



wwPDB EM Validation Summary Report ⓘ

Jun 15, 2026 – 10:49 am BST

PDB ID : 9RHL / pdb_00009rhl
EMDB ID : EMD-53972
Title : Phospho-DH bound by Sld3-MBD on ARS1 DNA
Authors : Puehringer, T.; Couves, E.C.; Costa, A.
Deposited on : 2025-06-09
Resolution : 3.10 Å(reported)

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:

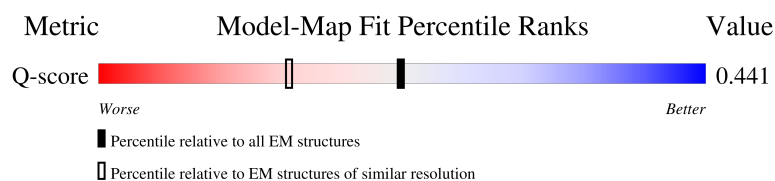
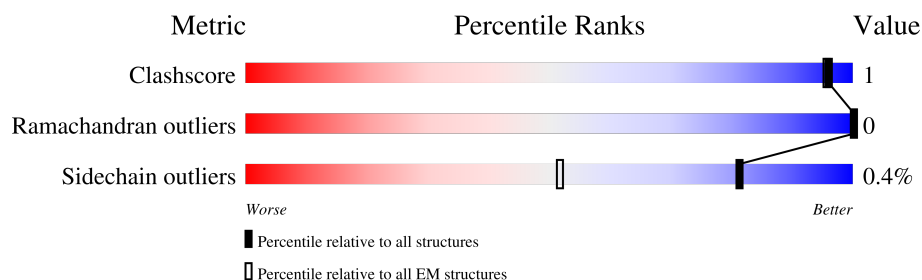
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 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	14724 (2.60 - 3.60)

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	<div> <div>23%</div> <div>70%</div> <div>28%</div> </div>
1	a	868	<div> <div>24%</div> <div>69%</div> <div>28%</div> </div>
2	3	1006	<div> <div>7%</div> <div>62%</div> <div>37%</div> </div>
2	b	1006	<div> <div>7%</div> <div>62%</div> <div>37%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	4	933	
3	c	933	
4	5	775	
4	d	775	
5	6	1017	
5	e	1017	
6	7	845	
6	f	845	
7	H	704	
7	I	704	
8	X	53	
9	Y	53	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 64409 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	623	Total	C	N	O	S	0	0
			4932	3109	877	927	19		
1	a	623	Total	C	N	O	S	0	0
			4932	3109	877	927	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	638	Total	C	N	O	S	0	0
			4994	3150	889	942	13		
2	b	638	Total	C	N	O	S	0	0
			4994	3150	889	942	13		

There are 70 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
3	-17	PHE	-	expression tag	UNP P24279
3	-16	LYS	-	expression tag	UNP P24279
3	-15	LYS	-	expression tag	UNP P24279
3	-14	ILE	-	expression tag	UNP P24279
3	-13	SER	-	expression tag	UNP P24279
3	-12	SER	-	expression tag	UNP P24279
3	-11	SER	-	expression tag	UNP P24279
3	-10	GLY	-	expression tag	UNP P24279
3	-9	ALA	-	expression tag	UNP P24279
3	-8	LEU	-	expression tag	UNP P24279
3	-7	GLU	-	expression tag	UNP P24279
3	-6	ASN	-	expression tag	UNP P24279
3	-5	LEU	-	expression tag	UNP P24279
3	-4	TYR	-	expression tag	UNP P24279
3	-3	PHE	-	expression tag	UNP P24279
3	-2	GLN	-	expression tag	UNP P24279
3	-1	GLY	-	expression tag	UNP P24279
3	0	GLU	-	expression tag	UNP P24279
b	-34	MET	-	initiating methionine	UNP P24279
b	-33	LYS	-	expression tag	UNP P24279
b	-32	ARG	-	expression tag	UNP P24279
b	-31	ARG	-	expression tag	UNP P24279
b	-30	TRP	-	expression tag	UNP P24279
b	-29	LYS	-	expression tag	UNP P24279
b	-28	LYS	-	expression tag	UNP P24279
b	-27	ASN	-	expression tag	UNP P24279
b	-26	PHE	-	expression tag	UNP P24279
b	-25	ILE	-	expression tag	UNP P24279
b	-24	ALA	-	expression tag	UNP P24279
b	-23	VAL	-	expression tag	UNP P24279
b	-22	SER	-	expression tag	UNP P24279
b	-21	ALA	-	expression tag	UNP P24279
b	-20	ALA	-	expression tag	UNP P24279
b	-19	ASN	-	expression tag	UNP P24279
b	-18	ARG	-	expression tag	UNP P24279
b	-17	PHE	-	expression tag	UNP P24279
b	-16	LYS	-	expression tag	UNP P24279
b	-15	LYS	-	expression tag	UNP P24279
b	-14	ILE	-	expression tag	UNP P24279
b	-13	SER	-	expression tag	UNP P24279
b	-12	SER	-	expression tag	UNP P24279
b	-11	SER	-	expression tag	UNP P24279

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	672	Total	C	N	O	S	0	0
			5356	3357	926	1043	30		
3	c	672	Total	C	N	O	S	0	0
			5356	3357	926	1043	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	651	Total	C	N	O	S	0	0
			5097	3195	872	1005	25		
4	d	651	Total	C	N	O	S	0	0
			5097	3195	872	1005	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	637	Total	C	N	O	S	0	0
			5041	3174	879	963	25		
5	e	637	Total	C	N	O	S	0	0
			5041	3174	879	963	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	700	Total	C	N	O	S	0	0
			5513	3468	953	1060	32		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	700	Total	C	N	O	S	0	0
			5513	3468	953	1060	32		

- Molecule 7 is a protein called DNA replication regulator SLD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	15	Total	C	N	O	S	0	0
			124	76	24	23	1		
7	I	15	Total	C	N	O	S	0	0
			124	76	24	23	1		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	669	GLU	-	expression tag	UNP P53135
H	670	ASN	-	expression tag	UNP P53135
H	671	LEU	-	expression tag	UNP P53135
H	672	TYR	-	expression tag	UNP P53135
H	673	PHE	-	expression tag	UNP P53135
H	674	GLN	-	expression tag	UNP P53135
H	675	GLY	-	expression tag	UNP P53135
H	676	TRP	-	expression tag	UNP P53135
H	677	SER	-	expression tag	UNP P53135
H	678	HIS	-	expression tag	UNP P53135
H	679	PRO	-	expression tag	UNP P53135
H	680	GLN	-	expression tag	UNP P53135
H	681	PHE	-	expression tag	UNP P53135
H	682	GLU	-	expression tag	UNP P53135
H	683	LYS	-	expression tag	UNP P53135
H	684	GLY	-	expression tag	UNP P53135
H	685	GLY	-	expression tag	UNP P53135
H	686	GLY	-	expression tag	UNP P53135
H	687	SER	-	expression tag	UNP P53135
H	688	GLY	-	expression tag	UNP P53135
H	689	GLY	-	expression tag	UNP P53135
H	690	GLY	-	expression tag	UNP P53135
H	691	SER	-	expression tag	UNP P53135
H	692	GLY	-	expression tag	UNP P53135
H	693	GLY	-	expression tag	UNP P53135
H	694	SER	-	expression tag	UNP P53135
H	695	SER	-	expression tag	UNP P53135
H	696	ALA	-	expression tag	UNP P53135

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	697	TRP	-	expression tag	UNP P53135
H	698	SER	-	expression tag	UNP P53135
H	699	HIS	-	expression tag	UNP P53135
H	700	PRO	-	expression tag	UNP P53135
H	701	GLN	-	expression tag	UNP P53135
H	702	PHE	-	expression tag	UNP P53135
H	703	GLU	-	expression tag	UNP P53135
H	704	LYS	-	expression tag	UNP P53135
I	669	GLU	-	expression tag	UNP P53135
I	670	ASN	-	expression tag	UNP P53135
I	671	LEU	-	expression tag	UNP P53135
I	672	TYR	-	expression tag	UNP P53135
I	673	PHE	-	expression tag	UNP P53135
I	674	GLN	-	expression tag	UNP P53135
I	675	GLY	-	expression tag	UNP P53135
I	676	TRP	-	expression tag	UNP P53135
I	677	SER	-	expression tag	UNP P53135
I	678	HIS	-	expression tag	UNP P53135
I	679	PRO	-	expression tag	UNP P53135
I	680	GLN	-	expression tag	UNP P53135
I	681	PHE	-	expression tag	UNP P53135
I	682	GLU	-	expression tag	UNP P53135
I	683	LYS	-	expression tag	UNP P53135
I	684	GLY	-	expression tag	UNP P53135
I	685	GLY	-	expression tag	UNP P53135
I	686	GLY	-	expression tag	UNP P53135
I	687	SER	-	expression tag	UNP P53135
I	688	GLY	-	expression tag	UNP P53135
I	689	GLY	-	expression tag	UNP P53135
I	690	GLY	-	expression tag	UNP P53135
I	691	SER	-	expression tag	UNP P53135
I	692	GLY	-	expression tag	UNP P53135
I	693	GLY	-	expression tag	UNP P53135
I	694	SER	-	expression tag	UNP P53135
I	695	SER	-	expression tag	UNP P53135
I	696	ALA	-	expression tag	UNP P53135
I	697	TRP	-	expression tag	UNP P53135
I	698	SER	-	expression tag	UNP P53135
I	699	HIS	-	expression tag	UNP P53135
I	700	PRO	-	expression tag	UNP P53135
I	701	GLN	-	expression tag	UNP P53135
I	702	PHE	-	expression tag	UNP P53135

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	703	GLU	-	expression tag	UNP P53135
I	704	LYS	-	expression tag	UNP P53135

- Molecule 8 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	53	Total	C	N	O	P	0	0
			1086	515	199	319	53		

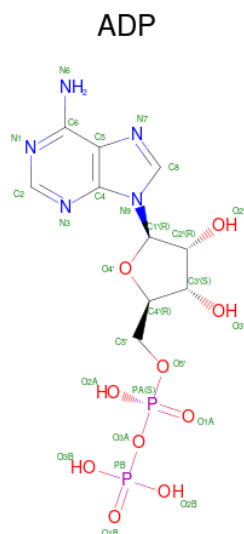
- Molecule 9 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Y	53	Total	C	N	O	P	0	0
			1087	515	202	317	53		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	2	1	Total	Zn	0
			1	1	
10	4	1	Total	Zn	0
			1	1	
10	5	1	Total	Zn	0
			1	1	
10	6	1	Total	Zn	0
			1	1	
10	7	1	Total	Zn	0
			1	1	
10	a	1	Total	Zn	0
			1	1	
10	c	1	Total	Zn	0
			1	1	
10	d	1	Total	Zn	0
			1	1	
10	e	1	Total	Zn	0
			1	1	
10	f	1	Total	Zn	0
			1	1	

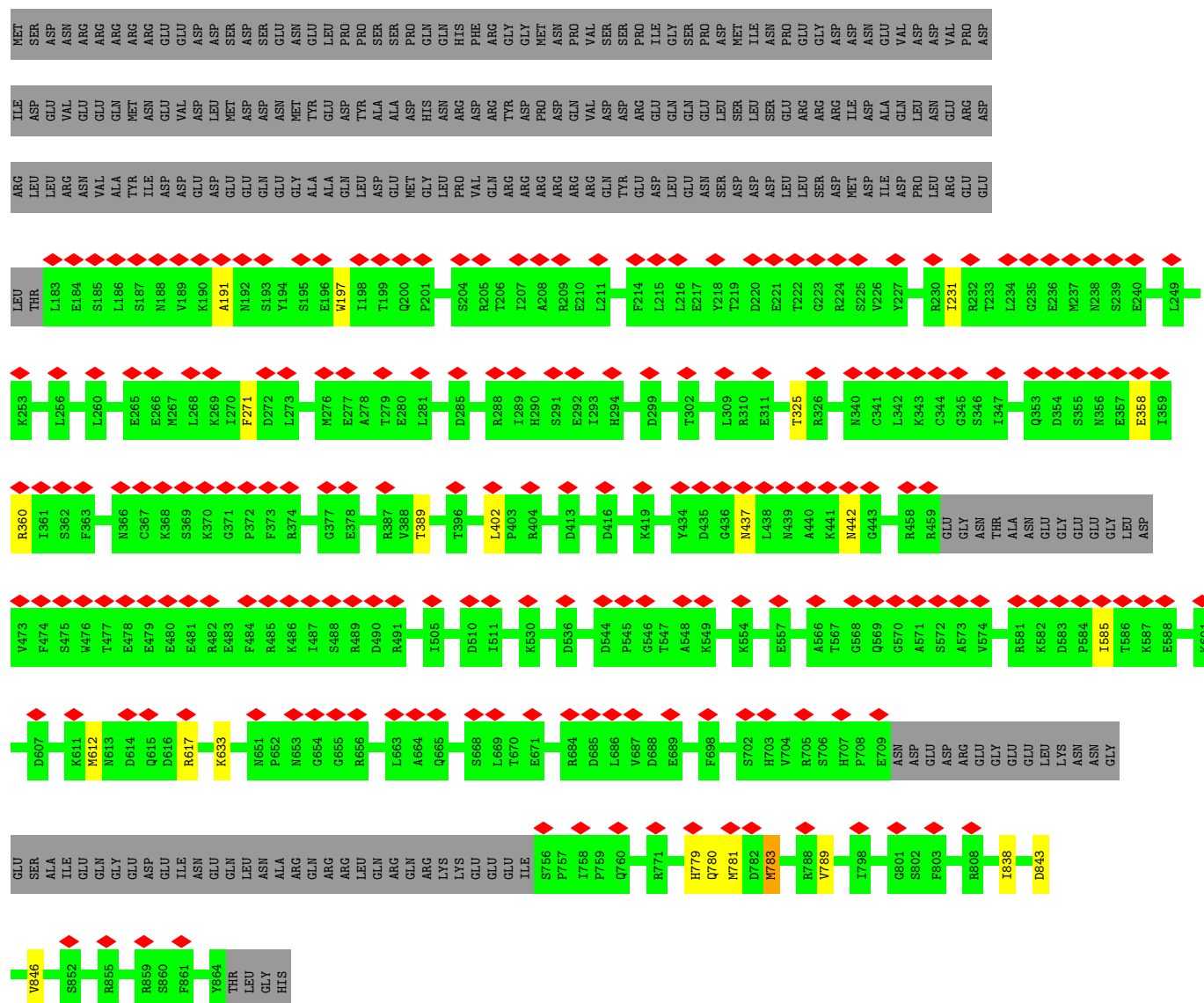
- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
11	3	1	Total 27	C 10	N 5	O 10	P 2	0
11	5	1	Total 27	C 10	N 5	O 10	P 2	0
11	b	1	Total 27	C 10	N 5	O 10	P 2	0
11	d	1	Total 27	C 10	N 5	O 10	P 2	0

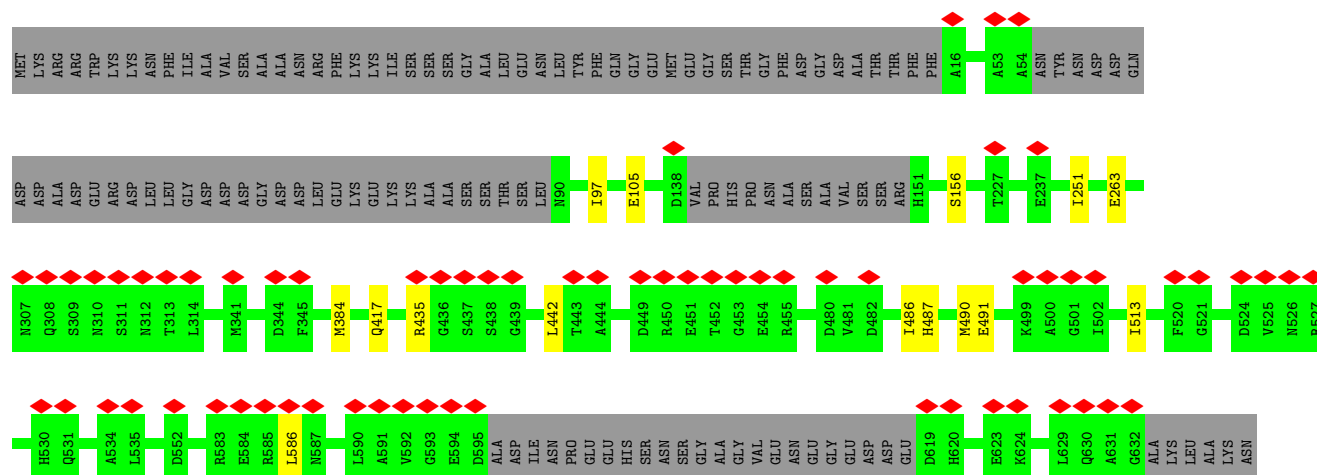
- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
12	3	1	Total Mg 1 1	0
12	5	1	Total Mg 1 1	0
12	b	1	Total Mg 1 1	0
12	d	1	Total Mg 1 1	0

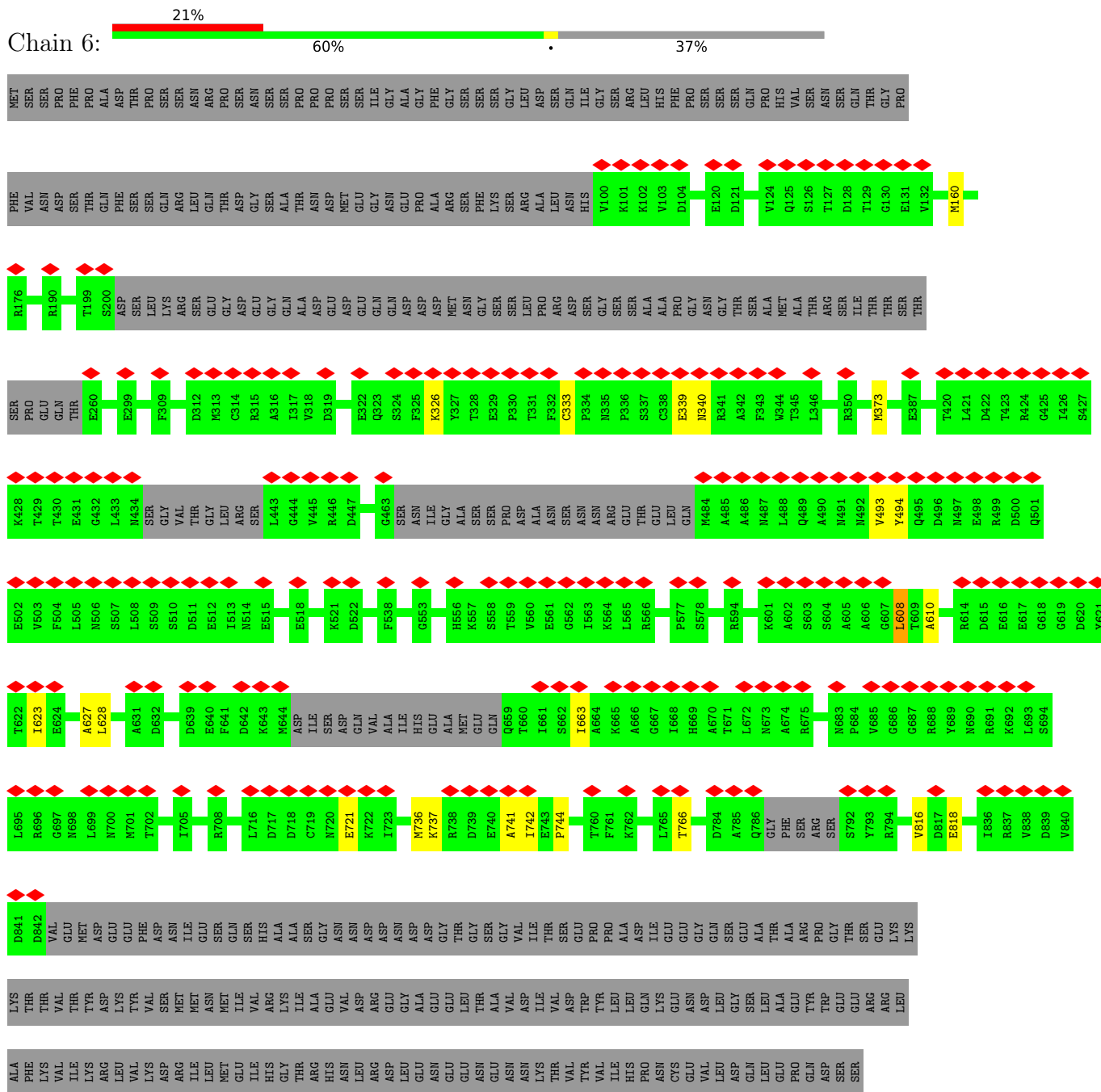


• Molecule 2: DNA replication licensing factor MCM3

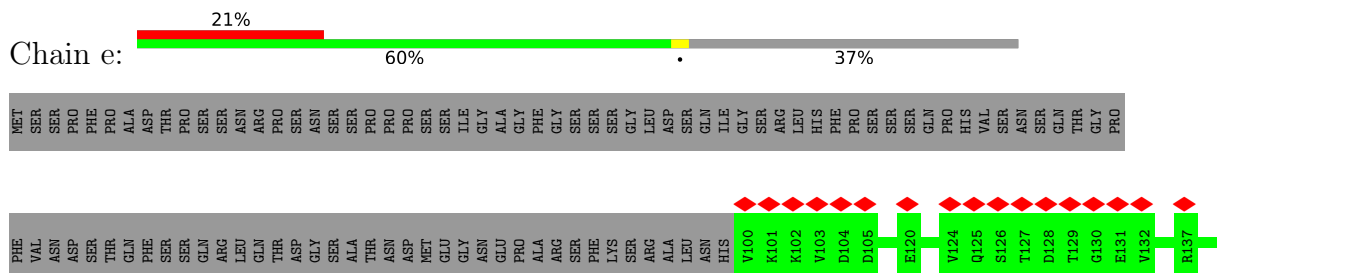
Chain 3: 7% 62% 37%

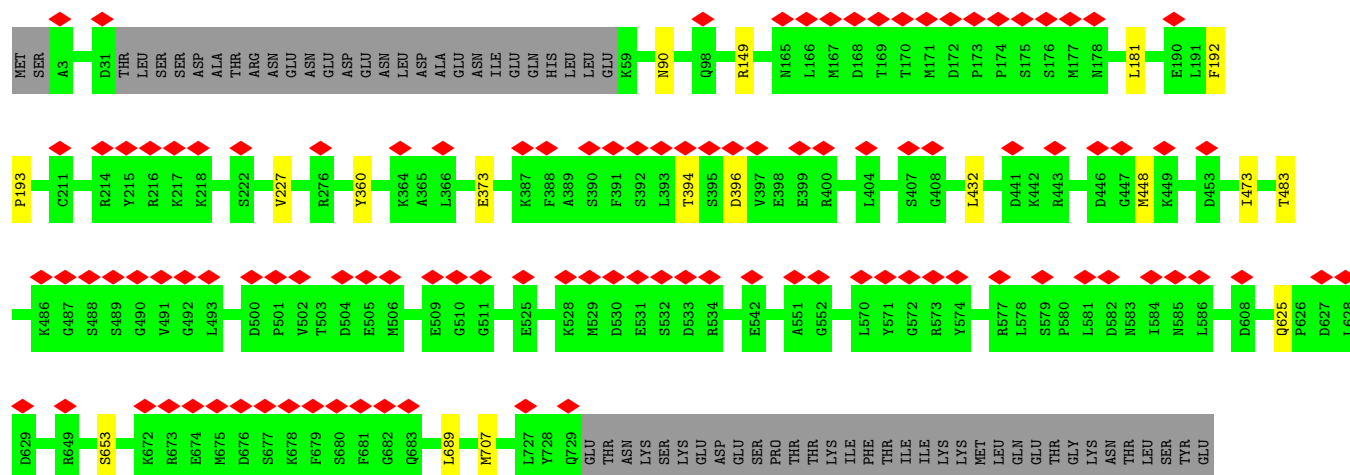
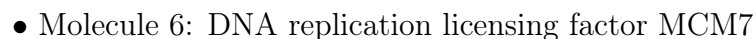


Chain 6:

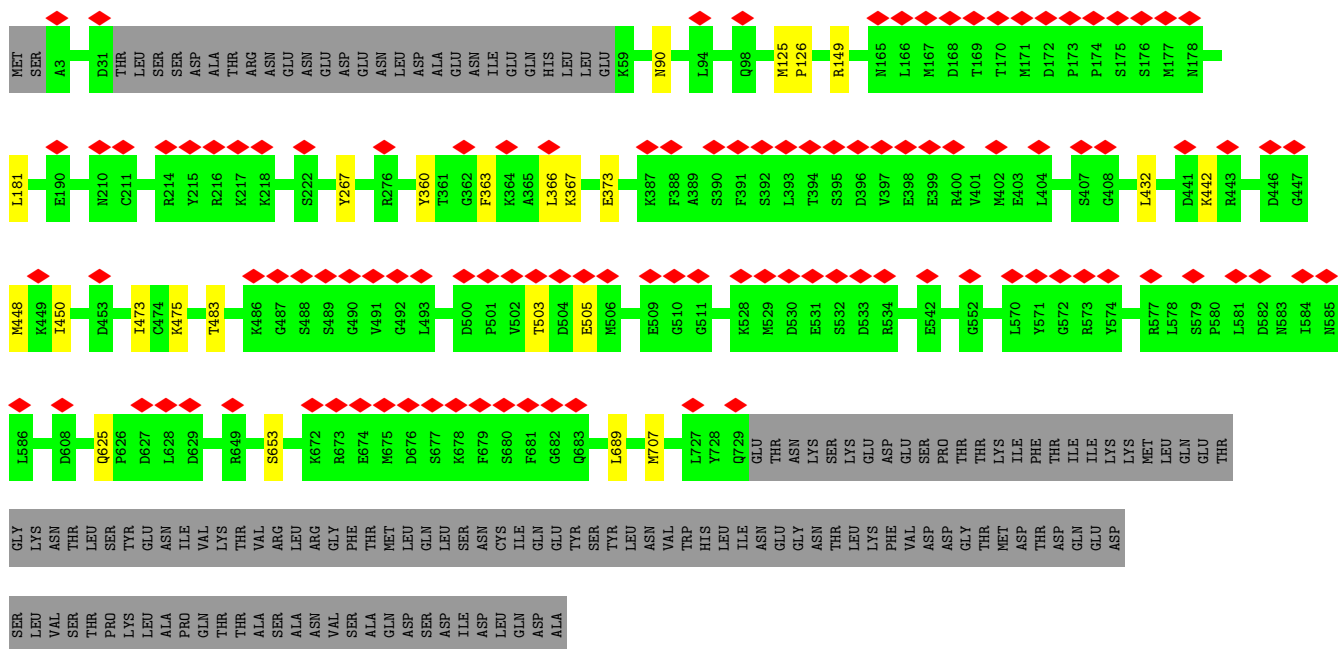
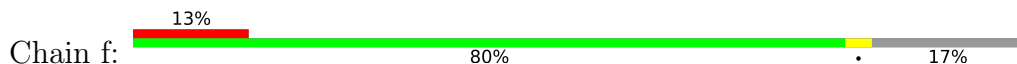


Chain e:

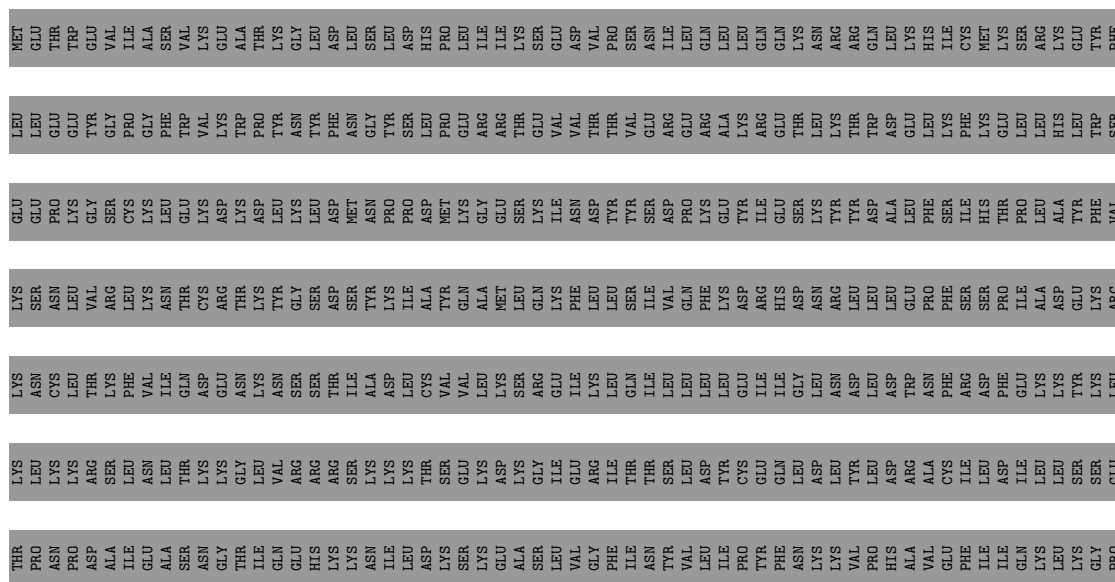


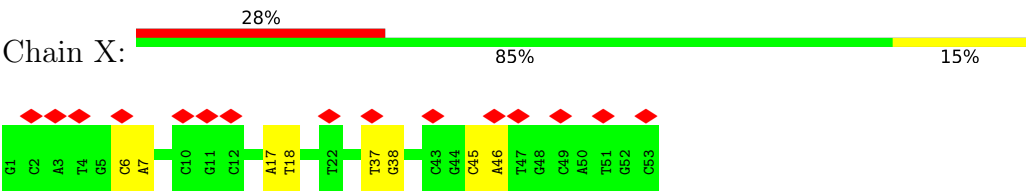


- Molecule 6: DNA replication licensing factor MCM7

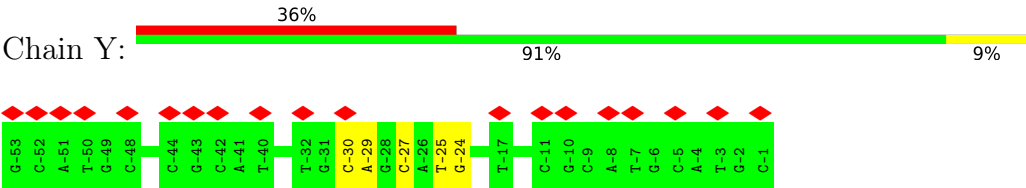


- Molecule 7: DNA replication regulator SLD3





• Molecule 9: DNA (53-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	359025	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.8	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.737	Depositor
Minimum map value	-0.273	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.17	Depositor
Map size (\AA)	483.84003, 483.84003, 483.84003	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	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: ZN, MG, 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	0.30	0/5019	0.66	0/6781
1	a	0.29	0/5019	0.65	0/6781
2	3	0.27	0/5081	0.58	0/6889
2	b	0.27	0/5081	0.59	0/6889
3	4	0.27	0/5434	0.62	2/7345 (0.0%)
3	c	0.28	0/5434	0.63	2/7345 (0.0%)
4	5	0.29	0/5170	0.64	1/6992 (0.0%)
4	d	0.29	0/5170	0.63	0/6992
5	6	0.28	0/5119	0.62	2/6906 (0.0%)
5	e	0.29	0/5119	0.63	2/6906 (0.0%)
6	7	0.27	0/5599	0.61	1/7569 (0.0%)
6	f	0.27	0/5599	0.60	1/7569 (0.0%)
7	H	0.27	0/125	0.72	0/165
7	I	0.26	0/125	0.71	0/165
8	X	0.21	0/1217	0.46	0/1876
9	Y	0.23	0/1219	0.48	0/1879
All	All	0.28	0/65530	0.62	11/89049 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	339	GLU	CA-CB-CG	7.32	128.74	114.10
5	6	339	GLU	CA-CB-CG	6.61	127.32	114.10
5	6	339	GLU	CB-CA-C	6.41	121.56	112.07
5	e	339	GLU	CB-CA-C	6.02	120.98	112.07
3	4	312	LYS	CB-CG-CD	5.23	123.33	111.30

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	4932	0	4985	10	0
1	a	4932	0	4985	11	0
2	3	4994	0	5059	8	0
2	b	4994	0	5059	6	0
3	4	5356	0	5410	11	0
3	c	5356	0	5410	8	0
4	5	5097	0	5143	15	0
4	d	5097	0	5143	10	0
5	6	5041	0	5065	15	0
5	e	5041	0	5065	13	0
6	7	5513	0	5575	7	0
6	f	5513	0	5575	12	0
7	H	124	0	122	0	0
7	I	124	0	122	0	0
8	X	1086	0	596	4	0
9	Y	1087	0	595	3	0
10	2	1	0	0	0	0
10	4	1	0	0	0	0
10	5	1	0	0	0	0
10	6	1	0	0	0	0
10	7	1	0	0	0	0
10	a	1	0	0	0	0
10	c	1	0	0	0	0
10	d	1	0	0	0	0
10	e	1	0	0	0	0
10	f	1	0	0	0	0
11	3	27	0	12	0	0
11	5	27	0	12	1	0
11	b	27	0	12	0	0
11	d	27	0	12	1	0
12	3	1	0	0	0	0
12	5	1	0	0	0	0
12	b	1	0	0	0	0
12	d	1	0	0	0	0
All	All	64409	0	63957	118	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 1.

The worst 5 of 118 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)
3:4:616:LEU:HB3	5:6:373:MET:HE3	1.77	0.64
4:5:209:ARG:HH22	9:Y:-27:DC:H4'	1.62	0.63
4:d:194:ILE:HG12	4:d:205:VAL:HG21	1.84	0.59
5:e:608:LEU:HD13	5:e:627:ALA:HB3	1.85	0.59
4:5:194:ILE:HG12	4:5:205:VAL:HG21	1.84	0.58

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	617/868 (71%)	610 (99%)	7 (1%)	0	100	100
1	a	617/868 (71%)	610 (99%)	7 (1%)	0	100	100
2	3	628/1006 (62%)	621 (99%)	7 (1%)	0	100	100
2	b	628/1006 (62%)	619 (99%)	9 (1%)	0	100	100
3	4	668/933 (72%)	657 (98%)	11 (2%)	0	100	100
3	c	668/933 (72%)	658 (98%)	10 (2%)	0	100	100
4	5	643/775 (83%)	632 (98%)	11 (2%)	0	100	100
4	d	643/775 (83%)	632 (98%)	11 (2%)	0	100	100
5	6	625/1017 (62%)	614 (98%)	11 (2%)	0	100	100
5	e	625/1017 (62%)	613 (98%)	12 (2%)	0	100	100
6	7	696/845 (82%)	688 (99%)	8 (1%)	0	100	100
6	f	696/845 (82%)	688 (99%)	8 (1%)	0	100	100
7	H	13/704 (2%)	13 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	I	13/704 (2%)	13 (100%)	0	0	100	100
All	All	7780/12296 (63%)	7668 (99%)	112 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	547/770 (71%)	545 (100%)	2 (0%)	84	86
1	a	547/770 (71%)	542 (99%)	5 (1%)	70	80
2	3	550/864 (64%)	548 (100%)	2 (0%)	84	86
2	b	550/864 (64%)	548 (100%)	2 (0%)	84	86
3	4	611/848 (72%)	610 (100%)	1 (0%)	87	89
3	c	611/848 (72%)	611 (100%)	0	100	100
4	5	583/688 (85%)	582 (100%)	1 (0%)	87	89
4	d	583/688 (85%)	580 (100%)	3 (0%)	81	85
5	6	557/886 (63%)	555 (100%)	2 (0%)	84	86
5	e	557/886 (63%)	556 (100%)	1 (0%)	87	89
6	7	619/753 (82%)	614 (99%)	5 (1%)	73	81
6	f	619/753 (82%)	615 (99%)	4 (1%)	78	83
7	H	15/654 (2%)	15 (100%)	0	100	100
7	I	15/654 (2%)	15 (100%)	0	100	100
All	All	6964/10926 (64%)	6936 (100%)	28 (0%)	81	86

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	271	PHE
6	f	483	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	783	MET
6	f	90	ASN
1	a	585	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	424	GLN
6	f	554	ASN
4	d	585	ASN
5	e	799	GLN
5	6	157	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 18 ligands modelled in this entry, 14 are monoatomic - leaving 4 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	$\# Z > 2$
11	ADP	3	1001	12	27,29,29	1.38	4 (14%)	42,45,45	1.98	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	ADP	5	801	12	27,29,29	1.41	4 (14%)	42,45,45	2.01	10 (23%)
11	ADP	d	801	12	27,29,29	1.41	4 (14%)	42,45,45	2.01	10 (23%)
11	ADP	b	1001	12	27,29,29	1.38	4 (14%)	42,45,45	1.98	10 (23%)

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
11	ADP	3	1001	12	-	6/16/32/32	0/3/3/3
11	ADP	5	801	12	-	6/16/32/32	0/3/3/3
11	ADP	d	801	12	-	6/16/32/32	0/3/3/3
11	ADP	b	1001	12	-	6/16/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	5	801	ADP	C5-C4	4.75	1.47	1.39
11	d	801	ADP	C5-C4	4.75	1.47	1.39
11	3	1001	ADP	C5-C4	4.68	1.47	1.39
11	b	1001	ADP	C5-C4	4.68	1.47	1.39
11	d	801	ADP	C5-C6	2.79	1.48	1.41

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	5	801	ADP	C5-C4-N3	-6.57	118.17	126.75
11	d	801	ADP	C5-C4-N3	-6.57	118.18	126.75
11	3	1001	ADP	C5-C4-N3	-6.18	118.69	126.75
11	b	1001	ADP	C5-C4-N3	-6.17	118.70	126.75
11	d	801	ADP	N3-C4-N9	5.12	135.52	127.08

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	3	1001	ADP	PA-O3A-PB-O2B
11	3	1001	ADP	C5'-O5'-PA-O1A
11	3	1001	ADP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

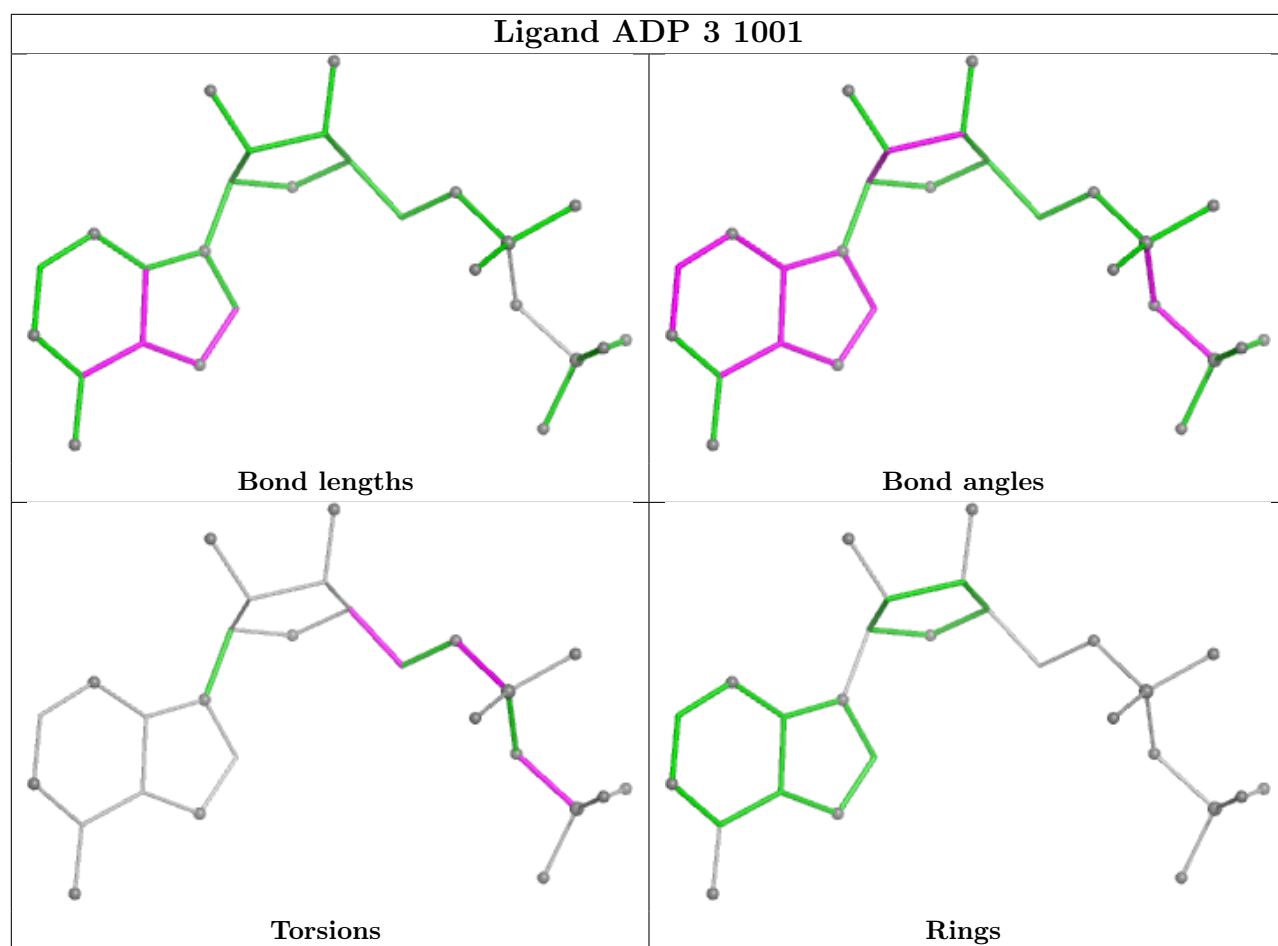
Mol	Chain	Res	Type	Atoms
11	5	801	ADP	PA-O3A-PB-O2B
11	5	801	ADP	C5'-O5'-PA-O3A

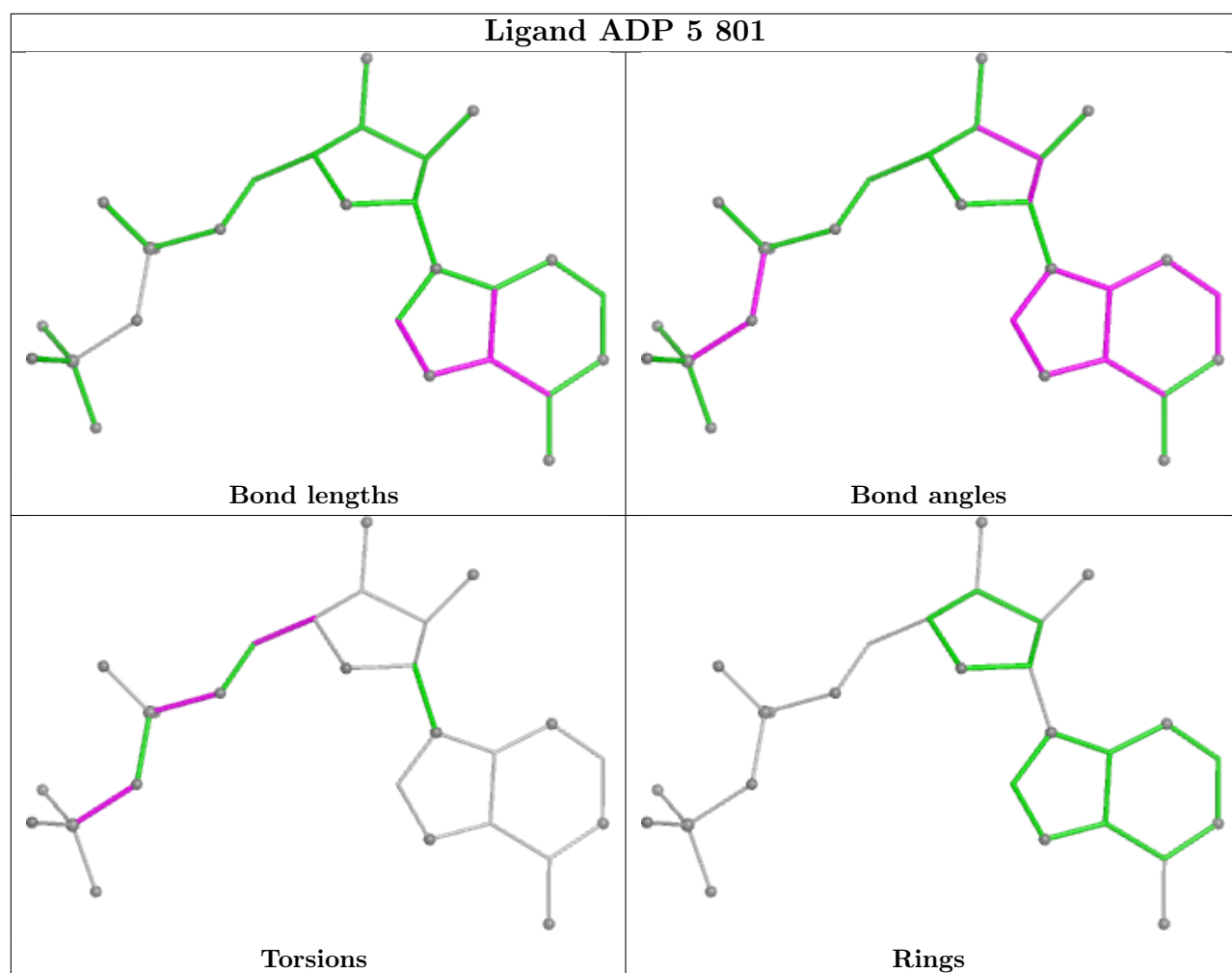
There are no ring outliers.

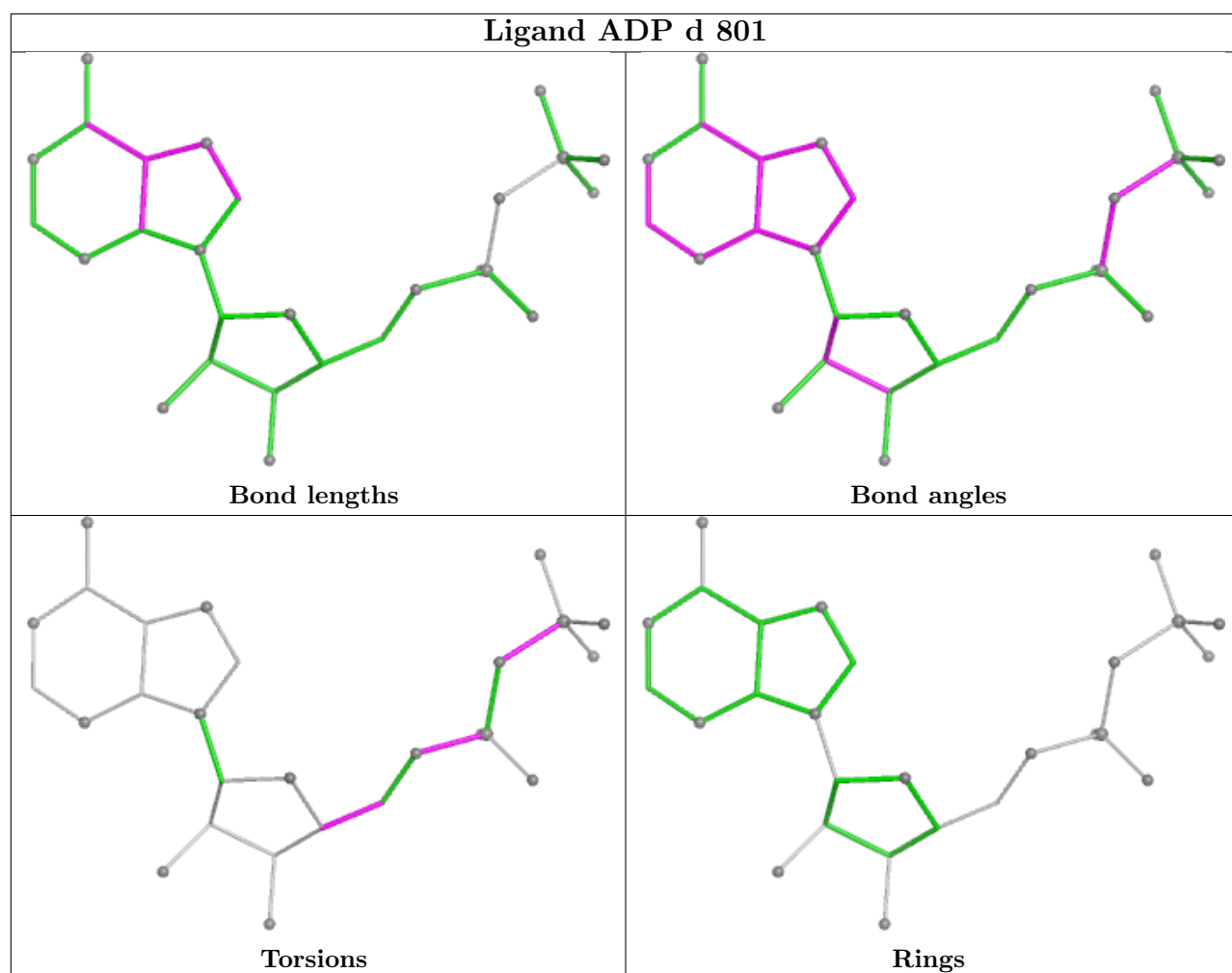
2 monomers are involved in 2 short contacts:

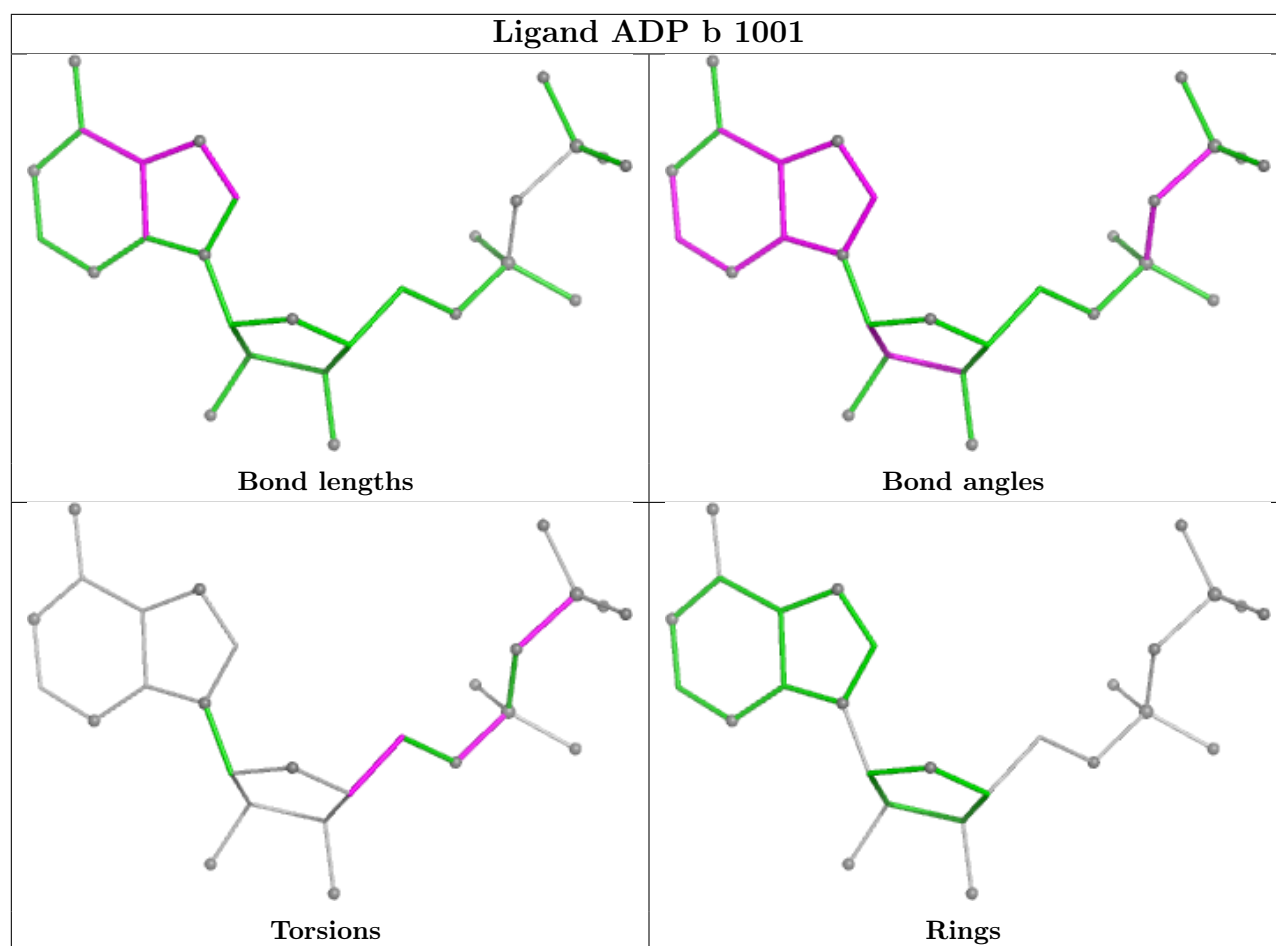
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	5	801	ADP	1	0
11	d	801	ADP	1	0

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.

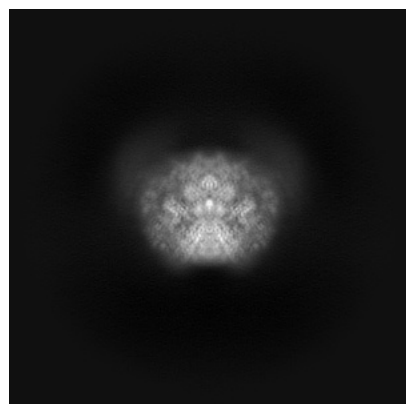
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53972. These allow visual inspection of the internal detail of the map and identification of artifacts.

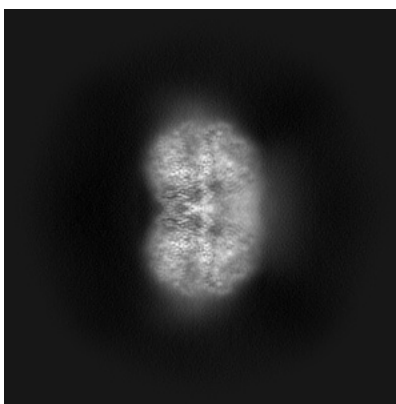
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

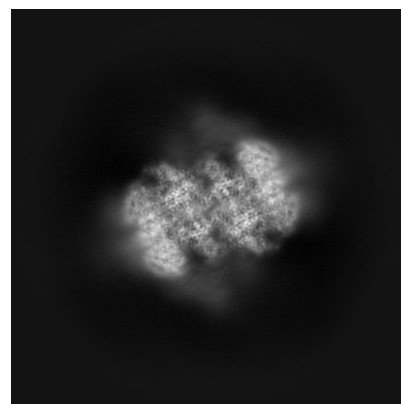
6.1.1 Primary map



X

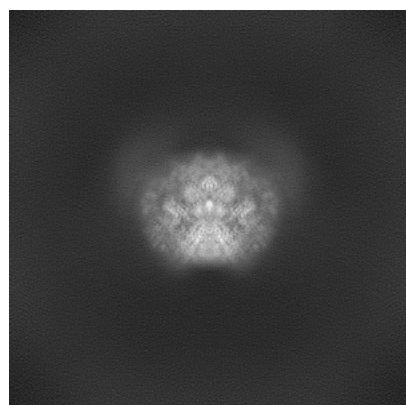


Y

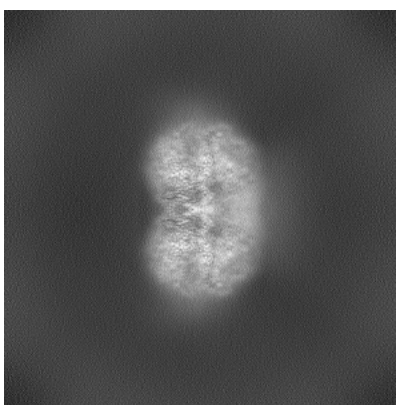


Z

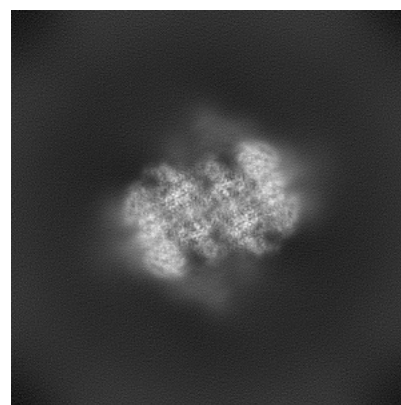
6.1.2 Raw map



X



Y

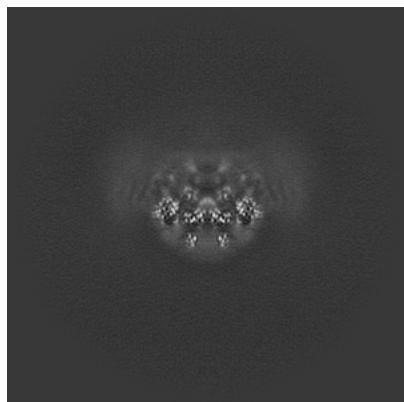


Z

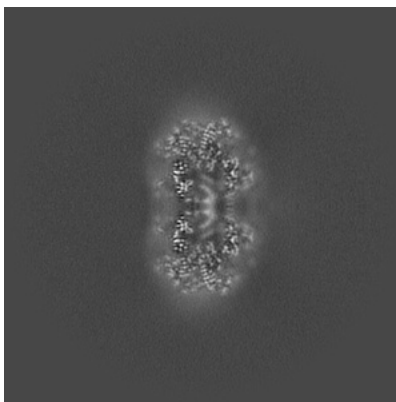
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

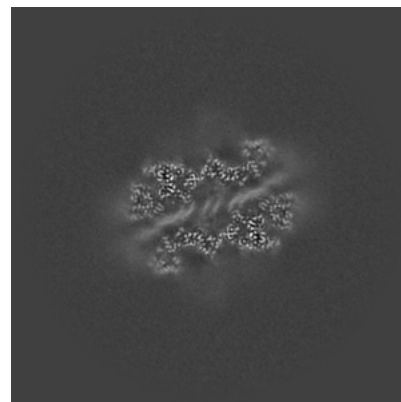
6.2.1 Primary map



X Index: 224

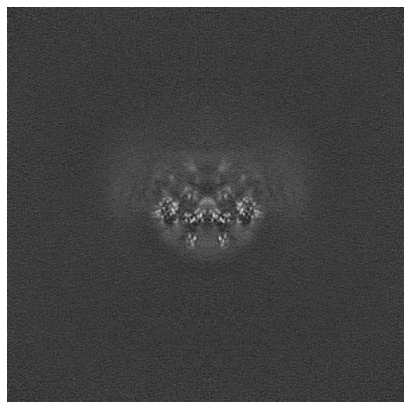


Y Index: 224

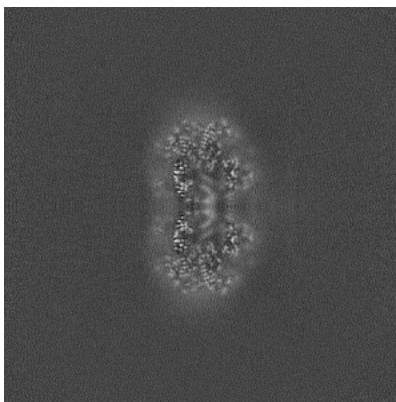


Z Index: 224

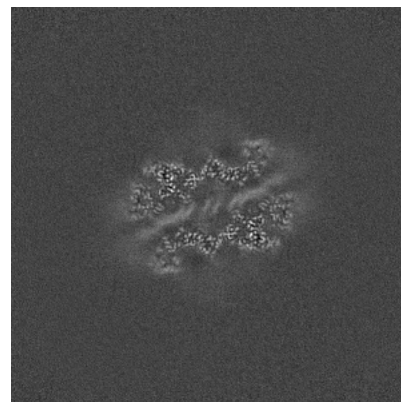
6.2.2 Raw map



X Index: 224



Y Index: 224

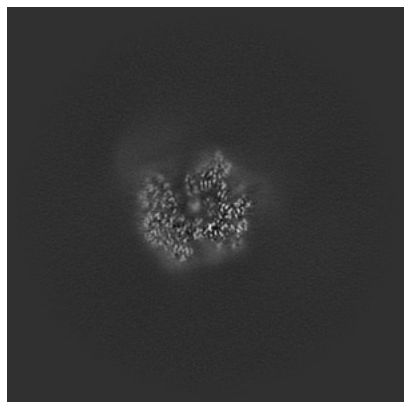


Z Index: 224

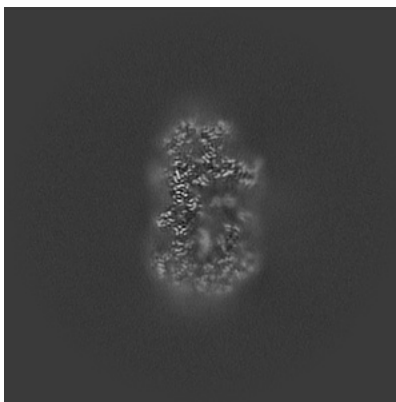
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

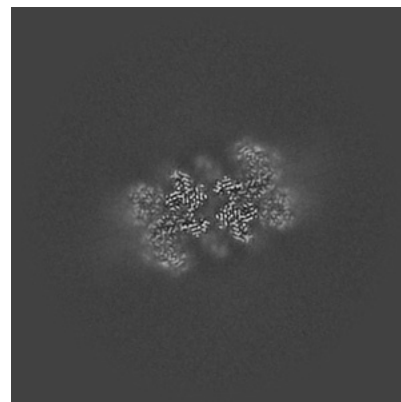
6.3.1 Primary map



X Index: 182

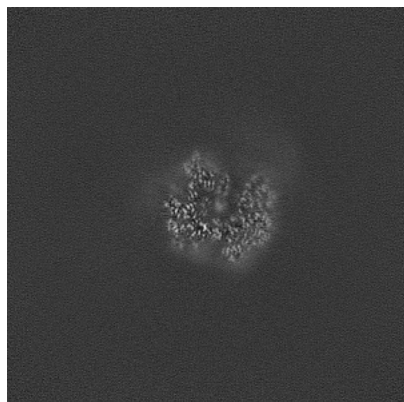


Y Index: 213

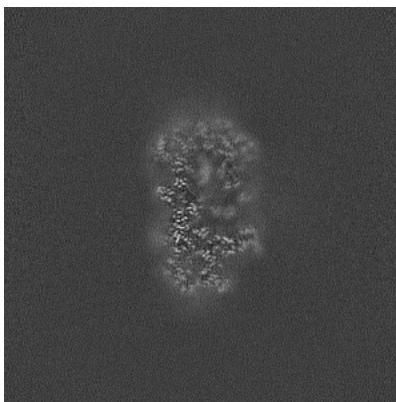


Z Index: 195

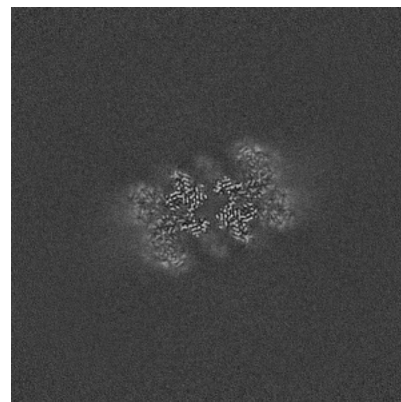
6.3.2 Raw map



X Index: 266



Y Index: 235

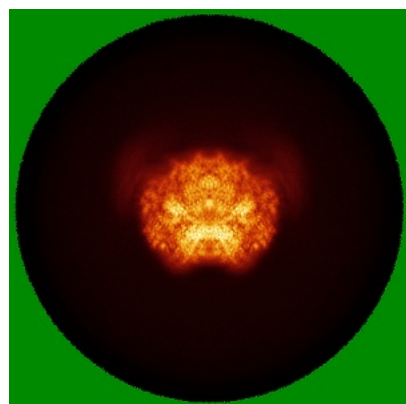


Z Index: 195

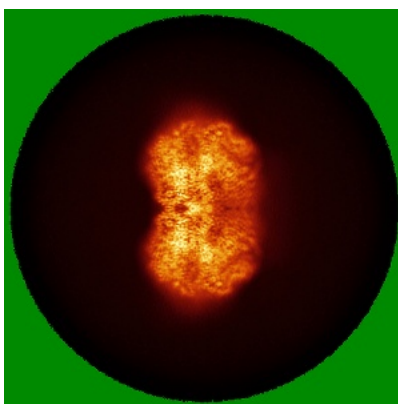
The images above show the largest variance slices of the map in three orthogonal directions.

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

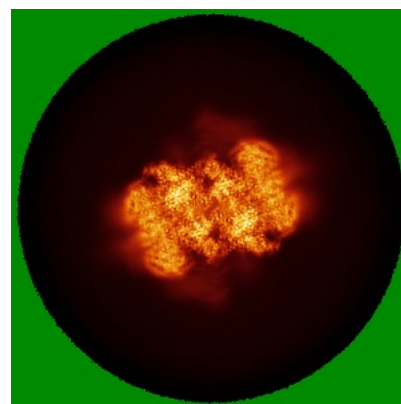
6.4.1 Primary map



X

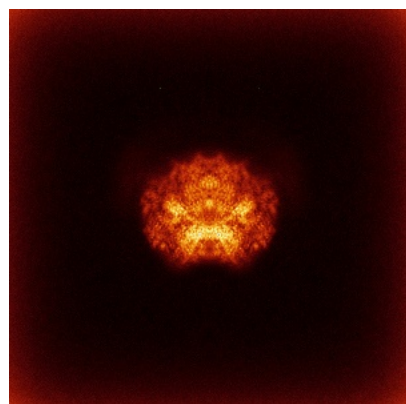


Y

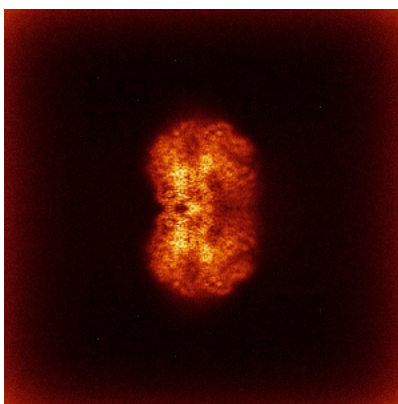


Z

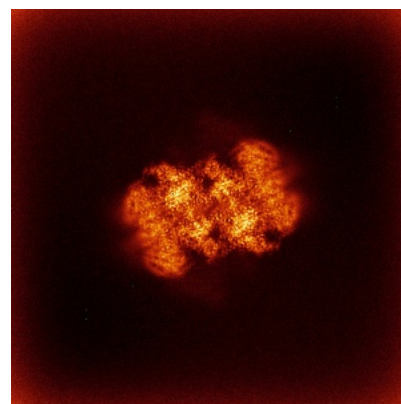
6.4.2 Raw map



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 0.17. 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.

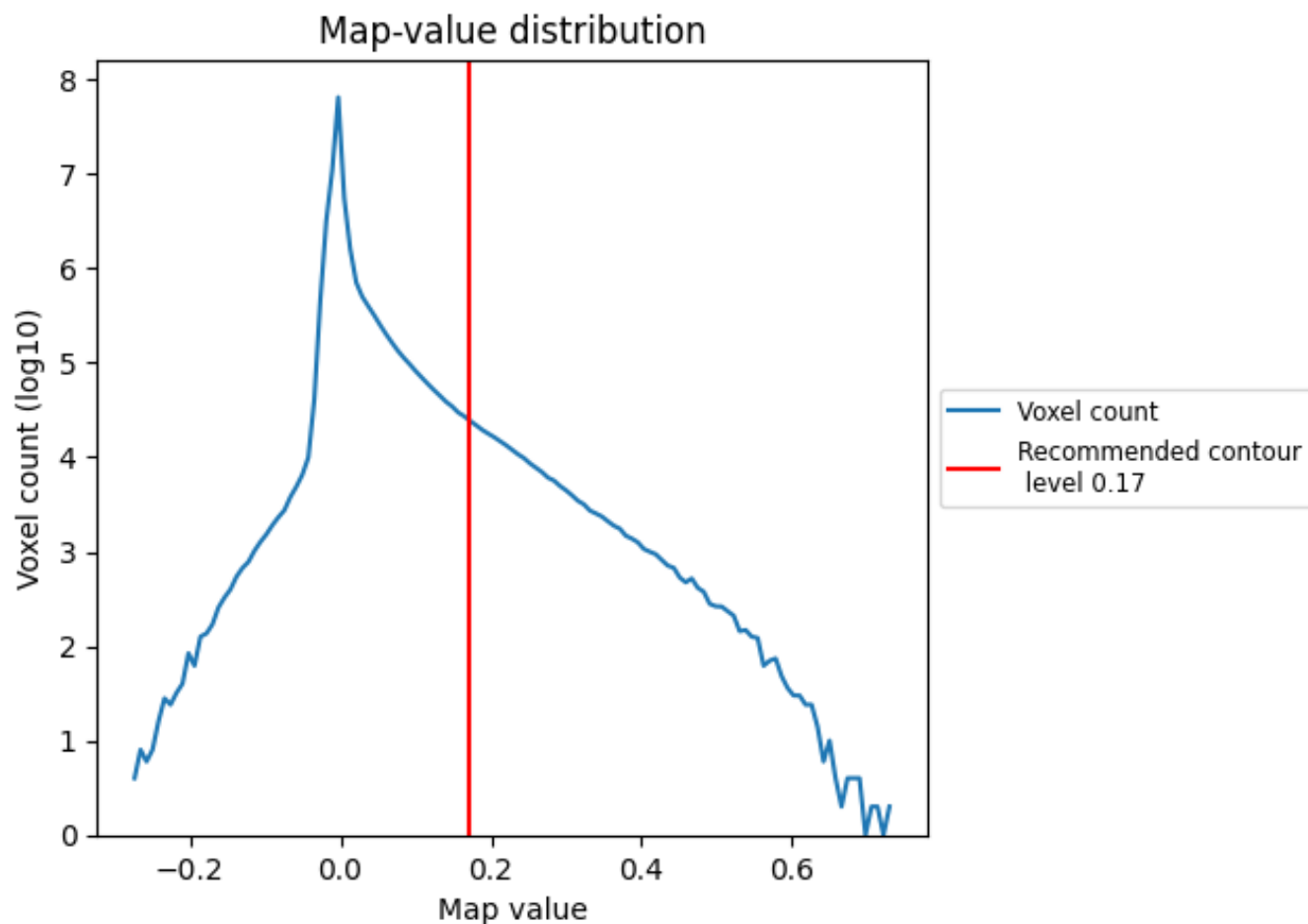
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

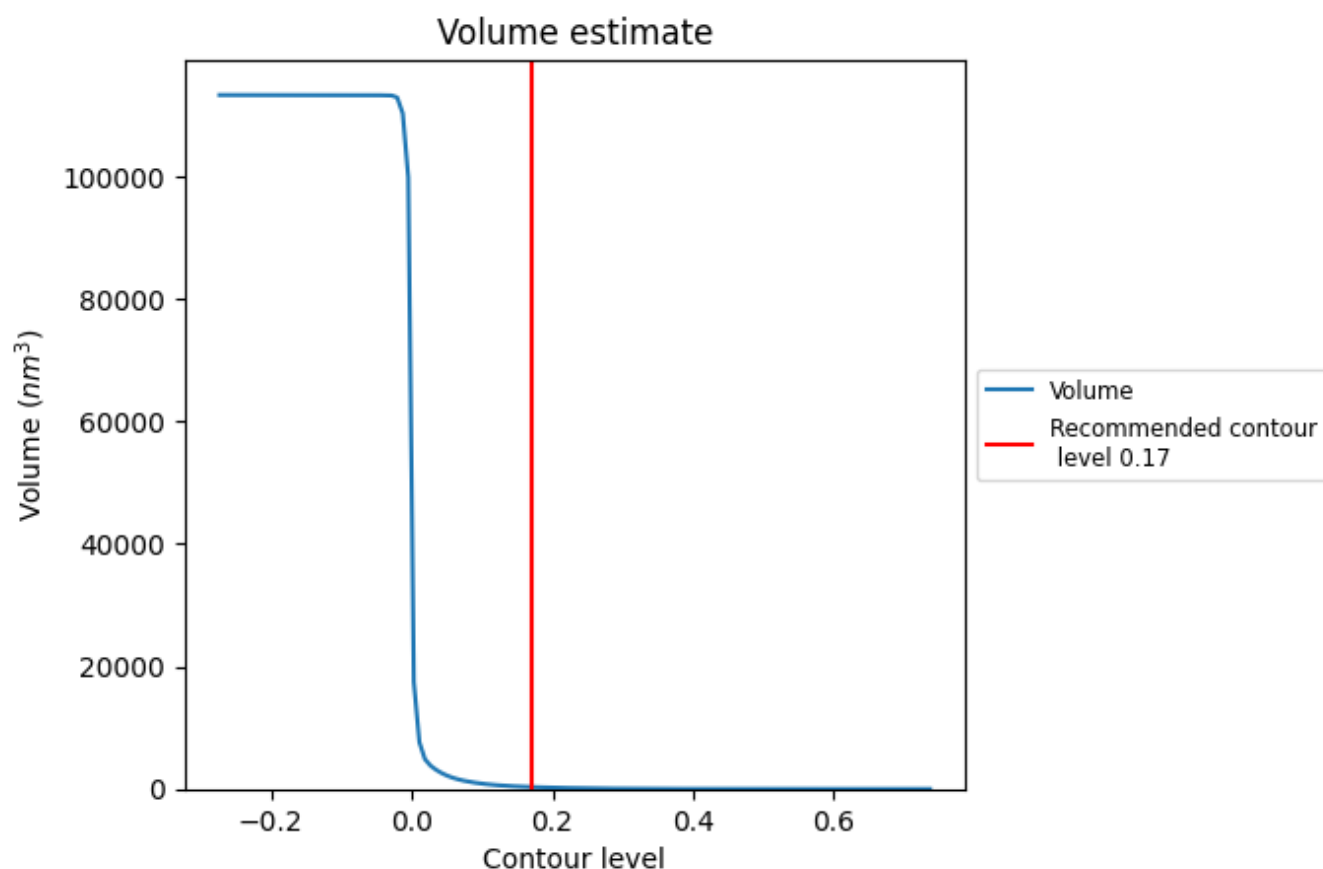
This section contains the results of statistical analysis of the map.

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.

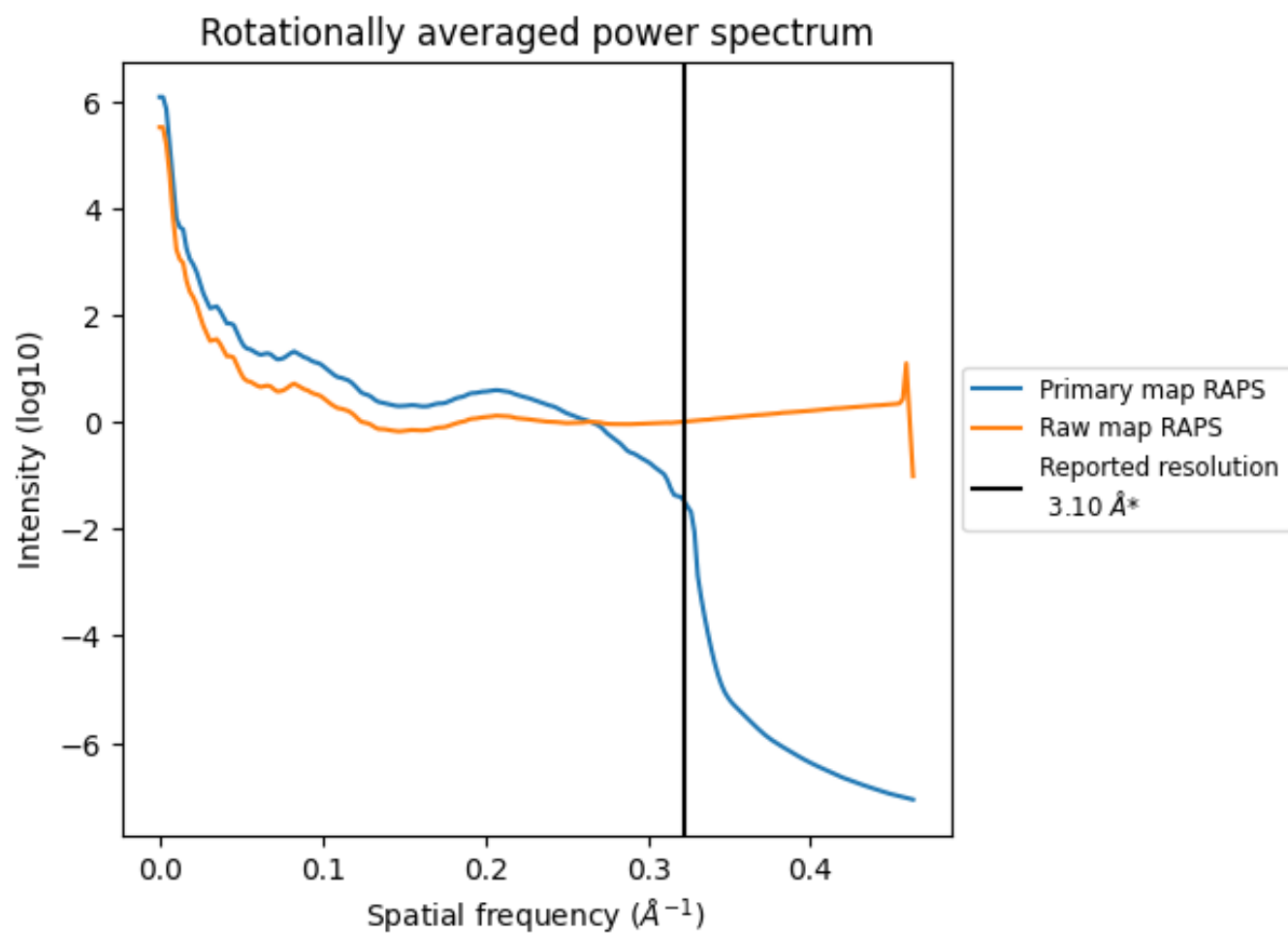
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 315 nm^3 ; this corresponds to an approximate mass of 284 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 ⓘ

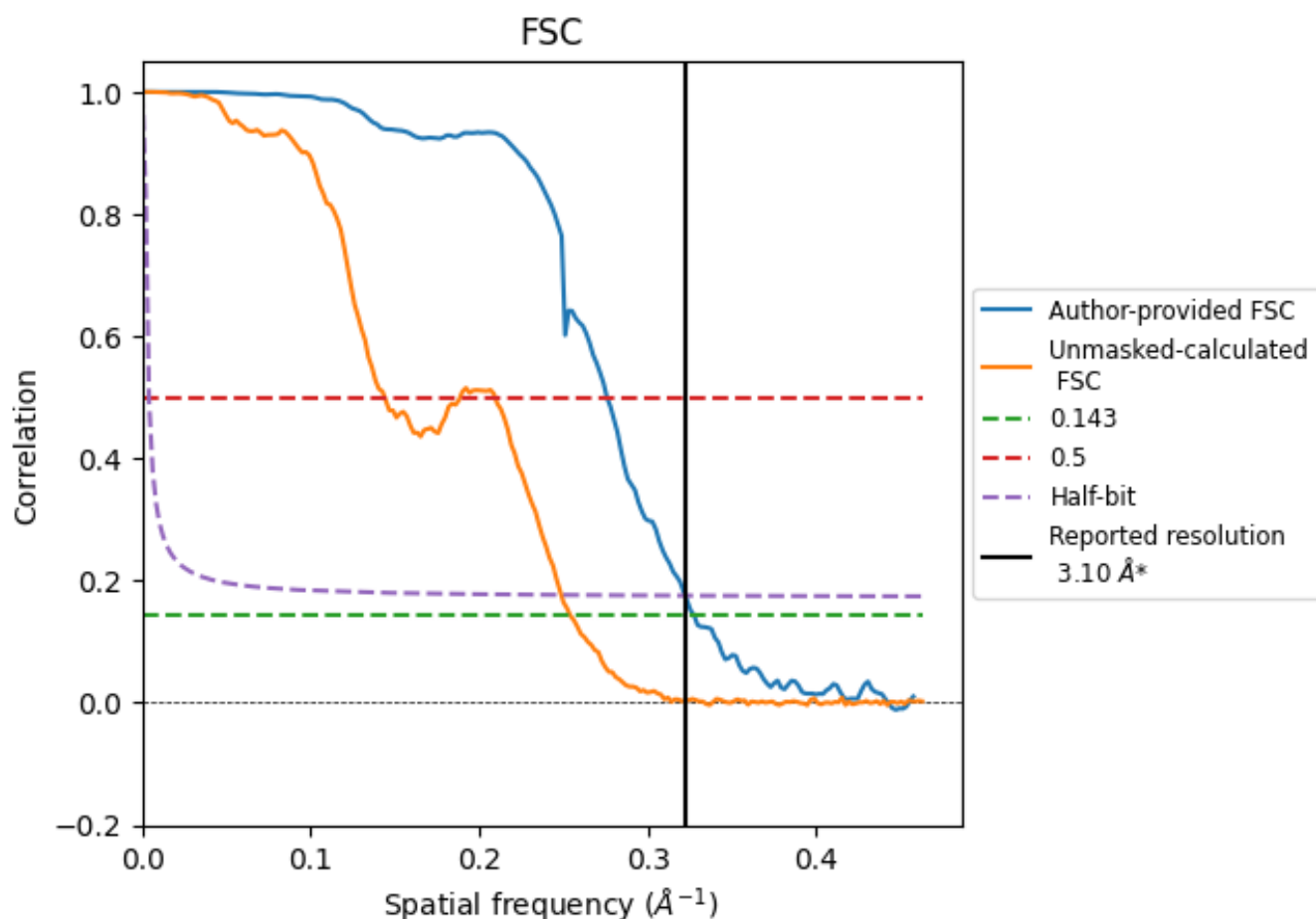


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

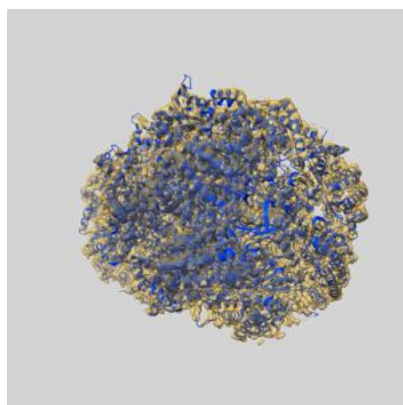
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.05	3.62	3.10
Unmasked-calculated*	3.94	6.95	4.02

*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 3.94 differs from the reported value 3.1 by more than 10 %

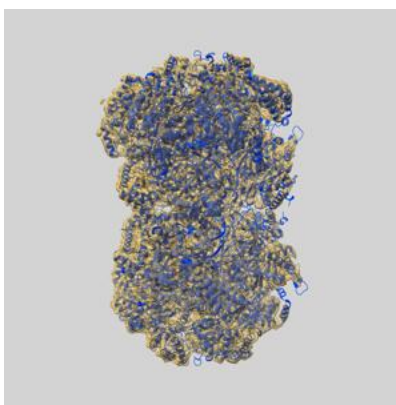
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53972 and PDB model 9RHL. Per-residue inclusion information can be found in section 3 on page 11.

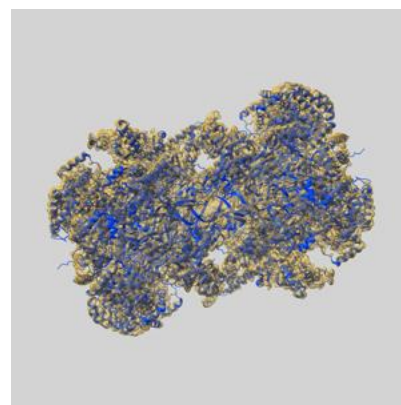
9.1 Map-model overlay [i](#)



X



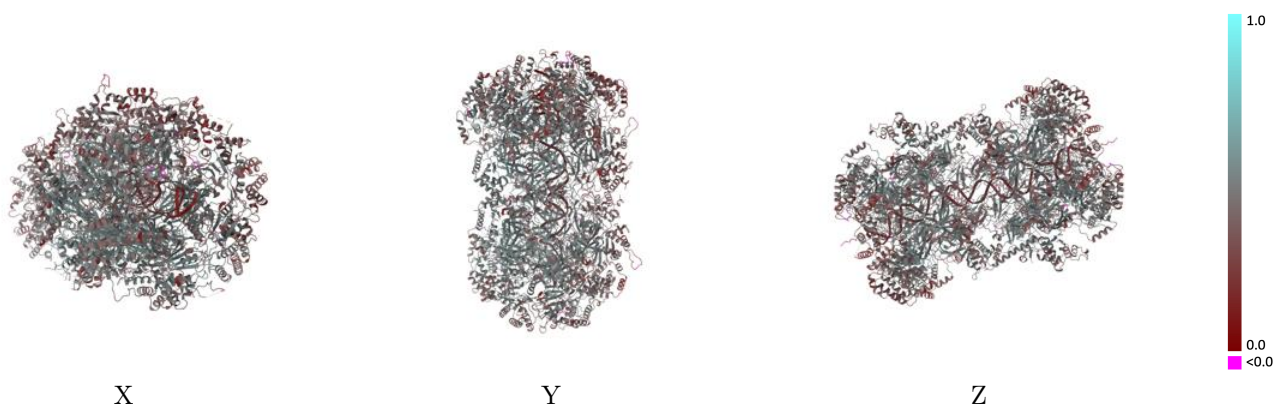
Y



Z

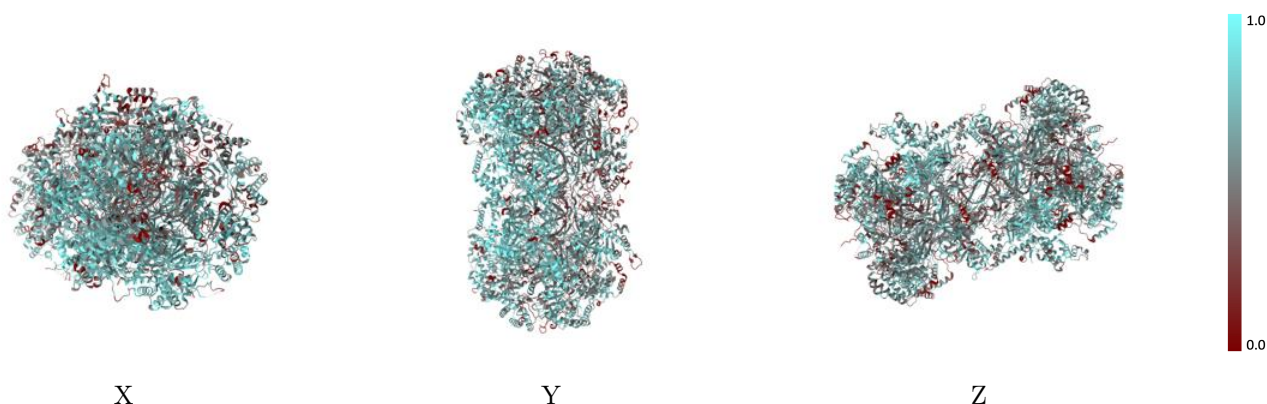
The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



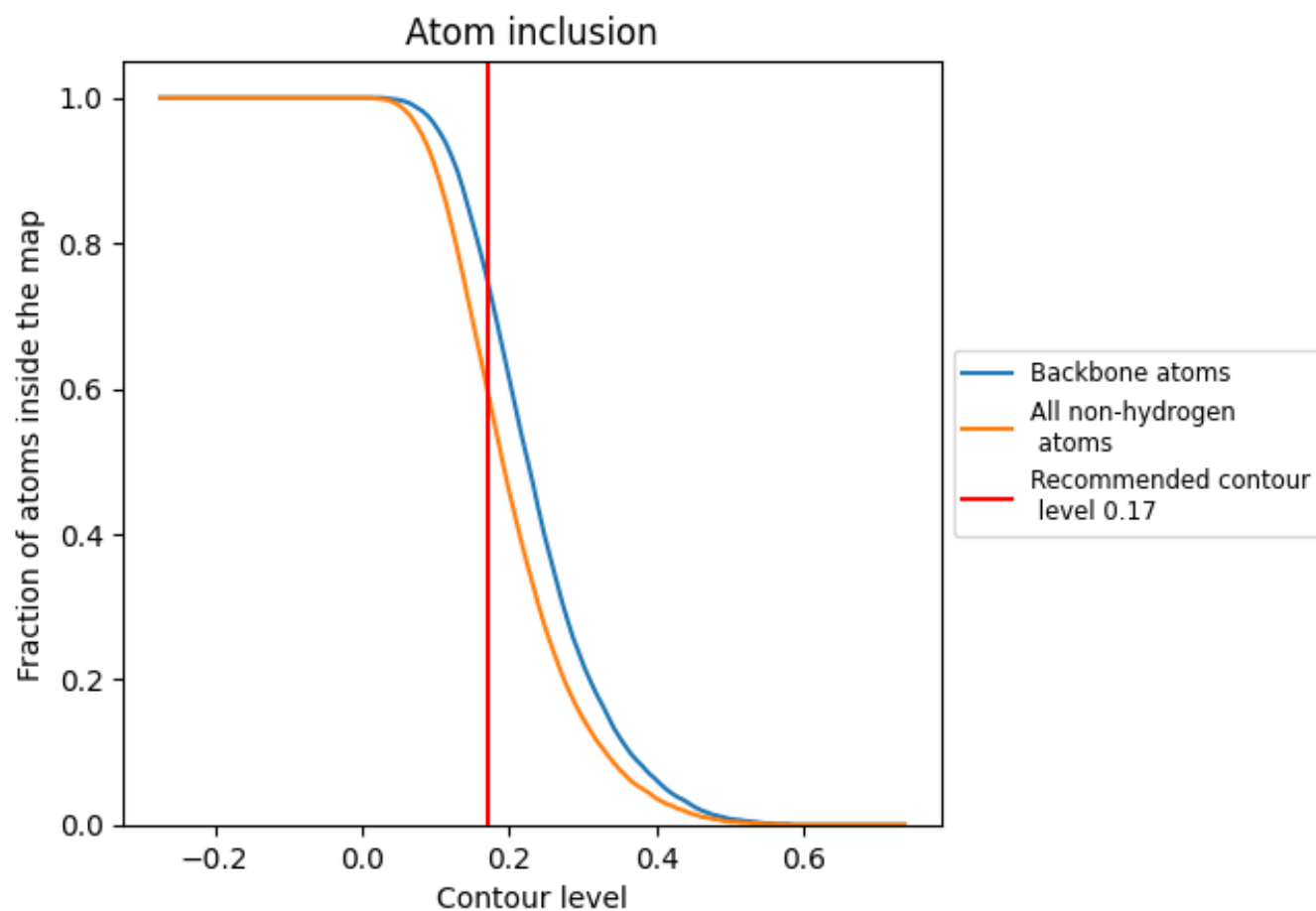
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.17).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 60% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6010	 0.4410
2	 0.4870	 0.4150
3	 0.7250	 0.4920
4	 0.6150	 0.4480
5	 0.6380	 0.4560
6	 0.5020	 0.4050
7	 0.6680	 0.4740
H	 0.3770	 0.4040
I	 0.3610	 0.4020
X	 0.4640	 0.2630
Y	 0.4600	 0.2590
a	 0.4800	 0.4100
b	 0.7250	 0.4890
c	 0.6160	 0.4490
d	 0.6360	 0.4500
e	 0.4990	 0.4040
f	 0.6680	 0.4750

