:HG13	1.77	0.49
4:4:910:LEU:HB3	4:4:915:LYS:HB2	1.93	0.49
5:6:144:LYS:HA	5:6:196:LEU:HD21	1.94	0.49
9:D:268:VAL:HG12	9:D:268:VAL:O	2.12	0.49
6:7:451:ARG:NH1	6:7:540:VAL:O	2.46	0.49
14:8:231:HIS:NE2	14:8:247:SER:O	2.39	0.49
5:6:923:VAL:HG13	5:6:928:ALA:HB3	1.94	0.49
7:B:432:SER:HB2	10:E:239:GLU:HB3	1.93	0.49
11:F:129:PHE:HA	11:F:165:LYS:HB2	1.93	0.49
1:2:323:VAL:HG22	1:2:423:GLU:HG2	1.95	0.49
7:B:374:PRO:O	7:B:378:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:484:THR:OG1	6:7:485:GLY:N	2.45	0.49
9:D:437:ASP:N	9:D:437:ASP:OD1	2.45	0.49
1:2:565:PHE:HA	1:2:605:LEU:HB2	1.95	0.49
2:3:410:ASP:O	2:3:413:THR:OG1	2.27	0.49
6:7:157:ARG:NH1	6:7:287:GLU:OE2	2.46	0.49
3:5:143:ALA:O	3:5:161:ARG:NH1	2.44	0.48
4:4:234:ARG:O	14:8:582:ARG:NH1	2.43	0.48
6:7:482:TYR:HA	6:7:522:CYS:HB2	1.95	0.48
7:B:467:ILE:HG12	7:B:560:THR:HG21	1.94	0.48
9:D:471:ARG:HD2	12:G:411:ILE:HG12	1.93	0.48
3:5:416:GLY:O	3:5:422:LYS:NZ	2.45	0.48
7:B:718:GLU:OE1	10:E:84:ARG:NH2	2.47	0.48
7:B:878:ILE:HG23	7:B:896:ILE:HG12	1.96	0.48
6:7:737:ASP:N	6:7:737:ASP:OD1	2.47	0.48
3:5:183:CYS:HB3	3:5:188:HIS:H	1.79	0.48
6:7:466:LYS:NZ	6:7:568:ASN:OD1	2.45	0.48
7:B:688:ALA:HB1	7:B:778:VAL:HG21	1.96	0.48
14:8:530:THR:HG22	14:8:580:VAL:HG22	1.94	0.48
3:5:409:ASP:OD2	3:5:500:GLN:NE2	2.47	0.47
8:C:551:ARG:HG3	8:C:553:GLY:H	1.79	0.47
8:C:363:LEU:HB2	8:C:424:VAL:HA	1.96	0.47
2:3:638:ASN:HB3	2:3:641:ASN:HB2	1.95	0.47
6:7:245:ILE:HD13	6:7:343:LEU:HB3	1.96	0.47
7:B:487:LEU:HD22	17:B:1001:ATP:H2'	1.95	0.47
13:I:252:PRO:C	13:I:254:VAL:H	2.22	0.47
7:B:806:TYR:O	7:B:810:ASN:ND2	2.47	0.47
13:I:122:ILE:HA	13:I:126:PHE:HB2	1.97	0.47
7:B:886:ASN:ND2	10:E:470:THR:OG1	2.47	0.47
9:D:423:ASN:HB3	9:D:426:GLU:HG2	1.95	0.47
11:F:8:VAL:HB	11:F:11:ARG:HB2	1.95	0.47
2:3:276:VAL:HG11	2:3:294:VAL:HG11	1.95	0.47
2:3:400:ARG:NH2	2:3:544:ASP:OD1	2.48	0.47
2:3:843:ARG:O	2:3:845:SER:N	2.47	0.47
4:4:237:GLY:O	4:4:299:LYS:NZ	2.48	0.47
5:6:294:VAL:HG21	5:6:389:ALA:HB1	1.97	0.47
6:7:260:TYR:HB3	6:7:298:LEU:HB3	1.97	0.47
8:C:316:PHE:HB3	8:C:480:ILE:HD11	1.97	0.47
10:E:228:GLN:HB3	10:E:231:LEU:HB2	1.97	0.47
14:8:45:LEU:HB2	14:8:228:LEU:HB2	1.96	0.47
5:6:297:THR:HG22	5:6:359:VAL:HG22	1.97	0.47
6:7:261:THR:HG22	6:7:268:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:313:LEU:HD11	12:G:319:LEU:HD22	1.97	0.47
14:8:66:LEU:HB2	14:8:72:GLY:HA3	1.97	0.47
6:7:459:MET:HG2	6:7:567:ALA:HB3	1.98	0.46
9:D:213:PHE:HZ	9:D:247:ILE:HG22	1.80	0.46
11:F:86:LYS:HD2	11:F:86:LYS:HA	1.72	0.46
7:B:500:SER:OG	7:B:507:ASP:OD1	2.33	0.46
8:C:556:LEU:HB2	8:C:598:GLU:HB3	1.96	0.46
10:E:124:LYS:HG3	10:E:125:GLU:HG2	1.97	0.46
11:F:337:ILE:HG23	11:F:341:LEU:HD12	1.97	0.46
3:5:724:ILE:HA	3:5:772:ARG:HD3	1.96	0.46
14:8:235:LEU:HB2	14:8:283:LEU:HD21	1.97	0.46
3:5:35:ILE:HG23	3:5:46:TYR:HB3	1.97	0.46
5:6:120:GLU:O	5:6:134:LYS:NZ	2.44	0.46
2:3:368:ALA:HB3	2:3:378:LYS:HE2	1.97	0.46
7:B:423:PHE:HB2	7:B:718:GLU:HG3	1.97	0.46
5:6:933:ALA:HA	5:6:936:ILE:HD12	1.97	0.46
7:B:836:ASN:HB2	7:B:842:VAL:HG21	1.98	0.46
9:D:86:GLU:HG2	9:D:266:LEU:HD11	1.97	0.46
1:2:342:LEU:HD12	1:2:372:PRO:HG2	1.98	0.46
4:4:599:VAL:HG21	16:P:49:DG:H3'	1.98	0.46
8:C:322:LYS:NZ	8:C:457:ASP:OD1	2.46	0.46
14:8:30:LEU:HB2	14:8:31:PRO:HD3	1.98	0.46
6:7:247:ARG:NH1	6:7:500:ASP:OD1	2.48	0.46
1:2:231:ILE:HG23	1:2:279:THR:HG22	1.98	0.46
1:2:803:PHE:HB3	1:2:845:PHE:HE1	1.81	0.46
8:C:536:MET:HE2	8:C:606:TYR:HB3	1.97	0.46
10:E:76:GLN:O	10:E:79:GLN:NE2	2.49	0.46
5:6:497:ASN:OD1	5:6:762:LYS:NZ	2.44	0.45
9:D:240:ILE:HD12	9:D:247:ILE:HG21	1.98	0.45
2:3:185:ILE:HG13	2:3:261:MET:HG2	1.98	0.45
2:3:415:LYS:HD2	2:3:515:ALA:HB1	1.97	0.45
6:7:193:PRO:HG2	6:7:196:LEU:HB2	1.97	0.45
6:7:333:ILE:HD13	6:7:351:VAL:HG11	1.97	0.45
7:B:565:LEU:HB2	7:B:597:ALA:HA	1.98	0.45
8:C:409:ASP:OD1	8:C:409:ASP:N	2.49	0.45
4:4:406:VAL:HG21	4:4:412:PRO:HB3	1.99	0.45
13:I:226:ASP:OD1	13:I:226:ASP:N	2.50	0.45
8:C:463:LEU:HD13	11:F:421:PHE:HD1	1.82	0.45
2:3:46:GLN:NE2	2:3:137:ASP:OD2	2.50	0.45
2:3:536:PRO:HD2	2:3:539:LEU:HD12	1.99	0.45
6:7:457:CYS:HB3	6:7:597:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:512:VAL:HG22	4:4:515:ARG:HH21	1.82	0.45
8:C:427:LEU:HB3	8:C:456:THR:HG22	1.99	0.45
16:P:69:DA:H2''	16:P:70:DA:C8	2.51	0.45
4:4:411:THR:HG22	6:7:555:THR:HG21	1.98	0.45
10:E:128:ILE:HD11	10:E:212:VAL:HG13	1.97	0.45
2:3:417:GLN:OE1	2:3:420:ARG:NH1	2.49	0.45
8:C:448:ARG:HA	8:C:448:ARG:HD2	1.81	0.45
16:P:78:DT:H2'	16:P:79:DA:C8	2.51	0.45
5:6:641:PHE:HB3	5:6:682:ALA:HB2	1.98	0.45
7:B:514:ASN:HB3	7:B:517:LYS:HB2	1.99	0.45
9:D:83:LEU:HD13	9:D:268:VAL:HG11	1.99	0.45
10:E:72:PHE:HD2	10:E:75:LEU:HD12	1.82	0.44
3:5:440:SER:OG	3:5:441:GLY:N	2.50	0.44
5:6:589:VAL:HG21	5:6:597:TYR:HB2	1.99	0.44
7:B:783:ASN:O	7:B:787:ASN:ND2	2.50	0.44
8:C:356:ASN:ND2	8:C:357:SER:O	2.50	0.44
2:3:784:LYS:O	2:3:788:ARG:NE	2.43	0.44
4:4:294:ASP:OD1	4:4:294:ASP:N	2.50	0.44
9:D:287:THR:HG23	9:D:288:VAL:HG13	1.97	0.44
11:F:67:LEU:HD13	11:F:73:LEU:HA	1.99	0.44
14:8:20:LEU:HD23	14:8:45:LEU:HD22	2.00	0.44
4:4:425:ASP:OD1	5:6:375:ARG:NH2	2.44	0.44
4:4:327:ASN:HA	4:4:436:THR:HA	1.99	0.44
7:B:394:PHE:O	7:B:397:ASN:ND2	2.50	0.44
9:D:270:SER:OG	9:D:313:ASN:ND2	2.51	0.44
4:4:618:SER:HB3	4:4:622:VAL:HB	1.99	0.44
13:I:149:LEU:HD23	13:I:152:LEU:HD11	1.98	0.44
14:8:23:VAL:HG22	14:8:29:LEU:HB2	1.98	0.44
5:6:522:ASP:OD2	5:6:528:LYS:NZ	2.50	0.44
9:D:125:TYR:OH	9:D:153:ALA:O	2.33	0.44
3:5:53:ASN:ND2	3:5:60:SER:O	2.51	0.44
4:4:530:ILE:O	4:4:537:LYS:NZ	2.46	0.44
8:C:331:ILE:O	8:C:335:SER:OG	2.31	0.44
10:E:63:THR:HG21	11:F:27:ASP:HA	1.98	0.44
10:E:275:MET:HE3	10:E:275:MET:HB3	1.85	0.44
11:F:45:TYR:HB2	17:F:1001:ATP:H2'	2.00	0.44
14:8:197:THR:HB	14:8:231:HIS:HB3	2.00	0.44
1:2:339:PHE:HB3	1:2:373:PHE:HB3	2.00	0.43
5:6:816:VAL:HG12	5:6:818:GLU:H	1.83	0.43
5:6:754:TYR:OH	5:6:813:ALA:O	2.32	0.43
4:4:543:GLN:NE2	4:4:562:ILE:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:252:PRO:O	13:I:253:THR:HG22	2.19	0.43
1:2:424:VAL:HG12	1:2:458:ARG:HG2	1.99	0.43
10:E:124:LYS:HE2	10:E:124:LYS:HB2	1.80	0.43
13:I:439:HIS:HA	13:I:442:LYS:HE2	2.00	0.43
16:P:71:DC:H2'	16:P:72:DA:C8	2.54	0.43
5:6:591:PHE:HA	5:6:752:ARG:HH21	1.83	0.43
16:P:67:DC:H2'	16:P:68:DA:C8	2.54	0.43
1:2:806:THR:HG22	3:5:529:ARG:HH21	1.84	0.43
4:4:283:LEU:O	4:4:287:ASN:ND2	2.50	0.43
6:7:437:VAL:HG22	6:7:642:ILE:HG23	2.00	0.43
8:C:590:ILE:C	8:C:591:THR:HG23	2.43	0.43
11:F:62:LEU:HA	11:F:62:LEU:HD23	1.86	0.43
6:7:494:THR:OG1	6:7:495:ALA:N	2.51	0.43
5:6:632:ASP:OD2	5:6:633:ASN:ND2	2.52	0.42
12:G:278:CYS:H	12:G:316:PRO:HG2	1.84	0.42
11:F:192:TYR:HB3	11:F:196:GLU:HB2	2.00	0.42
2:3:659:TYR:OH	2:3:715:VAL:O	2.32	0.42
4:4:446:ALA:HA	4:4:454:LYS:HE3	2.01	0.42
9:D:356:ARG:HB3	12:G:413:VAL:HB	2.01	0.42
11:F:49:LYS:HA	11:F:49:LYS:HD3	1.92	0.42
6:7:456:VAL:HG13	6:7:596:ILE:HB	2.00	0.42
8:C:554:VAL:HA	8:C:558:LEU:HD23	2.01	0.42
9:D:309:ASN:HB3	9:D:313:ASN:HB3	2.01	0.42
11:F:88:LEU:HD23	11:F:88:LEU:HA	1.93	0.42
6:7:749:LYS:HA	6:7:749:LYS:HD2	1.91	0.42
13:I:150:GLN:NE2	13:I:190:GLN:O	2.52	0.42
14:8:193:THR:HA	14:8:286:GLN:HE21	1.85	0.42
5:6:947:ASP:OD1	5:6:947:ASP:N	2.53	0.42
7:B:414:GLN:HG3	7:B:416:HIS:H	1.84	0.42
9:D:224:LYS:HE2	9:D:258:LEU:HD22	2.01	0.42
11:F:437:MET:HB3	11:F:441:ILE:HG23	2.01	0.42
9:D:62:HIS:O	9:D:66:SER:OG	2.32	0.42
10:E:506:MET:HE3	10:E:506:MET:HB3	1.80	0.42
14:8:235:LEU:HD12	14:8:282:LEU:HD23	2.02	0.42
1:2:534:ARG:NH1	1:2:624:MET:O	2.45	0.42
3:5:62:THR:HA	3:5:138:ILE:HB	2.02	0.42
5:6:566:ARG:O	5:6:805:ARG:NE	2.47	0.42
8:C:274:PHE:HD1	9:D:582:ILE:HG12	1.84	0.42
9:D:266:LEU:HD23	9:D:268:VAL:CG2	2.48	0.42
9:D:356:ARG:NE	12:G:413:VAL:O	2.46	0.42
14:8:527:GLN:H	14:8:527:GLN:HG3	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:22:DT:H2"	15:O:23:DG:H8	1.84	0.42
5:6:143:MET:HG2	5:6:148:LEU:HB2	2.02	0.41
7:B:799:PHE:HE2	7:B:849:LEU:HD11	1.84	0.41
9:D:535:ILE:HB	9:D:608:VAL:HG23	2.01	0.41
10:E:278:ILE:HG21	10:E:284:MET:HG3	2.02	0.41
4:4:564:ILE:HG23	4:4:704:LEU:HB2	2.02	0.41
5:6:965:ILE:HD12	5:6:968:LEU:HD12	2.01	0.41
11:F:59:ALA:HA	11:F:129:PHE:HB2	2.01	0.41
14:8:99:GLN:HG3	14:8:102:PHE:HB2	2.01	0.41
4:4:329:LYS:O	4:4:402:THR:OG1	2.37	0.41
8:C:250:ARG:HG2	9:D:533:MET:HB2	2.02	0.41
11:F:332:LEU:HD23	11:F:332:LEU:HA	1.93	0.41
11:F:430:LEU:HB2	11:F:432:LEU:HG	2.02	0.41
13:I:429:SER:OG	13:I:430:ASP:N	2.52	0.41
14:8:448:GLN:O	14:8:449:THR:HG22	2.20	0.41
13:I:193:ASN:OD1	13:I:193:ASN:N	2.53	0.41
13:I:246:PHE:HD1	13:I:246:PHE:HA	1.78	0.41
14:8:92:TYR:HB3	14:8:152:LEU:HB2	2.02	0.41
6:7:520:ILE:HA	6:7:562:SER:HB2	2.02	0.41
1:2:501:MET:HG3	1:2:516:ALA:HB2	2.01	0.41
2:3:420:ARG:HA	2:3:423:LEU:HD12	2.01	0.41
11:F:11:ARG:O	11:F:15:THR:OG1	2.31	0.41
2:3:141:HIS:HB3	2:3:144:ALA:HB3	2.01	0.41
7:B:811:LEU:O	7:B:815:ASN:ND2	2.54	0.41
8:C:241:ASP:O	8:C:242:THR:HG22	2.21	0.41
8:C:516:SER:HB2	13:I:109:PRO:HD3	2.03	0.41
13:I:183:GLN:HE22	13:I:198:GLN:HA	1.85	0.41
3:5:755:LEU:O	3:5:760:THR:OG1	2.38	0.41
4:4:607:ARG:NH2	15:O:45:DT:OP1	2.54	0.41
11:F:289:ILE:HD12	11:F:289:ILE:HA	1.88	0.41
14:8:72:GLY:N	14:8:93:ILE:O	2.53	0.41
14:8:203:LYS:HD3	14:8:221:SER:HB3	2.02	0.41
7:B:411:LYS:HE3	10:E:207:ILE:HD11	2.03	0.41
9:D:229:TYR:HB3	9:D:231:HIS:CE1	2.56	0.41
9:D:465:LEU:HD21	12:G:412:LEU:HD21	2.03	0.41
13:I:201:ASN:HB2	13:I:202:MET:H	1.66	0.41
15:O:43:DT:H3	16:P:47:DA:H61	1.69	0.41
9:D:205:PHE:HE2	9:D:236:LEU:HB3	1.86	0.41
12:G:293:GLU:HB3	12:G:332:PHE:HZ	1.86	0.41
13:I:282:LEU:HD23	13:I:282:LEU:H	1.85	0.40
6:7:236:GLY:N	6:7:355:PHE:O	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:604:LEU:HB3	7:B:605:PRO:HD3	2.03	0.40
7:B:797:LEU:HB3	7:B:801:ALA:HB3	2.04	0.40
11:F:433:ILE:HG22	11:F:452:VAL:HA	2.03	0.40
13:I:96:ILE:HG12	13:I:217:THR:HG21	2.03	0.40
4:4:248:LEU:O	4:4:254:THR:OG1	2.36	0.40
4:4:330:GLY:HA3	4:4:399:LEU:HD21	2.02	0.40
6:7:81:ASP:HA	6:7:205:LYS:HB3	2.03	0.40
1:2:543:GLY:O	1:2:549:LYS:NZ	2.43	0.40
4:4:341:ASP:O	4:4:392:ALA:N	2.50	0.40
6:7:231:LYS:H	6:7:234:PHE:HD2	1.69	0.40
11:F:136:ASP:N	11:F:136:ASP:OD1	2.52	0.40
5:6:596:VAL:HG23	5:6:631:ALA:HB2	2.04	0.40
7:B:486:THR:N	17:B:1001:ATP:O2A	2.55	0.40
8:C:571:ASN:OD1	8:C:571:ASN:N	2.55	0.40
14:8:216:ASP:OD1	14:8:216:ASP:N	2.55	0.40

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	615/868 (71%)	587 (95%)	28 (5%)	0	100	100
2	3	616/971 (63%)	577 (94%)	38 (6%)	1 (0%)	43	77
3	5	625/775 (81%)	587 (94%)	38 (6%)	0	100	100
4	4	668/933 (72%)	621 (93%)	43 (6%)	4 (1%)	21	59
5	6	674/1017 (66%)	631 (94%)	40 (6%)	3 (0%)	30	67
6	7	674/845 (80%)	621 (92%)	51 (8%)	2 (0%)	36	72
7	B	445/914 (49%)	421 (95%)	23 (5%)	1 (0%)	43	77
8	C	318/620 (51%)	293 (92%)	24 (8%)	1 (0%)	36	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	D	530/616 (86%)	490 (92%)	39 (7%)	1 (0%)	43	77
10	E	426/529 (80%)	409 (96%)	17 (4%)	0	100	100
11	F	399/479 (83%)	377 (94%)	20 (5%)	2 (0%)	24	63
12	G	146/435 (34%)	139 (95%)	7 (5%)	0	100	100
13	I	338/513 (66%)	312 (92%)	23 (7%)	3 (1%)	14	50
14	8	425/604 (70%)	378 (89%)	41 (10%)	6 (1%)	9	40
All	All	6899/10119 (68%)	6443 (93%)	432 (6%)	24 (0%)	37	72

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	6	271	PRO
4	4	501	ILE
4	4	840	PRO
4	4	856	VAL
11	F	68	VAL
14	8	67	PRO
14	8	134	VAL
14	8	390	ASN
2	3	786	THR
8	C	242	THR
13	I	509	LYS
14	8	41	ASP
14	8	69	THR
4	4	602	THR
5	6	369	PRO
5	6	609	THR
6	7	494	THR
13	I	252	PRO
13	I	253	THR
14	8	204	ALA
7	B	727	TYR
11	F	139	GLN
6	7	463	GLY
9	D	400	ASN

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	512/770 (66%)	512 (100%)	0	100	100
2	3	519/835 (62%)	518 (100%)	1 (0%)	87	87
3	5	550/688 (80%)	549 (100%)	1 (0%)	87	87
4	4	590/848 (70%)	586 (99%)	4 (1%)	76	81
5	6	573/886 (65%)	572 (100%)	1 (0%)	87	87
6	7	603/753 (80%)	602 (100%)	1 (0%)	87	87
7	B	396/813 (49%)	395 (100%)	1 (0%)	86	85
8	C	299/573 (52%)	296 (99%)	3 (1%)	68	78
9	D	488/576 (85%)	484 (99%)	4 (1%)	73	80
10	E	395/488 (81%)	390 (99%)	5 (1%)	61	74
11	F	376/440 (86%)	373 (99%)	3 (1%)	73	80
12	G	138/406 (34%)	135 (98%)	3 (2%)	45	64
13	I	307/470 (65%)	302 (98%)	5 (2%)	55	70
14	8	389/545 (71%)	380 (98%)	9 (2%)	44	64
All	All	6135/9091 (68%)	6094 (99%)	41 (1%)	73	81

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3	197	ILE
3	5	391	LEU
4	4	495	VAL
4	4	604	TYR
4	4	856	VAL
4	4	873	LEU
5	6	831	LEU
6	7	410	VAL
7	B	808	LEU
8	C	242	THR
8	C	298	LYS
8	C	446	VAL
9	D	115	LYS
9	D	397	VAL
9	D	461	ILE

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Mol	Chain	Res	Type
9	D	540	PHE
10	E	76	GLN
10	E	98	VAL
10	E	187	LEU
10	E	261	GLU
10	E	349	LYS
11	F	152	LEU
11	F	194	VAL
11	F	452	VAL
12	G	274	VAL
12	G	359	VAL
12	G	414	THR
13	I	239	VAL
13	I	248	LEU
13	I	253	THR
13	I	311	ILE
13	I	387	LEU
14	8	17	VAL
14	8	20	LEU
14	8	57	LEU
14	8	139	LEU
14	8	143	ILE
14	8	258	VAL
14	8	320	VAL
14	8	449	THR
14	8	537	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	313	ASN
1	2	508	HIS
1	2	748	GLN
1	2	779	HIS
1	2	809	HIS
2	3	46	GLN
2	3	177	ASN
2	3	351	ASN
2	3	809	GLN
3	5	560	HIS
3	5	765	HIS
4	4	229	GLN

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Mol	Chain	Res	Type
4	4	242	ASN
4	4	387	ASN
4	4	646	HIS
4	4	666	ASN
4	4	858	GLN
5	6	139	GLN
5	6	149	ASN
5	6	274	HIS
5	6	633	ASN
5	6	649	GLN
5	6	833	GLN
5	6	978	HIS
6	7	89	GLN
6	7	107	GLN
6	7	544	GLN
6	7	615	HIS
6	7	620	HIS
6	7	622	HIS
6	7	623	ASN
7	B	397	ASN
7	B	576	GLN
7	B	783	ASN
7	B	789	HIS
7	B	810	ASN
8	C	284	ASN
8	C	356	ASN
8	C	515	GLN
8	C	560	ASN
9	D	246	ASN
9	D	279	GLN
9	D	311	ASN
9	D	470	ASN
9	D	477	GLN
9	D	490	ASN
9	D	536	ASN
10	E	79	GLN
10	E	80	GLN
10	E	96	HIS
10	E	121	GLN
10	E	126	GLN
10	E	270	GLN
10	E	371	GLN

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Mol	Chain	Res	Type
10	E	489	ASN
10	E	493	GLN
11	F	32	ASN
11	F	58	HIS
11	F	248	HIS
12	G	290	ASN
13	I	124	GLN
13	I	150	GLN
13	I	204	HIS
13	I	237	GLN
13	I	313	GLN
13	I	423	GLN
14	8	598	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z > 2$
17	ATP	E	1001	18	32,33,33	0.28	0	48,52,52	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	ATP	F	1001	18	32,33,33	0.28	0	48,52,52	0.38	0
17	ATP	B	1001	18	32,33,33	0.28	0	48,52,52	0.38	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
17	ATP	E	1001	18	-	8/22/38/38	0/3/3/3
17	ATP	F	1001	18	-	1/22/38/38	0/3/3/3
17	ATP	B	1001	18	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

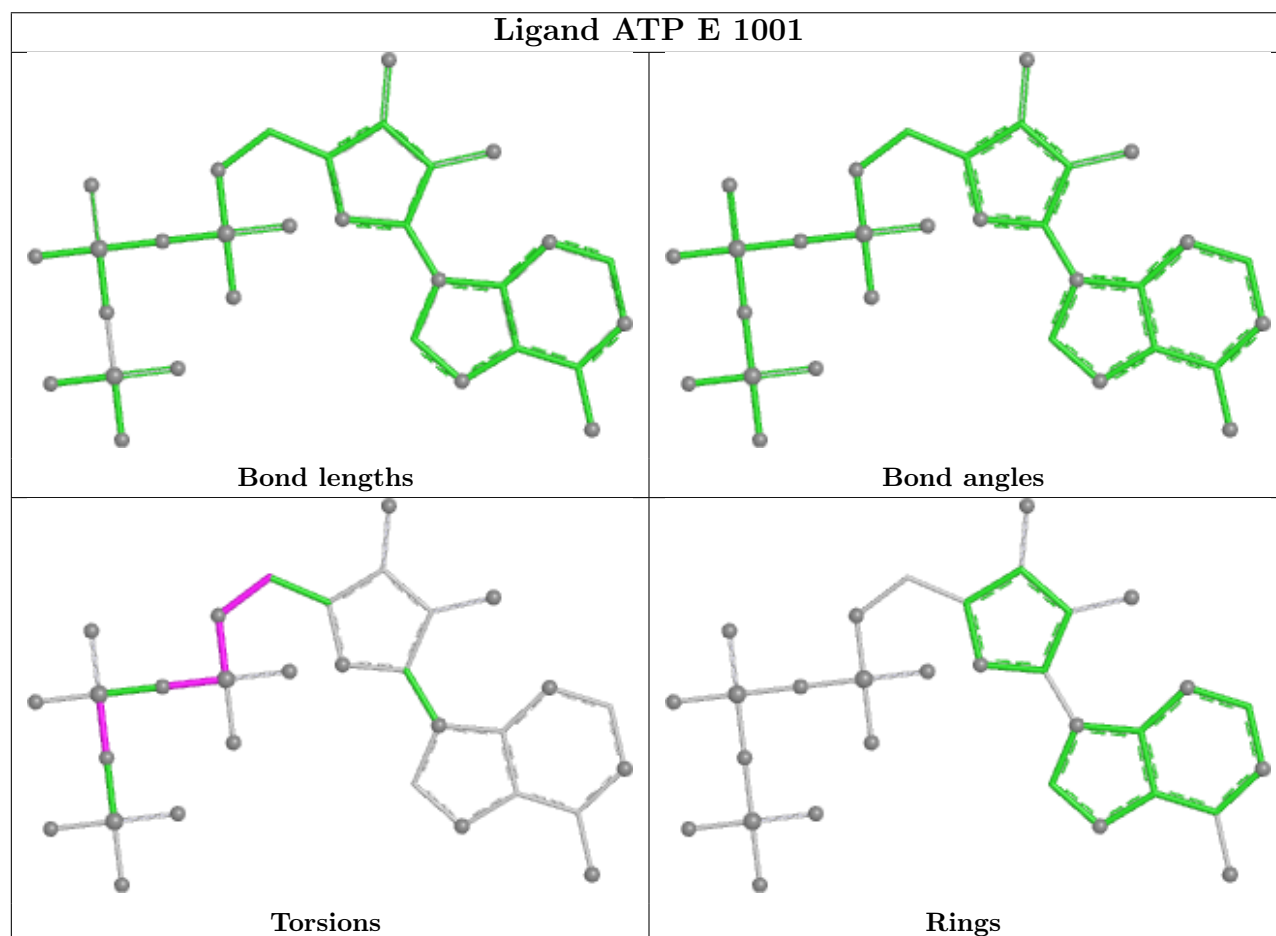
Mol	Chain	Res	Type	Atoms
17	B	1001	ATP	PB-O3B-PG-O2G
17	B	1001	ATP	C5'-O5'-PA-O1A
17	E	1001	ATP	C5'-O5'-PA-O1A
17	E	1001	ATP	C5'-O5'-PA-O3A
17	E	1001	ATP	C5'-O5'-PA-O2A
17	E	1001	ATP	C4'-C5'-O5'-PA
17	B	1001	ATP	PG-O3B-PB-O1B
17	E	1001	ATP	PB-O3A-PA-O1A
17	E	1001	ATP	PB-O3A-PA-O2A
17	B	1001	ATP	PB-O3B-PG-O1G
17	B	1001	ATP	PB-O3B-PG-O3G
17	B	1001	ATP	PB-O3A-PA-O1A
17	E	1001	ATP	PG-O3B-PB-O1B
17	E	1001	ATP	PG-O3B-PB-O2B
17	F	1001	ATP	C4'-C5'-O5'-PA
17	B	1001	ATP	PB-O3A-PA-O2A

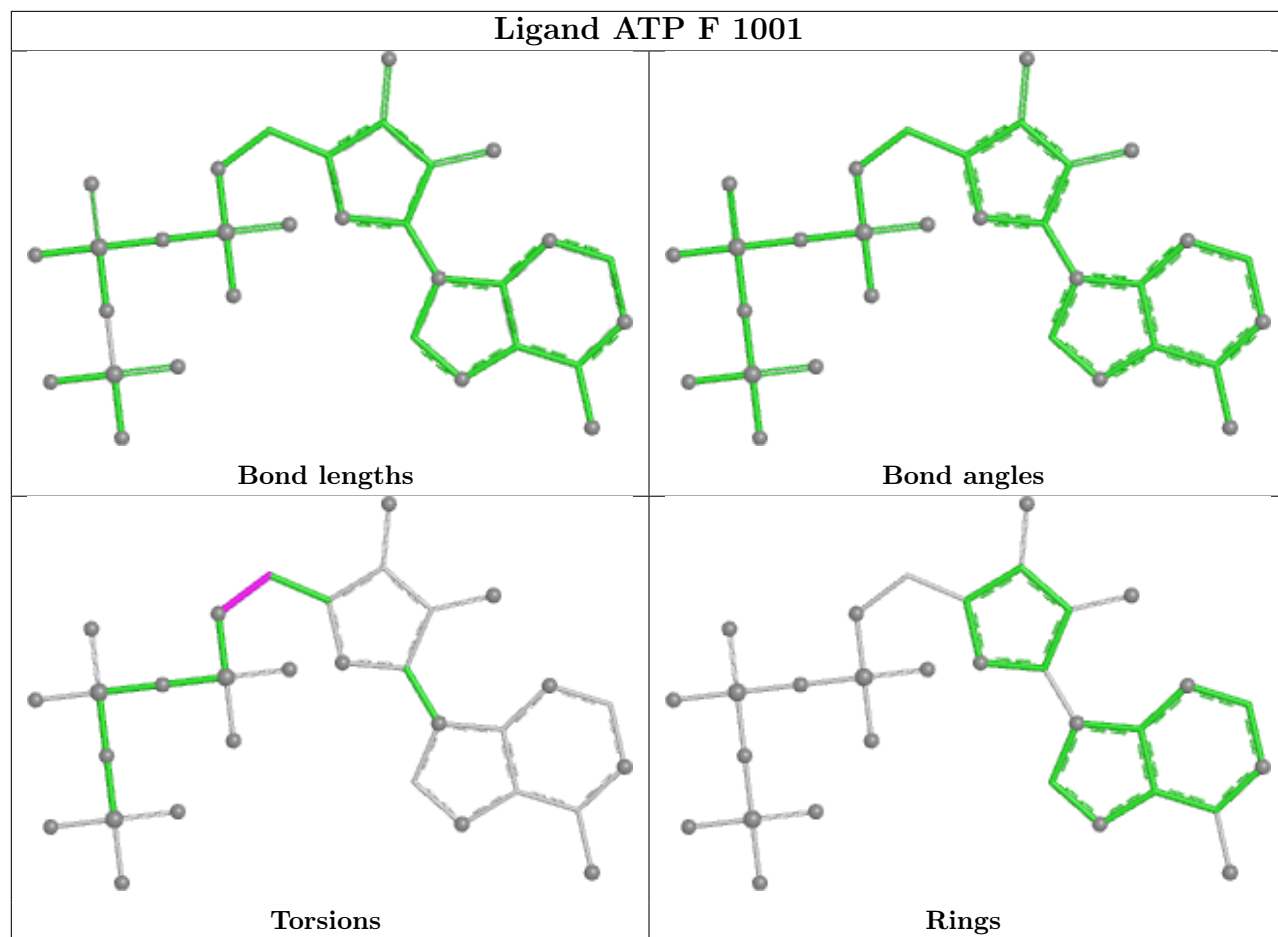
There are no ring outliers.

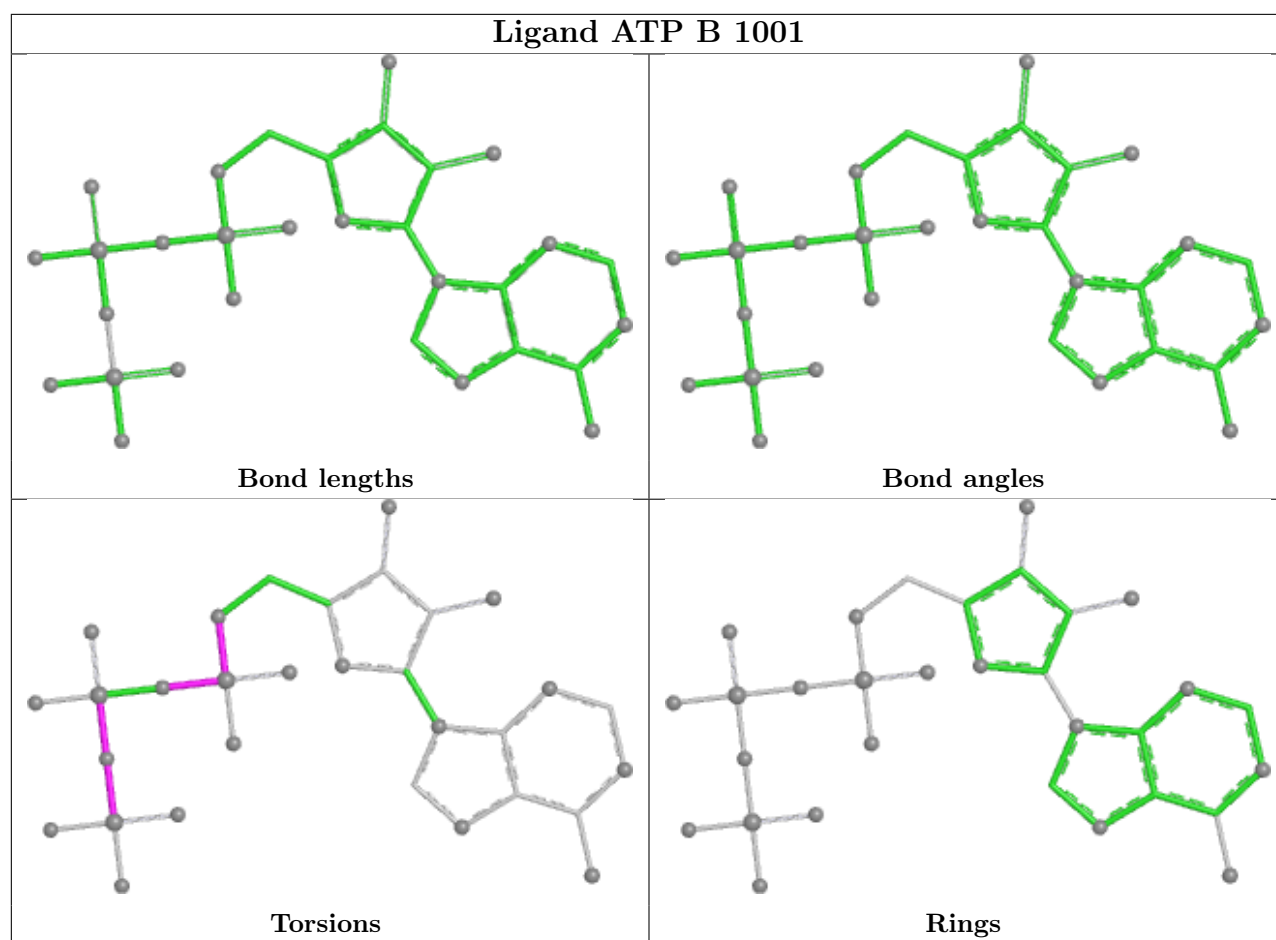
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	F	1001	ATP	1	0
17	B	1001	ATP	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.

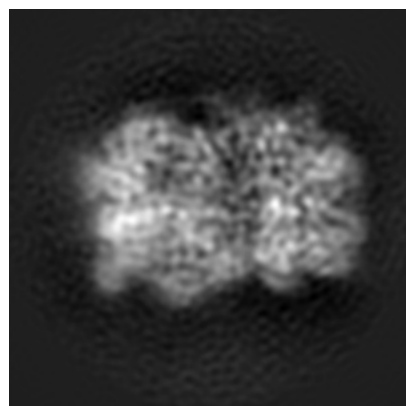
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44441. These allow visual inspection of the internal detail of the map and identification of artifacts.

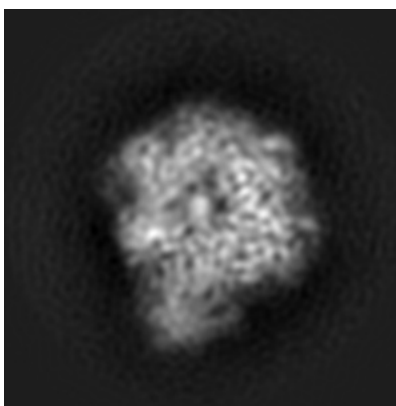
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

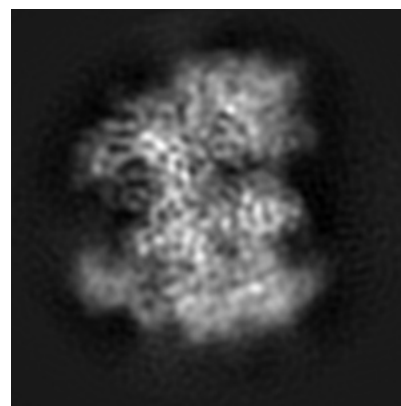
6.1.1 Primary map



X

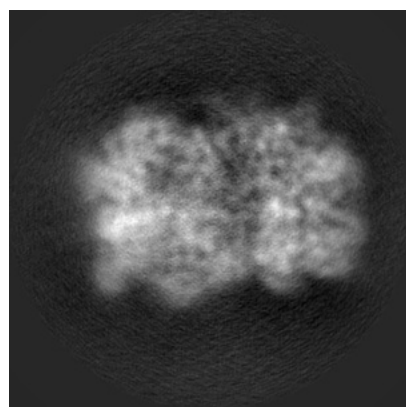


Y

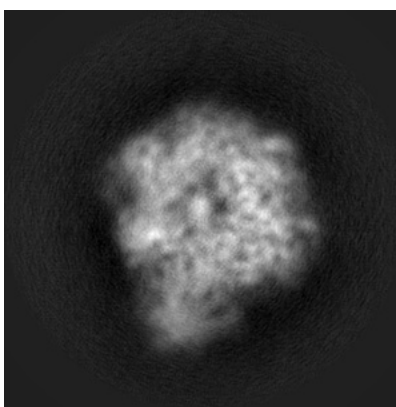


Z

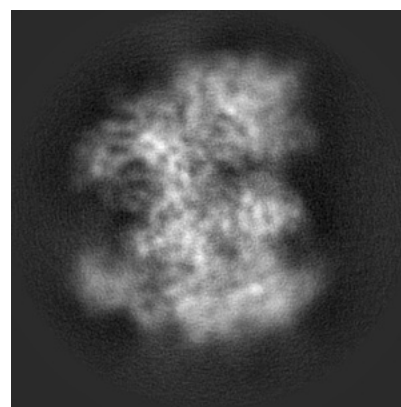
6.1.2 Raw map



X



Y

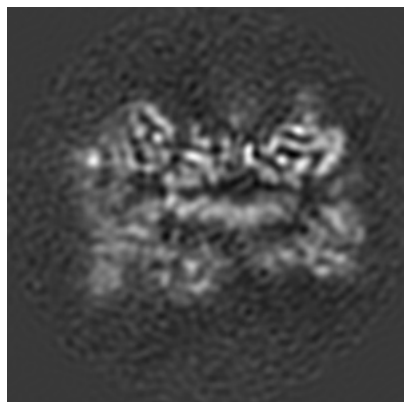


Z

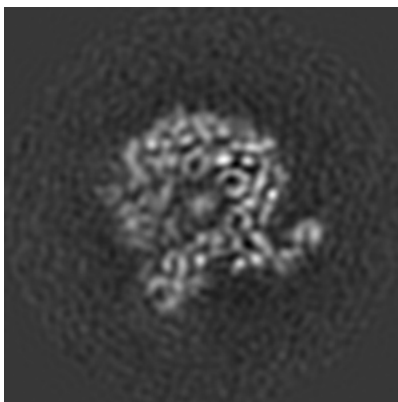
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

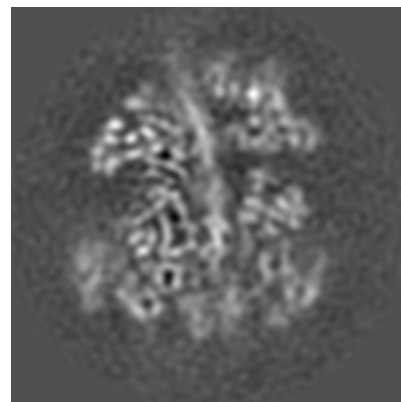
6.2.1 Primary map



X Index: 128

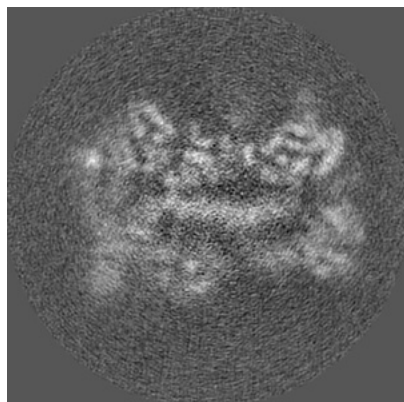


Y Index: 128

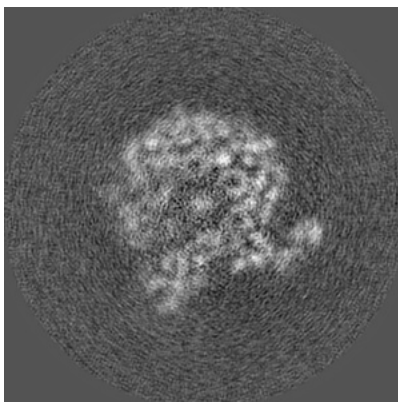


Z Index: 128

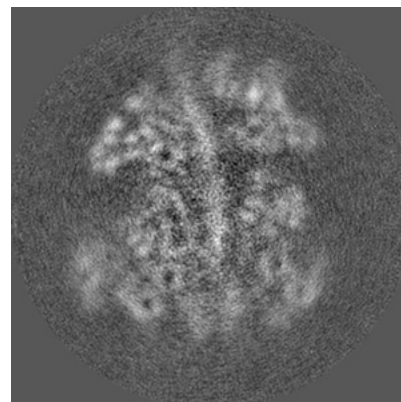
6.2.2 Raw map



X Index: 128



Y Index: 128

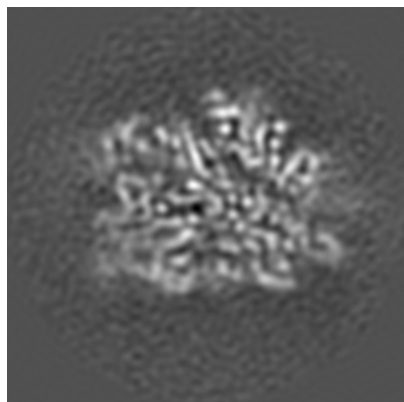


Z Index: 128

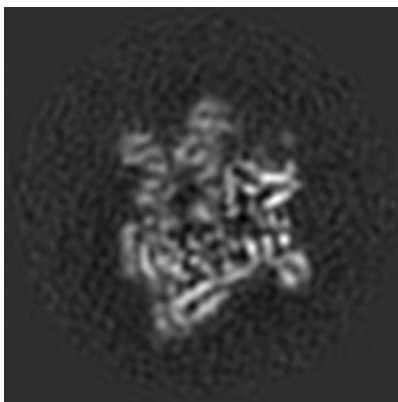
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

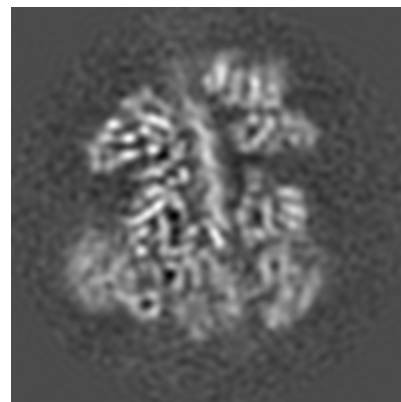
6.3.1 Primary map



X Index: 104

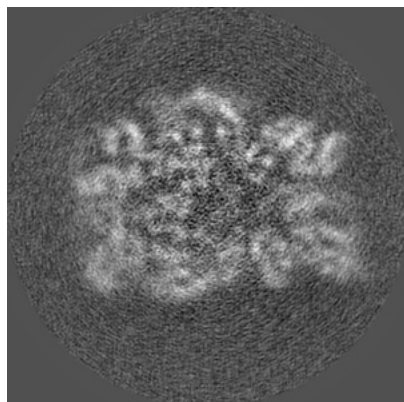


Y Index: 172

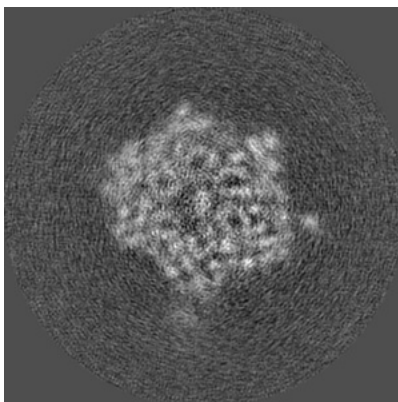


Z Index: 125

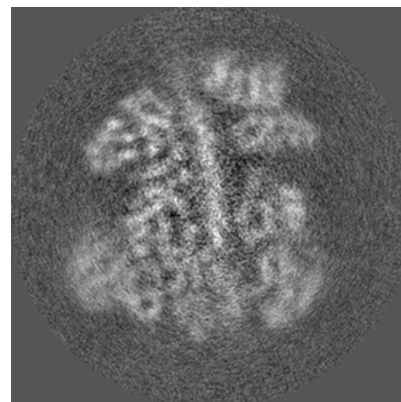
6.3.2 Raw map



X Index: 115



Y Index: 117

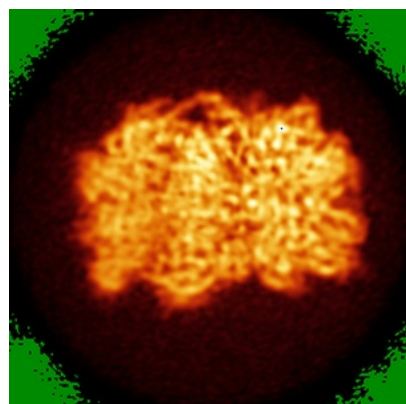


Z Index: 125

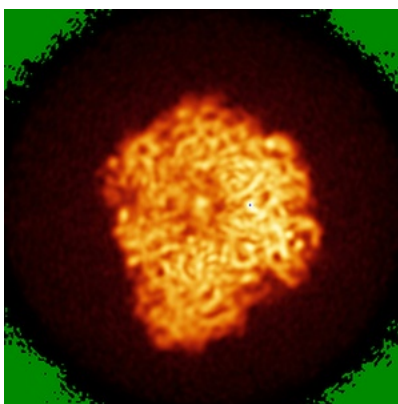
The images above show the largest variance slices of the map in three orthogonal directions.

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

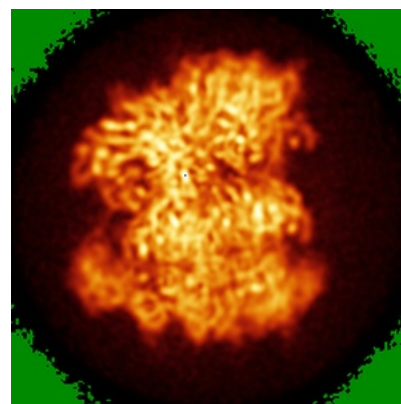
6.4.1 Primary map



X

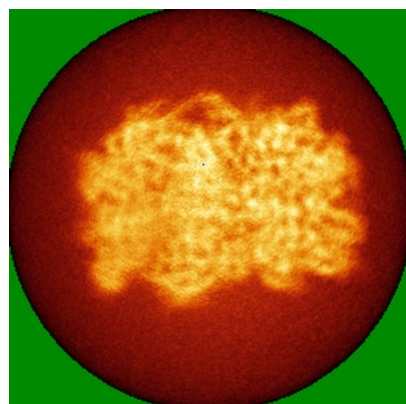


Y

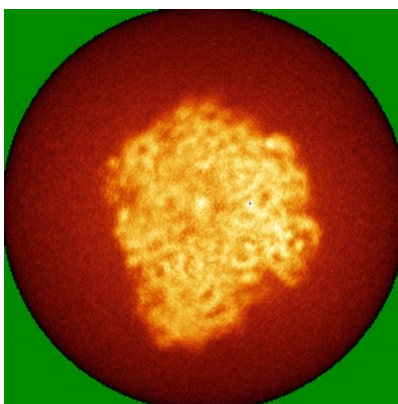


Z

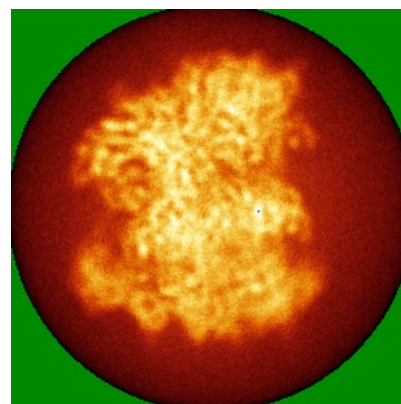
6.4.2 Raw map



X



Y

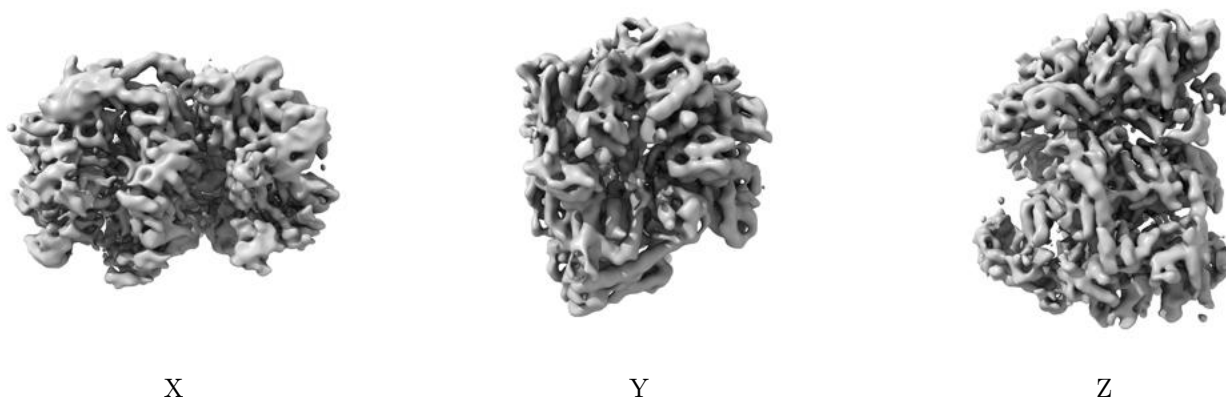


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

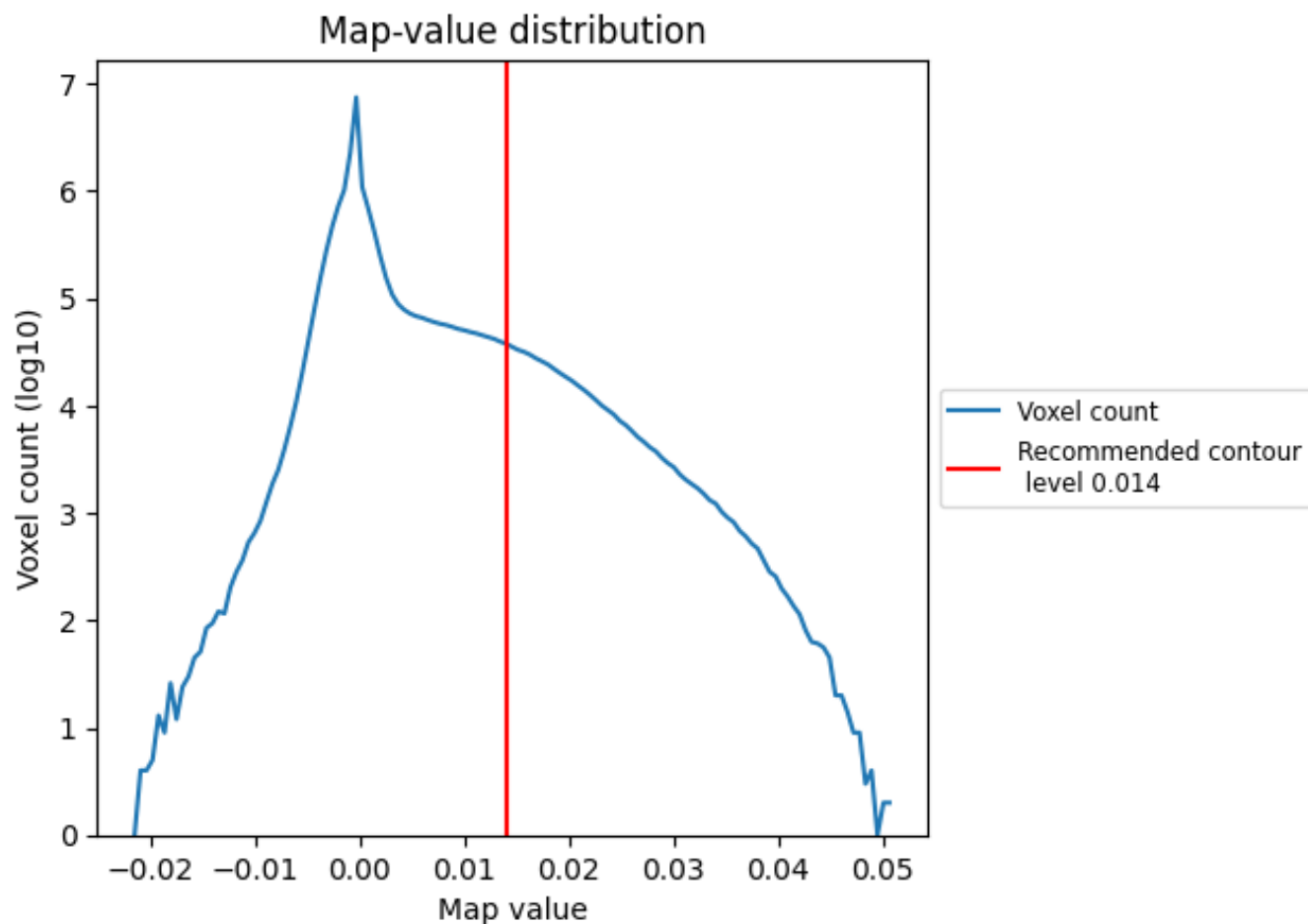
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

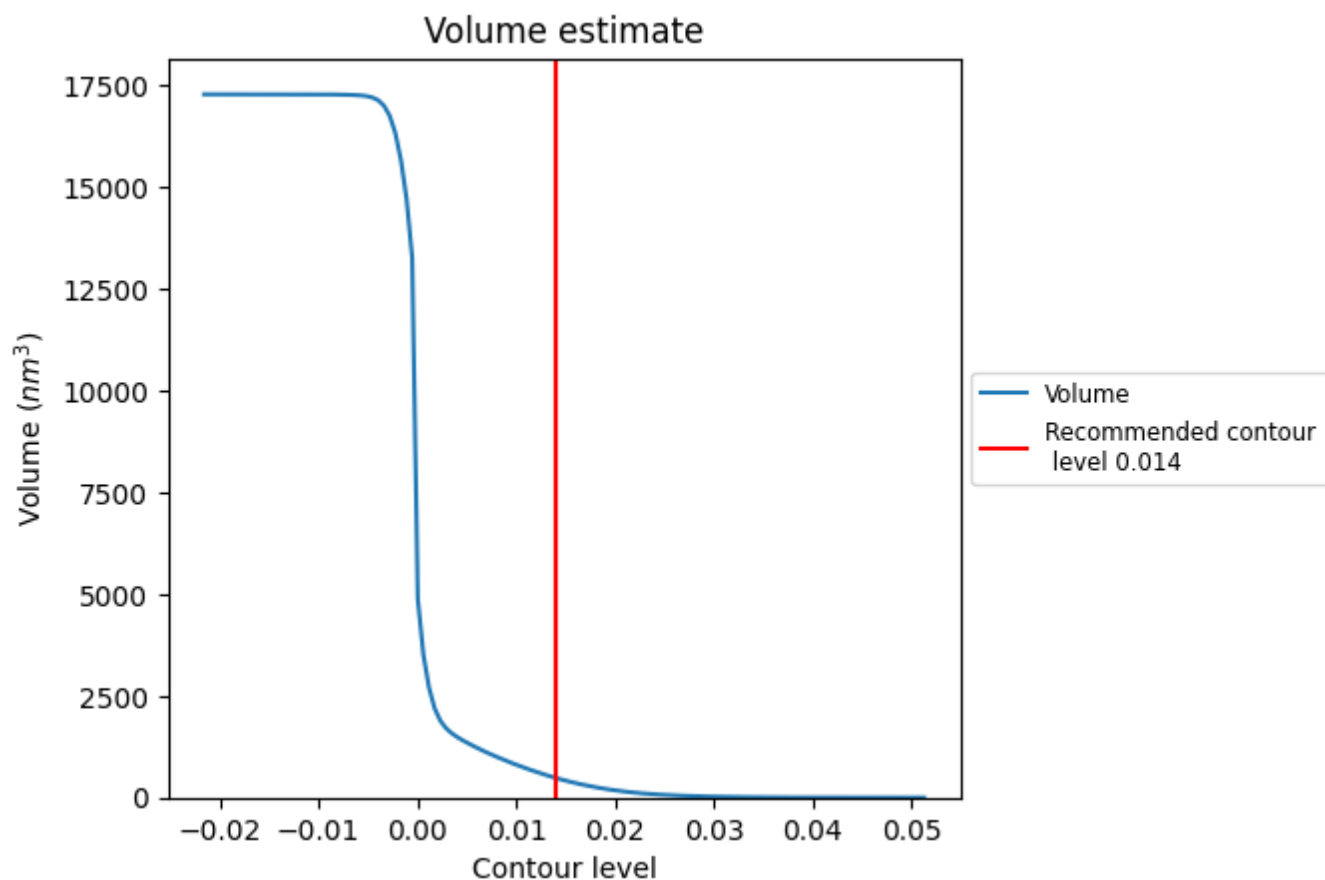
This section contains the results of statistical analysis of the map.

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.

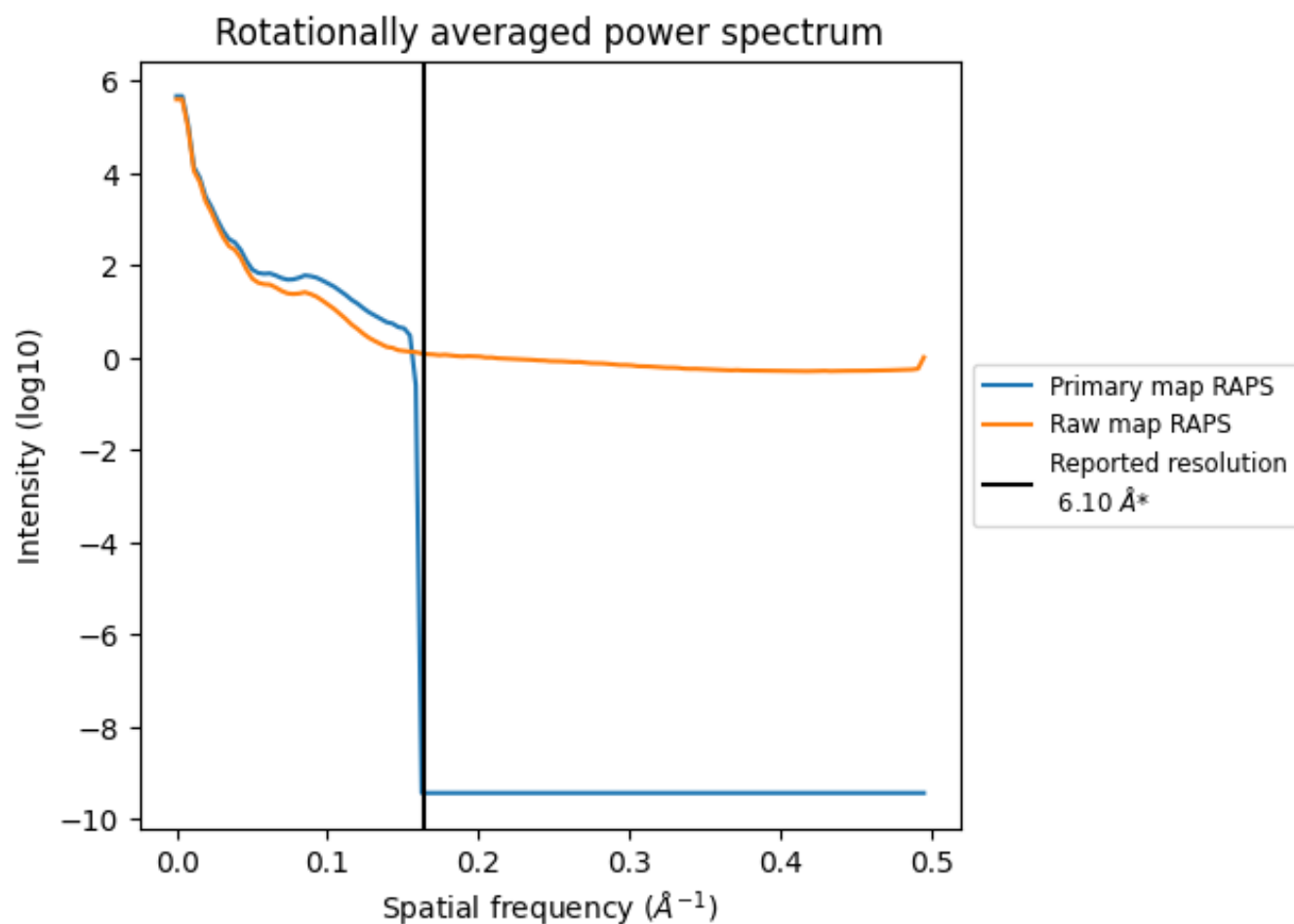
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 482 nm³; this corresponds to an approximate mass of 435 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 ⓘ

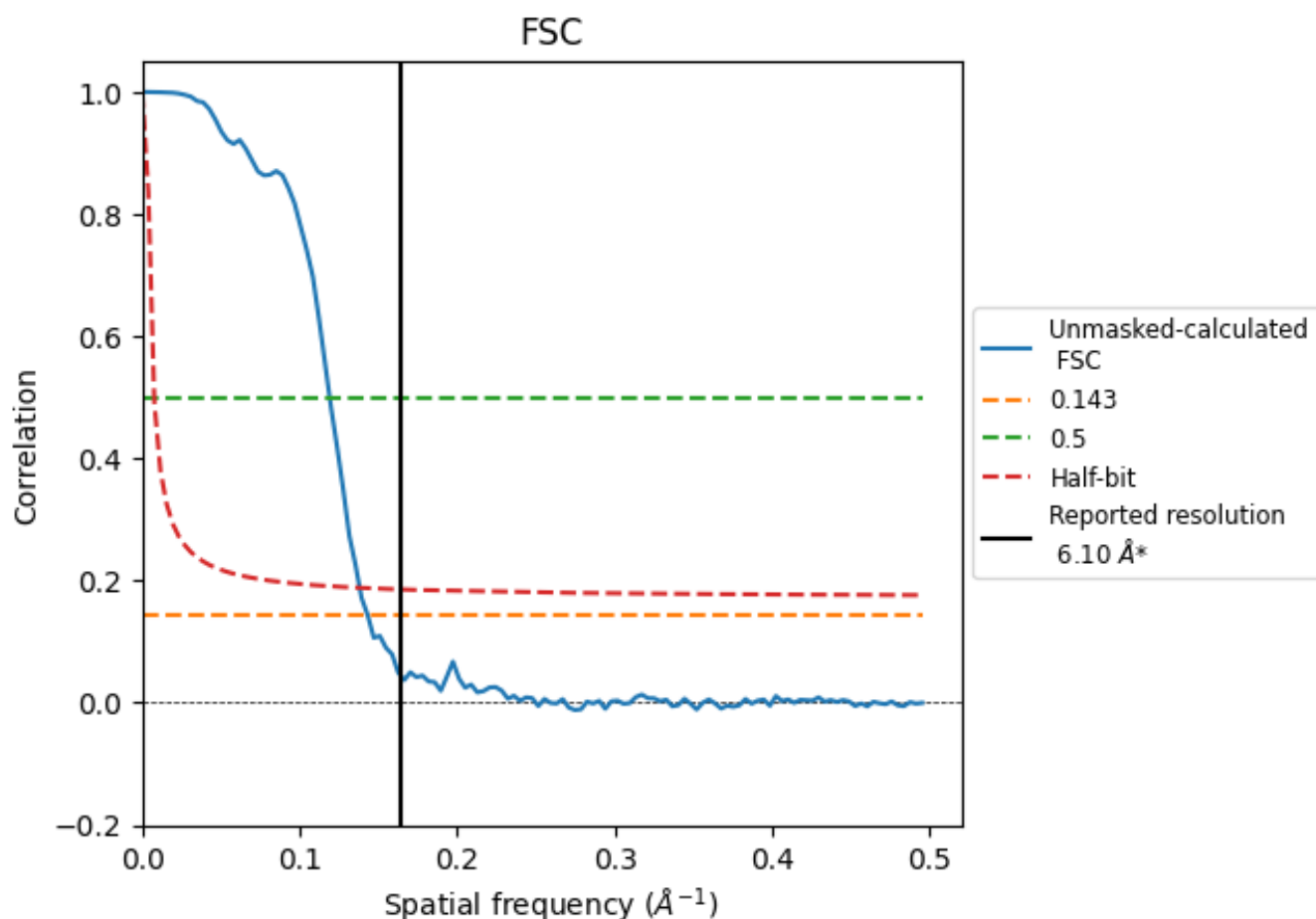


*Reported resolution corresponds to spatial frequency of 0.164 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.164 Å⁻¹

8.2 Resolution estimates [i](#)

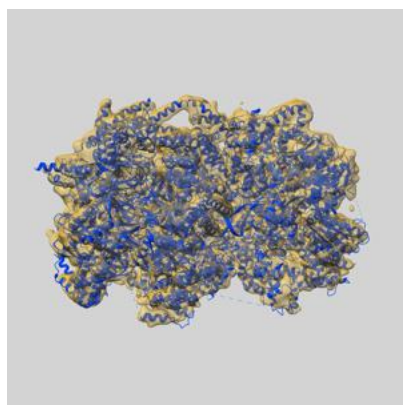
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.99	8.40	7.25

*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 6.99 differs from the reported value 6.1 by more than 10 %

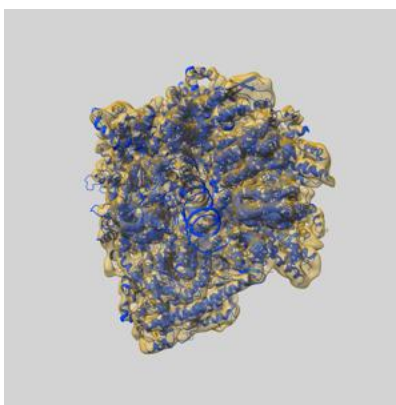
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44441 and PDB model 9BCX. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

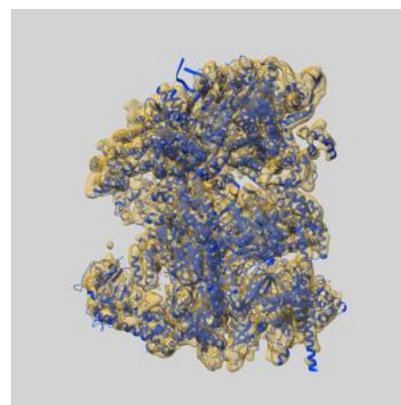
9.1 Map-model overlay [i](#)



X



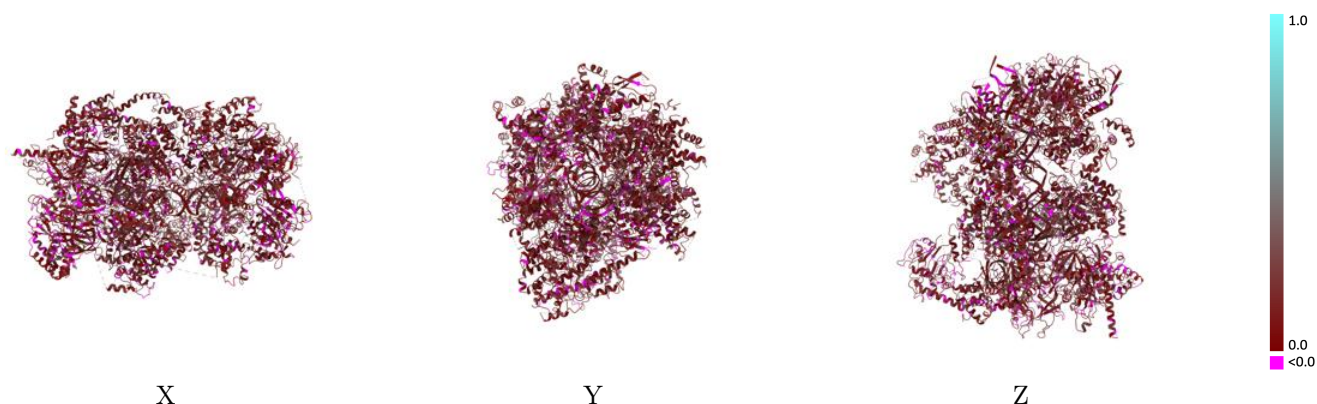
Y



Z

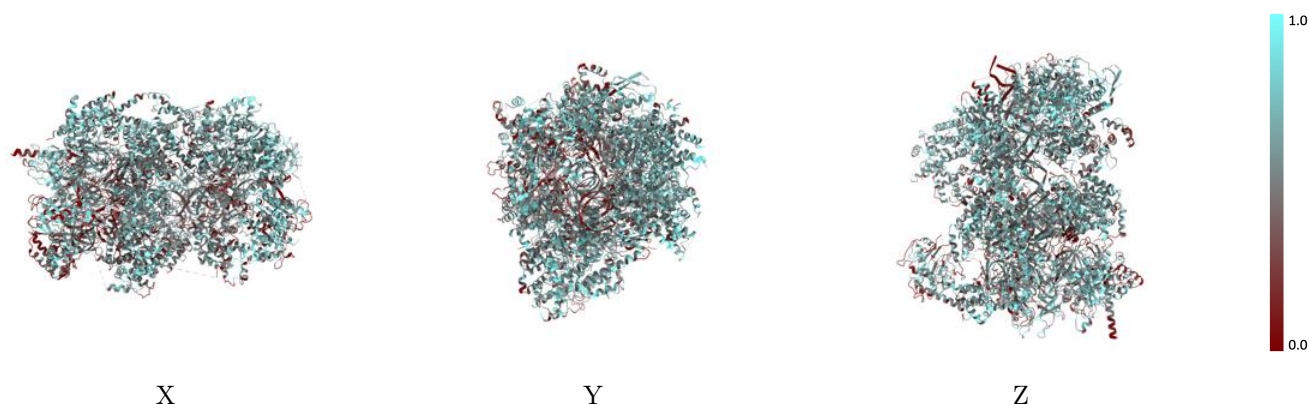
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



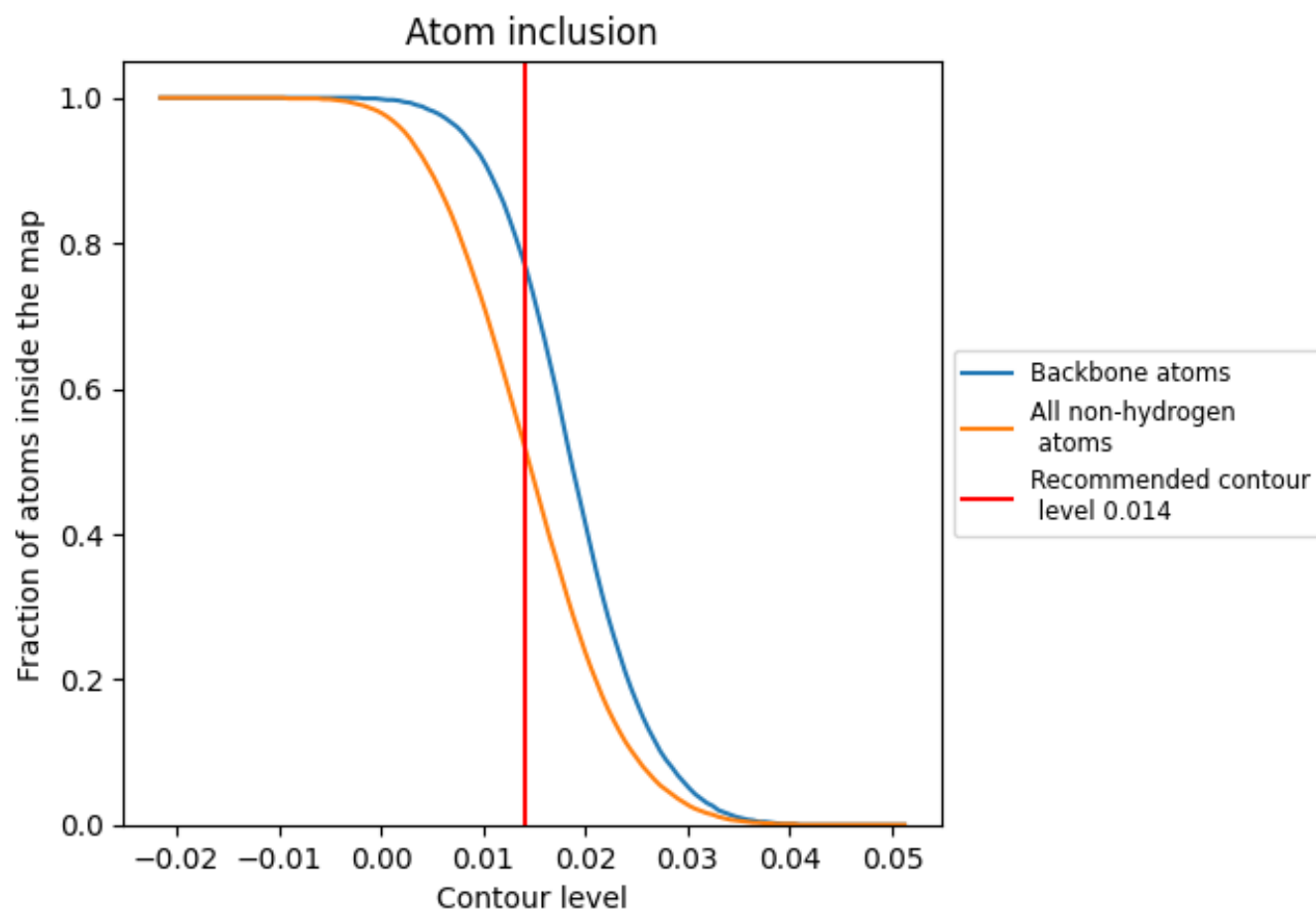
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 52% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5230	0.1330
2	0.5040	0.1310
3	0.4850	0.1300
4	0.5620	0.1450
5	0.4480	0.1220
6	0.5500	0.1290
7	0.4660	0.1320
8	0.4680	0.1190
B	0.5680	0.1280
C	0.5400	0.1400
D	0.5860	0.1340
E	0.6060	0.1440
F	0.6130	0.1490
G	0.5150	0.1350
I	0.4600	0.1270
O	0.4280	0.1420
P	0.4800	0.1590

1.0

0.0

<0.0