



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 06:50 pm BST

PDB ID : 6RAZ / pdb_00006raz
EMDB ID : EMD-4788
Title : D. melanogaster CMG-DNA, State 2B
Authors : Eickhoff, P.; Martino, F.; Costa, A.
Deposited on : 2019-04-08
Resolution : 4.46 Å(reported)

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

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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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

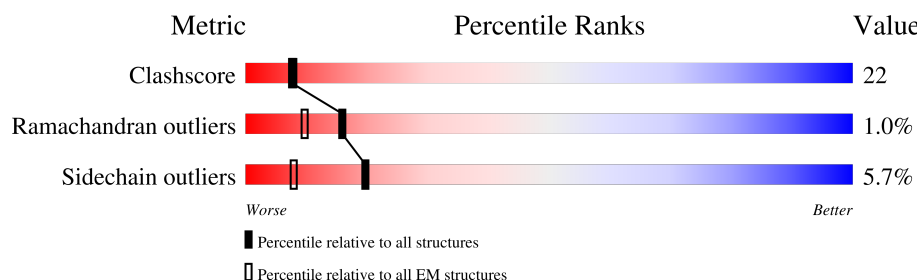
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.46 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	X	21	<div> <div>67%</div> <div>29% 52% 19%</div> </div>
2	Y	2	<div> <div>100%</div> <div>100%</div> </div>
3	A	575	<div> <div>6%</div> <div>55% 33% 10%</div> </div>
4	H	202	<div> <div>14%</div> <div>51% 41%</div> </div>
5	L	203	<div> <div>52% 33% 12%</div> </div>
6	M	212	<div> <div>6%</div> <div>37% 31% 29%</div> </div>
7	N	228	<div> <div>9%</div> <div>55% 32% 10%</div> </div>
8	2	887	<div> <div>11%</div> <div>37% 24% 37%</div> </div>

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Mol	Chain	Length	Quality of chain
9	5	733	
10	6	817	
11	3	819	
12	4	866	
13	7	720	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	ATP	7	801	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 38294 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 DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	21	Total	C	N	O	P	0	0
			425	209	58	137	21		

- Molecule 2 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	2	Total	C	N	O	P	0	0
			41	19	8	12	2		

- Molecule 3 is a protein called CDC45L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	519	Total	C	N	O	S	0	0
			4190	2685	718	765	22		

- Molecule 4 is a protein called IP07275p.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	195	Total	C	N	O	S	0	0
			1583	1007	279	289	8		

- Molecule 5 is a protein called Probable DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	179	Total	C	N	O	S	0	0
			1457	939	243	262	13		

- Molecule 6 is a protein called AT18545p.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	150	Total	C	N	O	S	0	0
			1259	806	220	229	4		

- Molecule 7 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	206	Total	C	N	O	S	0	0
			1661	1032	283	333	13		

- Molecule 8 is a protein called DNA replication licensing factor Mcm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	559	Total	C	N	O	S	0	0
			4442	2811	781	823	27		

- Molecule 9 is a protein called DNA replication licensing factor Mcm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	5	571	Total	C	N	O	S	0	0
			4459	2801	790	841	27		

- Molecule 10 is a protein called DNA replication licensing factor Mcm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	6	588	Total	C	N	O	S	0	0
			4609	2891	804	892	22		

- Molecule 11 is a protein called DNA replication licensing factor Mcm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	3	590	Total	C	N	O	S	0	0
			4585	2857	825	877	26		

- Molecule 12 is a protein called DNA replication licensing factor MCM4.

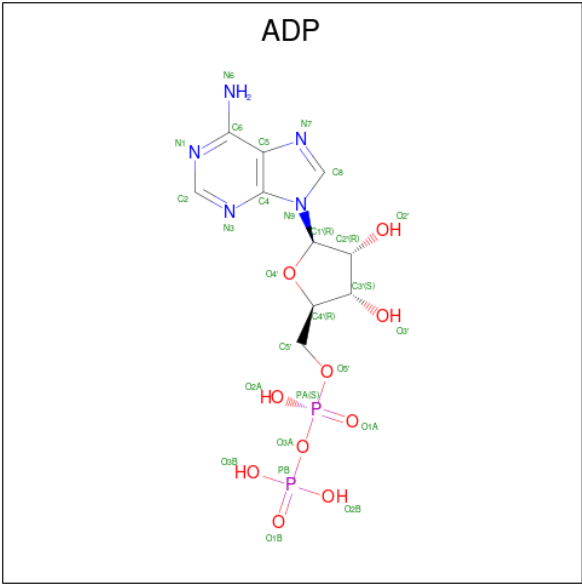
Mol	Chain	Residues	Atoms					AltConf	Trace
12	4	606	Total	C	N	O	S	0	0
			4811	3022	854	913	22		

- Molecule 13 is a protein called DNA replication licensing factor Mcm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	7	601	Total	C	N	O	S	0	0
			4594	2876	818	875	25		

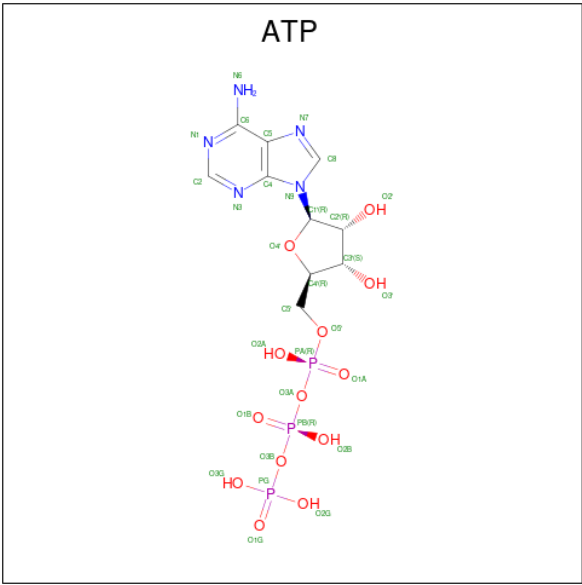
- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂)

(labeled as "Ligand of Interest" by depositor).

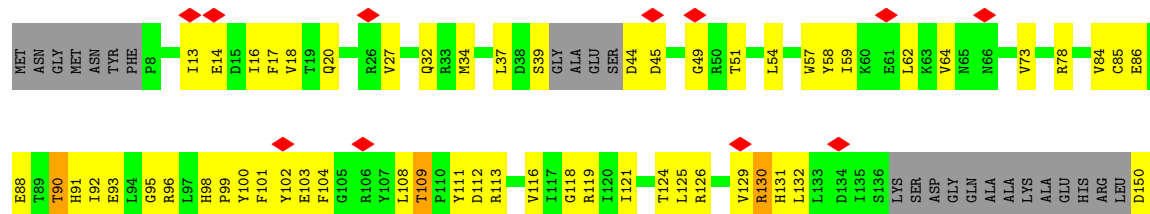


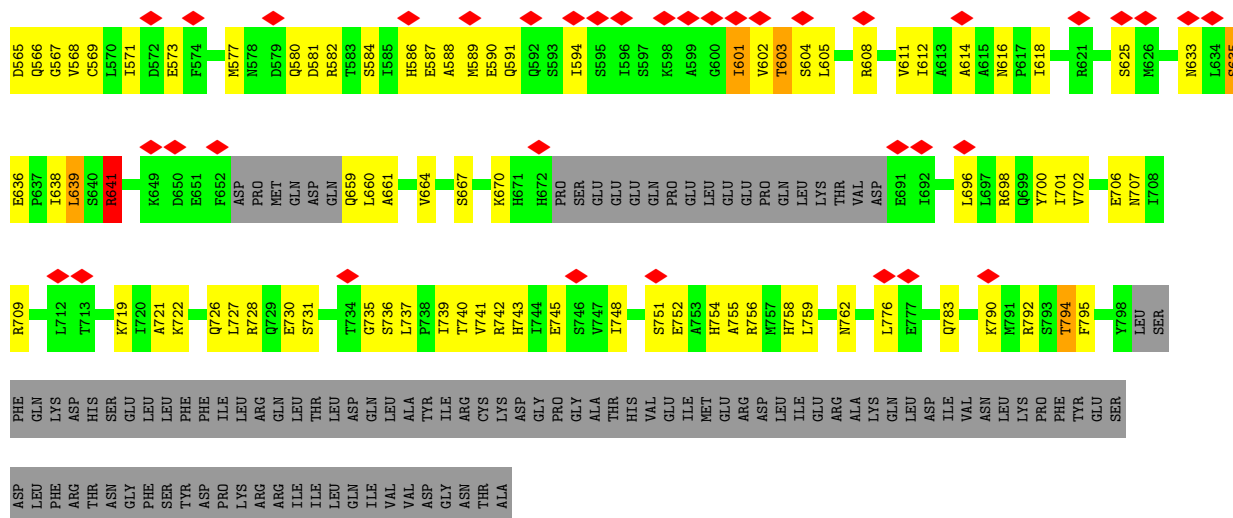
Mol	Chain	Residues	Atoms					AltConf
14	5	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	6	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

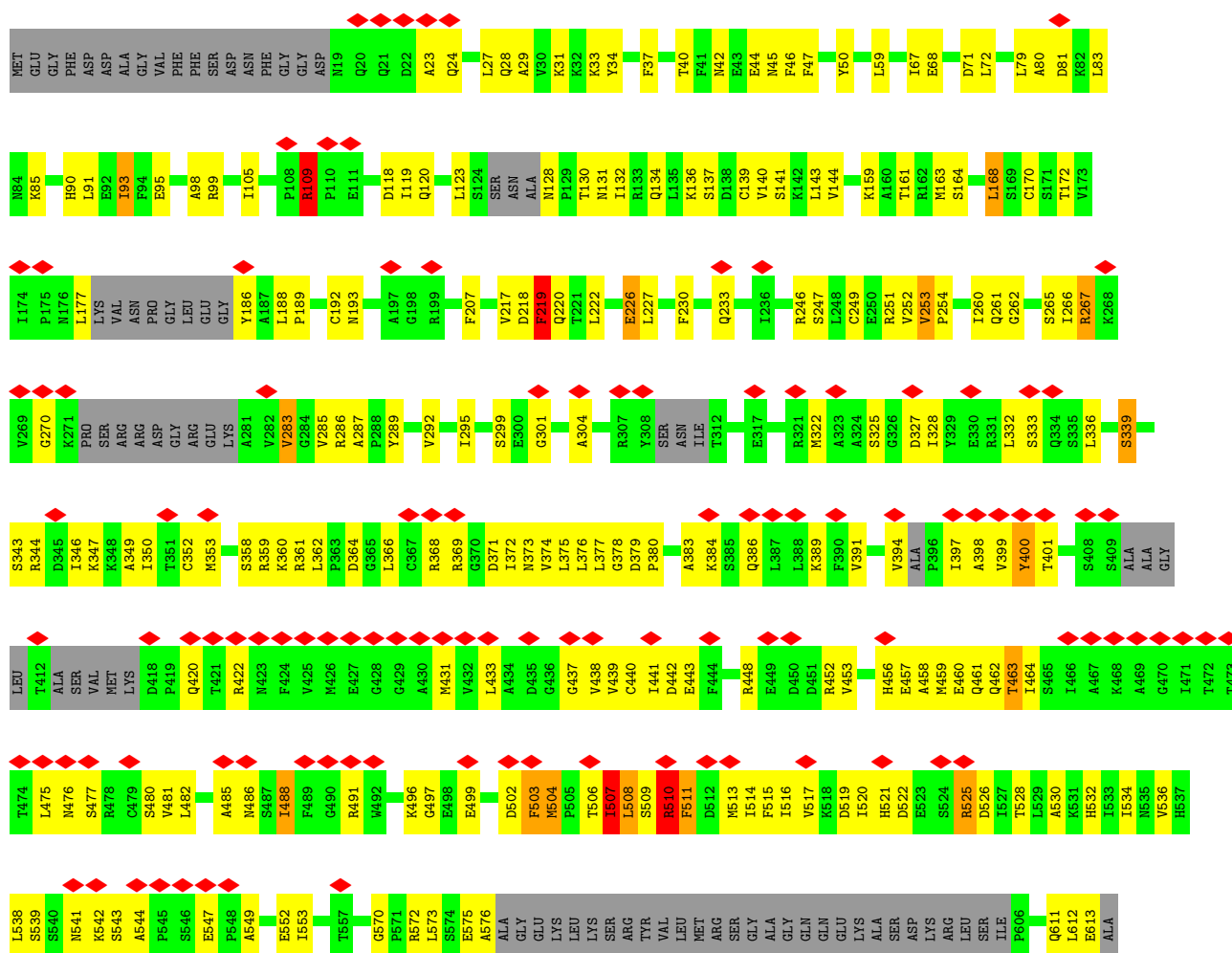
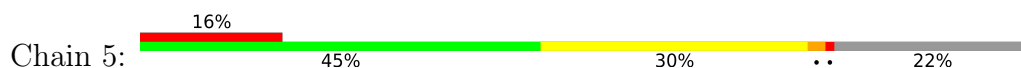


Mol	Chain	Residues	Atoms					AltConf
15	6	1	Total 31	C 10	N 5	O 13	P 3	0
15	3	1	Total 31	C 10	N 5	O 13	P 3	0
15	4	1	Total 31	C 10	N 5	O 13	P 3	0
15	7	1	Total 31	C 10	N 5	O 13	P 3	0

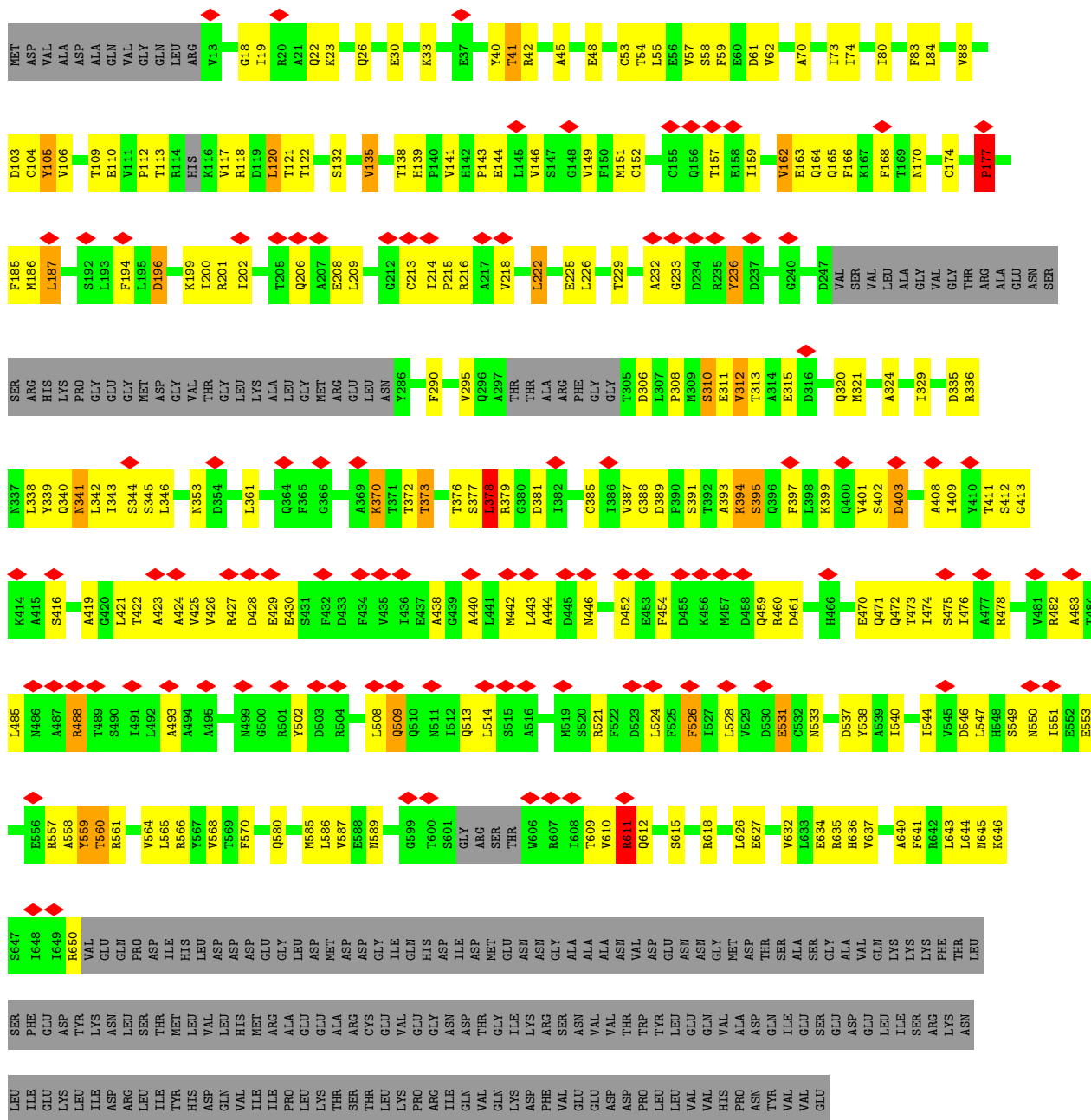
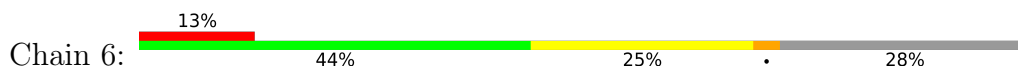




• Molecule 9: DNA replication licensing factor Mcm5

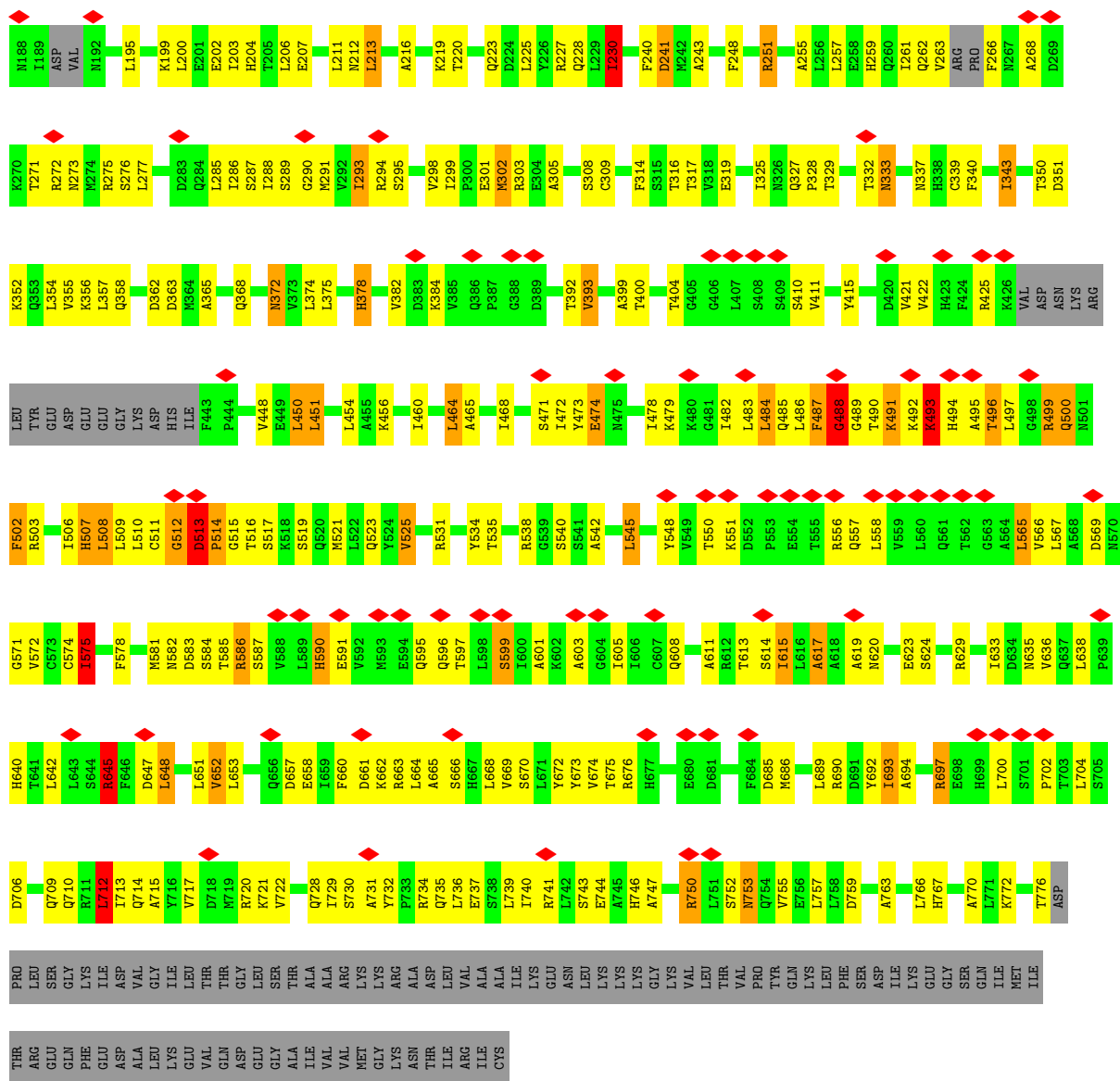


- Molecule 10: DNA replication licensing factor Mcm6

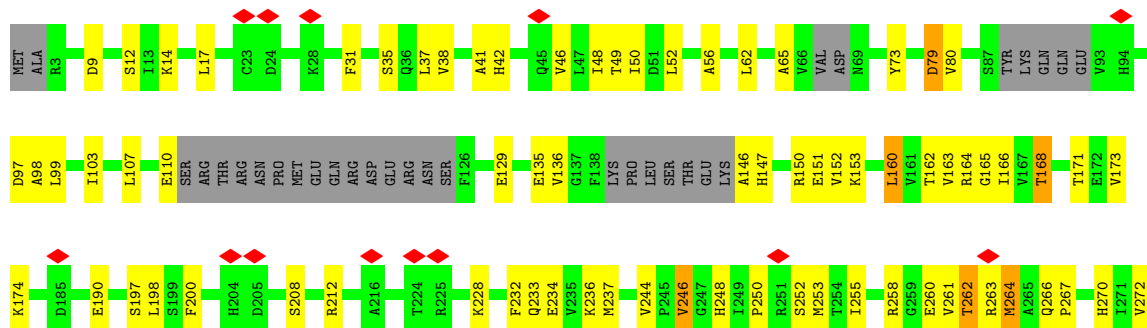


- Molecule 11: DNA replication licensing factor Mcm3





• Molecule 13: DNA replication licensing factor Mcm7



LEU	ALA	GLY	SER	GLY	LYS	ALA	VAL	LYS	ILE	SER	ASP	ILE	MET	ASP	ARG	CYS	THR	THR	LYS	GLY	PHE	LYS	PRO	ASP	GLN	VAL	ASP	LYS	ILE	CYS	ASP	TYR	GLU	GLU	LEU	ASN	VAL	TRP	HIS	GLN	VAL	ASN	MET	GLY	ARG	THR	LYS	ILE	THR	ASN	THR	ASP	PHE	MET					
G605	L606	L607	G608	G609	L610	R611	L612	S613	T614	A615	L616	A617	R618	L619	R620	L621	S622	D623	S624	V625	E626		D629	V630	A631	E632	A633	L634	R635	L636	L637	S640	L644	N645	Q646	ILE	HIS	TRP	GLN	VAL	HIS	GLN	LYS	MET	GLY	HIS	VAL	PRO	ASN	THR	THR	LYS	ILE	THR	ASN	THR	ASP	PHE	MET
S468	A534	K535	T538	Y539	V540	H541	S544	K545	Q546	P547	P548	T549	R550	V551	K552	A553	L554	D555	M556	N557	L558	M559	R560	R561	N564	L565	C566	K567	R568	K569	N570	P571	T572	I573	P574	D575	E576	L577	T578	D579	Y580	L581	V582	G583	A584	Y585	V586	E587	L588	R589	E591	K596	R604						
I469	A470	K471	A472	G473	L474	M475	T476	L477	L478	N479	A480	R481	V482	S483	L484	L485	A486	A487	A488	N489	P490	A491	F492	G493	R494	Y495	R499	T500	V501	E502	Q503	N504	I505	A509	A510	L511	L512	S513	R514	F515	D516	L517	L518	W519	L520	I521	K524	P525	D526	R527	D528	N529	D530	L531	R532				
T404	G406	R407	G408	S409	S410	G411	V412	G413	L414	T415	A416	A417	K420	D421	P422	L423	T424	G425	E426	M427	T428	L429	G430	G431	G432	A433	L434	V435	L436	A437	D438	Q439	G440	V441	C442	C443	E446	F447	D448	K449	M450	A451	D452	Q453	D454	R455	H459	E460	V461	M462	E463	Q464	Q465	T466	I467				
A341	P342	E343	I344	Y345		D349	V350	K351		L354	L355	L356	L357	L358	V359	G360	G361	V362	D363	K364	R365	P366	D367	G368	M369	K370	I371	R372	G373	N374	I375	N376	I377	C378	L379	M380	G381	D382	P383	V385	A386	K387	S388	Q389	L390	L391	G392	Y393	I394		L397	A398	V399	R400	S401	Q402	Y403		
G275	V276	F277	L278	P279	I280	M281	F285	A286	Q287	M288	I289	Q290	G291	L292	L293	S294	E295	T296	F297	L298	Q299		R302	I303	I304	C305	I306	ASN	LYS	ASN	ASP	GLU	ILE	SER	ASP	LYS	ASP	ALA	GLU	LEU	THR	P321	E322	E323	L324	E325	E326	L327	A328	Q329		Y333	E334	R335	L336	A337	T338	S339	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61082	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.039	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0045	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 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	X	0.73	0/471	1.55	6/725 (0.8%)
2	Y	0.49	0/45	0.81	0/67
3	A	0.48	0/4280	0.78	2/5790 (0.0%)
4	H	0.52	1/1618 (0.1%)	0.83	2/2184 (0.1%)
5	L	0.54	0/1492	0.75	0/2017
6	M	0.61	0/1288	0.82	1/1745 (0.1%)
7	N	0.48	0/1685	0.76	1/2277 (0.0%)
8	2	0.48	0/4515	0.90	12/6089 (0.2%)
9	5	0.53	1/4526 (0.0%)	0.96	20/6092 (0.3%)
10	6	0.47	0/4678	0.81	3/6319 (0.0%)
11	3	0.49	0/4641	0.86	4/6251 (0.1%)
12	4	0.62	1/4896 (0.0%)	1.07	41/6626 (0.6%)
13	7	0.41	0/4661	0.71	4/6297 (0.1%)
All	All	0.51	3/38796 (0.0%)	0.88	96/52479 (0.2%)

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	A	0	4
4	H	0	6
5	L	0	1
6	M	0	2
7	N	0	2
8	2	0	5
9	5	0	15
10	6	0	6
11	3	0	12
12	4	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	7	0	1
All	All	0	66

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	4	491	LYS	C-N	-26.85	0.72	1.34
9	5	507	ILE	C-N	-12.81	1.04	1.34
4	H	122	TYR	CD1-CE1	-5.63	1.30	1.39

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	4	491	LYS	O-C-N	-17.88	94.09	122.70
9	5	507	ILE	C-N-CA	-17.54	77.85	121.70
9	5	507	ILE	CA-C-N	-15.93	82.15	117.20
11	3	610	ARG	NE-CZ-NH2	-15.38	112.61	120.30
1	X	27	DT	P-O3'-C3'	14.84	137.50	119.70

There are no chirality outliers.

5 of 66 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	101	HIS	Peptide
3	A	294	TYR	Peptide
3	A	490	THR	Peptide
3	A	82	ASP	Peptide
4	H	34	VAL	Peptide

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	X	425	0	247	26	0
2	Y	41	0	23	0	0
3	A	4190	0	4167	156	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1583	0	1567	63	0
5	L	1457	0	1476	59	0
6	M	1259	0	1233	59	0
7	N	1661	0	1609	62	0
8	2	4442	0	4503	166	0
9	5	4459	0	4452	205	0
10	6	4609	0	4509	212	0
11	3	4585	0	4624	197	0
12	4	4811	0	4768	242	0
13	7	4594	0	4509	386	0
14	5	27	0	11	5	0
14	6	27	0	12	5	0
15	3	31	0	12	7	0
15	4	31	0	10	6	0
15	6	31	0	11	6	0
15	7	31	0	9	11	0
All	All	38294	0	37752	1704	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 22.

The worst 5 of 1704 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:3:422:GLU:HG3	11:3:473:ARG:NH1	1.24	1.41
9:5:460:GLU:CG	9:5:510:ARG:HD2	1.54	1.34
11:3:418:HIS:NE2	11:3:473:ARG:NH2	1.77	1.31
10:6:611:ARG:NH1	14:6:901:ADP:O1B	1.64	1.30
9:5:506:THR:O	9:5:509:SER:CB	1.81	1.29

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	515/575 (90%)	424 (82%)	88 (17%)	3 (1%)	22	60
4	H	193/202 (96%)	155 (80%)	36 (19%)	2 (1%)	13	49
5	L	175/203 (86%)	143 (82%)	32 (18%)	0	100	100
6	M	144/212 (68%)	115 (80%)	28 (19%)	1 (1%)	19	56
7	N	202/228 (89%)	169 (84%)	32 (16%)	1 (0%)	25	64
8	2	543/887 (61%)	453 (83%)	88 (16%)	2 (0%)	30	68
9	5	550/733 (75%)	429 (78%)	117 (21%)	4 (1%)	19	56
10	6	578/817 (71%)	461 (80%)	107 (18%)	10 (2%)	7	36
11	3	570/819 (70%)	461 (81%)	103 (18%)	6 (1%)	12	46
12	4	598/866 (69%)	482 (81%)	105 (18%)	11 (2%)	7	34
13	7	589/720 (82%)	498 (85%)	86 (15%)	5 (1%)	16	54
All	All	4657/6262 (74%)	3790 (81%)	822 (18%)	45 (1%)	16	49

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	2	512	THR
9	5	508	LEU
10	6	233	GLY
11	3	376	ALA
11	3	387	ARG

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	
3	A	451/501 (90%)	438 (97%)	13 (3%)	37	58
4	H	170/176 (97%)	164 (96%)	6 (4%)	31	52
5	L	166/184 (90%)	156 (94%)	10 (6%)	16	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	M	138/188 (73%)	132 (96%)	6 (4%)	25	47
7	N	185/205 (90%)	178 (96%)	7 (4%)	28	50
8	2	492/781 (63%)	466 (95%)	26 (5%)	19	41
9	5	486/630 (77%)	458 (94%)	28 (6%)	17	38
10	6	494/718 (69%)	466 (94%)	28 (6%)	17	39
11	3	500/699 (72%)	465 (93%)	35 (7%)	12	33
12	4	531/759 (70%)	497 (94%)	34 (6%)	14	36
13	7	482/630 (76%)	440 (91%)	42 (9%)	8	26
All	All	4095/5471 (75%)	3860 (94%)	235 (6%)	20	39

5 of 235 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	6	429	GLU
13	7	494	ARG
11	3	341	ASP
13	7	482	VAL
13	7	246	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
11	3	47	ASN
12	4	337	ASN
11	3	199	GLN
11	3	490	GLN
12	4	379	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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
15	ATP	3	901	-	26,33,33	0.87	1 (3%)	31,52,52	1.56	4 (12%)
15	ATP	7	801	13	26,33,33	0.96	1 (3%)	31,52,52	1.79	7 (22%)
14	ADP	6	901	-	24,29,29	1.49	4 (16%)	29,45,45	1.83	4 (13%)
14	ADP	5	801	9	24,29,29	0.97	1 (4%)	29,45,45	1.56	6 (20%)
15	ATP	6	902	10	26,33,33	0.94	1 (3%)	31,52,52	1.87	5 (16%)
15	ATP	4	901	12,13	26,33,33	0.89	1 (3%)	31,52,52	1.62	7 (22%)

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
15	ATP	3	901	-	-	5/18/38/38	0/3/3/3
15	ATP	7	801	13	-	5/18/38/38	0/3/3/3
14	ADP	6	901	-	-	0/12/32/32	0/3/3/3
14	ADP	5	801	9	-	0/12/32/32	0/3/3/3
15	ATP	6	902	10	-	5/18/38/38	0/3/3/3
15	ATP	4	901	12,13	-	6/18/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	6	901	ADP	PB-O1B	3.32	1.61	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	6	901	ADP	O4'-C1'	3.21	1.45	1.41
14	6	901	ADP	PA-O1A	3.20	1.62	1.50
15	4	901	ATP	C5-C4	2.55	1.47	1.40
14	5	801	ADP	C5-C4	2.51	1.47	1.40

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	6	901	ADP	PA-O3A-PB	-6.58	110.23	132.83
15	7	801	ATP	PA-O3A-PB	-4.93	115.91	132.83
15	6	902	ATP	PA-O3A-PB	-4.80	116.37	132.83
15	6	902	ATP	PB-O3B-PG	-4.71	116.67	132.83
14	6	901	ADP	N3-C2-N1	-4.62	121.45	128.68

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	6	902	ATP	C5'-O5'-PA-O1A
15	6	902	ATP	C5'-O5'-PA-O2A
15	3	901	ATP	C5'-O5'-PA-O1A
15	3	901	ATP	C5'-O5'-PA-O2A
15	4	901	ATP	C5'-O5'-PA-O2A

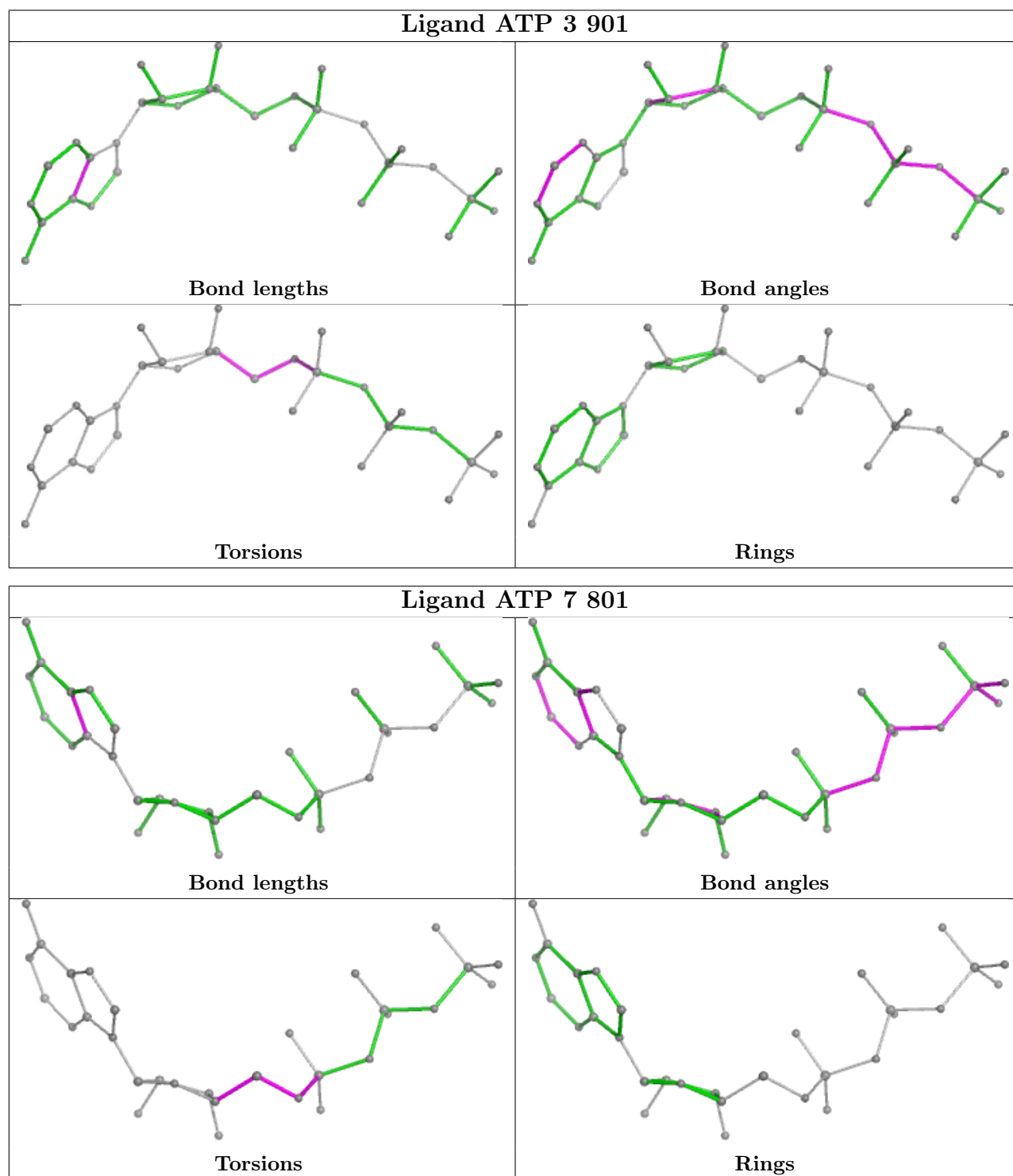
There are no ring outliers.

6 monomers are involved in 40 short contacts:

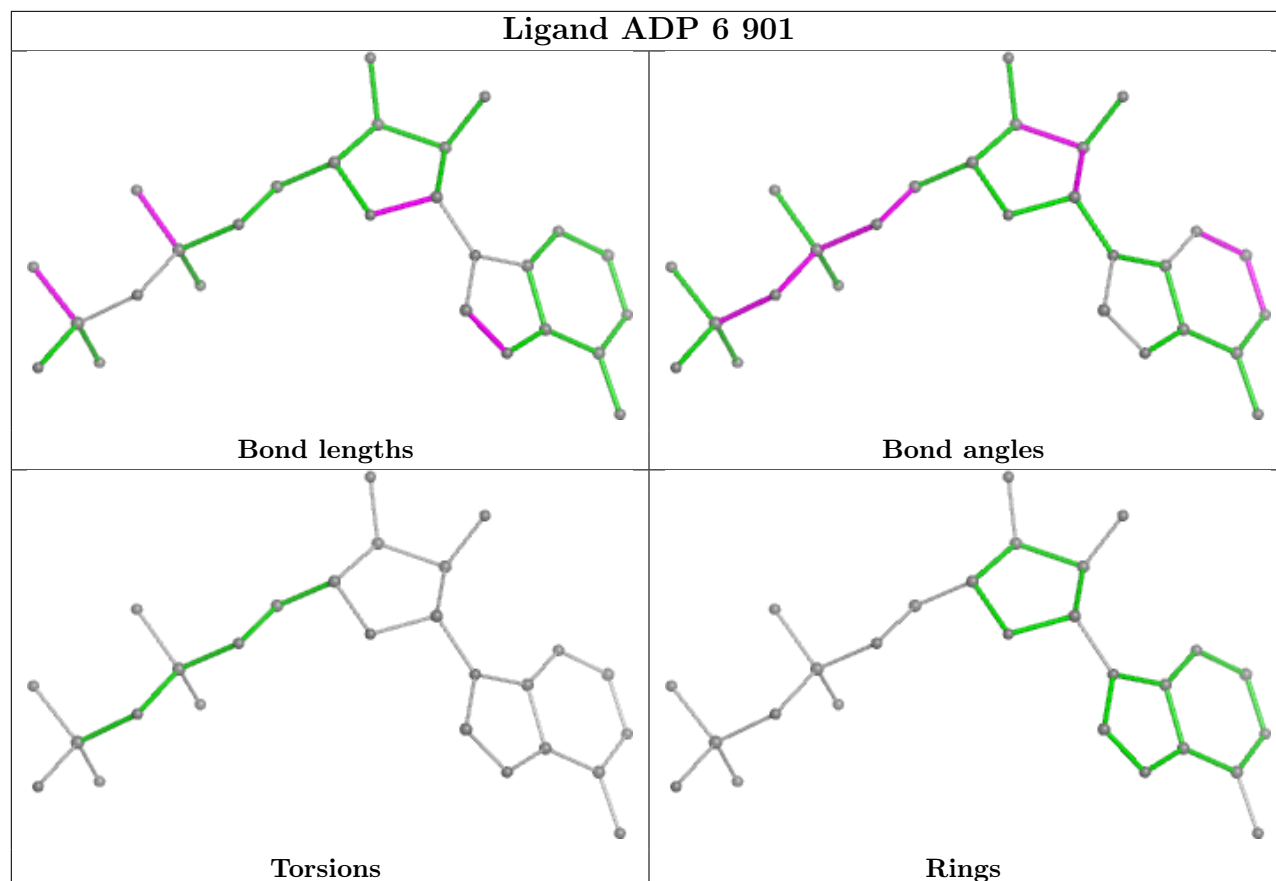
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3	901	ATP	7	0
15	7	801	ATP	11	0
14	6	901	ADP	5	0
14	5	801	ADP	5	0
15	6	902	ATP	6	0
15	4	901	ATP	6	0

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

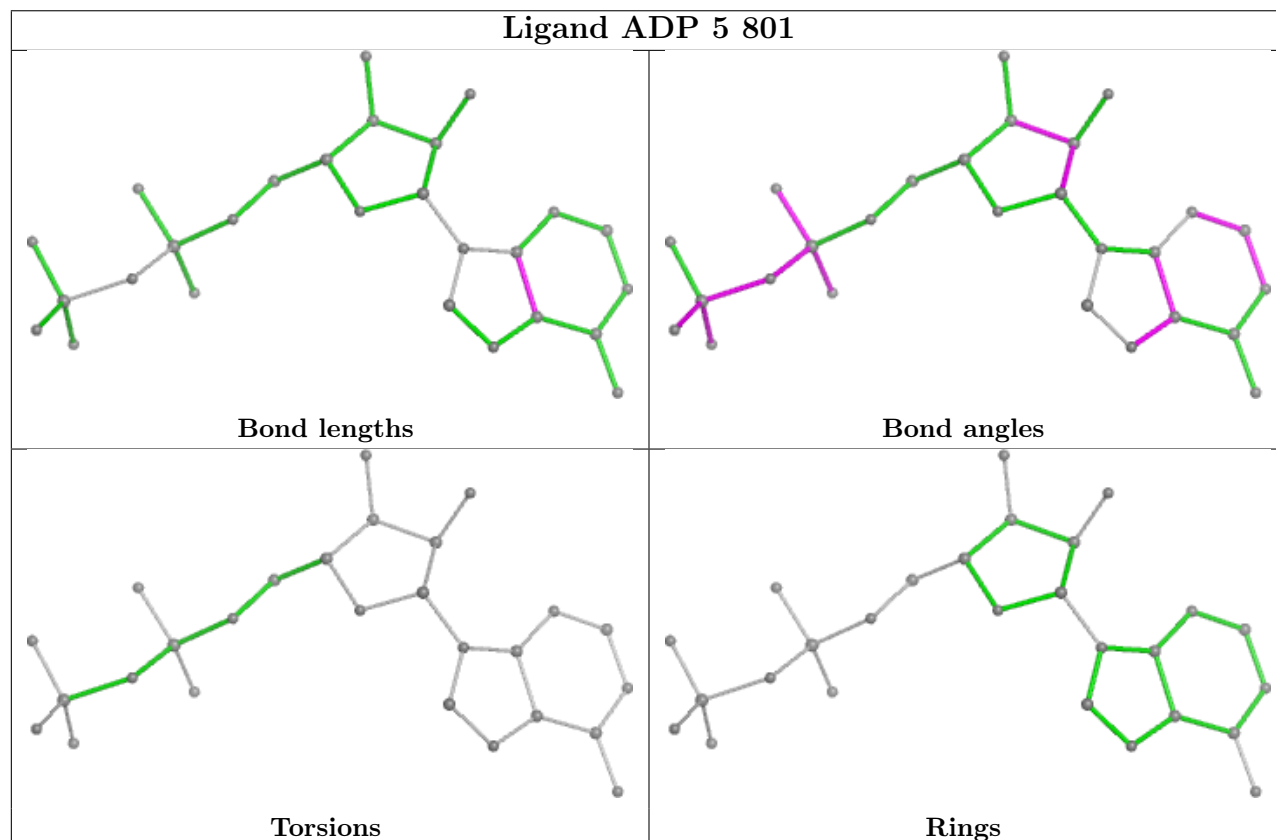
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

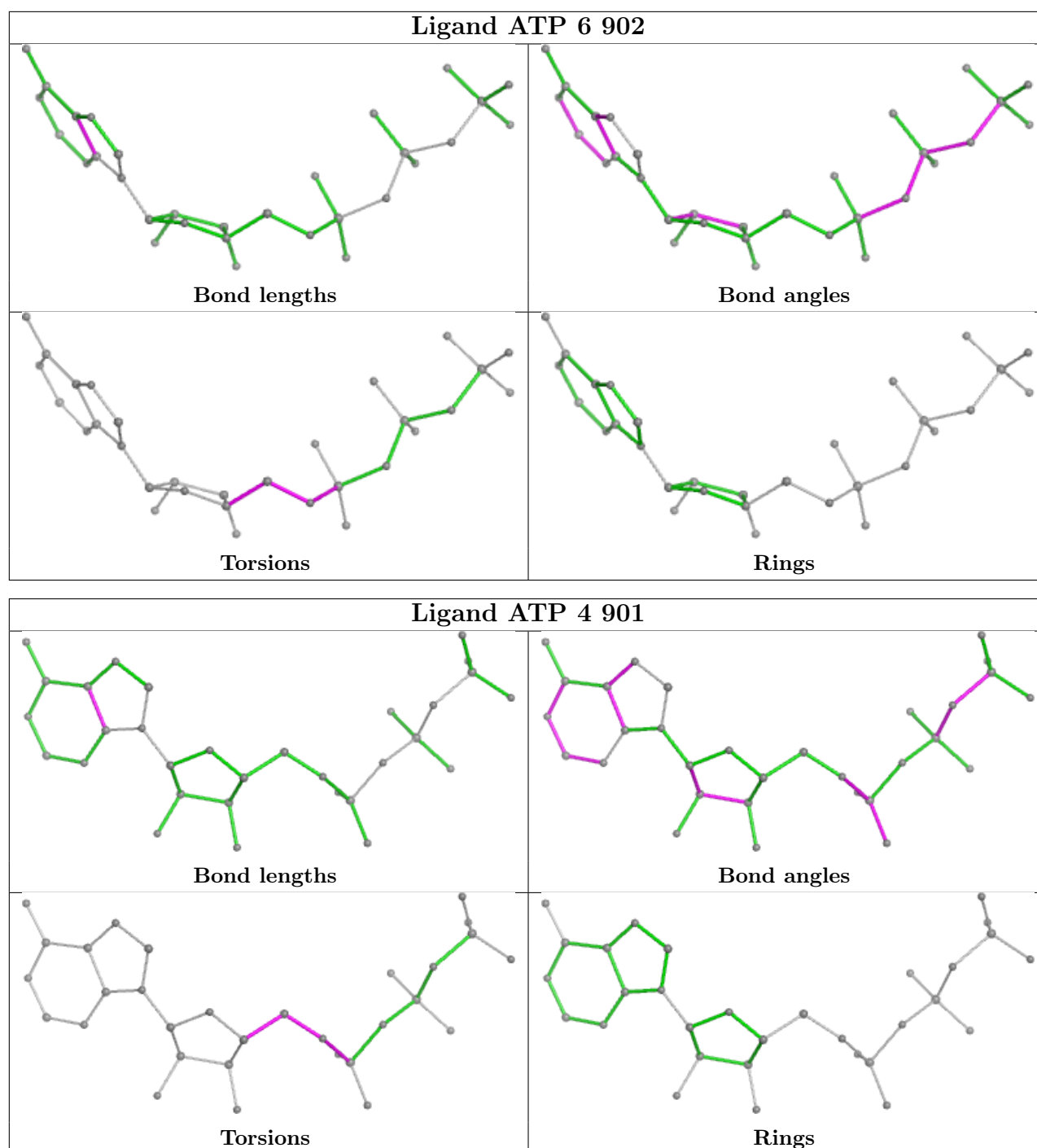


Ligand ADP 6 901



Ligand ADP 5 801





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	5	2
8	2	1
12	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	405:GLY	C	408:SER	N	5.55
1	2	435:LYS	C	436:GLN	N	4.80
1	5	507:ILE	C	508:LEU	N	1.04
1	4	491:LYS	C	492:LYS	N	0.72

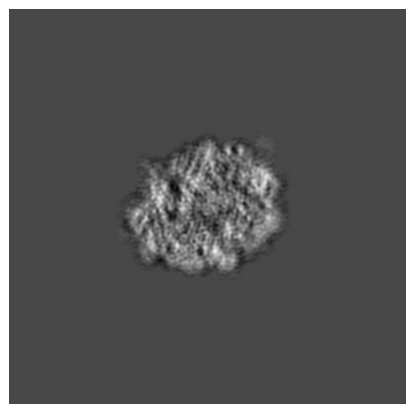
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4788. These allow visual inspection of the internal detail of the map and identification of artifacts.

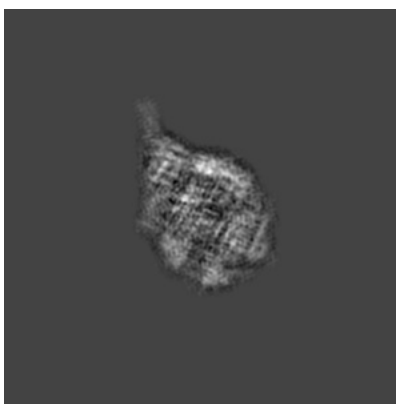
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

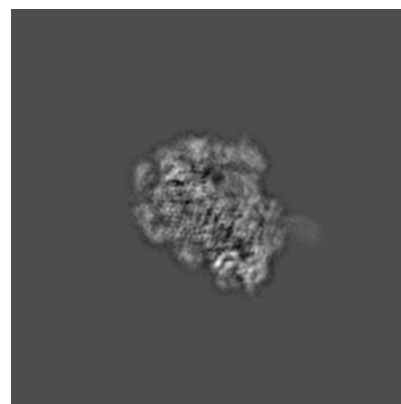
6.1.1 Primary map



X

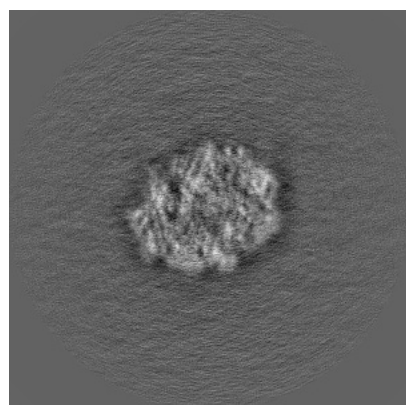


Y

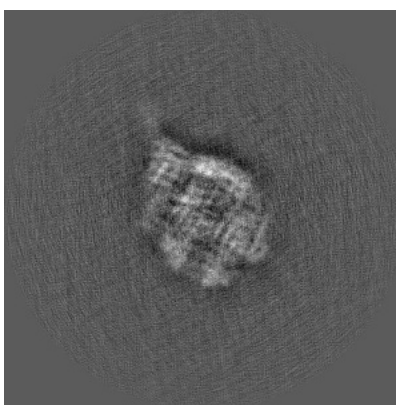


Z

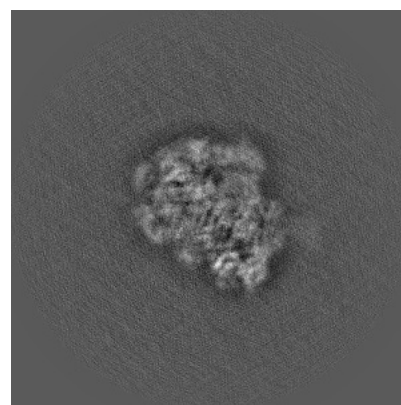
6.1.2 Raw map



X



Y

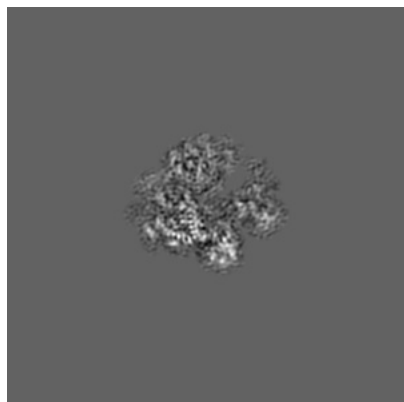


Z

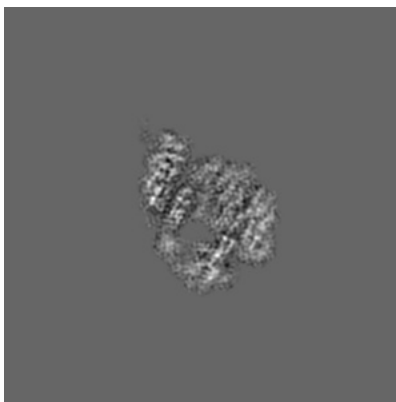
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

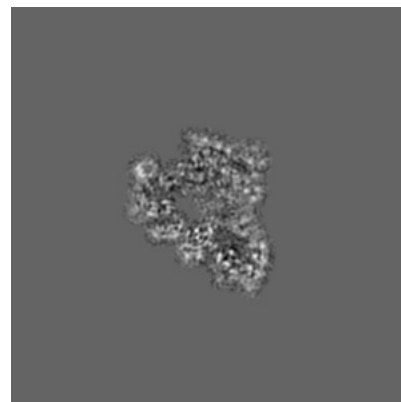
6.2.1 Primary map



X Index: 192

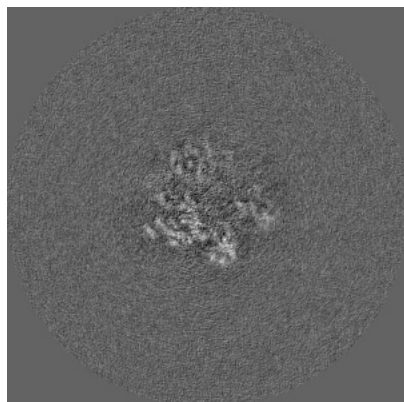


Y Index: 192

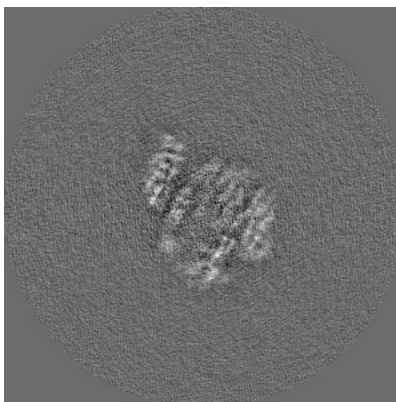


Z Index: 192

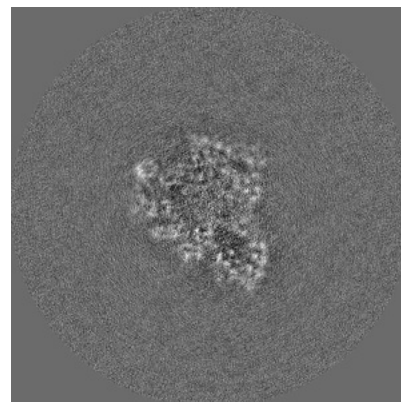
6.2.2 Raw map



X Index: 192



Y Index: 192

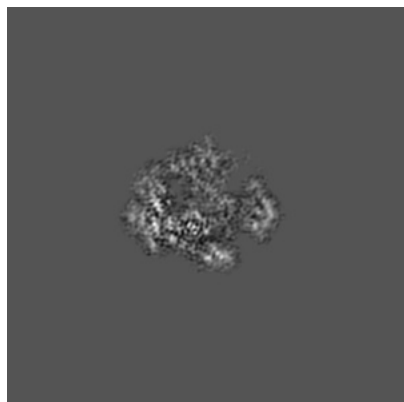


Z Index: 192

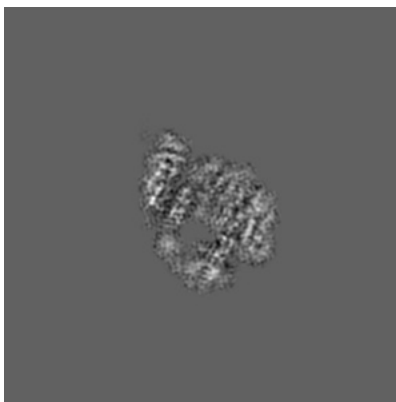
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

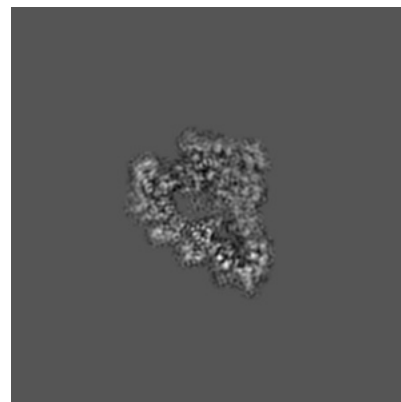
6.3.1 Primary map



X Index: 200

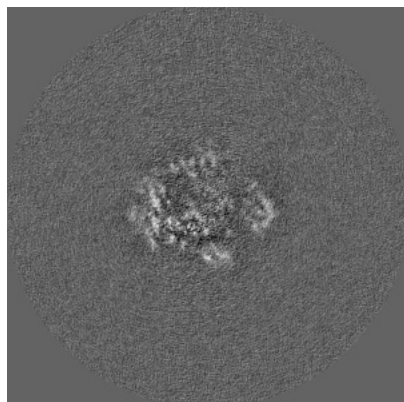


Y Index: 193

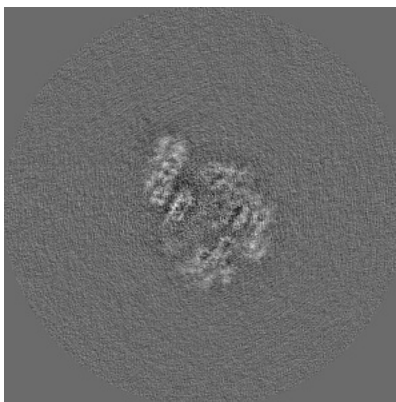


Z Index: 195

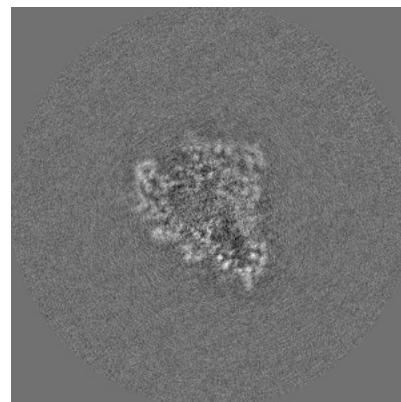
6.3.2 Raw map



X Index: 199



Y Index: 189

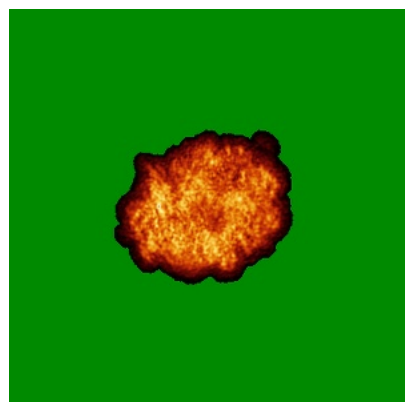


Z Index: 195

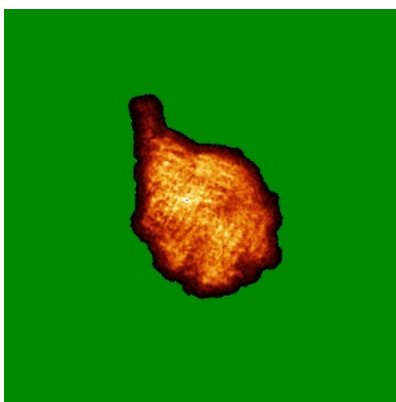
The images above show the largest variance slices of the map in three orthogonal directions.

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

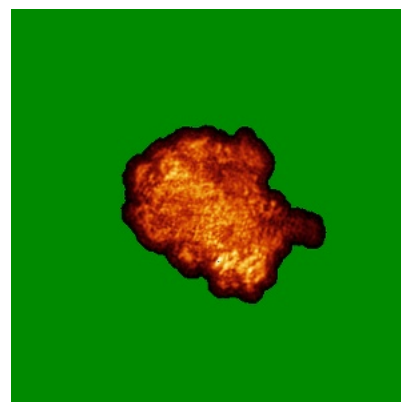
6.4.1 Primary map



X

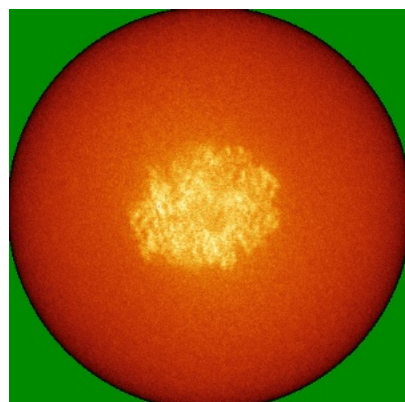


Y

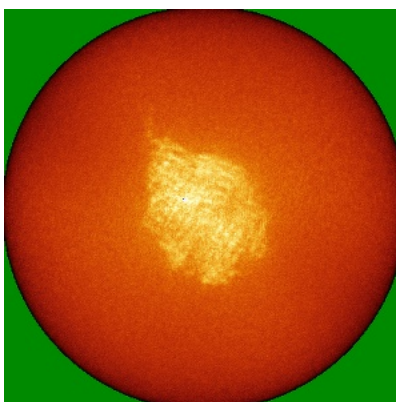


Z

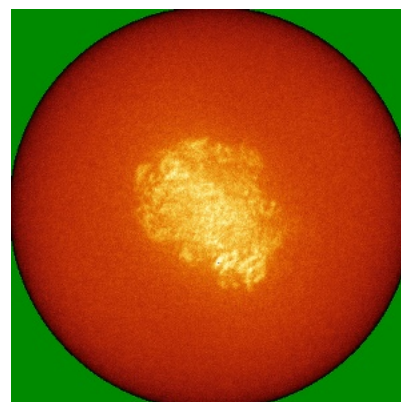
6.4.2 Raw map



X



Y

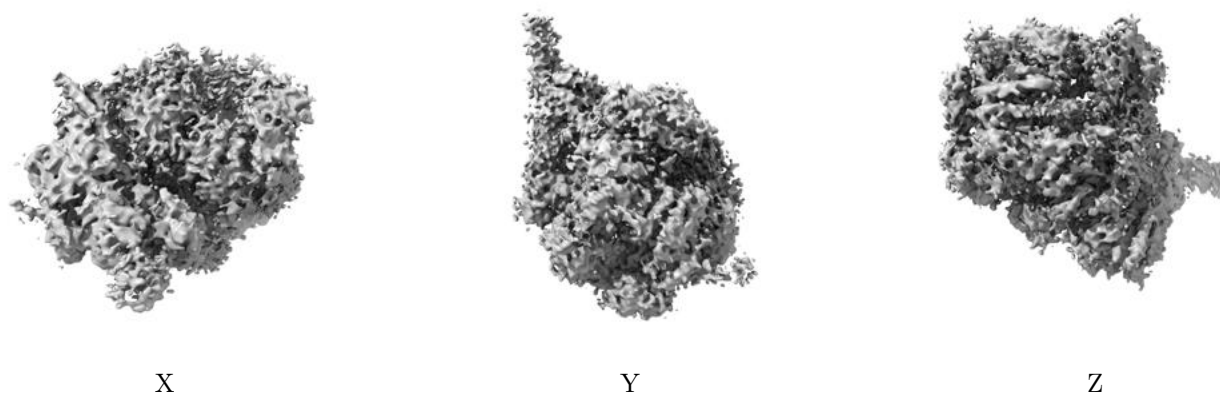


Z

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.

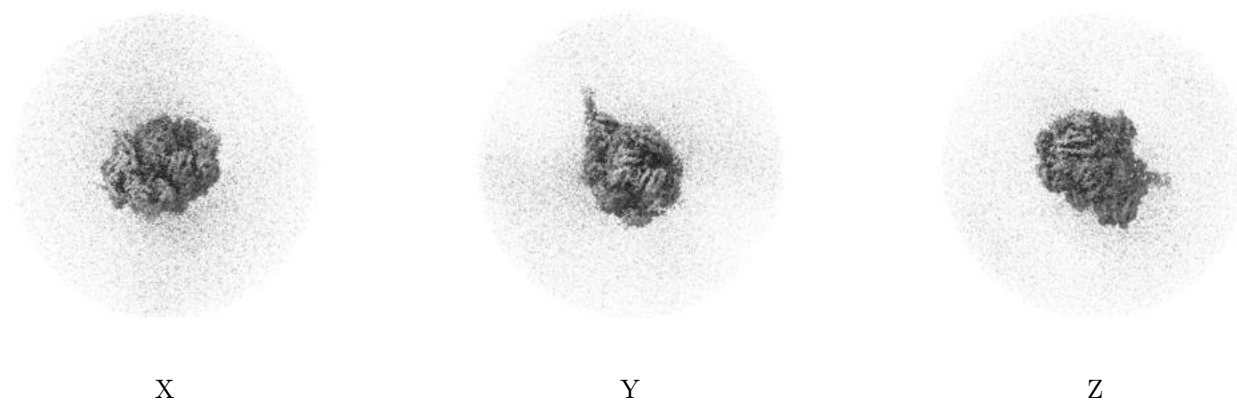
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0045. 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



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

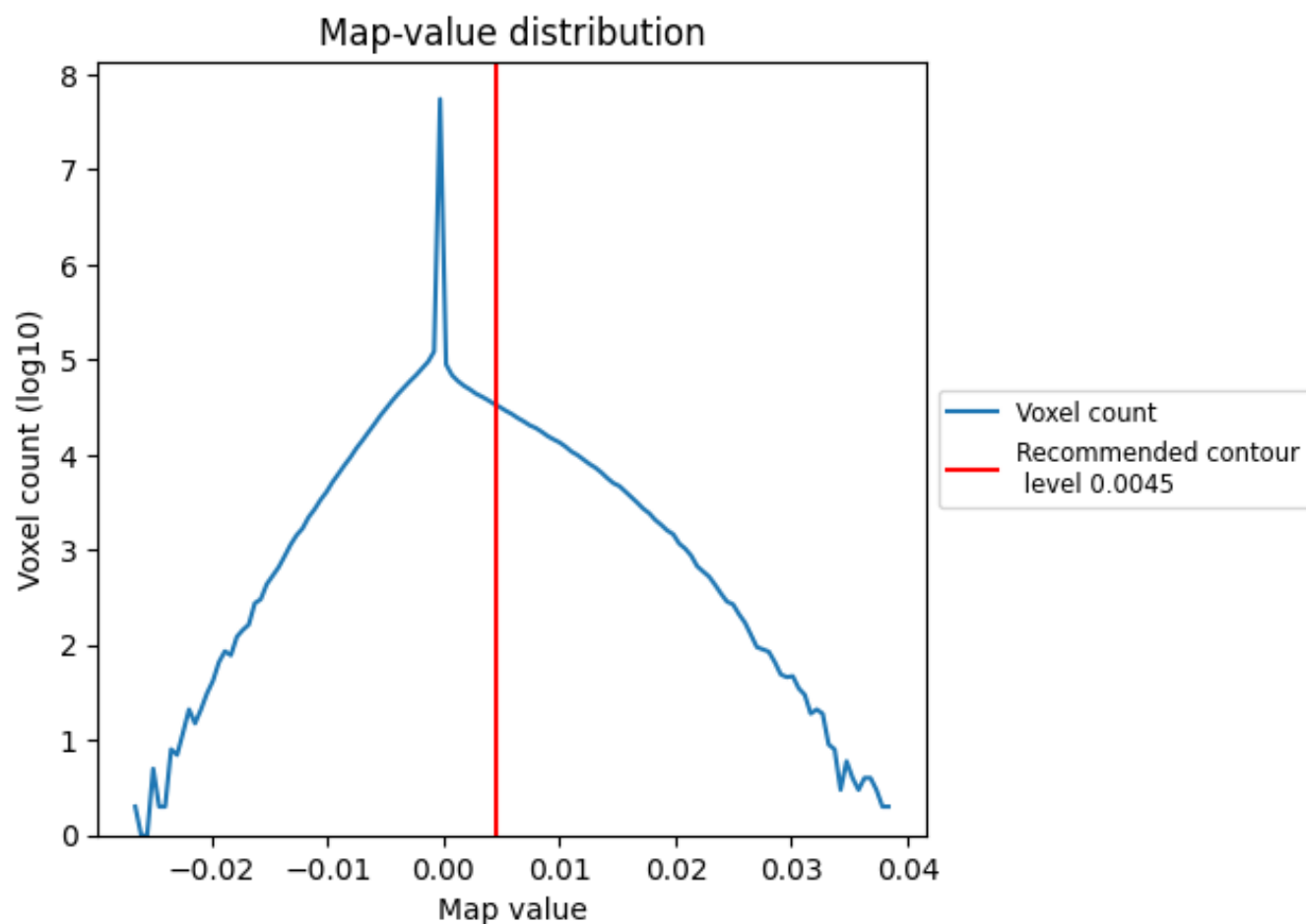
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

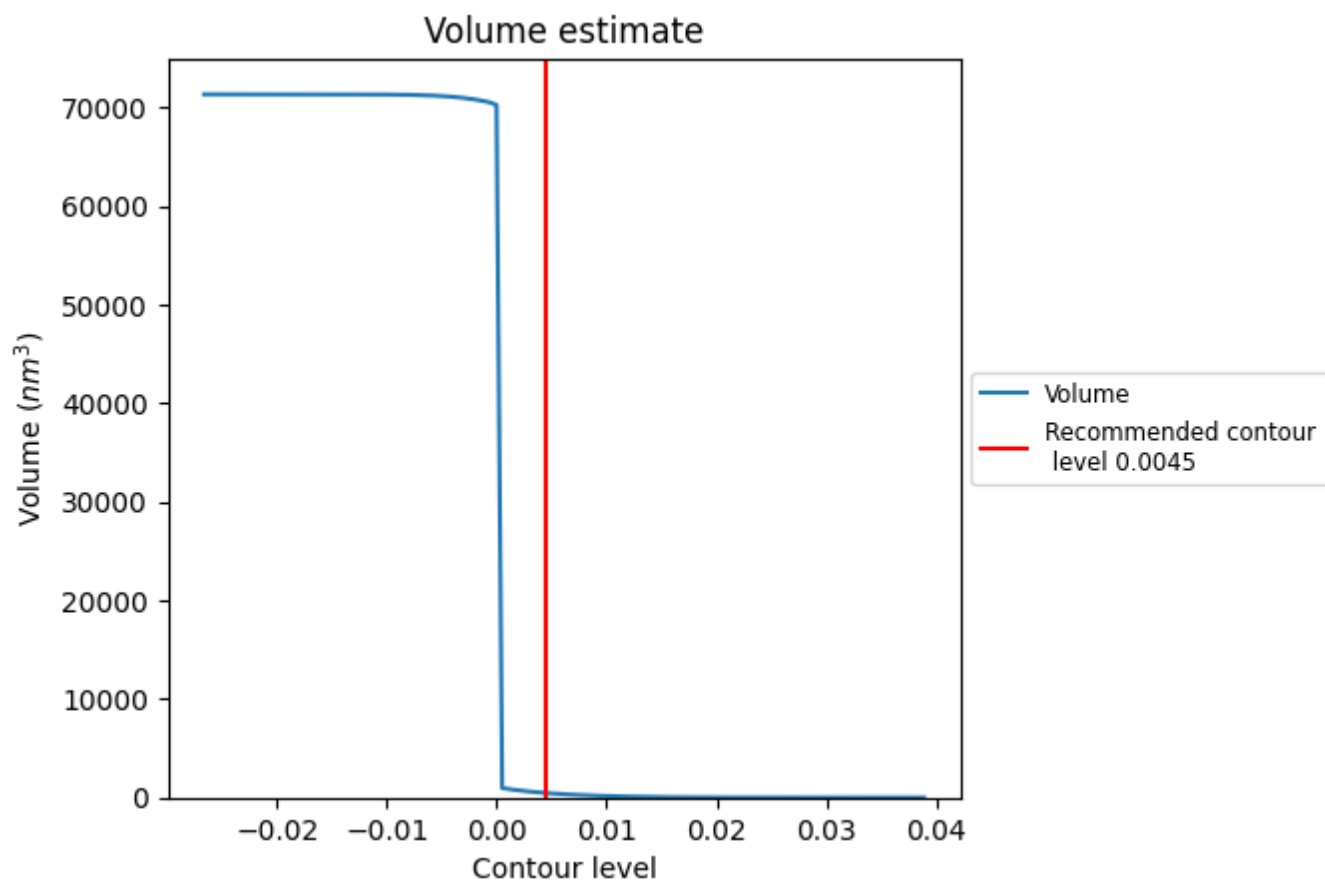
This section contains the results of statistical analysis of the map.

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.

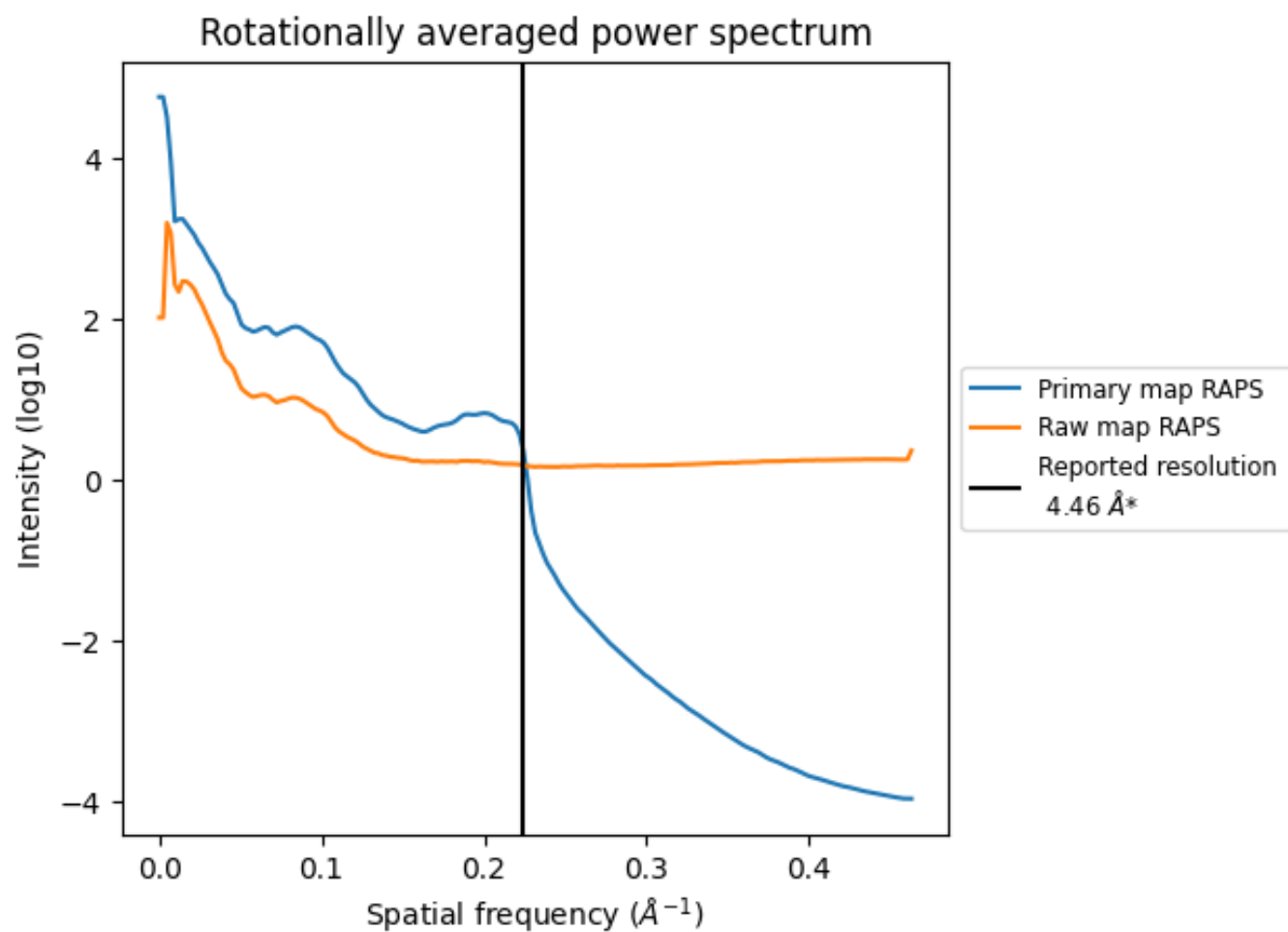
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 463 nm³; this corresponds to an approximate mass of 418 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 ⓘ

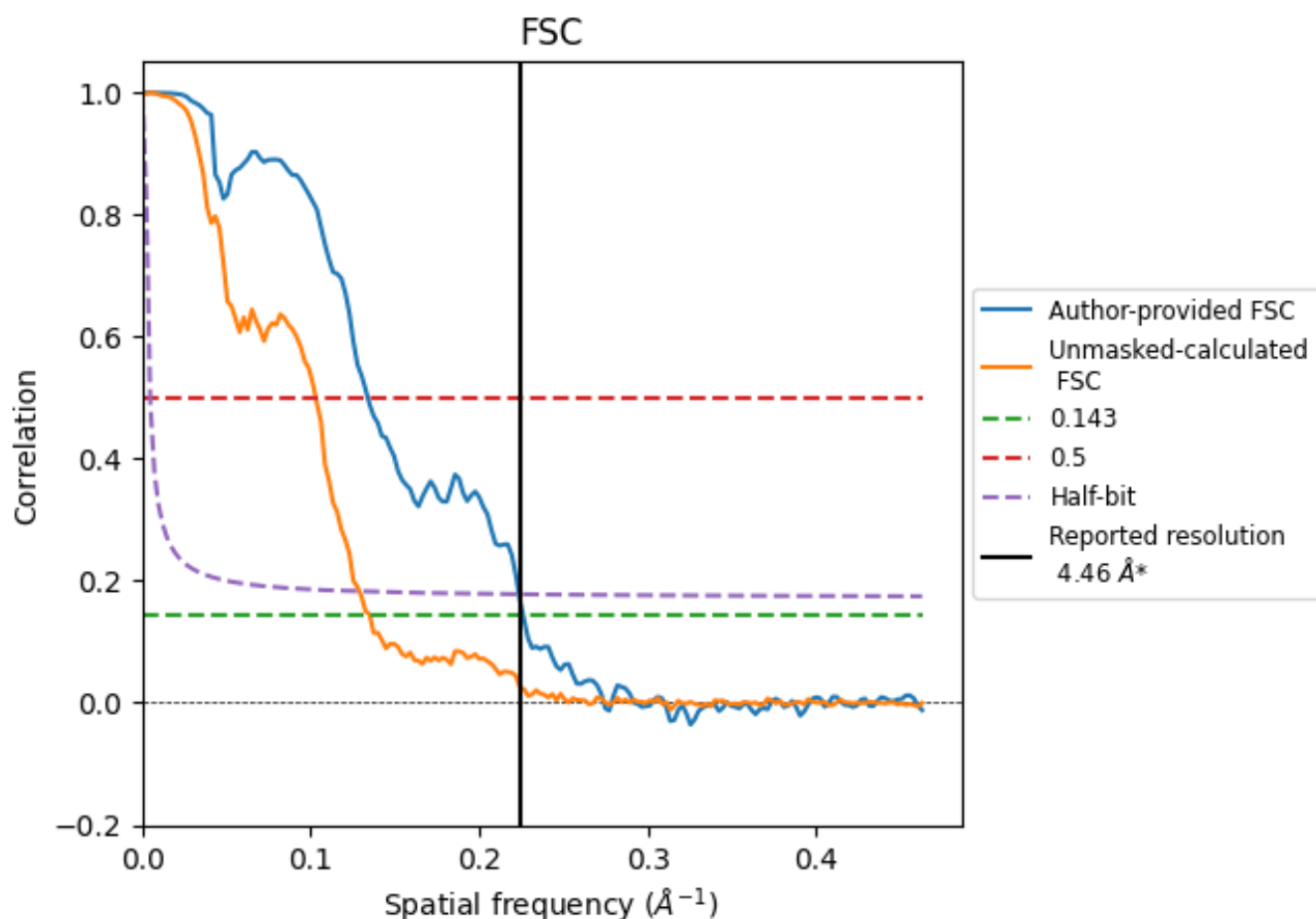


*Reported resolution corresponds to spatial frequency of 0.224 Å⁻¹

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 0.224 \AA^{-1}

8.2 Resolution estimates [i](#)

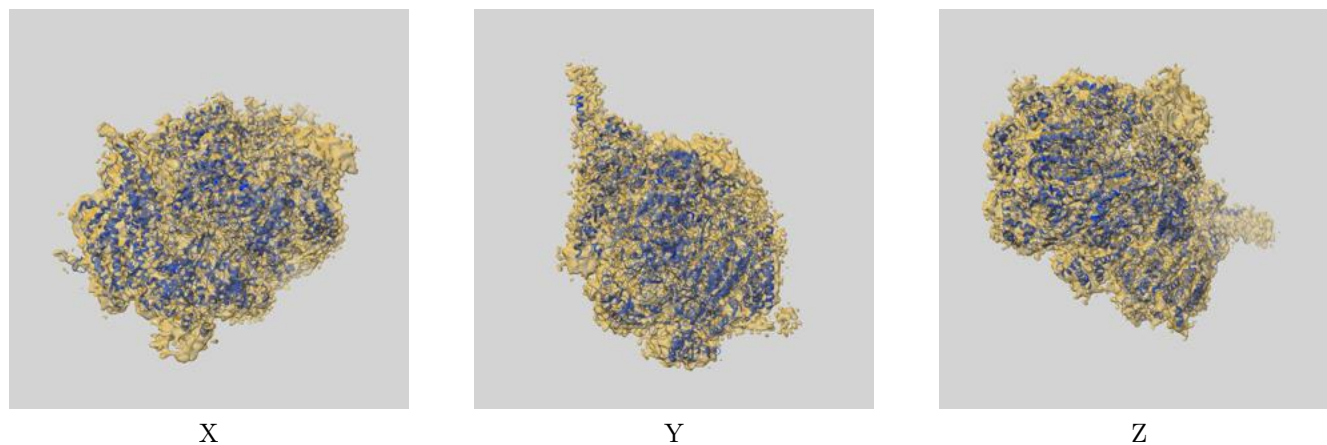
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.46	-	-
Author-provided FSC curve	4.42	7.46	4.47
Unmasked-calculated*	7.40	9.71	7.76

*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 7.40 differs from the reported value 4.46 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4788 and PDB model 6RAZ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



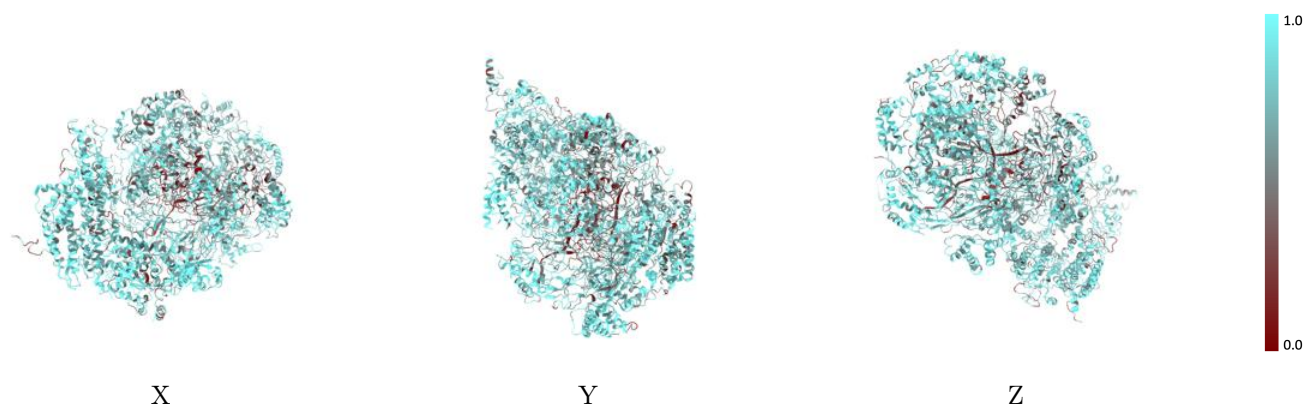
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



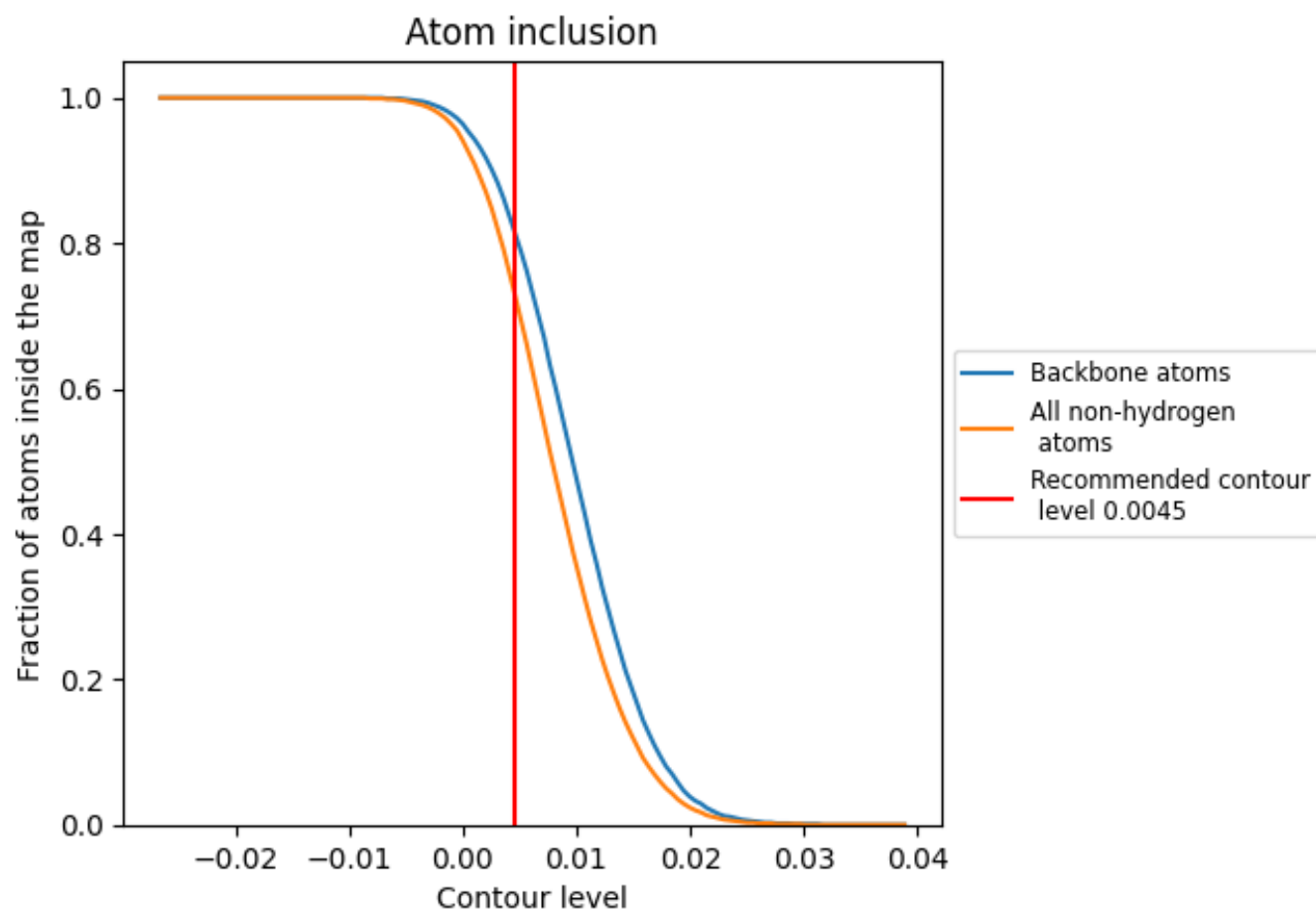
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0045).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7350	 0.2460
2	 0.7080	 0.2360
3	 0.7460	 0.2630
4	 0.7370	 0.2460
5	 0.6750	 0.2360
6	 0.6970	 0.2250
7	 0.7640	 0.2680
A	 0.8020	 0.2700
H	 0.7370	 0.1920
L	 0.8360	 0.2760
M	 0.7710	 0.2610
N	 0.7960	 0.2460
X	 0.2660	 0.0990
Y	 0.1950	 0.1090

