Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 05:56 AM EDT

PDB ID	:	9EAR / pdb_00009ear
EMDB ID	:	EMD-47841
Title	:	CHD1-nucleosome complex (closed state)
Authors	:	James, A.M.; Farnung, L.
Deposited on	:	2024-11-11
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

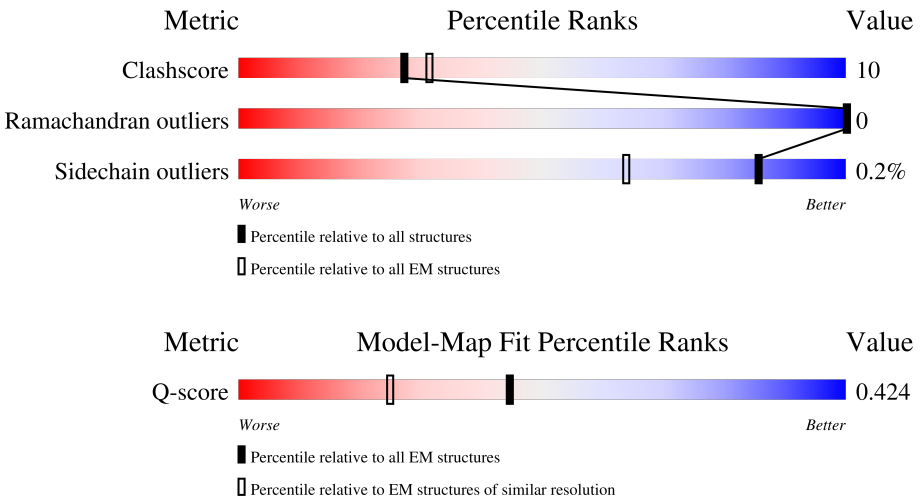
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 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 <=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	68% 7% 25%
1	E	136	67% 29%
2	B	86	7% 93% 7%
2	F	86	85% 6% 9%

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Mol	Chain	Length	Quality of chain
3	C	105	90% 9%
3	G	105	92% 8%
4	D	95	88% 12%
4	H	95	88% 9%
5	I	158	27% 68% 5%
6	J	158	51% 45%
7	W	1329	5% 43% 7% 50%

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
8	ADP	W	1501	-	-	X	-
9	BEF	W	1502	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 18004 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	102	845	532	165	145	3	0	0
1	E	97	800	504	155	139	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1
E	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	86	694	436	140	117	1	0	0
2	F	78	619	391	120	107	1	0	0

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	103	796	501	155	140	0	0
3	G	105	810	510	158	142	0	0

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	95	745	469	134	140	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	93	726	457	130	137	2	0	0

- Molecule 5 is a DNA chain called DNA (205-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	I	158	3219	1529	586	946	158	0	0

- Molecule 6 is a DNA chain called DNA (205-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	J	158	3259	1543	608	950	158	0	0

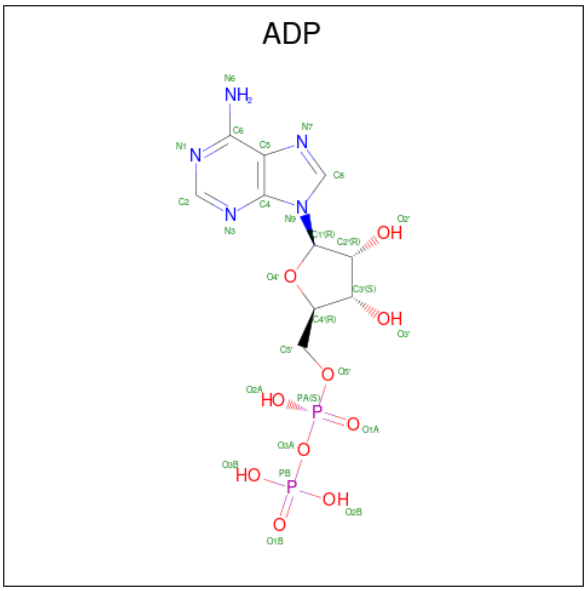
- Molecule 7 is a protein called Chromodomain-helicase-DNA-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	W	663	5460	3485	957	993	25	0	0

There are 3 discrepancies between the modelled and reference sequences:

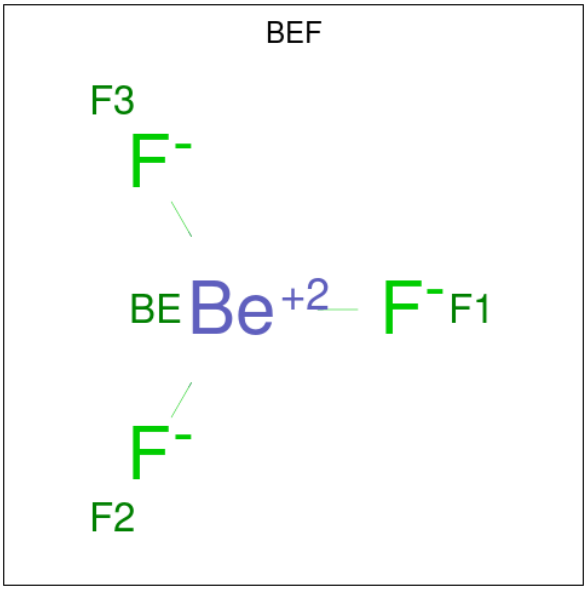
Chain	Residue	Modelled	Actual	Comment	Reference
W	-1	SER	-	expression tag	UNP O14646
W	0	ASN	-	expression tag	UNP O14646
W	1	ALA	-	expression tag	UNP O14646

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



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

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



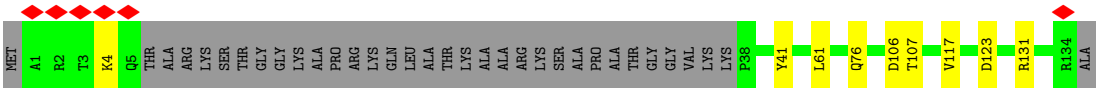
Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
9	W	1	4	1	3	0

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.

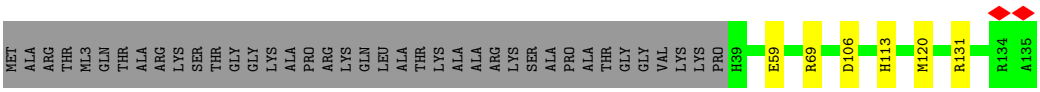
• Molecule 1: Histone H3

Chain A:



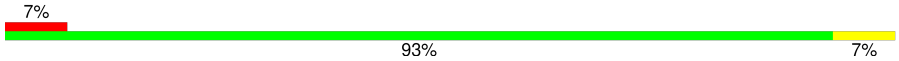
• Molecule 1: Histone H3

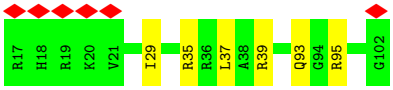
Chain E:



• Molecule 2: Histone H4

Chain B:



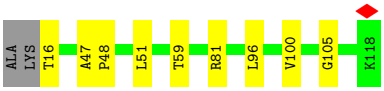


• Molecule 2: Histone H4

Chain F:

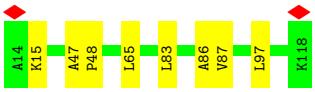
• Molecule 3: Histone H2A

Chain C:



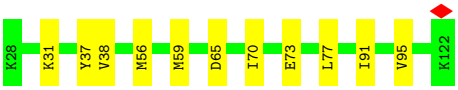
• Molecule 3: Histone H2A

Chain G:



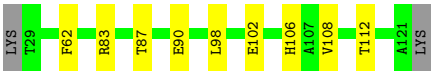
• Molecule 4: Histone H2B

Chain D:



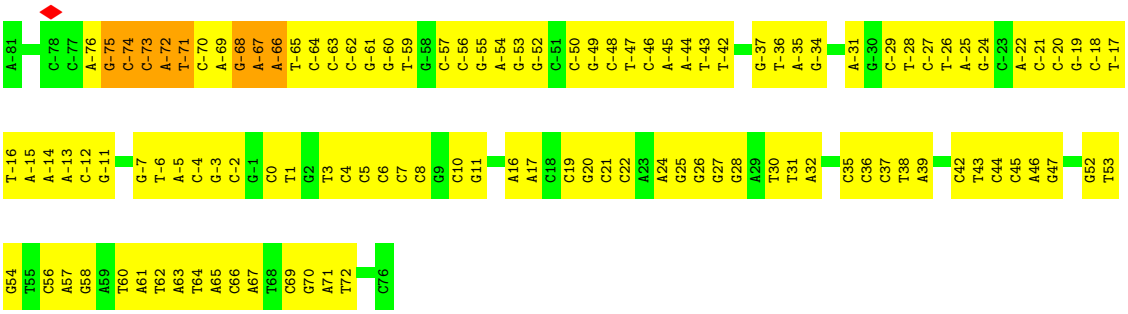
• Molecule 4: Histone H2B

Chain H:



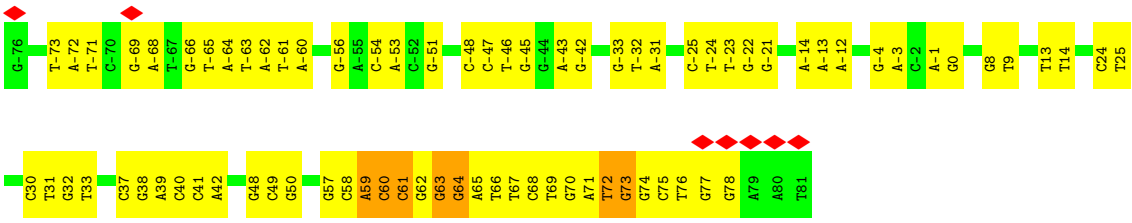
• Molecule 5: DNA (205-MER)

Chain I:



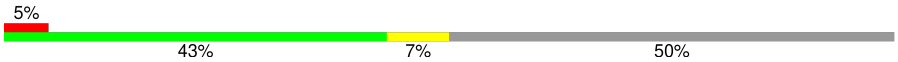
• Molecule 6: DNA (205-MER)

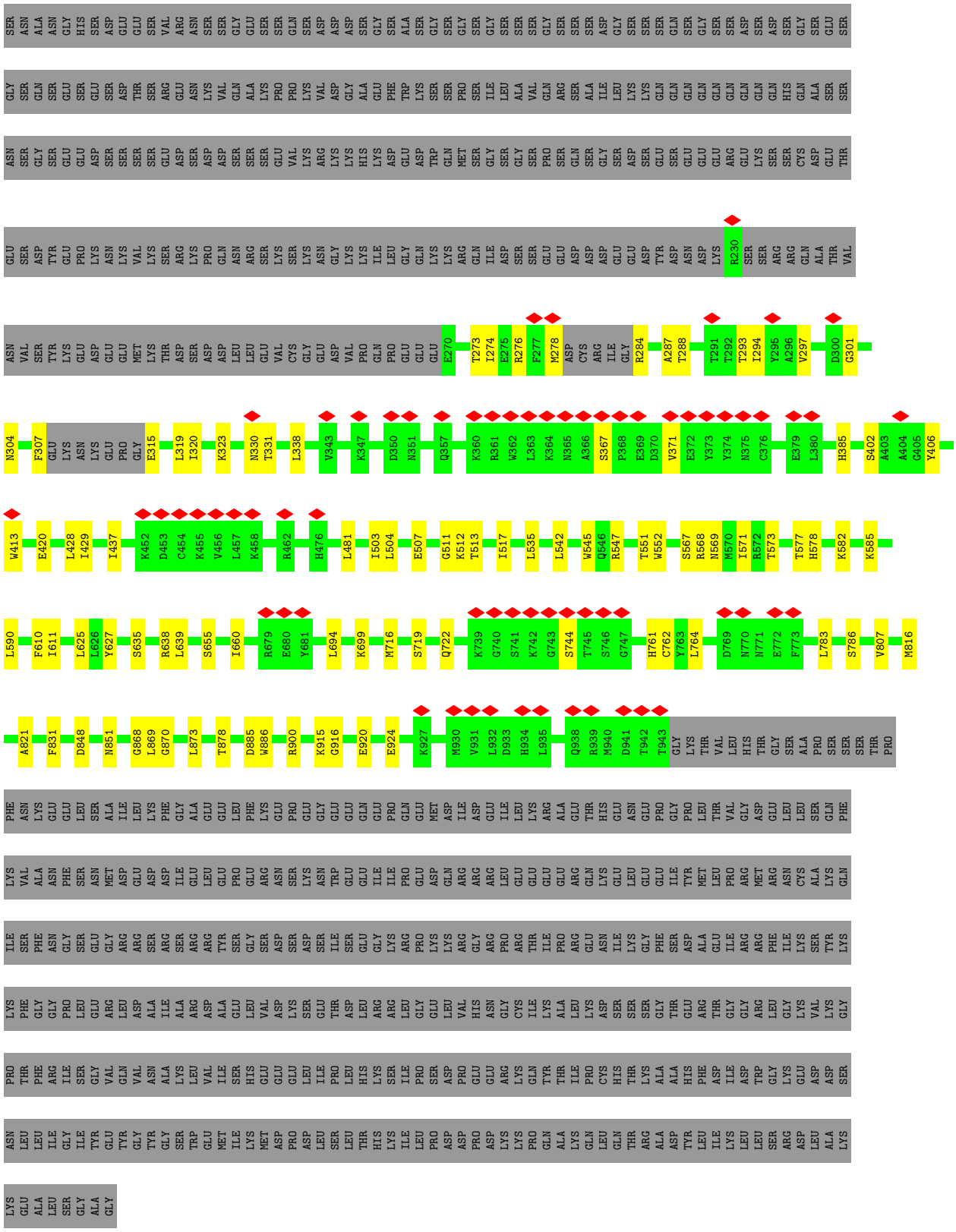
Chain J:



• Molecule 7: Chromodomain-helicase-DNA-binding protein 1

Chain W:




SER ASN ALA ASN GLY HIS SER ASP GLU GLU SER VAL ARG ASN SER SER GLY GLU SER SER GLN SER ASP ASP ASP SER GLY SER SER ASP SER SER GLY SER SER GLY SER GLY SER SER SER GLY SER SER SER GLN SER GLY SER SER ASP GLY SER SER SER GLN SER GLY SER SER ASP SER SER SER GLY SER GLN SER ASP GLU GLU SER THR SER ARG GLU ASN LYS VAL GLN ALA LYS PRO PRO LYS VAL ASP GLY ALA GLU PHE TRP LYS SER SER PRO SER ILE LEU ALA VAL GLN ARG SER ALA ILE LEU LYS LYS GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN GLN HIS GLN ALA SER SER
ASN SER GLY SER GLU GLU ASP SER SER SER GLU ASP SER ASP ASP SER SER SER GLU VAL LYS LYS HIS LYS ASP GLU ASP TRP GLN MET SER GLY SER GLY SER PRO SER GLU SER GLN SER GLY SER ASP SER GLU SER GLU GLU ARG GLU LYS SER SER CYS ASP GLU THR
GLU SER ASP TYR GLU PRO LYS ASN LYS VAL LYS SER ARG LYS PRO GLN ASN ARG SER LYS SER LYS ASN GLY LYS LYS LYS ILE LEU GLY GLN LYS LYS ARG GLN ILE ASP SER SER GLU GLU ASP ASP ASP GLU GLU GLU ASP TYR ASP ASN ASP LYS R230 SER SER ARG ARG GLN ALA THR VAL
ASN VAL SER TYR LYS GLU ASP GLU GLU MET LYS THR ASP SER ASP ASP LEU LEU GLU VAL CYS GLY GLU ASP VAL PRO GLN PRO GLU GLU GLU E270 T273 I274 E275 R276 F277 M278 ASP CYS ARG ILE GLY R284 A287 T288 T291 T292 T293 I294 Y295 A296 V297 D300 G301
N304 F307 GLU LYS ASN LYS GLU PRO GLY E315 L319 I320 K323 N330 T331 L338 V343 K347 D350 N351 Q357 K360 R361 W362 L363 K364 N365 A366 S367 P368 E369 D370 V371 E372 Y373 Y374 N375 C376 E379 L380 H385 S402 A403 A404 G405 Y406
W413 E420 L428 I429 I437 K452 D453 C454 K455 V456 L457 K458 R462 H476 L481 I503 L504 E507 G511 K512 T513 I517 L535 L542 W545 Q546 R547 T551 W552 S567 R568 N569 M570 I571 R572 T573 T577 H578 K582 K585
L590 F610 I611 L625 L626 Y627 S635 R638 L639 S655 I660 R679 E680 Y681 L694 K699 M716 S719 Q722 K739 G740 S741 K742 G743 S744 T745 S746 G747 H761 C762 Y763 L764 D769 N770 M771 E772 F773 L783 S786 V807 M816
A821 F831 D848 N851 G868 L869 G870 L873 T878 D885 W886 R900 K915 G916 E920 E924 K927 M930 V931 L932 D933 H934 L935 Q938 R939 M940 D941 T942 T943 GLY LYS THR VAL LEU HIS THR GLY SER ALA PRO SER SER SER THR PRO
PHE ASN LYS GLU GLU LEU SER ALA ILE LEU LYS PHE GLY ALA GLU GLU LEU PHE LYS GLU PRO GLU GLY GLU GLU GLU GLN GLU PRO GLN GLU MET ASP ILE ASP GLU ILE LEU LYS ARG ALA GLU THR HIS GLU ASN GLU PRO GLY PRO LEU THR VAL GLY ASP GLU LEU LEU SER GLN PHE
LYS VAL ALA ASN PHE SER ASN MET ASP GLU ASP ASP ILE GLU LEU GLU PRO GLU ARG ASN SER LYS ASN TRP GLU GLU GLU ILE ILE PRO GLU ASP GLN ARG ARG ARG ARG LEU GLU GLU GLU GLU GLU ILE TYR MET LEU PRO ARG MET ARG ASN CYS ALA LYS GLN
ILE SER PHE ASN GLY SER GLU GLY ARG ARG SER ARG SER ARG ARG ARG TYR SER GLY SER ASP SER ASP SER ILE SER GLU GLY LYS ARG PRO LYS LYS ARG GLY ARG PRO ARG THR ILE PRO ARG GLU ASN ILE LYS GLY PHE SER ASP ALA GLU ILE ARG ARG PHE ILE LYS SER TYR LYS
LYS PHE GLY GLY PRO LEU GLU ARG LEU ASP ALA ILE ALA ARG ASP ALA GLU LEU VAL ASP LYS SER GLU THR ASP LEU ARG ARG LEU GLY GLU LEU VAL HIS ASN GLY CYS ILE LYS ALA LEU LYS ASP SER SER SER GLY THR GLU ARG THR GLY GLY ARG LEU GLY LYS VAL LYS GLY
PRO THR PHE ARG ILE SER GLY VAL GLN VAL ASN ALA LYS LEU VAL ILE SER HIS GLU GLU GLU LEU ILE PRO LEU HIS LYS SER ILE PRO SER ASP PRO GLU GLU ARG LYS GLN TYR THR ILE PRO CYS HIS THR LYS ALA ALA HIS PHE ASP ILE ASP TRP GLY LYS GLU ASP SER
ASN LEU LEU ILE GLY ILE TYR GLU TYR GLY SER TRP GLU MET ILE LYS MET ASP PRO ASP LEU SER LEU THR HIS LYS ILE LEU PRO ASP ASP PRO ASP LYS LYS PRO GLN ALA LYS GLN LEU GLN THR ARG ALA ASP TYR LEU ILE LYS LEU LEU SER ARG ASP LEU ALA LYS
LYS GLU ALA LEU SER GLY ALA GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77190	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	54.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.828	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.0182	Depositor
Map size (Å)	249.0, 249.0, 249.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: ML3, BEF, 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	A	0.14	0/843	0.26	0/1128
1	E	0.14	0/811	0.26	0/1087
2	B	0.13	0/702	0.27	0/937
2	F	0.14	0/626	0.27	0/837
3	C	0.13	0/806	0.27	0/1088
3	G	0.13	0/820	0.25	0/1106
4	D	0.14	0/756	0.25	0/1015
4	H	0.13	0/737	0.24	0/993
5	I	0.31	0/3607	0.64	9/5559 (0.2%)
6	J	0.31	0/3659	0.64	7/5651 (0.1%)
7	W	0.11	0/5581	0.26	0/7514
All	All	0.22	0/18948	0.46	16/26915 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	60	DC	P-O3'-C3'	-9.98	105.23	120.20
6	J	64	DG	P-O3'-C3'	-9.71	105.64	120.20
5	I	-68	DG	P-O3'-C3'	-9.53	105.91	120.20
5	I	-66	DA	P-O3'-C3'	-9.13	106.51	120.20
5	I	-72	DA	P-O3'-C3'	-8.35	107.68	120.20
6	J	72	DT	P-O3'-C3'	-8.09	108.06	120.20
5	I	-74	DC	P-O3'-C3'	-7.34	109.19	120.20
5	I	-75	DG	P-O3'-C3'	-7.33	109.21	120.20
5	I	-73	DC	P-O3'-C3'	-7.23	109.36	120.20
6	J	61	DC	P-O3'-C3'	-6.88	109.88	120.20
6	J	73	DG	P-O3'-C3'	-6.66	110.21	120.20
6	J	63	DG	P-O3'-C3'	-5.59	111.81	120.20
5	I	-67	DA	P-O3'-C3'	-5.43	112.05	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	-73	DC	OP2-P-O3'	5.26	123.79	108.00
6	J	59	DA	P-O3'-C3'	-5.19	112.42	120.20
5	I	-71	DT	P-O3'-C3'	-5.09	112.57	120.20

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	845	0	892	7	0
1	E	800	0	838	4	0
2	B	694	0	742	4	0
2	F	619	0	659	6	0
3	C	796	0	846	6	0
3	G	810	0	864	6	0
4	D	745	0	773	12	0
4	H	726	0	747	6	0
5	I	3219	0	1773	132	0
6	J	3259	0	1775	97	0
7	W	5460	0	5447	72	0
8	W	27	0	10	10	0
9	W	4	0	0	6	0
All	All	18004	0	15366	322	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 10.

All (322) 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)
7:W:900:ARG:NH2	8:W:1501:ADP:O2B	1.72	1.22
7:W:511:GLY:HA2	8:W:1501:ADP:O2A	1.45	1.16
6:J:61:DC:H2"	6:J:62:DG:H5"	1.48	0.95
5:I:-69:DA:H2"	5:I:-68:DG:H5"	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:75:DC:H2'	6:J:76:DT:C6	2.14	0.82
6:J:75:DC:C6	6:J:76:DT:H72	2.17	0.80
7:W:900:ARG:CZ	9:W:1502:BEF:F1	2.20	0.79
7:W:722:GLN:NE2	7:W:762:CYS:SG	2.56	0.78
7:W:719:SER:OG	7:W:722:GLN:OE1	2.01	0.77
7:W:569:ASN:O	7:W:573:THR:HG23	1.88	0.73
5:I:-48:DC:H2"	5:I:-47:DT:H71	1.71	0.72
7:W:870:GLY:HA2	9:W:1502:BEF:F3	1.80	0.72
1:E:59:GLU:OE1	1:E:59:GLU:N	2.21	0.71
6:J:63:DG:H2"	6:J:64:DG:C8	2.25	0.71
5:I:-69:DA:C2'	5:I:-68:DG:H5"	2.19	0.71
7:W:315:GLU:N	7:W:315:GLU:OE1	2.23	0.71
7:W:402:SER:OG	7:W:406:TYR:O	2.08	0.69
5:I:-72:DA:H2'	5:I:-71:DT:C6	2.28	0.69
1:E:69:ARG:NH2	5:I:17:DA:OP1	2.26	0.69
7:W:294:ILE:HD11	7:W:428:LEU:HD11	1.75	0.67
6:J:66:DT:H2"	6:J:67:DT:H71	1.75	0.67
7:W:481:LEU:HA	8:W:1501:ADP:HN62	1.59	0.67
3:C:59:THR:HG23	4:D:59:MET:HE2	1.78	0.65
5:I:63:DA:H2'	5:I:64:DT:C6	2.32	0.65
6:J:65:DA:H2"	6:J:66:DT:OP1	1.96	0.65
6:J:-25:DC:H2"	6:J:-24:DT:H71	1.77	0.64
7:W:900:ARG:NH2	8:W:1501:ADP:PB	2.71	0.63
4:H:87:THR:OG1	4:H:90:GLU:OE1	2.03	0.63
5:I:-64:DC:H4'	5:I:-63:DC:OP1	1.99	0.63
6:J:64:DG:O5'	6:J:64:DG:H8	1.81	0.62
7:W:511:GLY:CA	8:W:1501:ADP:O2A	2.37	0.62
7:W:513:THR:CG2	8:W:1501:ADP:O1A	2.48	0.62
5:I:42:DC:H2'	5:I:43:DT:H72	1.82	0.61
7:W:547:ARG:NH2	7:W:848:ASP:OD2	2.33	0.61
6:J:59:DA:H2'	6:J:60:DC:O4'	2.01	0.61
6:J:66:DT:H2"	6:J:67:DT:C7	2.31	0.60
6:J:73:DG:C2	6:J:74:DG:C6	2.89	0.60
6:J:-24:DT:H2'	6:J:-23:DT:H71	1.82	0.60
7:W:367:SER:O	7:W:371:VAL:HG23	2.01	0.60
7:W:577:THR:O	7:W:585:LYS:NZ	2.34	0.60
7:W:278:MET:SD	7:W:385:HIS:ND1	2.75	0.60
7:W:885:ASP:OD1	7:W:886:TRP:N	2.35	0.60
6:J:64:DG:H2'	6:J:65:DA:C8	2.38	0.59
2:F:92:ARG:HH21	4:H:98:LEU:HD23	1.67	0.59
1:A:123:ASP:OD1	1:E:113:HIS:NE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-60:DG:H22	6:J:60:DC:H5	1.50	0.59
6:J:65:DA:H3'	6:J:66:DT:C7	2.32	0.59
7:W:294:ILE:CD1	7:W:428:LEU:HD11	2.33	0.59
1:A:106:ASP:OD2	1:A:131:ARG:NH1	2.36	0.59
2:F:68:ASP:OD2	2:F:92:ARG:NH1	2.36	0.58
7:W:627:TYR:OH	7:W:655:SER:O	2.21	0.58
5:I:70:DG:N2	6:J:-69:DG:C6	2.71	0.58
5:I:-36:DT:H2"	5:I:-35:DA:N7	2.17	0.58
7:W:512:LYS:NZ	8:W:1501:ADP:O2B	2.36	0.58
6:J:41:DC:H2'	6:J:42:DA:C8	2.37	0.58
4:D:38:VAL:HG21	4:D:56:MET:HE1	1.85	0.58
5:I:53:DT:H2"	5:I:54:DG:C8	2.38	0.57
4:D:65:ASP:OD2	2:F:98:TYR:OH	2.21	0.57
5:I:-63:DC:N4	6:J:62:DG:O6	2.38	0.57
5:I:-18:DC:H2'	5:I:-17:DT:H72	1.87	0.56
5:I:38:DT:H2"	5:I:39:DA:C8	2.41	0.56
7:W:578:HIS:O	7:W:582:LYS:N	2.39	0.56
5:I:56:DC:H2"	5:I:57:DA:N7	2.21	0.56
6:J:74:DG:H2"	6:J:75:DC:O4'	2.06	0.56
7:W:535:LEU:HD13	7:W:545:TRP:CZ3	2.40	0.56
5:I:-68:DG:H2"	5:I:-67:DA:C8	2.40	0.56
5:I:26:DG:H2"	5:I:27:DG:C8	2.41	0.56
6:J:68:DC:H2"	6:J:69:DT:O5'	2.06	0.56
7:W:900:ARG:NH2	9:W:1502:BEF:F1	2.29	0.55
6:J:-32:DT:H2'	6:J:-31:DA:C8	2.41	0.55
5:I:-44:DA:C2'	5:I:-43:DT:H71	2.36	0.55
5:I:71:DA:H2"	5:I:72:DT:H71	1.87	0.55
5:I:-54:DA:H2"	5:I:-53:DG:C8	2.41	0.55
6:J:30:DC:H2'	6:J:31:DT:H72	1.88	0.55
7:W:503:ILE:CD1	7:W:660:ILE:HD11	2.37	0.55
5:I:-67:DA:H2"	5:I:-66:DA:O5'	2.05	0.55
5:I:57:DA:C2	6:J:-56:DG:N2	2.75	0.55
7:W:284:ARG:NE	7:W:307:PHE:O	2.34	0.54
7:W:513:THR:HG21	8:W:1501:ADP:O1A	2.06	0.54
4:H:83:ARG:NH2	6:J:-33:DG:OP2	2.40	0.54
7:W:503:ILE:HD12	7:W:660:ILE:HD11	1.89	0.54
5:I:-12:DC:H2"	5:I:-11:DG:C8	2.43	0.53
5:I:-45:DA:H1'	5:I:-44:DA:C8	2.43	0.53
5:I:35:DC:H2"	5:I:36:DC:C5	2.44	0.53
6:J:-64:DA:H2"	6:J:-63:DT:C6	2.43	0.53
7:W:900:ARG:NH1	9:W:1502:BEF:F1	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:4:DC:H2"	5:I:5:DC:C6	2.44	0.53
6:J:75:DC:H6	6:J:75:DC:H5"	1.73	0.53
5:I:-70:DC:H2"	5:I:-69:DA:OP2	2.09	0.53
5:I:-54:DA:C2'	5:I:-53:DG:C8	2.91	0.53
6:J:-4:DG:H2"	6:J:-3:DA:C8	2.44	0.53
5:I:-68:DG:H1	6:J:68:DC:H42	1.55	0.52
6:J:-61:DT:H2'	6:J:-60:DA:C8	2.44	0.52
7:W:783:LEU:O	7:W:786:SER:OG	2.27	0.52
7:W:284:ARG:N	7:W:304:ASN:O	2.43	0.52
5:I:-73:DC:C2	5:I:-72:DA:C8	2.96	0.52
5:I:-71:DT:OP2	5:I:-71:DT:H6	1.92	0.52
6:J:65:DA:H3'	6:J:66:DT:H72	1.90	0.52
5:I:-65:DT:H2"	5:I:-64:DC:O5'	2.10	0.52
5:I:-21:DC:C2'	5:I:-20:DC:H5'	2.39	0.52
1:A:76:GLN:OE1	7:W:744:SER:OG	2.26	0.52
5:I:-4:DC:H2"	5:I:-3:DG:C8	2.45	0.52
5:I:-75:DG:H2"	5:I:-74:DC:O4'	2.10	0.52
6:J:62:DG:H2"	6:J:63:DG:O4'	2.10	0.52
5:I:-60:DG:H2"	5:I:-59:DT:O5'	2.11	0.51
6:J:75:DC:C6	6:J:75:DC:H5"	2.45	0.51
5:I:-74:DC:N3	5:I:-73:DC:C4	2.78	0.51
5:I:-29:DC:H2'	5:I:-28:DT:H71	1.91	0.51
7:W:413:TRP:NE1	7:W:420:GLU:O	2.43	0.51
5:I:-75:DG:N2	6:J:75:DC:O2	2.43	0.51
5:I:36:DC:H2"	5:I:37:DC:C5	2.46	0.51
3:C:96:LEU:O	3:C:96:LEU:HD23	2.11	0.51
5:I:25:DG:H1'	5:I:26:DG:C8	2.45	0.51
5:I:66:DC:N3	5:I:67:DA:C6	2.78	0.51
5:I:-72:DA:H2'	5:I:-71:DT:C5	2.45	0.51
6:J:-25:DC:H2"	6:J:-24:DT:C7	2.40	0.51
4:D:73:GLU:O	4:D:77:LEU:HD23	2.11	0.50
3:G:65:LEU:HB2	3:G:86:ALA:HB1	1.92	0.50
5:I:62:DT:C2	5:I:63:DA:C8	2.99	0.50
6:J:8:DG:H2'	6:J:9:DT:H71	1.92	0.50
3:C:81:ARG:NH2	3:C:105:GLY:O	2.44	0.50
4:D:38:VAL:CB	4:D:56:MET:HE1	2.40	0.50
5:I:16:DA:H2"	5:I:17:DA:C8	2.45	0.50
5:I:-5:DA:H2"	5:I:-4:DC:C6	2.45	0.50
5:I:-43:DT:C6	5:I:-42:DT:H72	2.47	0.50
7:W:297:VAL:O	7:W:301:GLY:N	2.38	0.50
5:I:-71:DT:C2	5:I:-70:DC:C5	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-21:DC:H2'	5:I:-20:DC:C6	2.47	0.50
7:W:294:ILE:HA	7:W:297:VAL:HG12	1.92	0.50
4:D:38:VAL:CG2	4:D:56:MET:HE1	2.41	0.50
5:I:-60:DG:H2'	5:I:-60:DG:N3	2.27	0.50
5:I:7:DC:H2"	5:I:8:DC:C6	2.47	0.50
6:J:-43:DA:H2"	6:J:-42:DG:C8	2.47	0.50
6:J:-47:DC:H2"	6:J:-46:DT:C5	2.47	0.49
6:J:-13:DA:C4	6:J:-12:DA:C8	2.99	0.49
6:J:60:DC:N3	6:J:61:DC:N4	2.60	0.49
5:I:5:DC:H2"	5:I:6:DC:C5	2.47	0.49
6:J:32:DG:H2"	6:J:33:DT:H71	1.94	0.49
5:I:-55:DG:H1'	5:I:-54:DA:C8	2.47	0.49
7:W:764:LEU:HD21	7:W:816:MET:SD	2.52	0.49
6:J:-48:DC:H2"	6:J:-47:DC:C5	2.48	0.49
5:I:19:DC:H2"	5:I:20:DG:C8	2.48	0.48
6:J:68:DC:H2'	6:J:69:DT:C6	2.48	0.48
7:W:320:ILE:HG22	7:W:331:THR:H	1.78	0.48
5:I:-25:DA:H1'	5:I:-24:DG:C8	2.48	0.48
6:J:73:DG:N2	6:J:74:DG:C6	2.81	0.48
4:H:108:VAL:O	4:H:112:THR:HG23	2.12	0.48
5:I:-71:DT:H2"	5:I:-70:DC:H6	1.79	0.48
5:I:-55:DG:H2"	5:I:-54:DA:C8	2.49	0.48
6:J:-14:DA:H2"	6:J:-13:DA:C8	2.48	0.48
5:I:-47:DT:H2"	5:I:-46:DC:C6	2.49	0.48
5:I:-7:DG:H2"	5:I:-6:DT:C7	2.44	0.48
6:J:-54:DC:H2"	6:J:-53:DA:C8	2.49	0.48
6:J:60:DC:N3	6:J:61:DC:C4	2.82	0.48
6:J:65:DA:H8	6:J:65:DA:P	2.36	0.48
7:W:319:LEU:HD12	7:W:319:LEU:H	1.78	0.48
5:I:-26:DT:H2'	5:I:-25:DA:C8	2.49	0.48
5:I:37:DC:C2'	5:I:38:DT:H72	2.44	0.48
6:J:30:DC:C2'	6:J:31:DT:H72	2.43	0.48
5:I:-76:DA:H1'	5:I:-75:DG:H5'	1.96	0.47
5:I:-48:DC:H2"	5:I:-47:DT:C7	2.41	0.47
5:I:-13:DA:C2	6:J:14:DT:O2	2.67	0.47
7:W:551:THR:HG1	7:W:552:TRP:CD1	2.32	0.47
6:J:74:DG:H1'	6:J:75:DC:OP1	2.14	0.47
7:W:851:ASN:ND2	7:W:873:LEU:O	2.47	0.47
5:I:24:DA:H2"	5:I:25:DG:C8	2.49	0.47
6:J:65:DA:C8	6:J:65:DA:O5'	2.68	0.47
7:W:611:ILE:HD12	7:W:635:SER:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:38:VAL:HB	4:D:56:MET:HE1	1.96	0.47
5:I:-69:DA:C3'	5:I:-68:DG:H5"	2.45	0.47
5:I:64:DT:H2"	5:I:65:DA:H8	1.80	0.47
6:J:64:DG:H3'	6:J:65:DA:C8	2.50	0.47
6:J:38:DG:H2"	6:J:39:DA:C8	2.50	0.47
5:I:-28:DT:H2"	5:I:-27:DC:O4'	2.14	0.47
6:J:76:DT:H2'	6:J:77:DG:N7	2.30	0.47
4:H:102:GLU:OE2	4:H:106:HIS:NE2	2.44	0.46
6:J:24:DC:H2"	6:J:25:DT:C6	2.51	0.46
5:I:-50:DC:H2"	5:I:-49:DG:C8	2.49	0.46
5:I:-43:DT:H2'	5:I:-42:DT:H72	1.96	0.46
5:I:70:DG:H2'	5:I:71:DA:C8	2.50	0.46
7:W:610:PHE:CZ	7:W:639:LEU:HD22	2.50	0.46
1:A:61:LEU:HD12	2:B:37:LEU:HD23	1.96	0.46
6:J:-73:DT:H4'	6:J:-72:DA:OP1	2.16	0.46
7:W:273:THR:O	7:W:323:LYS:N	2.40	0.46
5:I:3:DT:H2"	5:I:4:DC:C6	2.50	0.46
5:I:36:DC:H2"	5:I:37:DC:C6	2.50	0.46
5:I:-35:DA:H2"	5:I:-34:DG:C8	2.51	0.46
5:I:-27:DC:C2'	5:I:-26:DT:H72	2.46	0.46
6:J:13:DT:OP1	7:W:276:ARG:NH1	2.48	0.46
6:J:49:DC:H2'	6:J:50:DG:C8	2.50	0.46
7:W:870:GLY:O	9:W:1502:BEF:F1	2.24	0.46
5:I:-35:DA:C2'	5:I:-34:DG:C8	2.99	0.46
5:I:-27:DC:H2"	5:I:-26:DT:C6	2.51	0.46
5:I:-54:DA:H2'	5:I:-53:DG:C8	2.51	0.45
6:J:60:DC:O4'	6:J:60:DC:O2	2.34	0.45
3:C:51:LEU:HD13	4:D:70:ILE:HG21	1.98	0.45
4:D:91:ILE:O	4:D:95:VAL:HG23	2.16	0.45
5:I:-73:DC:H2"	5:I:-72:DA:O5'	2.16	0.45
5:I:-20:DC:H2"	5:I:-19:DG:H8	1.81	0.45
5:I:-18:DC:C2'	5:I:-17:DT:H72	2.45	0.45
7:W:610:PHE:CE2	7:W:639:LEU:HD22	2.52	0.45
7:W:807:VAL:HG13	7:W:878:THR:CG2	2.47	0.45
5:I:52:DG:C2	6:J:-51:DG:C2	3.05	0.45
1:E:106:ASP:OD2	1:E:131:ARG:NH2	2.49	0.45
5:I:-29:DC:H2'	5:I:-28:DT:C7	2.47	0.45
7:W:513:THR:HG22	8:W:1501:ADP:O1A	2.16	0.45
7:W:821:ALA:HB1	7:W:831:PHE:CZ	2.51	0.45
5:I:-53:DG:C4	5:I:-52:DG:N7	2.85	0.45
2:B:93:GLN:OE1	2:B:95:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:37:DC:H2"	5:I:38:DT:C7	2.47	0.45
6:J:74:DG:H2"	6:J:75:DC:C6	2.51	0.45
4:D:56:MET:HE3	4:D:56:MET:O	2.17	0.45
5:I:-16:DT:OP1	7:W:568:ARG:NH2	2.48	0.45
6:J:-66:DG:H2"	6:J:-65:DT:C6	2.52	0.45
5:I:-16:DT:H1'	5:I:-15:DA:C8	2.52	0.45
5:I:53:DT:C2'	5:I:54:DG:C8	3.00	0.45
6:J:64:DG:H3'	6:J:65:DA:H8	1.82	0.45
6:J:74:DG:C4	6:J:75:DC:C2	3.04	0.45
3:G:97:LEU:HD12	3:G:97:LEU:N	2.32	0.45
5:I:57:DA:H1'	5:I:58:DG:C8	2.52	0.45
5:I:44:DC:H2"	5:I:45:DC:C6	2.51	0.45
6:J:74:DG:C2'	6:J:75:DC:C6	3.00	0.45
6:J:-33:DG:H2"	6:J:-32:DT:O4'	2.17	0.44
6:J:75:DC:H2'	6:J:76:DT:C5	2.50	0.44
7:W:761:HIS:HB2	7:W:816:MET:HE1	2.00	0.44
4:D:37:TYR:OH	6:J:48:DG:OP1	2.34	0.44
5:I:-75:DG:C2	5:I:-74:DC:N4	2.85	0.44
5:I:-15:DA:H2"	5:I:-14:DA:C8	2.53	0.44
5:I:-71:DT:H2"	5:I:-70:DC:C6	2.53	0.44
5:I:-71:DT:H2"	5:I:-70:DC:OP2	2.18	0.44
5:I:-66:DA:C8	5:I:-65:DT:N3	2.85	0.44
5:I:61:DA:C2	6:J:-60:DA:C2	3.05	0.44
6:J:60:DC:C4	6:J:61:DC:C4	3.06	0.44
7:W:900:ARG:NH1	9:W:1502:BEF:F2	2.28	0.44
2:F:35:ARG:O	2:F:39:ARG:HG2	2.18	0.44
7:W:504:LEU:C	7:W:504:LEU:HD23	2.43	0.44
5:I:-7:DG:H4'	5:I:-6:DT:OP1	2.18	0.44
5:I:0:DC:H2'	5:I:1:DT:H72	2.00	0.43
6:J:39:DA:H2"	6:J:40:DC:C6	2.53	0.43
7:W:513:THR:O	7:W:517:ILE:HG13	2.18	0.43
7:W:916:GLY:N	7:W:920:GLU:OE2	2.48	0.43
5:I:10:DC:H2"	5:I:11:DG:C8	2.53	0.43
6:J:71:DA:H2"	6:J:72:DT:C6	2.53	0.43
7:W:319:LEU:HD23	7:W:330:ASN:OD1	2.19	0.43
1:A:107:THR:HG23	1:A:123:ASP:CB	2.47	0.43
5:I:-22:DA:H2"	5:I:-21:DC:H6	1.84	0.43
5:I:71:DA:H1'	5:I:72:DT:C6	2.53	0.43
5:I:-56:DC:H2"	5:I:-55:DG:N7	2.34	0.43
7:W:694:LEU:C	7:W:694:LEU:HD23	2.43	0.43
5:I:-75:DG:N2	6:J:76:DT:N3	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-67:DA:H2'	5:I:-66:DA:C2	2.52	0.43
5:I:57:DA:C4	5:I:58:DG:C5	3.07	0.43
7:W:429:ILE:HG22	7:W:437:ILE:HD11	2.00	0.43
7:W:507:GLU:OE1	7:W:699:LYS:N	2.40	0.43
7:W:567:SER:O	7:W:571:ILE:HG13	2.19	0.43
7:W:716:MET:O	7:W:915:LYS:N	2.46	0.43
7:W:920:GLU:O	7:W:924:GLU:HG2	2.19	0.43
5:I:-69:DA:C2	6:J:70:DG:N2	2.87	0.43
5:I:60:DT:H2"	5:I:61:DA:H8	1.84	0.43
6:J:-1:DA:H2"	6:J:0:DG:C8	2.54	0.43
6:J:65:DA:H8	6:J:65:DA:O5'	2.02	0.43
3:G:97:LEU:HD11	4:H:62:PHE:CE1	2.54	0.42
4:D:31:LYS:HD2	4:D:31:LYS:O	2.18	0.42
6:J:-73:DT:H2"	6:J:-72:DA:C8	2.54	0.42
6:J:-69:DG:O5'	6:J:-69:DG:C8	2.72	0.42
5:I:-37:DG:H2"	5:I:-36:DT:C6	2.54	0.42
7:W:287:ALA:O	7:W:288:THR:HG23	2.18	0.42
7:W:761:HIS:CB	7:W:816:MET:HE1	2.49	0.42
5:I:-7:DG:H2"	5:I:-6:DT:H71	2.00	0.42
5:I:61:DA:H2"	5:I:62:DT:O4'	2.19	0.42
6:J:-69:DG:H3'	6:J:-68:DA:C5'	2.49	0.42
7:W:437:ILE:HD12	7:W:437:ILE:H	1.84	0.42
6:J:74:DG:N3	6:J:74:DG:H2'	2.35	0.42
7:W:900:ARG:HH21	8:W:1501:ADP:PB	2.42	0.42
3:C:100:VAL:HG11	2:F:98:TYR:CE2	2.53	0.42
5:I:70:DG:N2	6:J:-69:DG:O6	2.52	0.42
2:F:35:ARG:NH2	5:I:8:DC:OP2	2.40	0.42
5:I:-37:DG:H2"	5:I:-36:DT:H72	2.02	0.42
6:J:76:DT:H2"	6:J:77:DG:C8	2.54	0.42
3:G:83:LEU:O	3:G:87:VAL:HG23	2.19	0.42
5:I:-62:DC:H2'	5:I:-61:DG:C8	2.55	0.42
5:I:-44:DA:H2'	5:I:-43:DT:H71	2.01	0.42
5:I:21:DC:C2	5:I:22:DC:C6	3.08	0.42
6:J:37:DC:H2"	6:J:38:DG:C8	2.55	0.42
5:I:30:DT:H2'	5:I:31:DT:H71	2.02	0.41
7:W:635:SER:OG	7:W:638:ARG:NE	2.53	0.41
1:A:41:TYR:HA	5:I:69:DC:H1'	2.03	0.41
5:I:46:DA:H1'	5:I:47:DG:N7	2.35	0.41
3:G:15:LYS:O	6:J:-43:DA:H4'	2.20	0.41
2:B:35:ARG:O	2:B:39:ARG:HG2	2.20	0.41
5:I:-3:DG:H2"	5:I:-2:DC:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:-62:DA:H2'	6:J:-61:DT:C6	2.55	0.41
7:W:293:THR:O	7:W:297:VAL:HG12	2.19	0.41
3:C:47:ALA:N	3:C:48:PRO:HD2	2.35	0.41
5:I:-13:DA:C2	5:I:-12:DC:C2	3.09	0.41
2:B:29:ILE:N	2:B:29:ILE:HD12	2.36	0.41
5:I:-37:DG:H2"	5:I:-36:DT:C7	2.50	0.41
7:W:274:ILE:HD11	7:W:338:LEU:HD13	2.03	0.41
5:I:16:DA:H2"	5:I:17:DA:O5'	2.21	0.41
6:J:-69:DG:H3'	6:J:-68:DA:H5"	2.03	0.41
5:I:-64:DC:H2"	5:I:-63:DC:O5'	2.21	0.41
5:I:-31:DA:C2	6:J:32:DG:C2	3.09	0.41
5:I:37:DC:C6	5:I:38:DT:H72	2.56	0.41
6:J:77:DG:H2"	6:J:78:DG:C8	2.56	0.41
5:I:-69:DA:C6	5:I:-68:DG:C6	3.08	0.41
5:I:-57:DC:H2"	5:I:-56:DC:C6	2.55	0.41
6:J:64:DG:C3'	6:J:65:DA:H8	2.34	0.41
1:A:117:VAL:O	1:A:117:VAL:HG12	2.22	0.40
3:G:47:ALA:HB3	3:G:48:PRO:HD3	2.04	0.40
6:J:-72:DA:C4	6:J:-71:DT:O4	2.75	0.40
6:J:-65:DT:H2"	6:J:-64:DA:H5'	2.02	0.40
6:J:57:DG:H1'	6:J:58:DC:O4'	2.22	0.40
6:J:67:DT:H2"	6:J:68:DC:C6	2.57	0.40
5:I:31:DT:C2	5:I:32:DA:C5	3.09	0.40
6:J:39:DA:H2"	6:J:40:DC:H6	1.85	0.40
7:W:542:LEU:HD11	7:W:590:LEU:HB3	2.04	0.40
5:I:27:DG:H2"	5:I:28:DG:C8	2.56	0.40
6:J:-46:DT:H2"	6:J:-45:DG:C8	2.56	0.40
6:J:66:DT:H2"	6:J:67:DT:C5	2.57	0.40
5:I:5:DC:H2"	5:I:6:DC:C6	2.57	0.40
6:J:-22:DG:C2	6:J:-21:DG:C5	3.09	0.40
7:W:868:GLY:C	7:W:869:LEU:HD12	2.46	0.40

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	A	97/136 (71%)	96 (99%)	1 (1%)	0	100	100
1	E	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
2	B	84/86 (98%)	84 (100%)	0	0	100	100
2	F	76/86 (88%)	76 (100%)	0	0	100	100
3	C	101/105 (96%)	101 (100%)	0	0	100	100
3	G	103/105 (98%)	103 (100%)	0	0	100	100
4	D	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
4	H	91/95 (96%)	89 (98%)	2 (2%)	0	100	100
7	W	656/1329 (49%)	639 (97%)	17 (3%)	0	100	100
All	All	1396/2173 (64%)	1374 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	87/109 (80%)	87 (100%)	0	100	100
1	E	83/109 (76%)	82 (99%)	1 (1%)	63	78
2	B	71/71 (100%)	71 (100%)	0	100	100
2	F	63/71 (89%)	63 (100%)	0	100	100
3	C	82/83 (99%)	81 (99%)	1 (1%)	63	78
3	G	83/83 (100%)	83 (100%)	0	100	100
4	D	81/81 (100%)	81 (100%)	0	100	100
4	H	79/81 (98%)	79 (100%)	0	100	100
7	W	591/1181 (50%)	590 (100%)	1 (0%)	87	89
All	All	1220/1869 (65%)	1217 (100%)	3 (0%)	85	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	16	THR
1	E	120	MET
7	W	625	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
3	C	24	GLN
3	C	38	ASN
4	D	92	GLN
4	H	44	GLN
7	W	525	HIS
7	W	578	HIS
7	W	617	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	ML3	A	4	1	10,11,12	3.44	2 (20%)	11,14,16	1.03	1 (9%)

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
1	ML3	A	4	1	-	3/8/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	ML3	CD-SG	-7.65	1.52	1.81
1	A	4	ML3	CB-SG	-7.58	1.51	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4	ML3	CB-SG-CD	2.61	110.00	102.26

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	4	ML3	N-CA-CB-SG
1	A	4	ML3	C-CA-CB-SG
1	A	4	ML3	CE-CD-SG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
9	BEF	W	1502	8	0,3,3	-	-	-		
8	ADP	W	1501	7,9	28,29,29	1.42	4 (14%)	43,45,45	1.85	9 (20%)

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	7,9	-	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	4.72	1.47	1.39
8	W	1501	ADP	C5-C6	2.76	1.48	1.41
8	W	1501	ADP	C8-N7	2.34	1.36	1.31
8	W	1501	ADP	C5-N7	-2.29	1.34	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	W	1501	ADP	C5-C4-N3	-5.85	118.67	126.72
8	W	1501	ADP	N3-C4-N9	4.63	135.03	127.17
8	W	1501	ADP	C2-N3-C4	3.70	120.86	111.83
8	W	1501	ADP	C4-C5-N7	-3.47	106.62	110.58
8	W	1501	ADP	N3-C2-N1	-3.22	123.72	128.58
8	W	1501	ADP	C4-N9-C8	2.62	108.49	105.74
8	W	1501	ADP	C5-N7-C8	2.55	107.47	103.45
8	W	1501	ADP	C3'-C2'-C1'	2.49	106.17	101.46
8	W	1501	ADP	C6-C5-N7	2.05	136.04	132.09

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

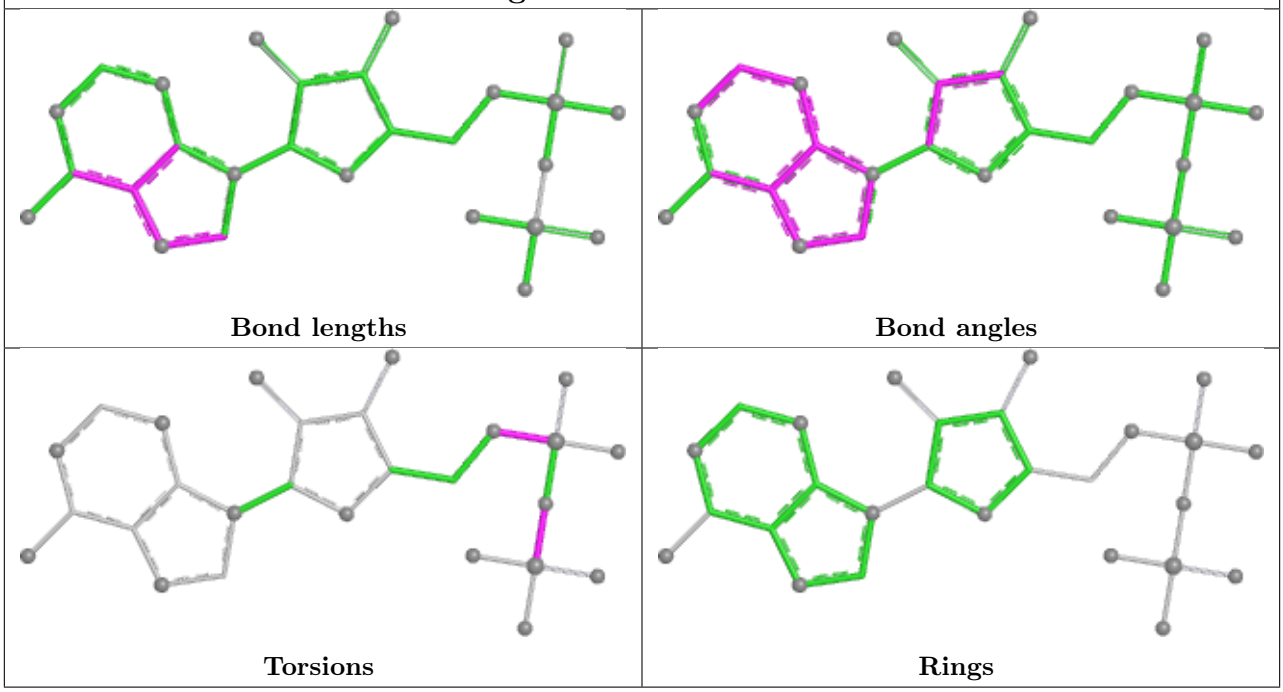
There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	W	1502	BEF	6	0
8	W	1501	ADP	10	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.

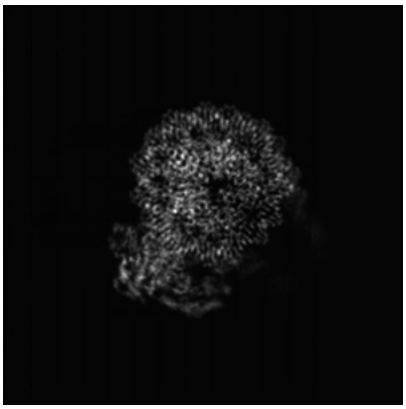
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-47841. These allow visual inspection of the internal detail of the map and identification of artifacts.

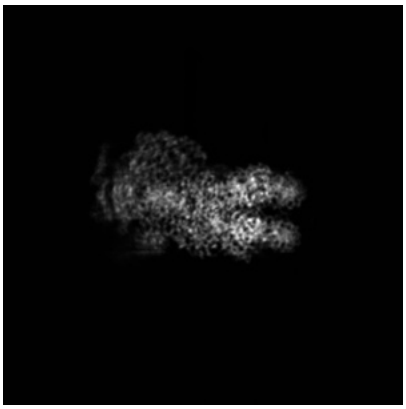
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

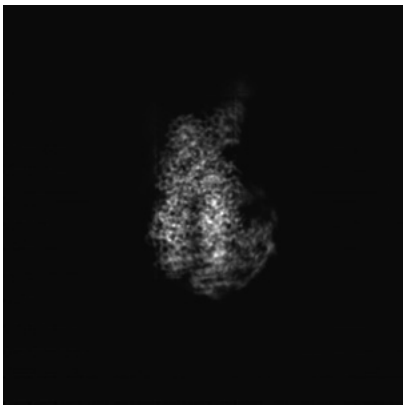
6.1.1 Primary map



X

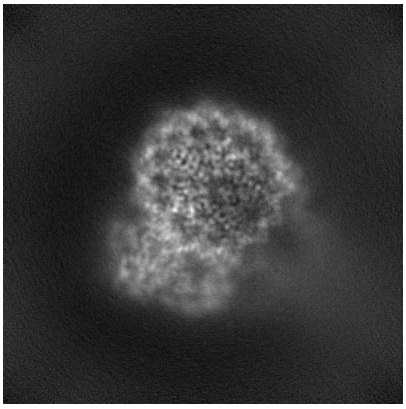


Y

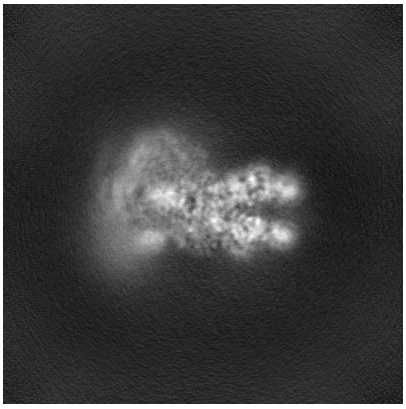


Z

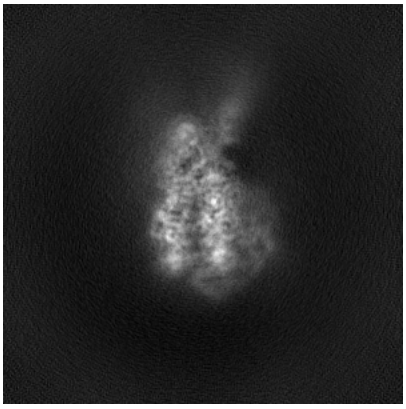
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

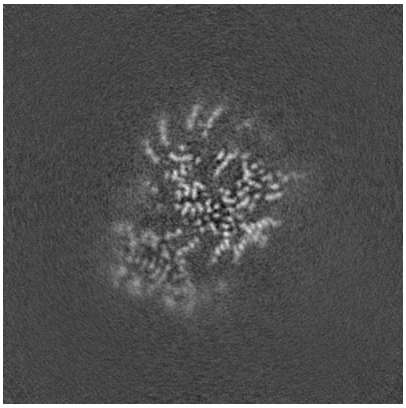
6.2.1 Primary map

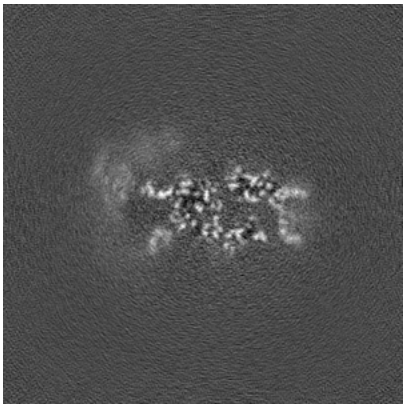
X Index: 150

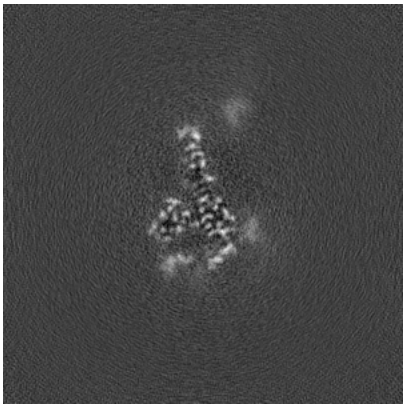
Y Index: 150

Z Index: 150

6.2.2 Raw map


X Index: 150


Y Index: 150


Z Index: 150

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

6.3 Largest variance slices (i)

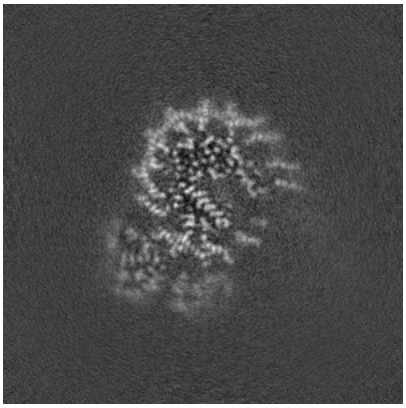
6.3.1 Primary map

X Index: 159

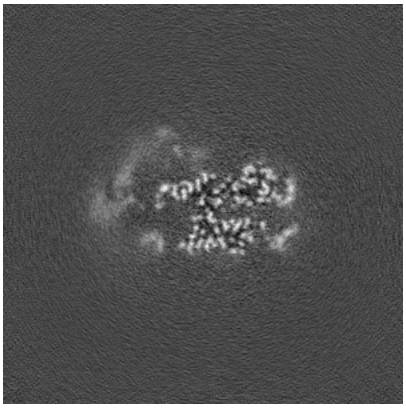
Y Index: 129

Z Index: 178

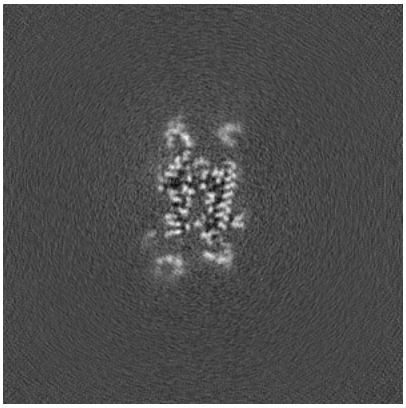
6.3.2 Raw map



X Index: 159



Y Index: 139

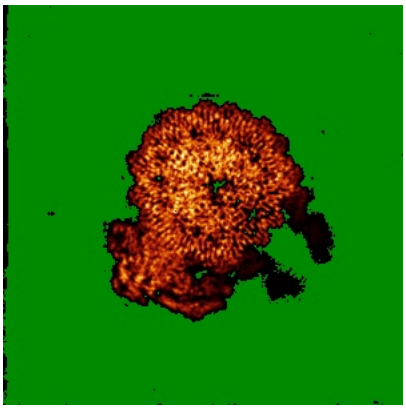


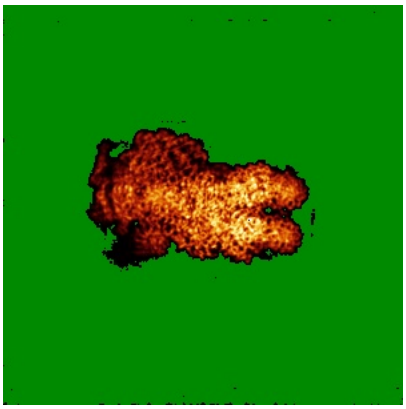
Z Index: 186

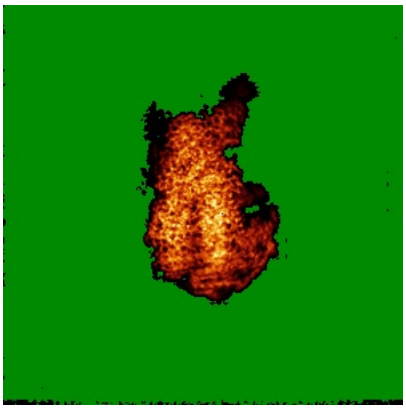
The images above show the largest variance slices of the map in three orthogonal directions.

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

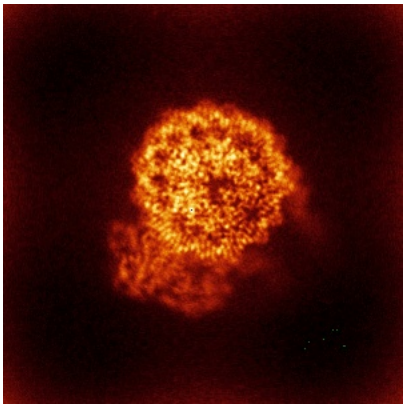
6.4.1 Primary map

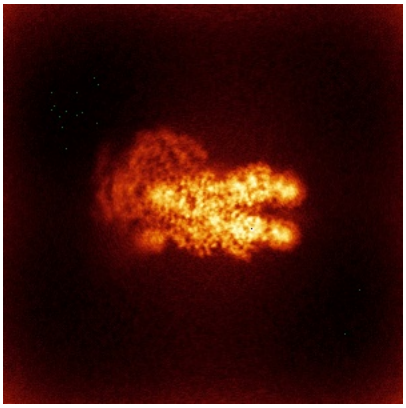

X

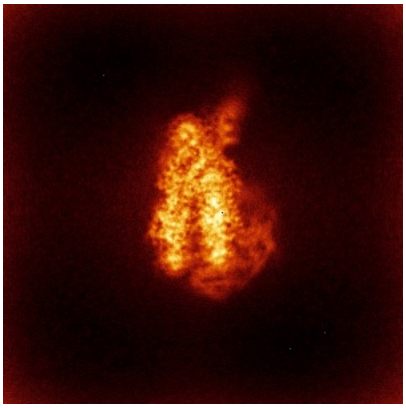

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0182. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

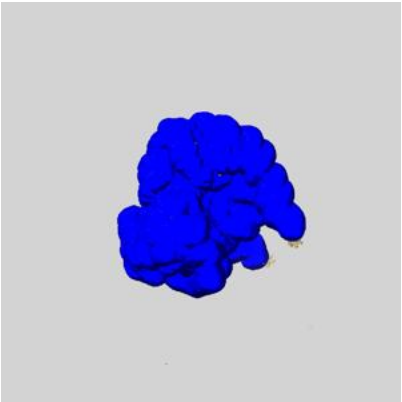
6.6 Mask visualisation (i)

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

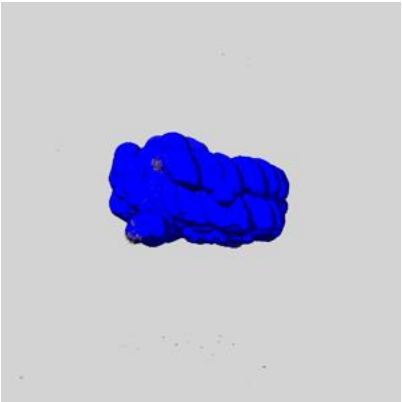
A mask typically either:

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

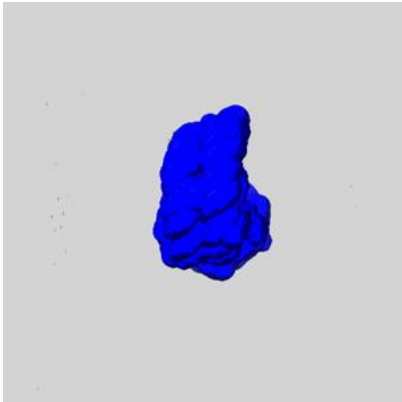
6.6.1 emd_47841_msk_1.map (i)



X



Y

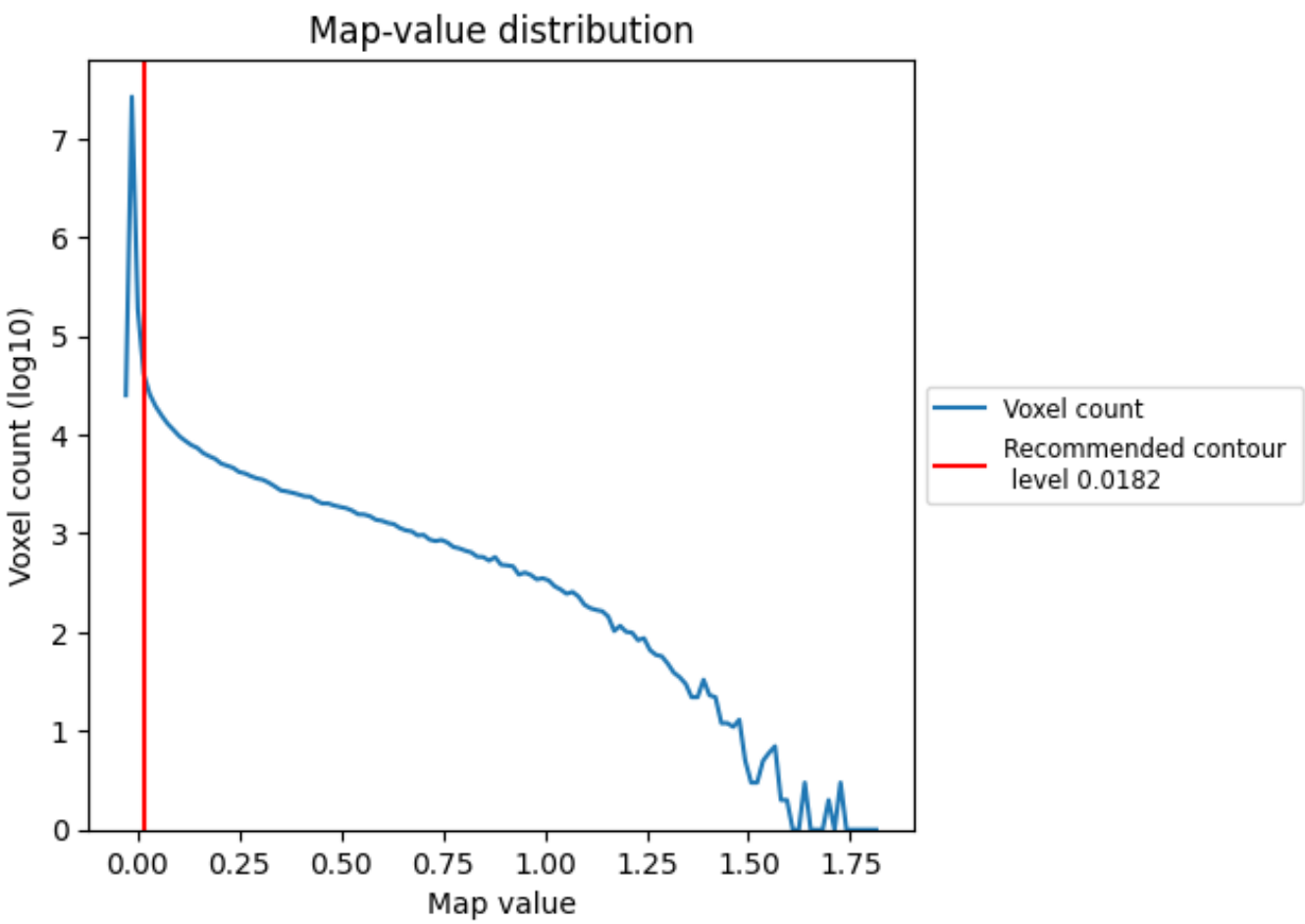


Z

7 Map analysis (i)

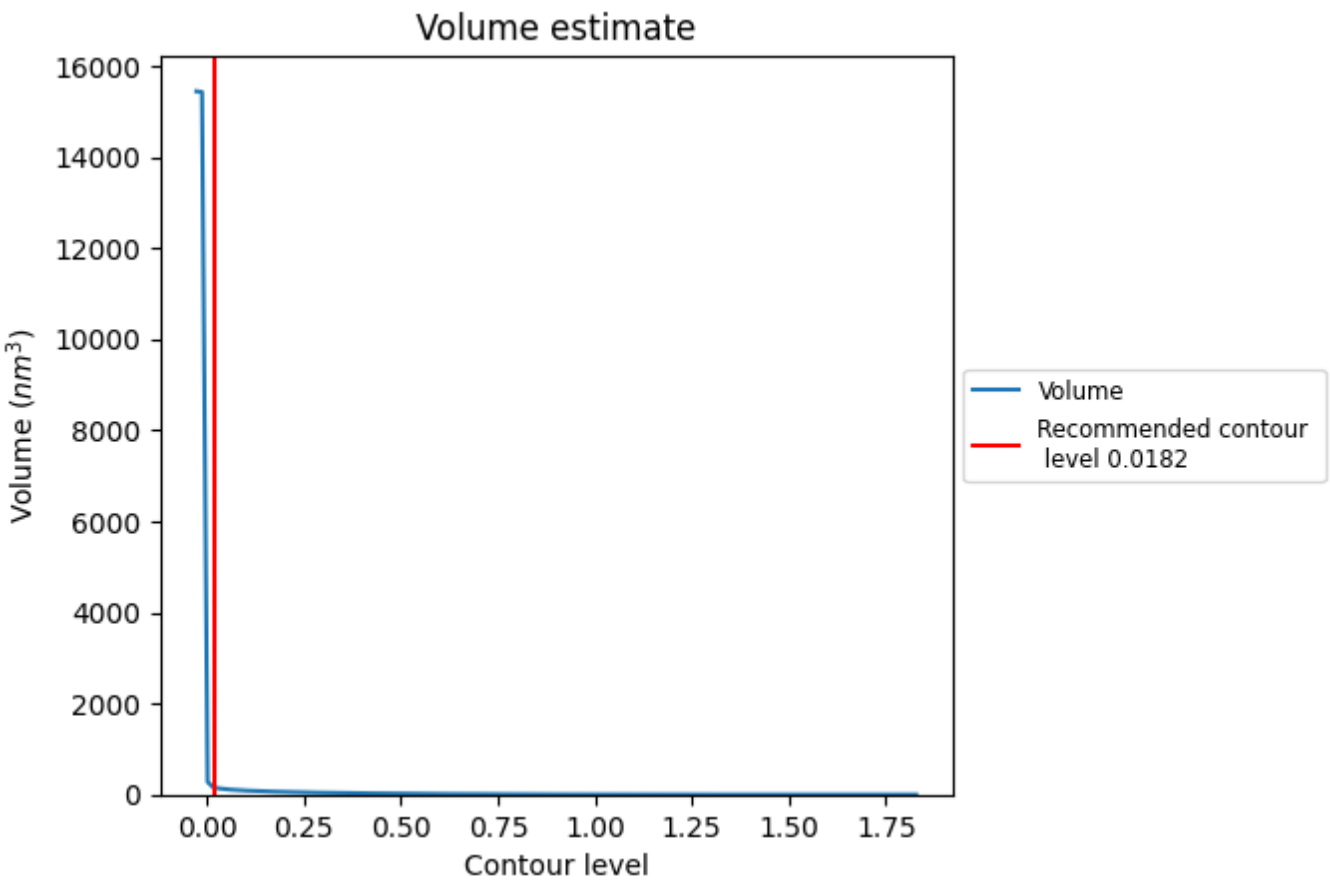
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

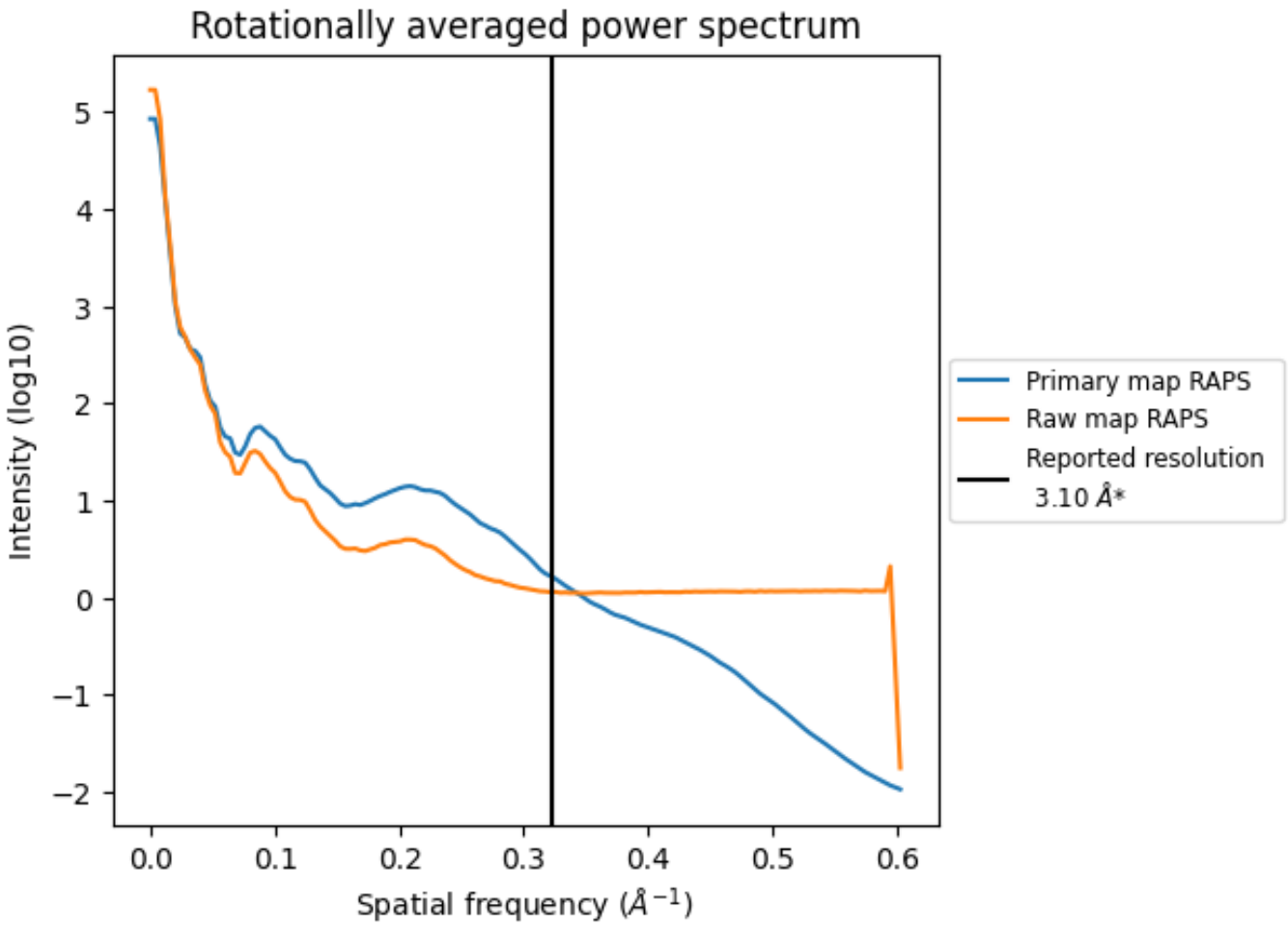
7.2 Volume estimate (i)



The volume at the recommended contour level is 155 nm^3; this corresponds to an approximate mass of 140 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)

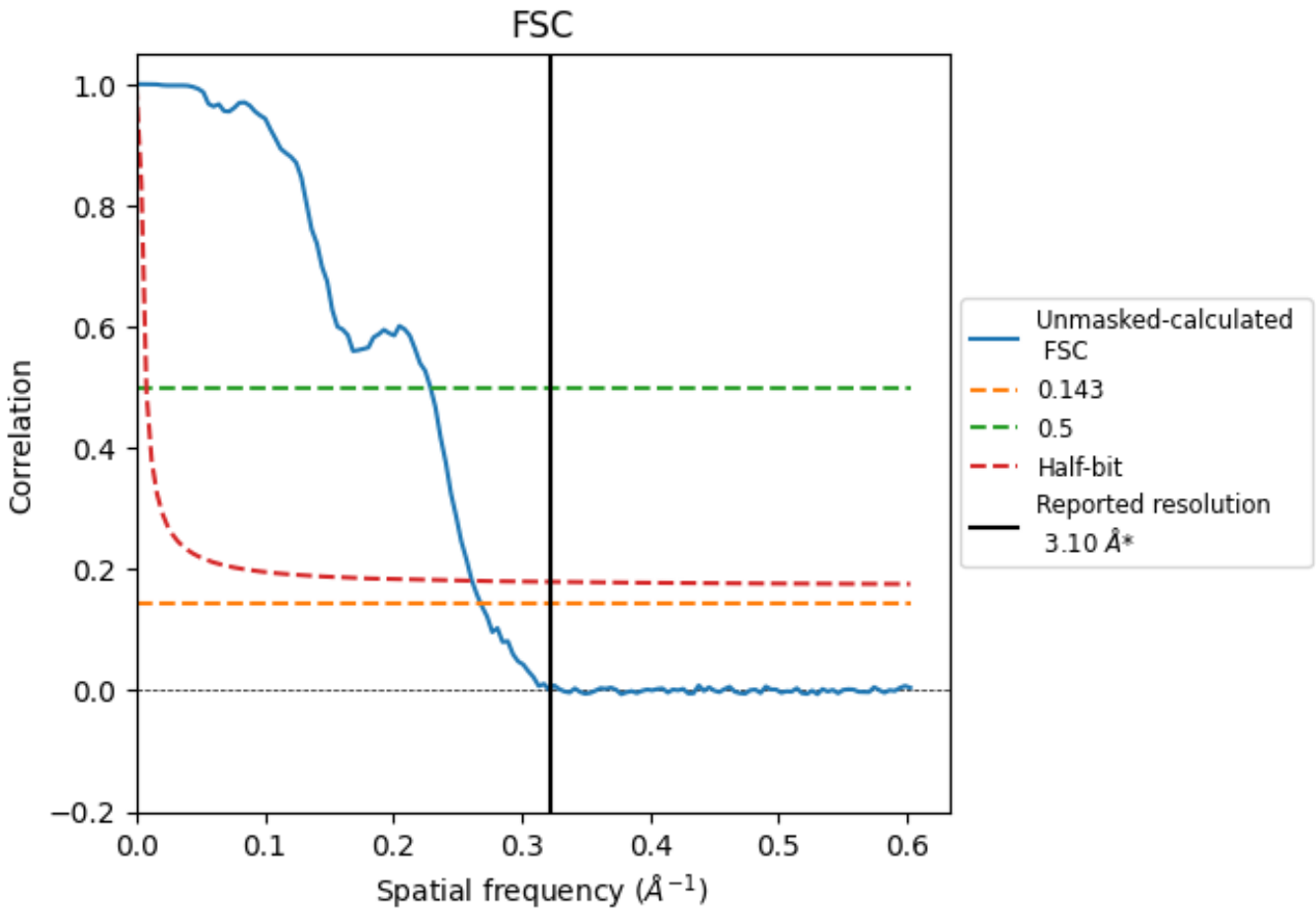


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 Å^{-1}

8.2 Resolution estimates (i)

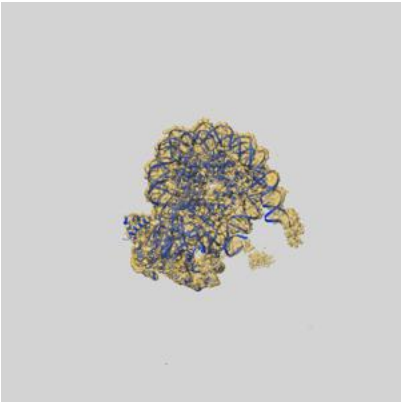
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.73	4.37	3.83

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

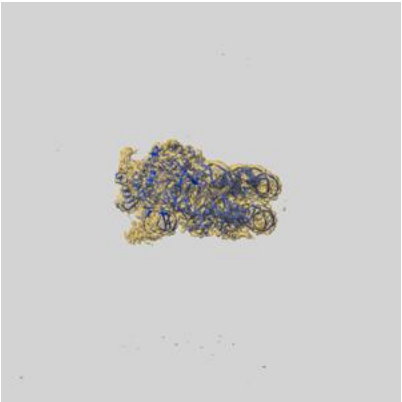
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-47841 and PDB model 9EAR. Per-residue inclusion information can be found in section 3 on page 7.

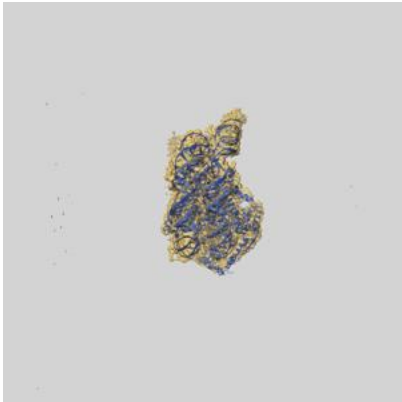
9.1 Map-model overlay (i)



X



Y



Z

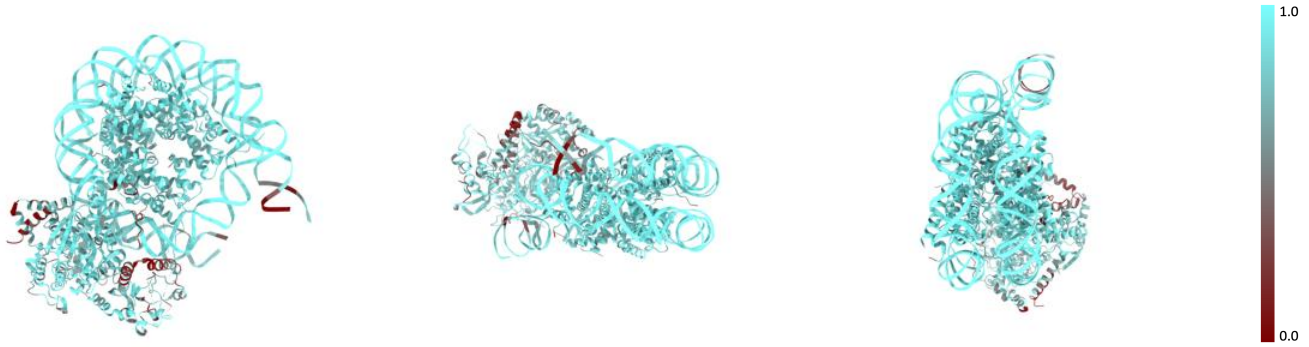
The images above show the 3D surface view of the map at the recommended contour level 0.0182 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

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.

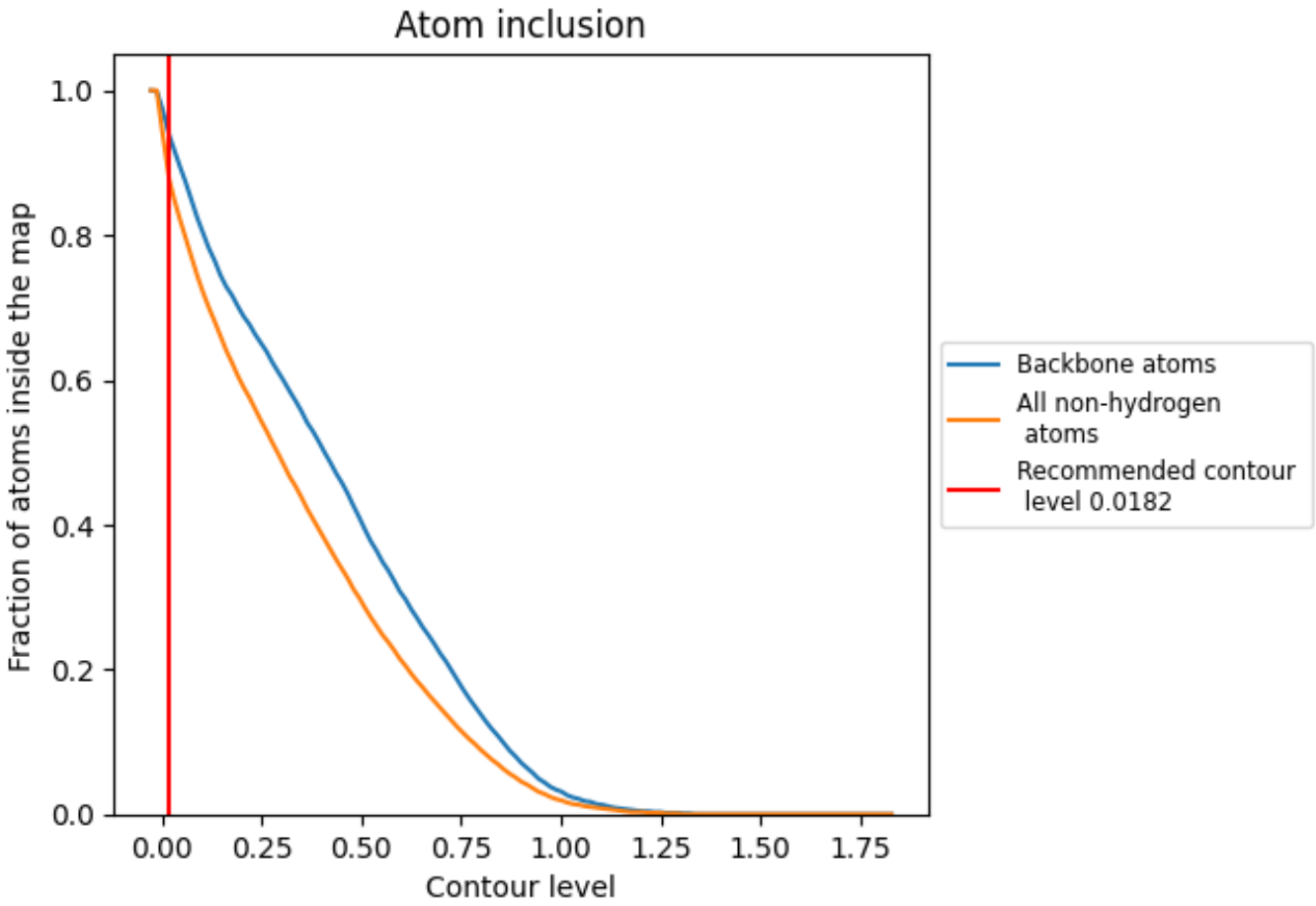
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0182).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0182) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8770	0.4240
A	0.8950	0.5170
B	0.8820	0.5210
C	0.9290	0.5310
D	0.9310	0.5110
E	0.9390	0.5420
F	0.9610	0.5560
G	0.9400	0.5330
H	0.9450	0.5210
I	0.9420	0.4520
J	0.9280	0.4610
W	0.7510	0.2690