wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 12:19 am BST

PDB ID	:	9GD1 / pdb_00009gd1
EMDB ID	:	EMD-51241
Title	:	Structure of Chd1 bound to a hexasome-nucleosome complex with a dyad-to-dyad distance of 103 bp.
Authors	:	Engeholm, M.; Roske, J.J.; Oberbeckmann, E.; Dienemann, C.; Lidschreiber, M.; Cramer, P.; Farnung, L.
Deposited on	:	2024-08-04
Resolution	:	4.00 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 (i) 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 (i)) were used in the production of this report:

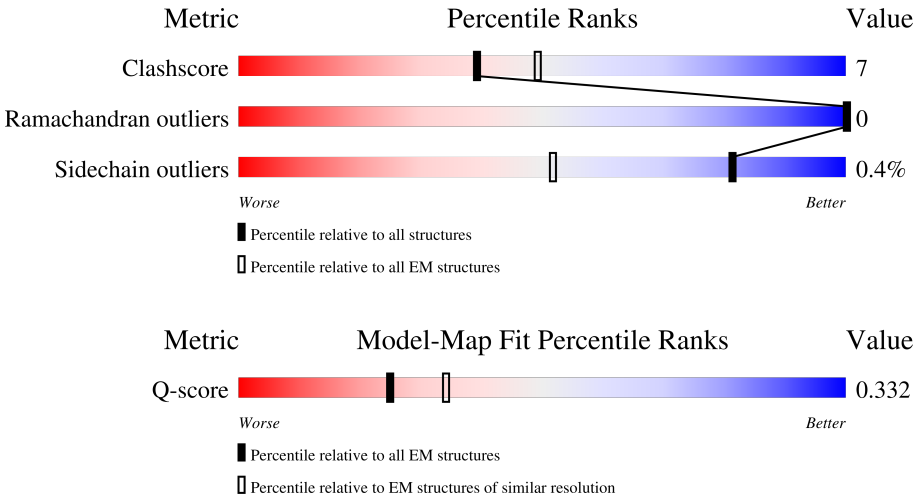
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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

Mol	Chain	Length	Quality of chain
1	A	136	65% · 32%
1	E	136	71% · 29%
1	K	136	50% · 46%
1	O	136	68% · 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	103	
2	F	103	
2	L	103	
2	P	103	
3	C	130	
3	G	130	
3	M	130	
4	D	123	
4	H	123	
4	N	123	
5	I	261	
6	J	261	
7	W	1468	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 27555 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	93	Total	C	N	O	S	0	0
			763	483	143	134	3		
1	E	97	Total	C	N	O	S	0	0
			796	503	152	138	3		
1	K	73	Total	C	N	O	S	0	0
			592	376	109	104	3		
1	O	96	Total	C	N	O	S	0	0
			795	501	154	137	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	conflict	UNP P84233
E	102	ALA	GLY	conflict	UNP P84233
K	102	ALA	GLY	conflict	UNP P84233
O	102	ALA	GLY	conflict	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	78	Total	C	N	O	S	0	0
			622	393	120	108	1		
2	F	77	Total	C	N	O	S	0	0
			614	389	119	105	1		
2	L	81	Total	C	N	O	S	0	0
			658	412	135	110	1		
2	P	80	Total	C	N	O	S	0	0
			644	408	125	110	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	102	Total	C	N	O	0	0
			786	495	153	138		
3	G	96	Total	C	N	O	0	0
			742	465	147	130		
3	M	103	Total	C	N	O	0	0
			795	501	155	139		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	conflict	UNP P06897
C	123	SER	ALA	conflict	UNP P06897
G	99	ARG	GLY	conflict	UNP P06897
G	123	SER	ALA	conflict	UNP P06897
M	99	ARG	GLY	conflict	UNP P06897
M	123	SER	ALA	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	92	Total	C	N	O	S	0	0
			721	454	129	136	2		
4	H	91	Total	C	N	O	S	0	0
			708	447	125	134	2		
4	N	90	Total	C	N	O	S	0	0
			699	441	123	133	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P02281
D	29	THR	SER	conflict	UNP P02281
H	0	MET	-	initiating methionine	UNP P02281
H	29	THR	SER	conflict	UNP P02281
N	0	MET	-	initiating methionine	UNP P02281
N	29	THR	SER	conflict	UNP P02281

- Molecule 5 is a DNA chain called DNA (261-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	259	Total	C	N	O	P	0	0
			5275	2506	953	1557	259		

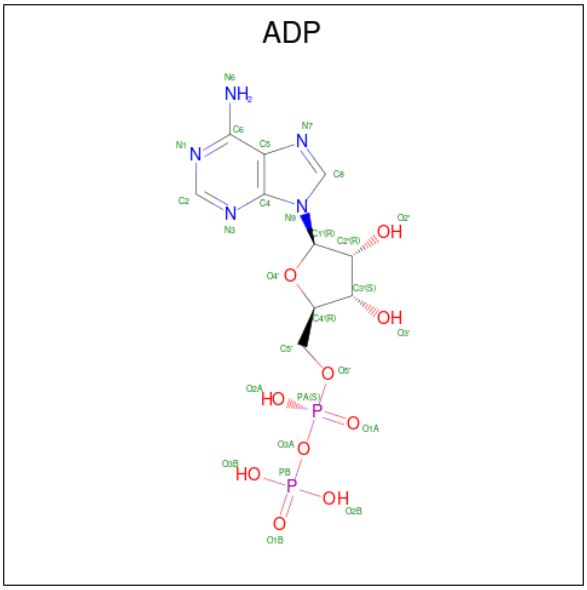
- Molecule 6 is a DNA chain called DNA (261-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	259	Total	C	N	O	P	0	0
			5344	2528	1006	1551	259		

- Molecule 7 is a protein called Chromo domain-containing protein 1.

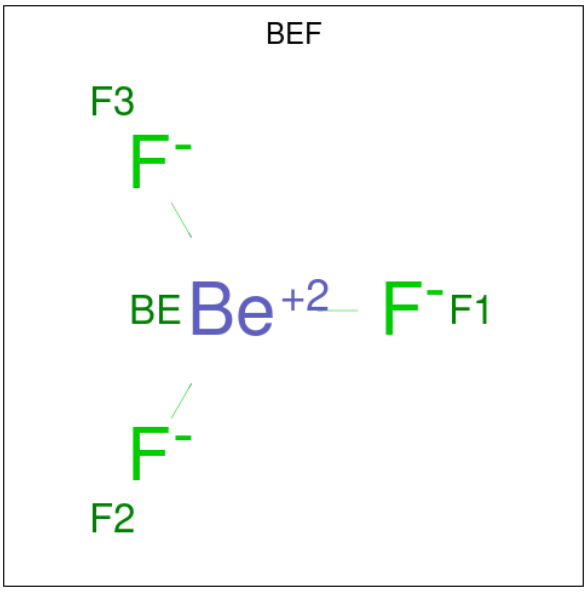
Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	849	Total	C	N	O	S	0	0
			6969	4431	1202	1308	28		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 9 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			AltConf
9	W	1	Total	Be	F	0
			4	1	3	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

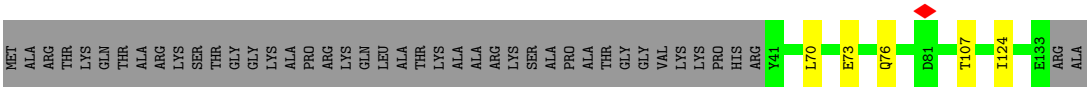
Mol	Chain	Residues	Atoms		AltConf
10	W	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

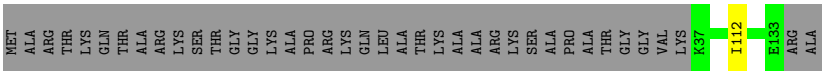
• Molecule 1: Histone H3.2

Chain A:



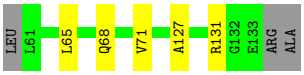
• Molecule 1: Histone H3.2

Chain E:



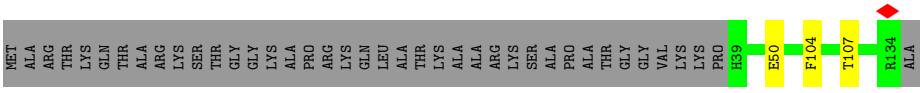
• Molecule 1: Histone H3.2

Chain K:



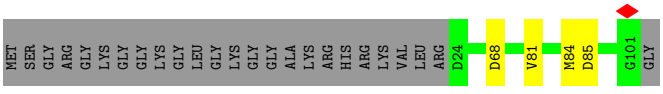
• Molecule 1: Histone H3.2

Chain O:



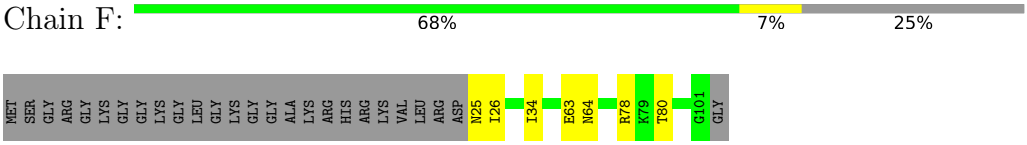
• Molecule 2: Histone H4

Chain B:



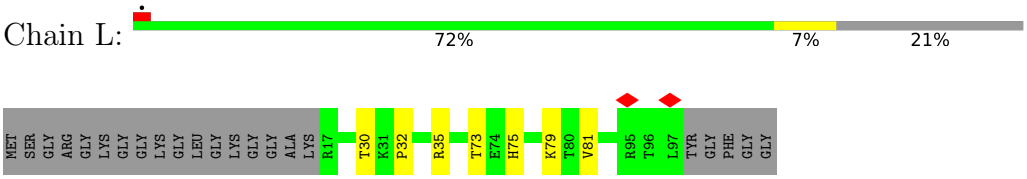
• Molecule 2: Histone H4

Chain F:



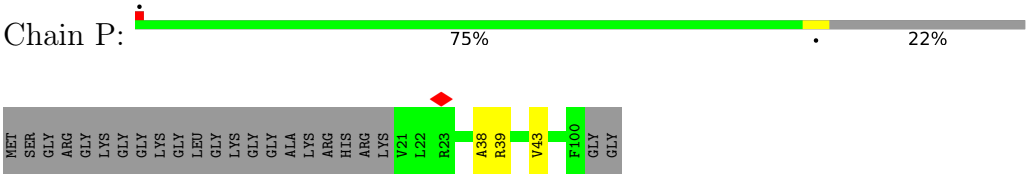
• Molecule 2: Histone H4

Chain L:



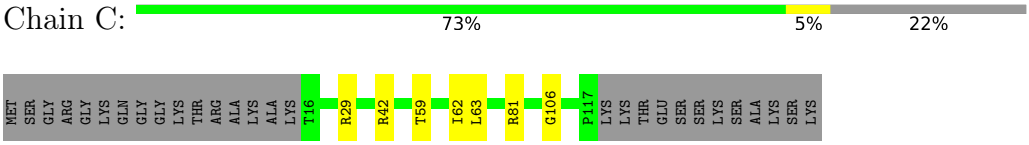
• Molecule 2: Histone H4

Chain P:



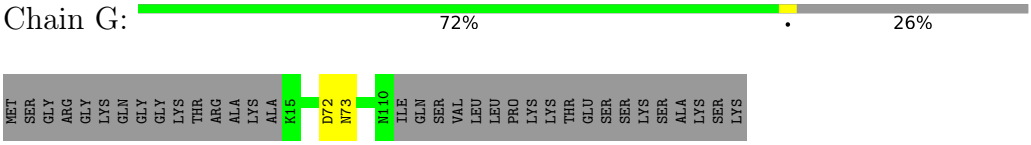
• Molecule 3: Histone H2A type 1

Chain C:



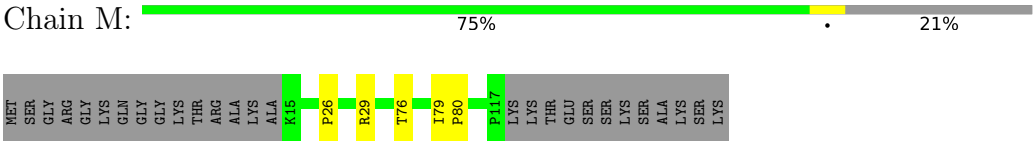
• Molecule 3: Histone H2A type 1

Chain G:



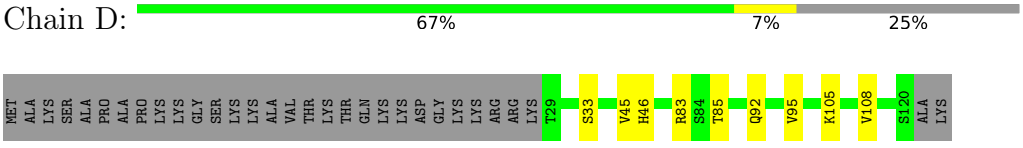
• Molecule 3: Histone H2A type 1

Chain M:



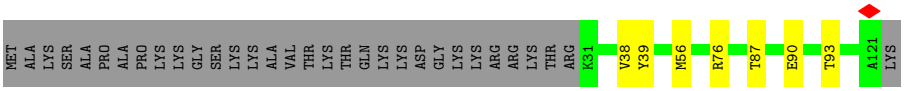
• Molecule 4: Histone H2B 1.1

Chain D:



• Molecule 4: Histone H2B 1.1

Chain H:

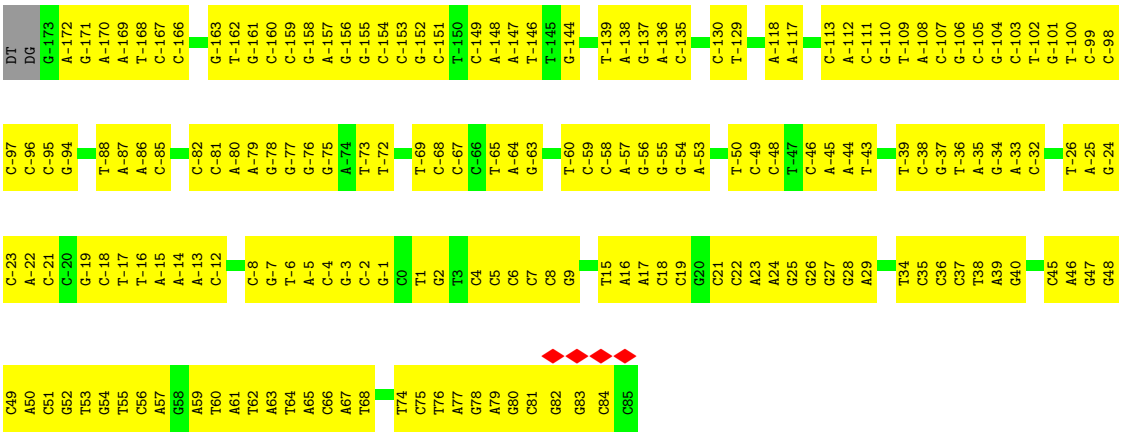


• Molecule 4: Histone H2B 1.1

Chain N:

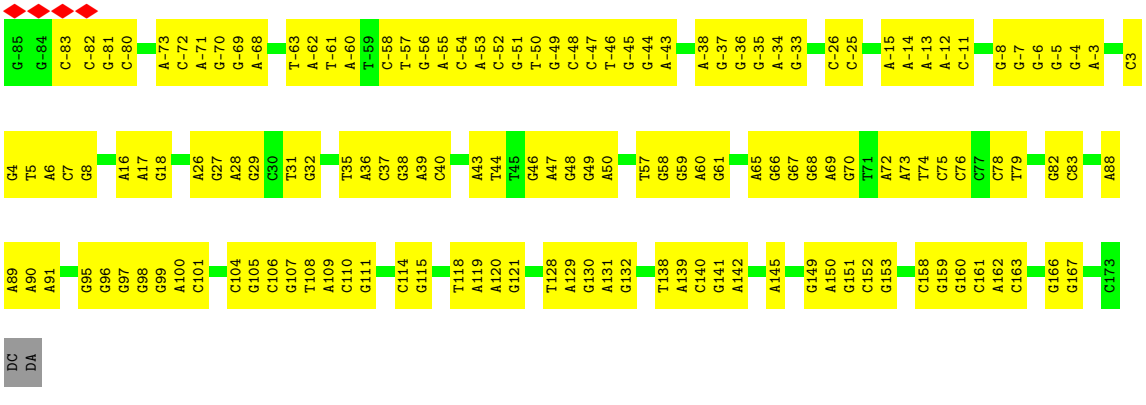
• Molecule 5: DNA (261-MER)

Chain I:



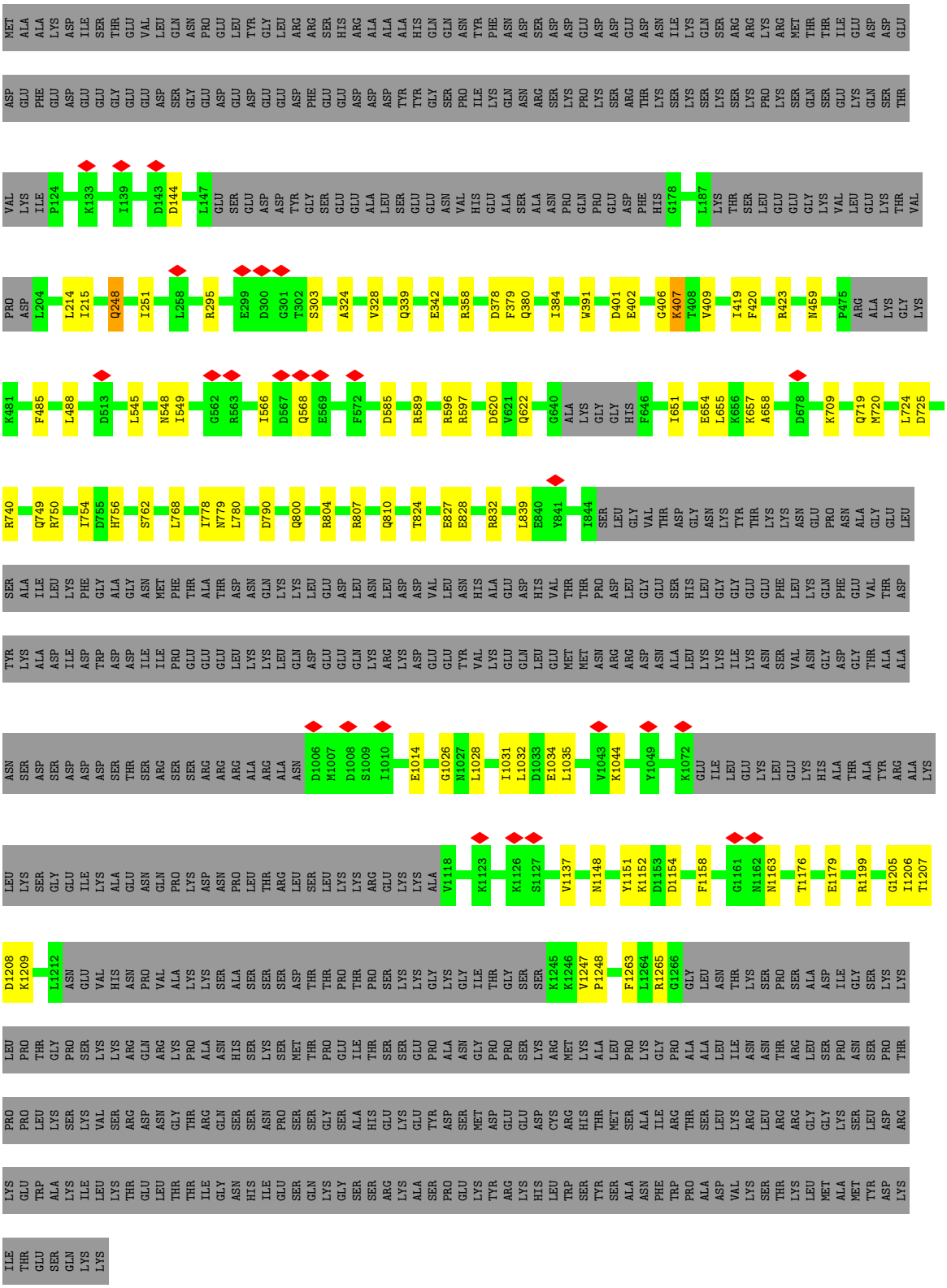
• Molecule 6: DNA (261-MER)

Chain J:



• Molecule 7: Chromo domain-containing protein 1

Chain W:


MET ALA ALA LYS ASP ILE SER THR GLU VAL LEU GLN ASN PRO GLU LEU TYR GLY LEU ARG ARG SER HIS ARG ALA ALA ALA HIS GLN GLN ASN TYR PHE ASN ASP SER ASP ASP GLU ASP GLU ASP ASN ILE LYS GLN SER ARG ARG LYS ARG MET THR THR ILE GLU ASP GLU
ASP GLU PHE GLU ASP GLU GLU GLY GLU GLU ASP SER GLY GLU ASP GLU ASP GLU GLU ASP PHE GLU GLU ASP ASP TYR TYR GLY SER PRO ILE LYS GLN ASN ARG SER LYS PRO LYS SER ARG THR LYS SER LYS SER LYS SER LYS PRO LYS SER GLN SER GLU LYS GLN SER THR
VAL LYS ILE P124 K133 I139 D143 D144 L147 GLU SER GLU ASP ASP TYR GLY SER GLU GLU ALA LEU SER GLU GLU ASN VAL HIS GLU ALA SER ALA ASN PRO GLN PRO GLU ASP PHE HIS G178 L187 LYS THR SER LEU GLU GLU GLY LYS VAL LEU GLU LYS THR VAL
PRO ASP L204 L214 I215 Q248 I251 L258 R295 E299 D300 G301 T302 S303 A324 V328 Q339 E342 R358 D378 F379 Q380 I384 W391 D401 E402 G406 K407 T408 V409 I419 F420 R423 N459 P475 ARG ALA LYS GLY LYS
K481 F485 L488 D513 L545 N548 I549 G562 R563 I566 D567 Q568 E569 F572 D585 R589 R596 R597 D620 V621 Q622 G640 ALA LYS GLY GLY HIS F646 I651 E654 L655 K656 K657 A658 D678 K709 Q719 M720 L724 D725
R740 Q749 R750 I754 D755 H756 S762 L768 I778 N779 L780 D790 Q800 R804 R807 Q810 T824 E827 E828 R832 L839 E840 Y841 I844 SER LEU GLY VAL THR ASP GLY ASN LYS TYR THR LYS LYS ASN GLU PRO ASN ALA GLY GLU LEU
SER ALA ILE LEU LYS PHE GLY ALA GLY ASN MET PHE THR ALA THR ASP ASN GLN LYS LYS LEU GLU ASP LEU ASN LEU ASP ASP VAL LEU ASN HIS ALA GLU ASP HIS VAL THR THR PRO ASP LEU GLY GLU SER HIS LEU GLY GLY GLU GLU PHE LEU LYS GLN PHE GLU VAL THR ASP
TYR LYS ALA ASP ILE ASP TRP ASP ASP ILE ILE PRO GLU GLU GLU LEU LYS LYS LEU GLN ASP GLU GLU GLN LYS ARG LYS ASP GLU GLU TYR VAL LYS GLU GLN LEU GLU MET MET ASN ARG ARG ASP ASN ALA LEU LYS LYS ILE LYS ASN SER VAL ASN GLY ASP GLY THR ALA ALA
ASN SER ASP SER ASP ASP SER THR SER ARG SER SER ARG ARG ARG ALA ALA ARG ALA ASN D1006 M1007 D1008 S1009 I1010 E1014 G1026 M1027 L1028 I1031 L1032 D1033 E1034 L1035 V1043 K1044 Y1049 K1072 GLU ILE LEU GLU LYS LEU GLU LYS HIS ALA THR ALA TYR ARG ALA LYS
LEU LYS SER GLY GLU ILE LYS ALA GLU ASN GLN PRO LYS ASP ASN PRO LEU THR ARG LEU SER LEU LYS LYS ARG GLU LYS LYS ALA V1118 K1123 K1126 S1127 V1137 N1148 Y1151 K1152 D1153 D1154 F1158 G1161 N1162 N1163 T1176 E1179 R1199 G1205 I1206 T1207
D1208 K1209 L1212 ASN GLU VAL HIS ASN PRO VAL ALA LYS LYS SER ALA SER SER SER ASP THR THR PRO THR PRO SER LYS LYS GLY LYS GLY ILE THR GLY SER SER K1245 K1246 V1247 P1248 F1263 L1264 R1265 G1266 GLY LEU ASN THR LYS SER PRO SER ALA ASP ILE GLY SER LYS LYS
LEU PRO THR GLY PRO SER LYS LYS ARG GLN ARG LYS PRO ALA ASN HIS SER LYS SER MET THR PRO GLU ILE THR SER SER GLU PRO ALA ASN GLY PRO PRO SER LYS ARG MET LYS ALA LEU PRO LYS GLY PRO ALA ALA LEU ILE ASN ASN THR ARG LEU SER PRO SER LEU PRO THR
PRO PRO LEU LYS SER VAL SER ARG ASP ASN GLY THR ARG SER ASN PRO SER SER GLY SER ALA HIS GLU LYS GLU SER MET ASP GLU GLU ASP CYS ARG HIS THR MET SER ALA ILE ARG THR SER LEU LYS ARG LEU ARG ARG GLY GLY LYS SER LEU ASP ARG
LYS GLU TRP ALA LYS ILE LEU LYS THR GLU LEU THR ILE GLY ASN HIS ILE GLU SER GLN LYS GLY SER SER ARG LYS ALA SER PRO GLU LYS TYR ARG LYS HIS LEU TRP SER TYR SER ALA ASN PHE TRP PRO ALA ASP VAL LYS SER THR SER LEU ARG LYS LEU MET ALA MET TYR ASP LYS
ILE THR GLU SER GLN LYS LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26819	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	350.28, 350.28, 350.28	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

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

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	A	0.13	0/773	0.34	0/1038
1	E	0.13	0/808	0.34	0/1086
1	K	0.14	0/599	0.30	0/804
1	O	0.14	0/806	0.32	0/1081
2	B	0.18	0/629	0.41	0/843
2	F	0.14	0/621	0.34	0/832
2	L	0.19	0/664	0.41	0/888
2	P	0.15	0/651	0.35	0/873
3	C	0.13	0/796	0.30	0/1077
3	G	0.14	0/751	0.31	0/1013
3	M	0.14	0/805	0.32	0/1088
4	D	0.15	0/732	0.34	0/986
4	H	0.15	0/719	0.37	0/969
4	N	0.16	0/710	0.33	0/958
5	I	0.31	0/5909	0.68	0/9109
6	J	0.31	0/6003	0.68	3/9272 (0.0%)
7	W	0.15	0/7103	0.38	0/9574
All	All	0.23	0/29079	0.53	3/41491 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	74	DT	C2'-C3'-O3'	-6.42	101.87	111.50
6	J	76	DC	C2'-C3'-O3'	-5.83	102.76	111.50
6	J	75	DC	C2'-C3'-O3'	-5.79	102.81	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	A	763	0	800	3	0
1	E	796	0	829	0	0
1	K	592	0	621	3	0
1	O	795	0	833	2	0
2	B	622	0	660	2	0
2	F	614	0	656	4	0
2	L	658	0	715	5	0
2	P	644	0	690	2	0
3	C	786	0	833	4	0
3	G	742	0	784	2	0
3	M	795	0	846	2	0
4	D	721	0	742	6	0
4	H	708	0	727	6	0
4	N	699	0	714	4	0
5	I	5275	0	2908	156	0
6	J	5344	0	2905	124	0
7	W	6969	0	6932	57	0
8	W	27	0	12	0	0
9	W	4	0	0	1	0
10	W	1	0	0	0	0
All	All	27555	0	23207	365	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 365 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)
6:J:-35:DG:H2”	6:J:-34:DA:C8	2.12	0.84
5:I:-118:DA:H2”	5:I:-117:DA:C8	2.12	0.84
6:J:99:DG:H2”	6:J:100:DA:C8	2.13	0.82
6:J:36:DA:H2”	6:J:37:DC:C6	2.15	0.80
5:I:-44:DA:H2’	5:I:-43:DT:H71	1.71	0.72

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	A	91/136 (67%)	90 (99%)	1 (1%)	0	100	100
1	E	95/136 (70%)	95 (100%)	0	0	100	100
1	K	71/136 (52%)	70 (99%)	1 (1%)	0	100	100
1	O	94/136 (69%)	92 (98%)	2 (2%)	0	100	100
2	B	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
2	F	75/103 (73%)	75 (100%)	0	0	100	100
2	L	79/103 (77%)	79 (100%)	0	0	100	100
2	P	78/103 (76%)	74 (95%)	4 (5%)	0	100	100
3	C	100/130 (77%)	97 (97%)	3 (3%)	0	100	100
3	G	94/130 (72%)	93 (99%)	1 (1%)	0	100	100
3	M	101/130 (78%)	100 (99%)	1 (1%)	0	100	100
4	D	90/123 (73%)	90 (100%)	0	0	100	100
4	H	89/123 (72%)	89 (100%)	0	0	100	100
4	N	88/123 (72%)	88 (100%)	0	0	100	100
7	W	833/1468 (57%)	819 (98%)	14 (2%)	0	100	100
All	All	2054/3183 (64%)	2026 (99%)	28 (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	A	81/111 (73%)	81 (100%)	0	100 100
1	E	84/111 (76%)	83 (99%)	1 (1%)	63 73
1	K	63/111 (57%)	63 (100%)	0	100 100
1	O	84/111 (76%)	84 (100%)	0	100 100
2	B	64/79 (81%)	62 (97%)	2 (3%)	35 56
2	F	63/79 (80%)	63 (100%)	0	100 100
2	L	69/79 (87%)	69 (100%)	0	100 100
2	P	67/79 (85%)	67 (100%)	0	100 100
3	C	81/102 (79%)	80 (99%)	1 (1%)	63 73
3	G	75/102 (74%)	75 (100%)	0	100 100
3	M	82/102 (80%)	81 (99%)	1 (1%)	63 73
4	D	79/103 (77%)	79 (100%)	0	100 100
4	H	77/103 (75%)	77 (100%)	0	100 100
4	N	76/103 (74%)	76 (100%)	0	100 100
7	W	769/1313 (59%)	767 (100%)	2 (0%)	86 85
All	All	1814/2688 (68%)	1807 (100%)	7 (0%)	81 84

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	112	ILE
3	M	76	THR
7	W	407	LYS
7	W	248	GLN
3	C	63	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
7	W	674	GLN
7	W	343	ASN
2	L	25	ASN
4	H	92	GLN
2	L	75	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
8	ADP	W	1501	9	27,29,29	1.33	4 (14%)	42,45,45	2.12	13 (30%)
9	BEF	W	1502	8	0,3,3	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	W	1501	9	-	4/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	1501	ADP	C5-C4	4.31	1.47	1.39
8	W	1501	ADP	C5-C6	2.48	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	1501	ADP	C8-N7	2.32	1.36	1.31
8	W	1501	ADP	C5-N7	-2.31	1.34	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	W	1501	ADP	C5-C4-N3	-6.21	118.65	126.75
8	W	1501	ADP	N3-C4-N9	5.14	135.55	127.08
8	W	1501	ADP	PA-O3A-PB	-4.50	117.38	132.83
8	W	1501	ADP	C2-N3-C4	3.99	121.19	111.75
8	W	1501	ADP	N3-C2-N1	-3.58	123.01	128.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	W	1501	ADP	PA-O3A-PB-O3B
8	W	1501	ADP	C5'-O5'-PA-O2A
8	W	1501	ADP	C5'-O5'-PA-O3A
8	W	1501	ADP	PA-O3A-PB-O2B

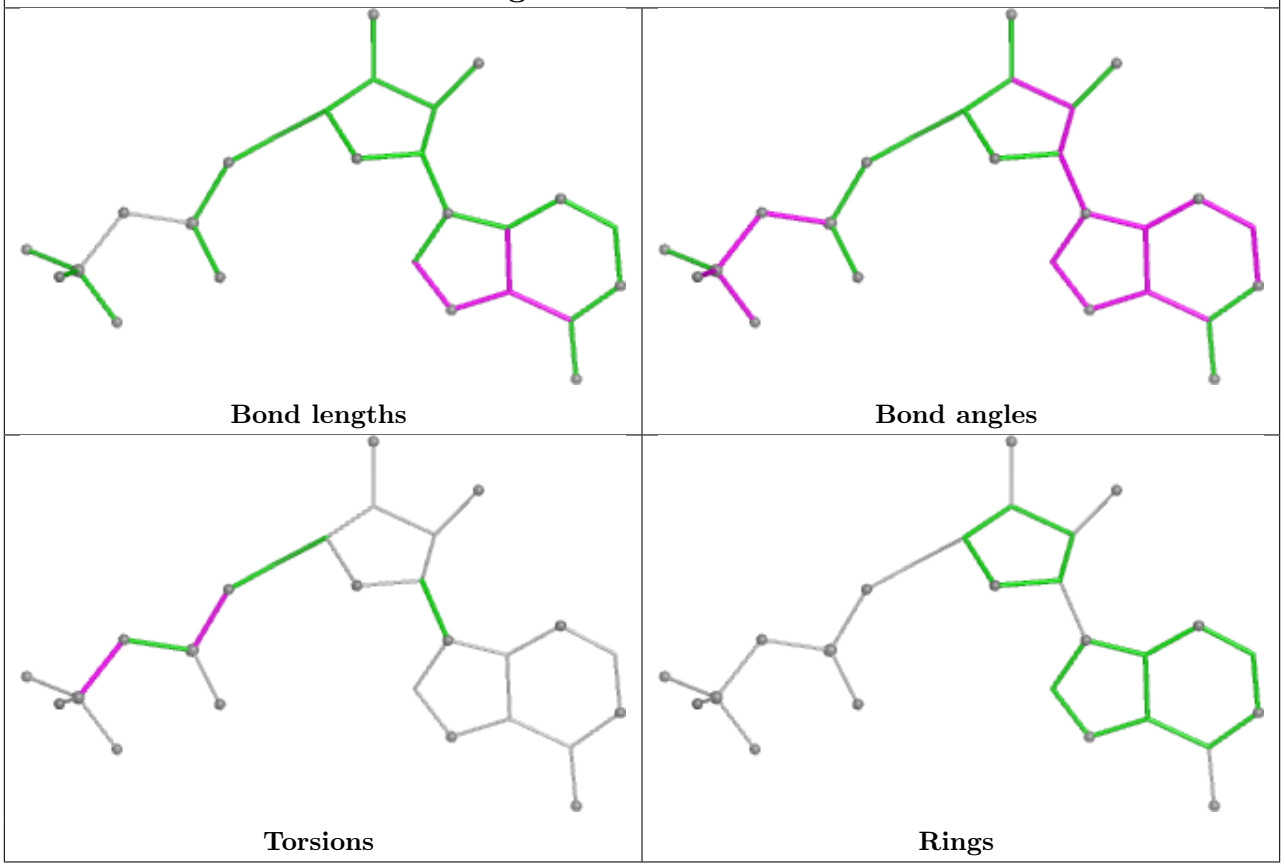
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	W	1502	BEF	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP W 1501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

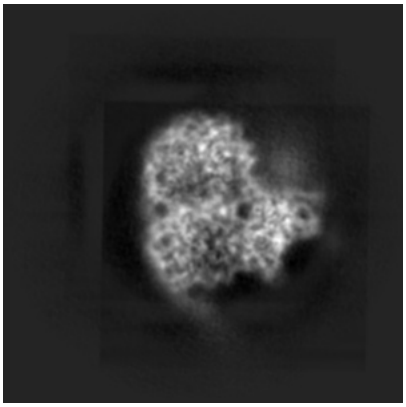
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51241. These allow visual inspection of the internal detail of the map and identification of artifacts.

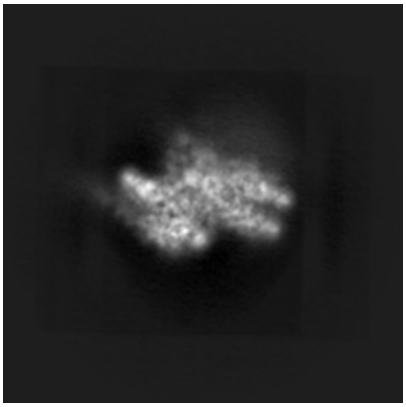
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

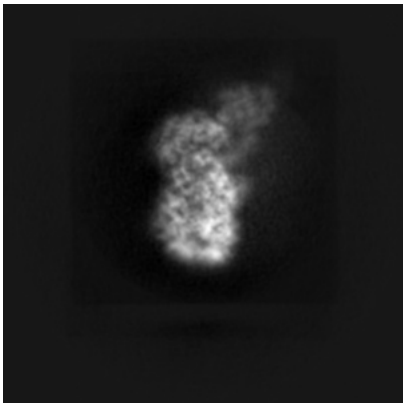
6.1.1 Primary map



X



Y

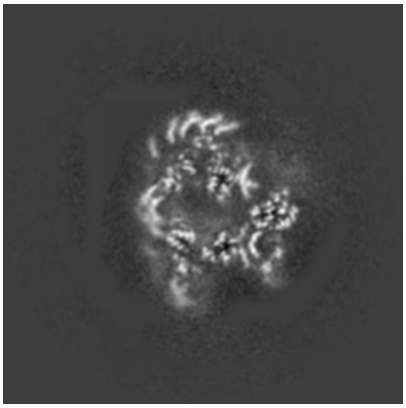


Z

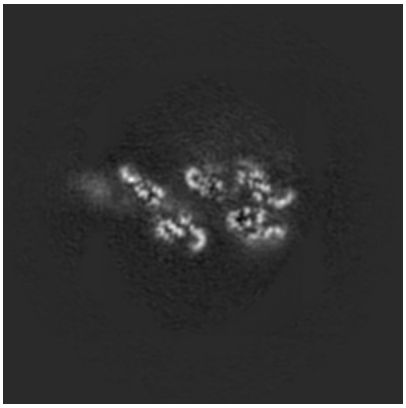
The images above show the map projected in three orthogonal directions.

6.2 Central slices

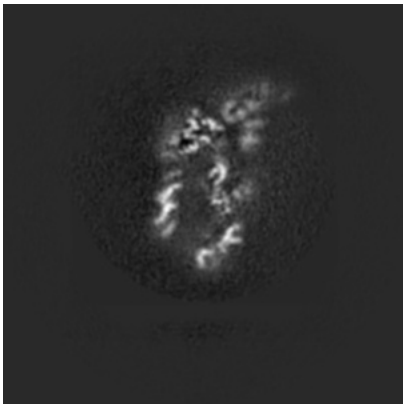
6.2.1 Primary map



X Index: 210



Y Index: 210

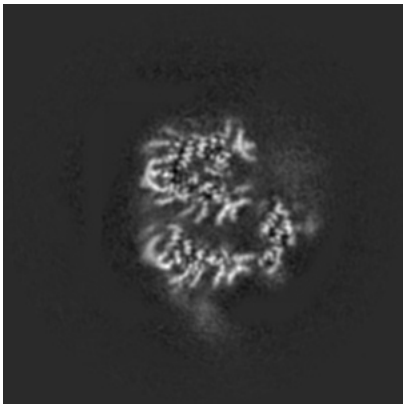


Z Index: 210

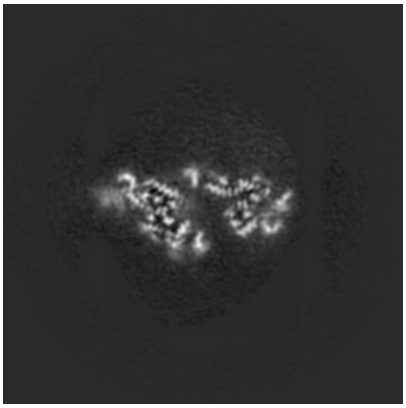
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

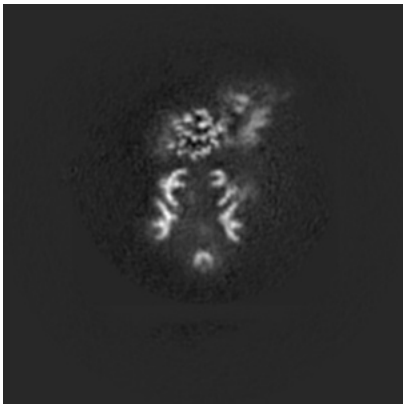
6.3.1 Primary map



X Index: 228



Y Index: 191

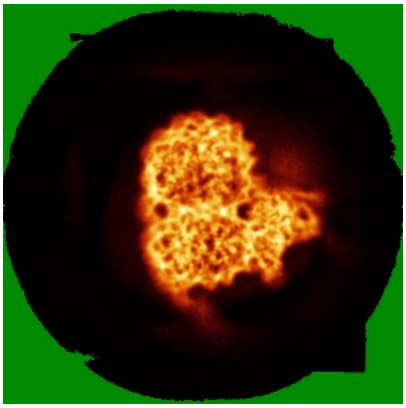


Z Index: 203

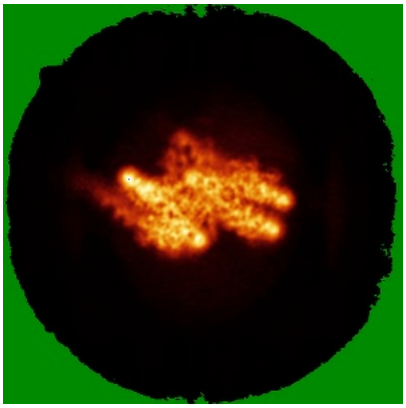
The images above show the largest variance slices of the map in three orthogonal directions.

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

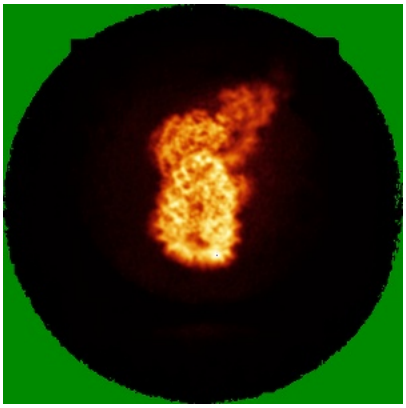
6.4.1 Primary map



X



Y

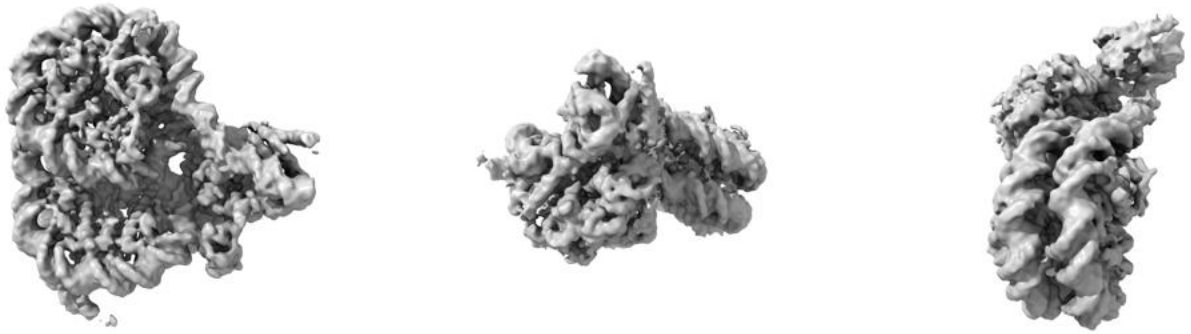


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

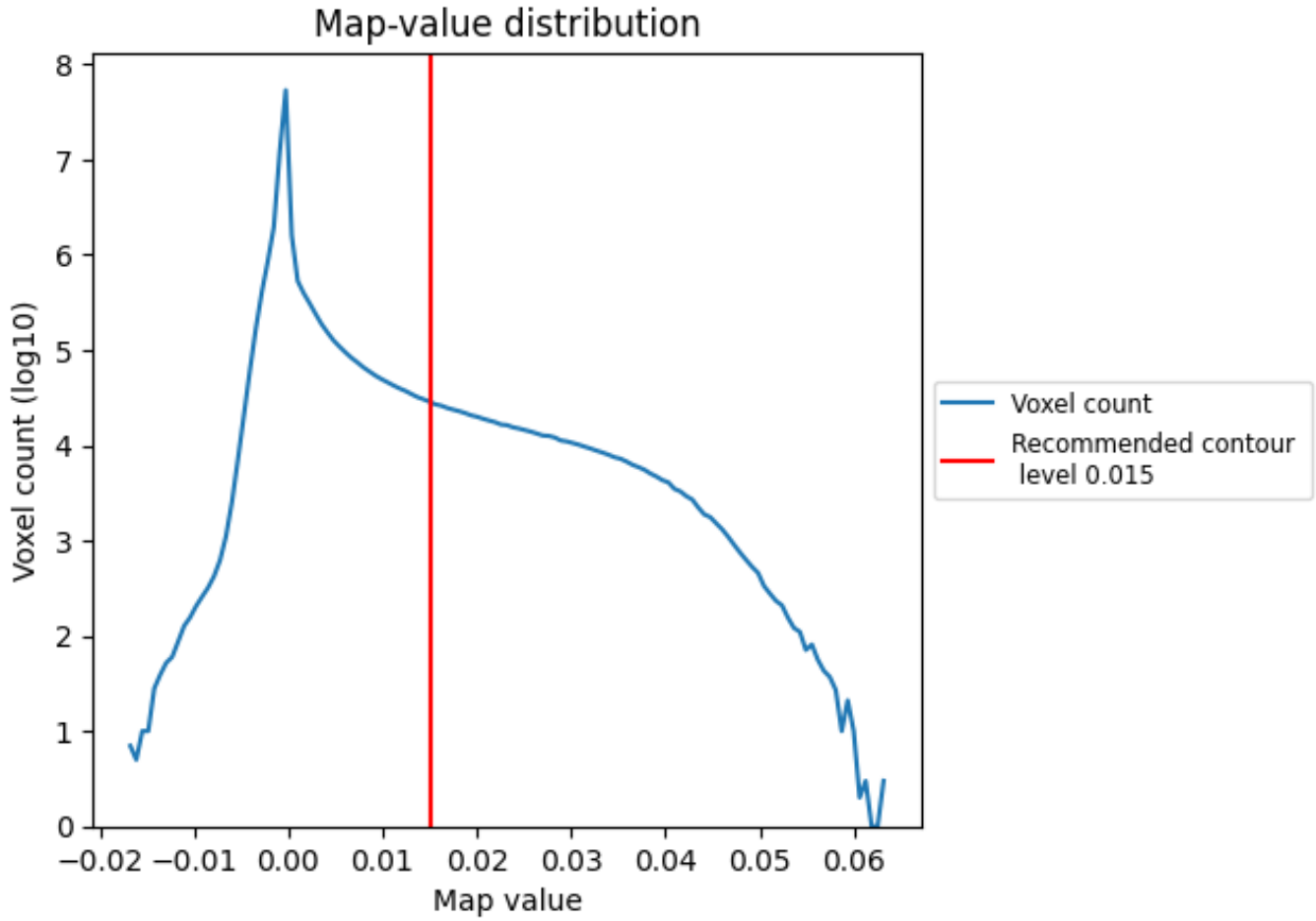
6.6 Mask visualisation (i)

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

7 Map analysis

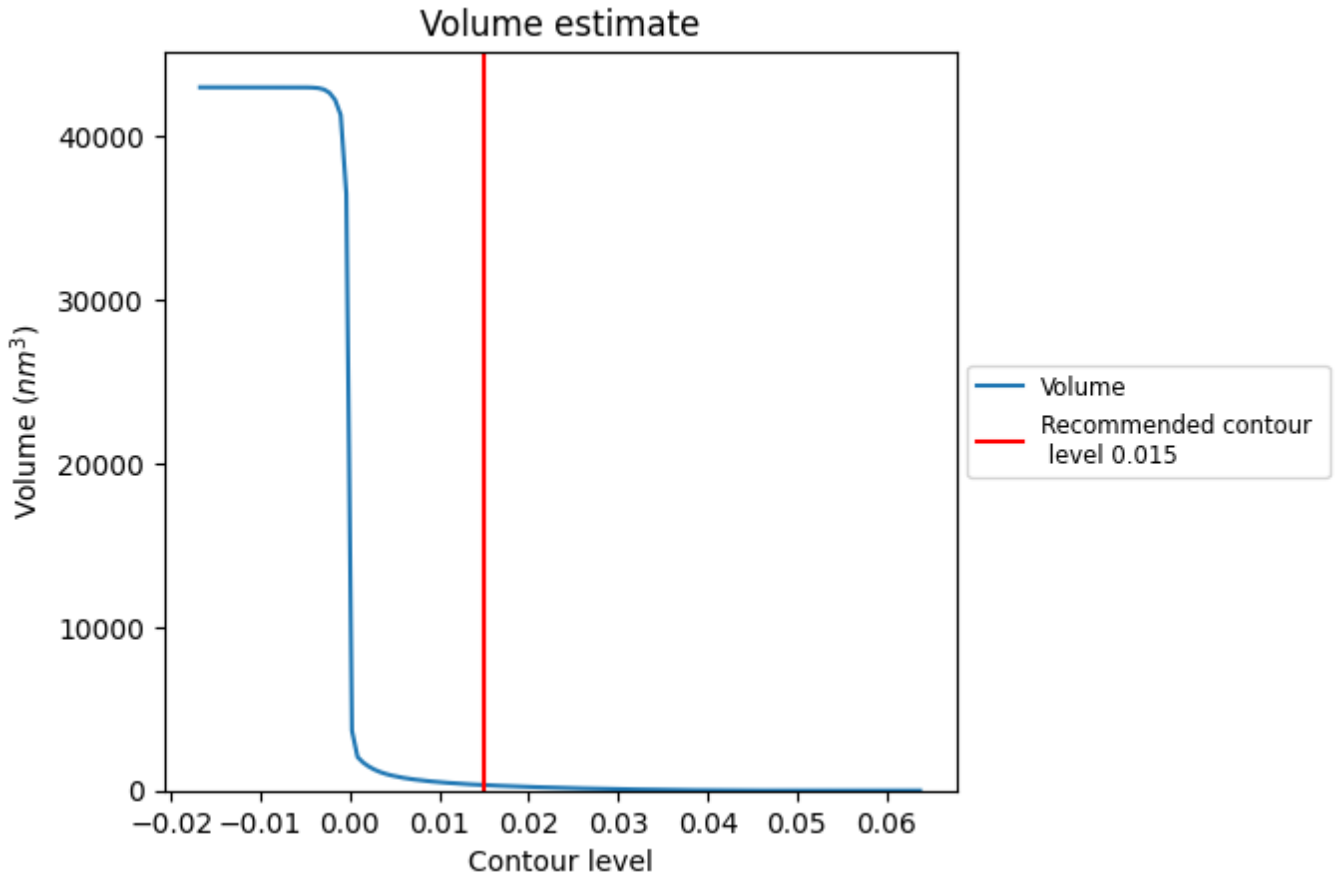
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

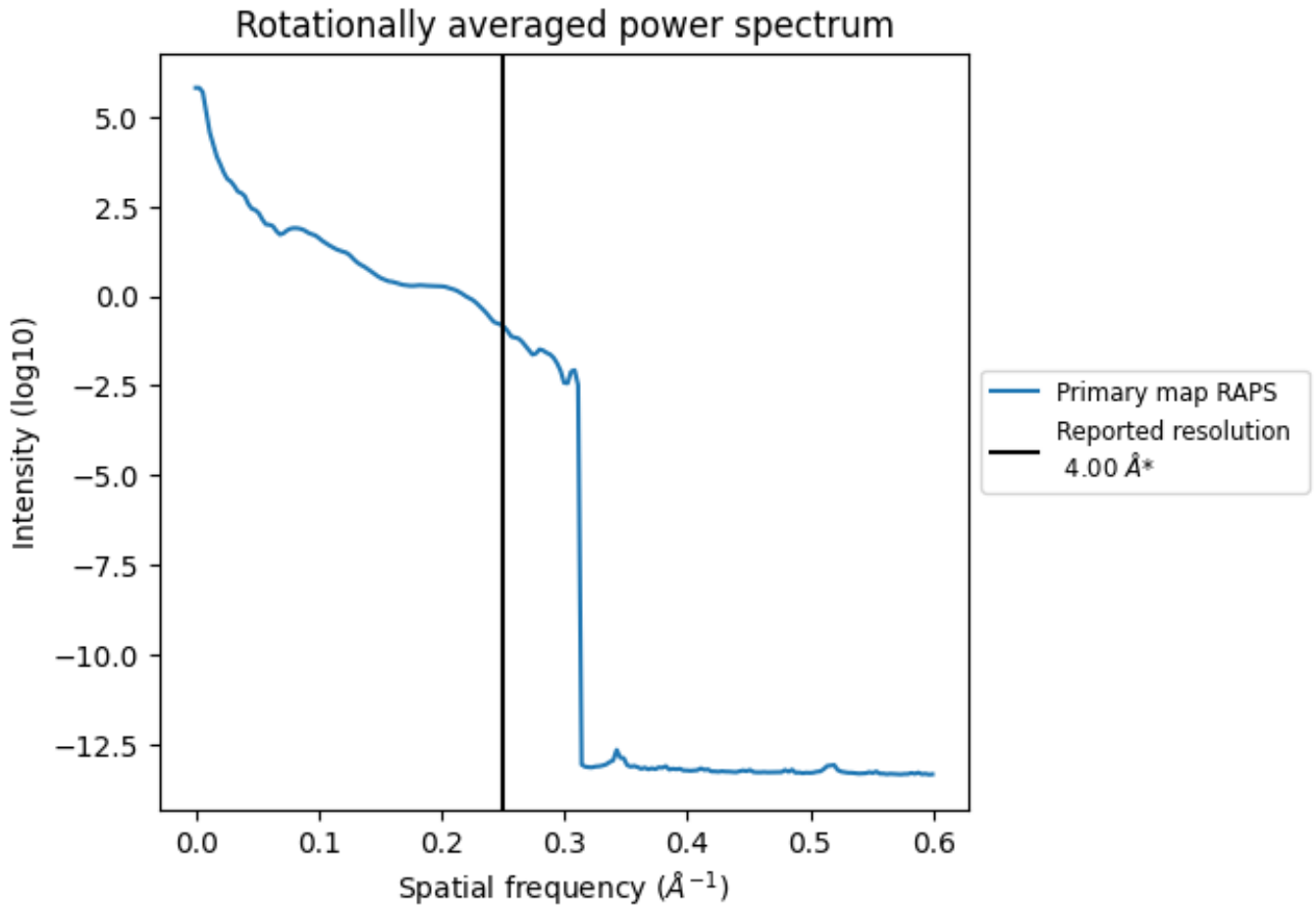
7.2 Volume estimate (i)



The volume at the recommended contour level is 337 nm^3; this corresponds to an approximate mass of 305 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.250 $Å^{-1}$

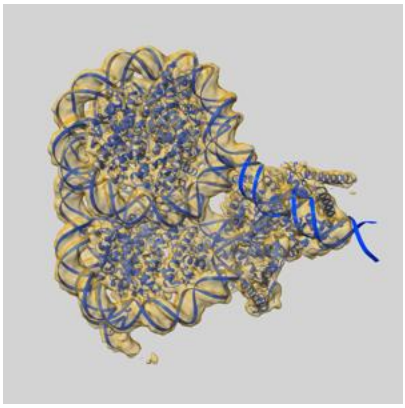
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

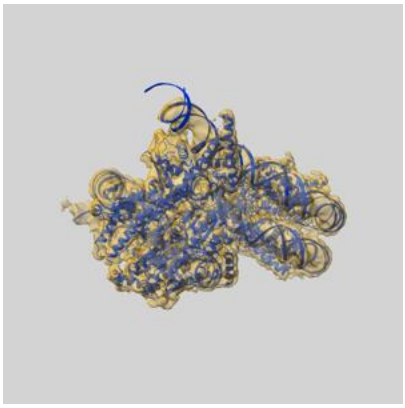
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51241 and PDB model 9GD1. Per-residue inclusion information can be found in section 3 on page 8.

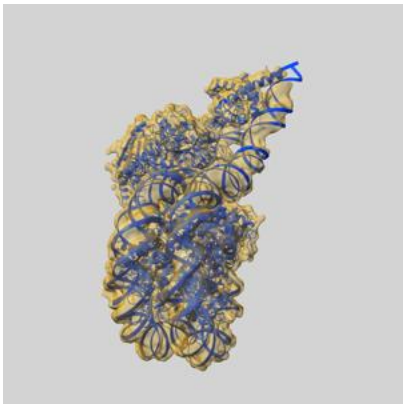
9.1 Map-model overlay



X



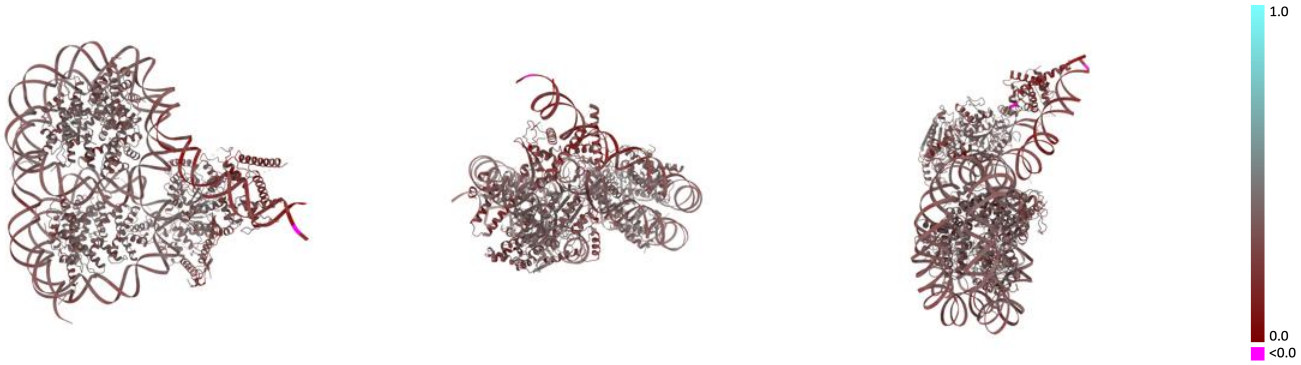
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

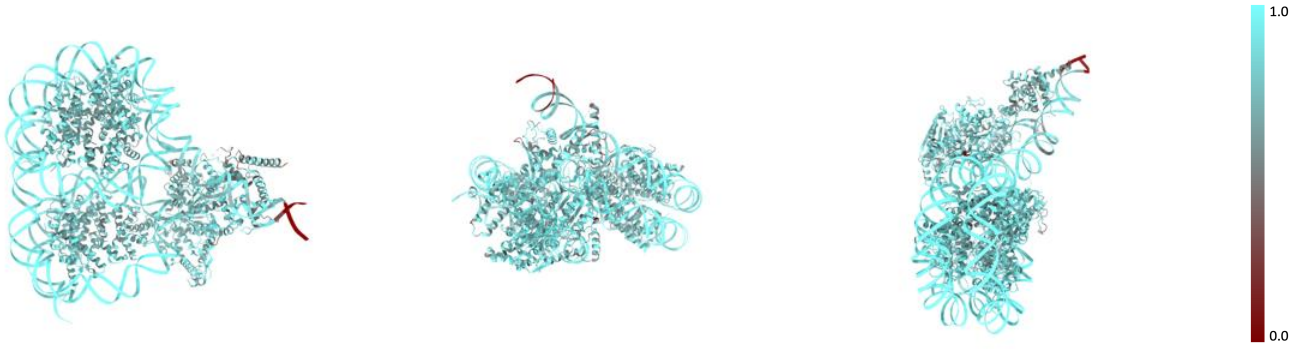
9.2 Q-score mapped to coordinate model



X Y Z

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

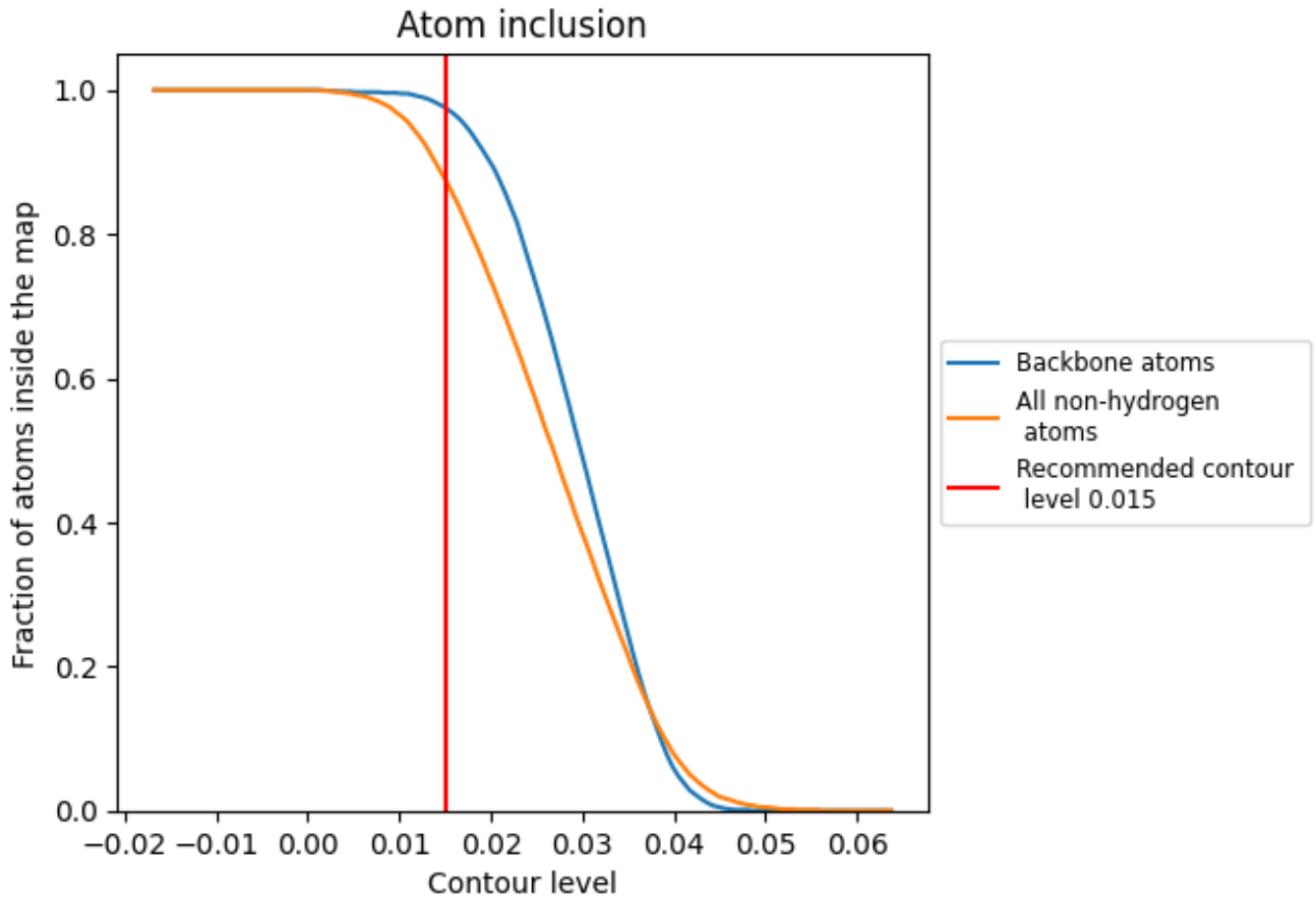
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 88% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8770	0.3320
A	0.8100	0.3520
B	0.8480	0.3780
C	0.8540	0.3770
D	0.8550	0.3630
E	0.8660	0.3610
F	0.8750	0.3850
G	0.8490	0.3680
H	0.8410	0.3600
I	0.9500	0.3100
J	0.9490	0.3130
K	0.8470	0.3730
L	0.8410	0.3560
M	0.8550	0.3570
N	0.8870	0.3440
O	0.8480	0.3370
P	0.8670	0.3500
W	0.7990	0.3210