wwPDB EM Validation Summary Report (i)

Mar 18, 2024 – 04:37 PM JST

PDB ID	:	6K1P
EMDB ID	:	EMD-9719
Title	:	The complex of ISWI-nucleosome in the ADP.BeF-bound state
Authors	:	Yan, L.J.; Wu, H.; Li, X.M.; Gao, N.; Chen, Z.C.
Deposited on	:	2019-05-10
Resolution	:	3.87 Å(reported)
Based on initial model	:	5X0Y

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 (1)) were used in the production of this report:

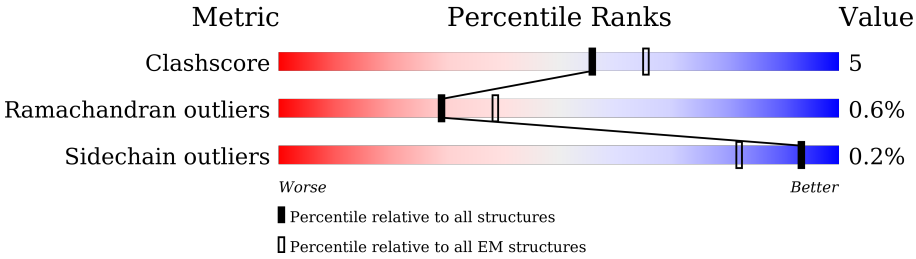
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.87 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	135	64% 7% • 27%
1	E	135	67% • 30%
2	B	102	• 79% 7% 14%
2	F	102	6% 82% • 16%
3	C	129	78% 5% 17%
3	G	129	81% • 17%
4	D	122	74% • 24%
4	H	122	73% • 24%

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Mol	Chain	Length	Quality of chain
5	I	167	73% 14% • 13%
6	J	167	70% 17% • 13%
7	K	1061	32% 11% 56%

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	BEF	K	1201	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 15841 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	98	801	506	153	139	3	0	0
1	E	95	779	492	148	136	3	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	88	707	445	143	118	1	0	0
2	F	86	672	424	130	117	1	0	0

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	107	811	510	158	143	0	0
3	G	107	815	513	159	143	0	0

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	93	718	451	128	137	2	0	0
4	H	93	726	457	130	137	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	conflict	UNP P02281

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Chain	Residue	Modelled	Actual	Comment	Reference
H	29	THR	SER	conflict	UNP P02281

- Molecule 5 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	I	146	2975	1413	540	876	146	0	0

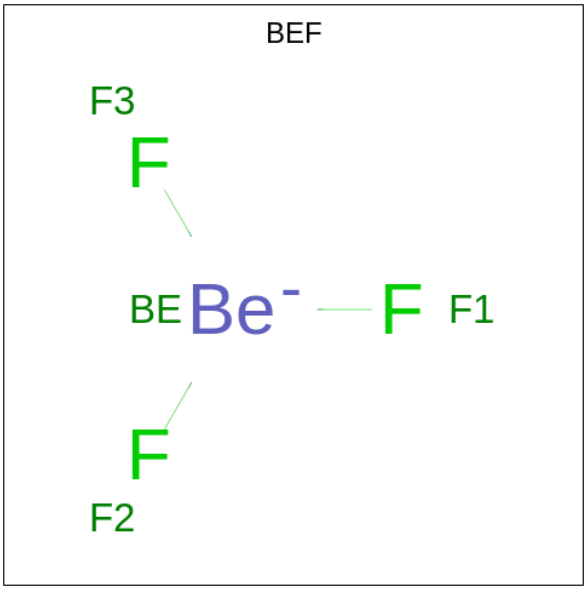
- Molecule 6 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	J	146	3011	1425	564	876	146	0	0

- Molecule 7 is a protein called ISWI chromatin-remodeling complex ATPase ISW1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	K	463	3794	2424	653	704	13	0	0

- Molecule 8 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).

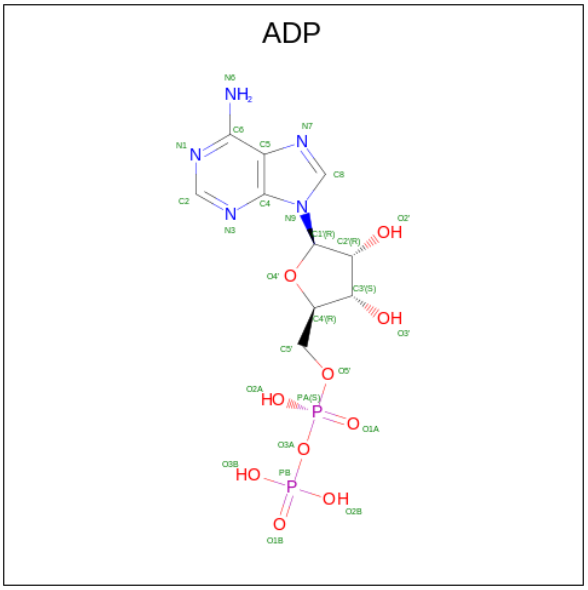


Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
8	K	1	4	1	3	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
9	K	1	1	1	0

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



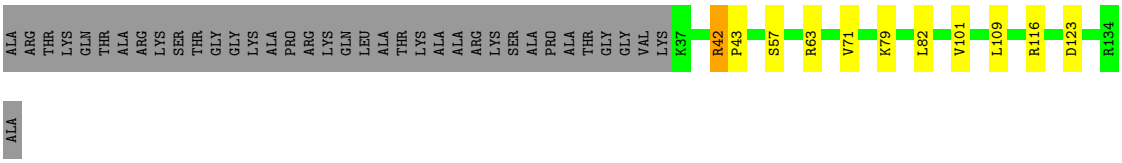
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	K	1	27	10	5	10	2	0

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.

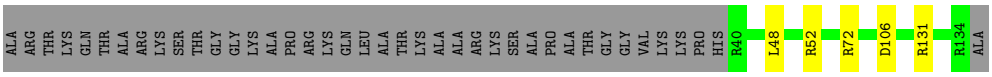
- Molecule 1: Histone H3

Chain A:



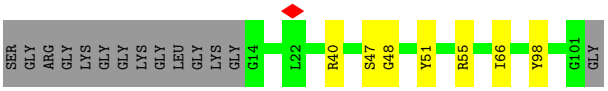
- Molecule 1: Histone H3

Chain E:



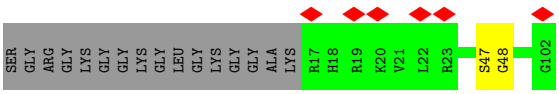
- Molecule 2: Histone H4

Chain B:



- Molecule 2: Histone H4

Chain F:

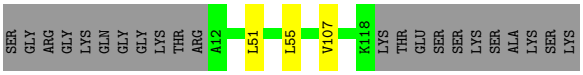


- Molecule 3: Histone H2A

Chain C:

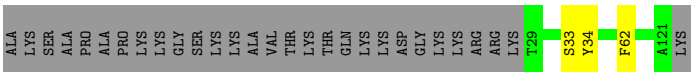
- Molecule 3: Histone H2A

Chain G:



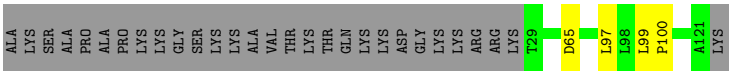
- Molecule 4: Histone H2B 1.1

Chain D:



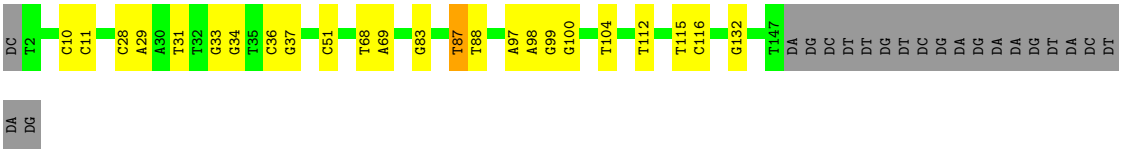
- Molecule 4: Histone H2B 1.1

Chain H:



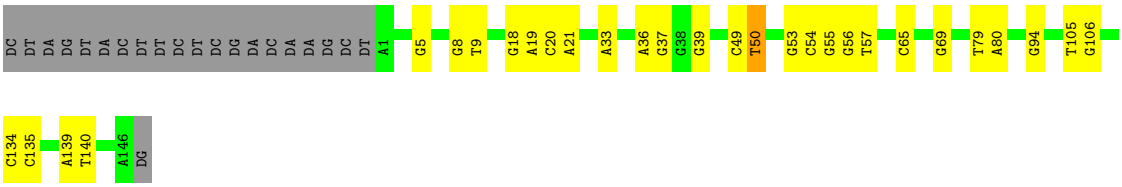
- Molecule 5: DNA (167-MER)

Chain I:



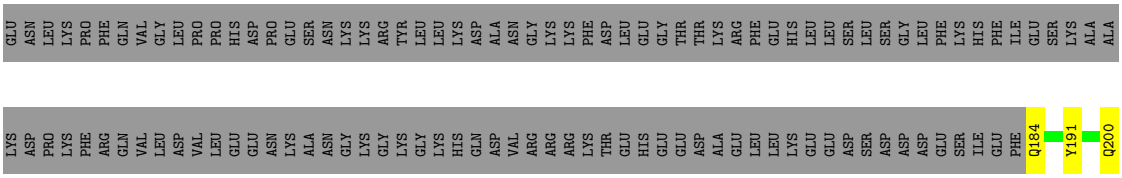
- Molecule 6: DNA (167-MER)

Chain J:



- Molecule 7: ISWI chromatin-remodeling complex ATPase ISW1

Chain K:



N205 V208 A216 G217 I218 L219 A220 Q230 S233 P247 V250 K254 R262 R266 I275 L276 I287 L291 W318 E319 I322 H327 N331 S334 R341 S345 R348 I351 T354 P355 L356 L360 W364 L367
N368 F369 L370 L371 W384 S389 T390 E391 E392 D393 V398 L401 V404 L405 Q406 P407 F408 R412 I413 K414 S415 D416 V417 E418 T419 S420 L421 L422 P423 Y430 K443 D448 LEU ASP ALA VAL ASN GLY SER ASN GLY SER LYS E460 L472 R473 K474 N477 H478
P479 Y480 D483 P489 P490 Y491 T492 T493 D494 E495 H496 L497 V498 Y499 K503 L504 Q505 V506 L507 V521 F524 S525 Q526 M527 S528 L531 D532 I533 C538 Y539 F540 R541 N542 Y543 R547 I548 D549 G550 E555 I558 L575 L576 T577 T578 G584 T588 S589
A590 D591 V592 V593 V594 S598 N601 P602 D605 M609 Q617 F624 R625 D629 V632 E633 E634 E638 K643 L649 V650 I651 N654 R655 T656 S657 LEU LYS LYS LYS GLU ASN LYS ALA ASP SER LYS ASP ALA LEU LEU SER MET ILE GLN HIS GLY ALA
ALA ASP VAL PHE LYS SER GLY THR SER THR GLY SER ALA GLY THR PRO GLU PRO GLY SER GLY GLU LYS GLY ASP ASP ILE ASP LEU ASP GLU LEU LEU LEU LYS SER GLU ASN LYS THR LYS SER LEU ASN ALA LYS TYR GLU THR LEU GLY LEU ASP ASP LEU LEU LYS PHE ASN GLN
ASP SER ALA TYR GLU TRP ASN GLY GLN ASP PHE LYS LYS LYS ILE GLN ARG ASP ILE ILE SER PRO LEU LEU LEU ASN PRO THR LYS ARG GLU ARG LYS GLU ASN TYR SER ILE ASP ASN TYR TYR TYR LYS ASP VAL LEU ASN THR GLY ARG SER SER THR PRO SER HIS PRO ARG MET PRO
LYS PRO HIS VAL PHE HIS SER HIS GLN LEU GLN PRO PRO GLN LEU LYS VAL LEU TYR GLU LYS GLU ARG MET TRP THR ALA LYS LYS THR GLY TYR VAL PRO THR MET ASP ASP VAL LYS ALA ALA TYR GLY ASP ILE SER ASP GLU GLU GLU LYS LYS GLN LYS LEU GLU LEU LEU LYS
LEU SER VAL ASN ASN SER GLN PRO LEU THR GLU GLU GLU GLU LYS MET LYS ALA ASP TRP GLU SER GLU GLY PHE THR ASN TRP ASN LYS LEU GLU PHE ARG LYS PHE ILE THR VAL SER GLY LYS TYR GLY ARG ASN SER ILE GLN ALA ILE ALA ARG GLU LEU ALA PRO GLY LYS THR
LEU GLU GLU VAL ARG ALA TYR ALA LYS ALA PHE TRP SER ASN ILE GLU ARG ILE GLU ASP TYR GLU LYS TYR LEU LYS ILE ILE GLU ASN GLU GLU GLU LYS LYS LYS ARG VAL LYS MET GLN GLN GLU ALA LEU ARG ARG LYS LEU SER GLU TYR GLY ASP CYS PRO LEU PHE GLU LEU LEU LYS
LEU LYS HIS PRO PRO SER SER ASN ASN LYS ARG THR TYR SER GLU GLU GLU ASP ARG PHE ILE LEU LEU MET LEU PHE LYS TYR GLY LEU ASP ARG ASP ASP VAL TYR GLU LEU VAL ARG ASP GLU ILE ARG GLU GLU ASP CYS PRO LEU PHE GLU LEU ASP PHE TYR PHE ARG SER ARG THR PRO
VAL GLU LEU ALA ARG ARG GLY ASN THR LEU LEU GLN CYS LEU GLU LYS GLU PHE ASN ALA GLY ILE VAL LEU ASP ALA THR LYS ASP ARG MET LYS LYS GLU ASP GLU ASN GLY LYS ARG ILE ARG GLU GLU PHE ALA ASP GLN THR ALA ASN GLU LYS GLU ASN VAL ASP GLY VAL
GLU SER LYS LYS ALA LYS ILE GLU ASP THR THR SER ASN VAL GLY THR GLU GLN LEU VAL ALA GLU LYS ILE PRO GLU ASN GLU THR THR HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62121	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.293	Depositor
Minimum map value	-0.185	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0253	Depositor
Map size (Å)	235.40001, 235.40001, 235.40001	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: 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	0.53	0/813	0.67	0/1093
1	E	0.50	0/789	0.63	0/1059
2	B	0.59	0/715	0.71	0/955
2	F	0.57	0/680	0.69	0/912
3	C	0.49	0/821	0.61	0/1112
3	G	0.52	0/825	0.66	1/1116 (0.1%)
4	D	0.54	0/729	0.61	0/985
4	H	0.57	0/737	0.67	0/993
5	I	0.91	0/3333	1.03	4/5137 (0.1%)
6	J	0.93	1/3381 (0.0%)	1.02	7/5221 (0.1%)
7	K	0.34	0/3867	0.57	0/5224
All	All	0.69	1/16690 (0.0%)	0.82	12/23807 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	94	DG	C3'-O3'	5.63	1.51	1.44

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	51	LEU	CB-CG-CD2	-5.84	101.07	111.00
6	J	94	DG	P-O3'-C3'	5.37	126.14	119.70
5	I	31	DT	N3-C4-O4	5.32	123.09	119.90
6	J	50	DT	N3-C4-O4	5.29	123.07	119.90
5	I	112	DT	N3-C4-O4	5.23	123.04	119.90

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	801	0	831	15	0
1	E	779	0	815	3	0
2	B	707	0	760	5	0
2	F	672	0	698	1	0
3	C	811	0	849	7	0
3	G	815	0	860	2	0
4	D	718	0	725	4	0
4	H	726	0	747	3	0
5	I	2975	0	1639	13	0
6	J	3011	0	1639	20	0
7	K	3794	0	3839	97	0
8	K	4	0	0	3	0
9	K	1	0	0	0	0
10	K	27	0	12	0	0
All	All	15841	0	13414	151	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 5.

The worst 5 of 151 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:K:489:PRO:HG2	7:K:492:THR:CG2	1.49	1.39
4:D:33:SER:O	4:D:34:TYR:CD1	1.84	1.29
4:D:33:SER:O	4:D:34:TYR:HD1	1.11	1.27
7:K:489:PRO:CG	7:K:492:THR:HG21	1.66	1.23
7:K:489:PRO:HG2	7:K:492:THR:HG22	1.25	1.10

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	96/135 (71%)	86 (90%)	9 (9%)	1 (1%)	15	52
1	E	93/135 (69%)	87 (94%)	6 (6%)	0	100	100
2	B	86/102 (84%)	78 (91%)	8 (9%)	0	100	100
2	F	84/102 (82%)	75 (89%)	9 (11%)	0	100	100
3	C	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
3	G	105/129 (81%)	101 (96%)	4 (4%)	0	100	100
4	D	91/122 (75%)	86 (94%)	5 (6%)	0	100	100
4	H	91/122 (75%)	87 (96%)	4 (4%)	0	100	100
7	K	459/1061 (43%)	398 (87%)	55 (12%)	6 (1%)	12	48
All	All	1210/2037 (59%)	1100 (91%)	103 (8%)	7 (1%)	29	63

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	K	275	ILE
7	K	542	ASN
7	K	492	THR
7	K	493	THR
7	K	494	ASP

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	84/110 (76%)	84 (100%)	0	100	100
1	E	82/110 (74%)	82 (100%)	0	100	100
2	B	72/78 (92%)	72 (100%)	0	100	100
2	F	67/78 (86%)	67 (100%)	0	100	100
3	C	81/101 (80%)	81 (100%)	0	100	100
3	G	82/101 (81%)	82 (100%)	0	100	100
4	D	77/102 (76%)	77 (100%)	0	100	100
4	H	79/102 (78%)	79 (100%)	0	100	100
7	K	421/958 (44%)	419 (100%)	2 (0%)	88	93
All	All	1045/1740 (60%)	1043 (100%)	2 (0%)	93	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	K	492	THR
7	K	540	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	75	HIS
7	K	230	GLN
7	K	526	GLN
7	K	613	HIS
7	K	617	GLN

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 monosaccharides 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	$\#\|Z\| > 2$
10	ADP	K	1203	-	24,29,29	0.92	1 (4%)	29,45,45	1.48	4 (13%)
8	BEF	K	1201	-	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
10	ADP	K	1203	-	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	1203	ADP	C5-C4	2.34	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	1203	ADP	PA-O3A-PB	-3.61	120.44	132.83
10	K	1203	ADP	N3-C2-N1	-3.46	123.28	128.68
10	K	1203	ADP	C3'-C2'-C1'	2.97	105.46	100.98
10	K	1203	ADP	C4-C5-N7	-2.16	107.15	109.40

There are no chirality outliers.

There are no torsion outliers.

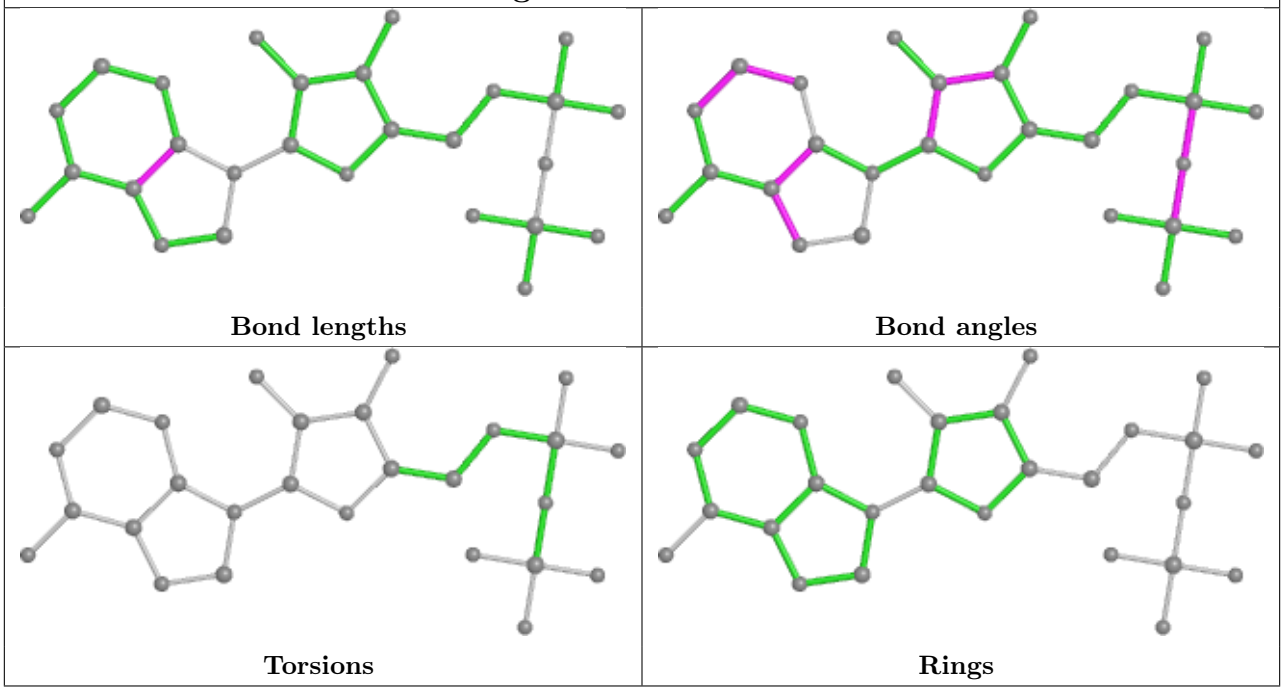
There are no ring outliers.

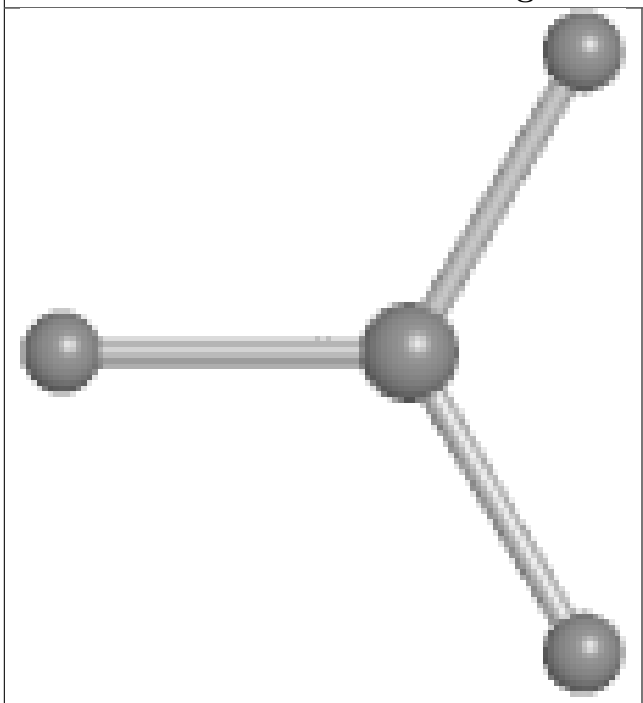
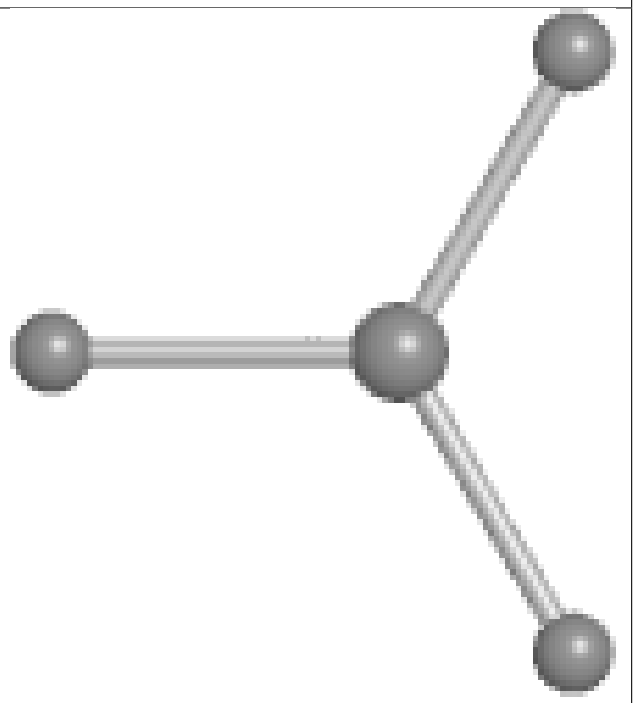
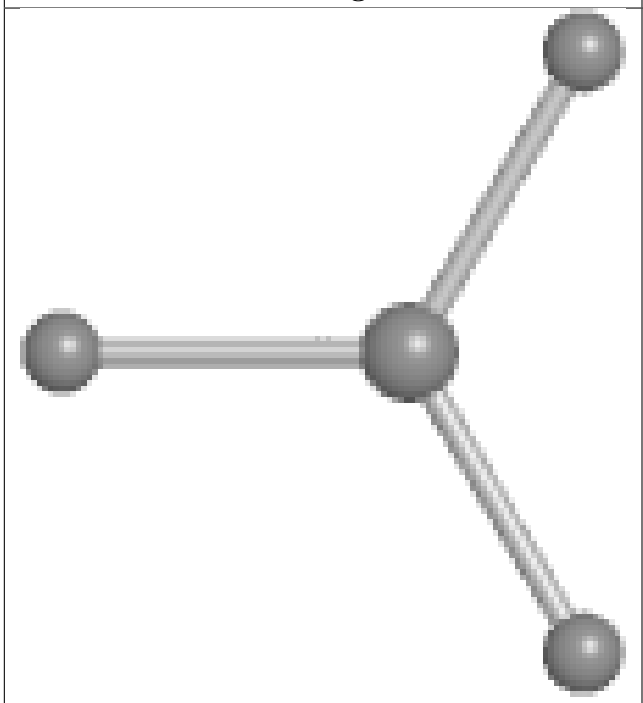
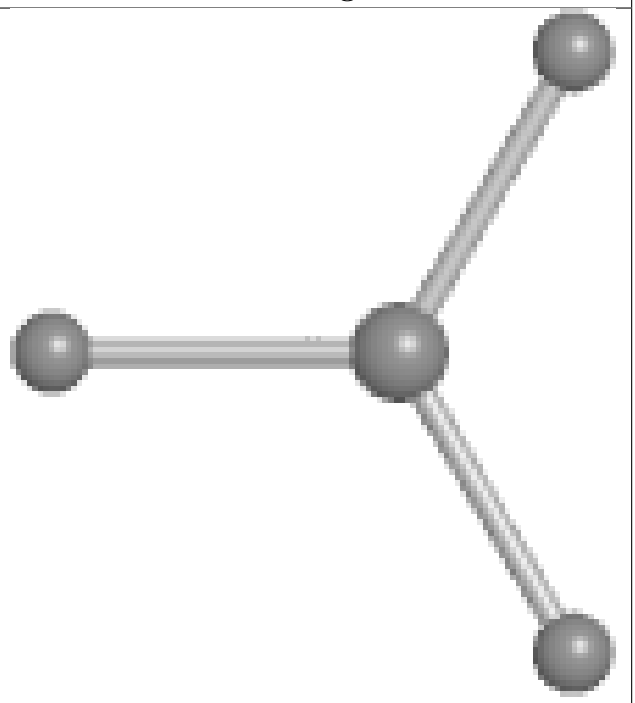
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	K	1201	BEF	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 K 1203



Ligand BEF K 1201	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

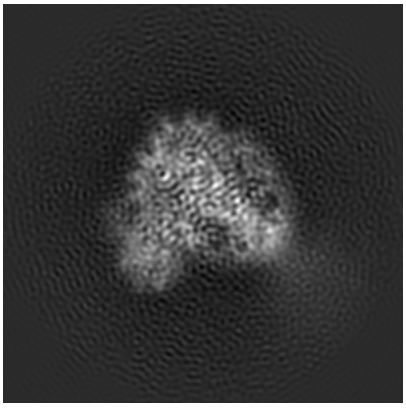
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9719. These allow visual inspection of the internal detail of the map and identification of artifacts.

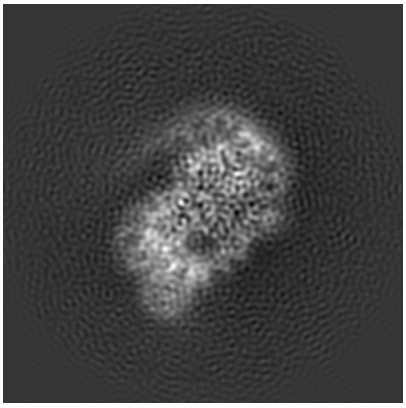
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

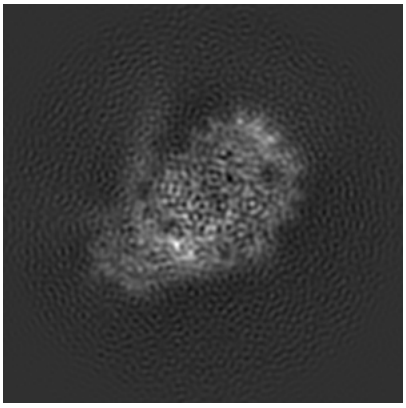
6.1.1 Primary map



X



Y

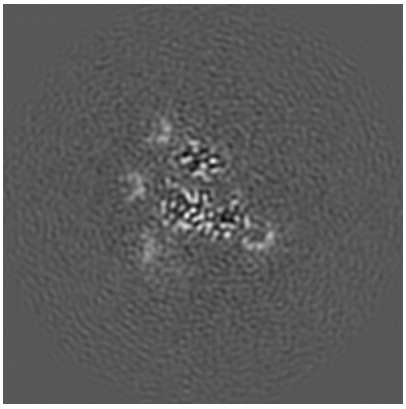


Z

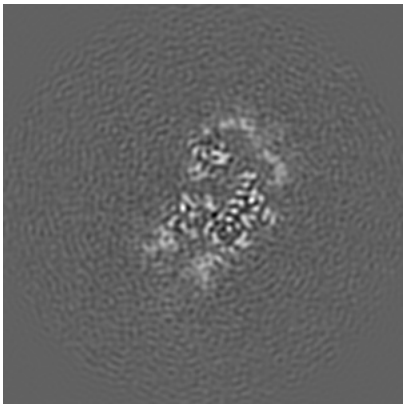
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

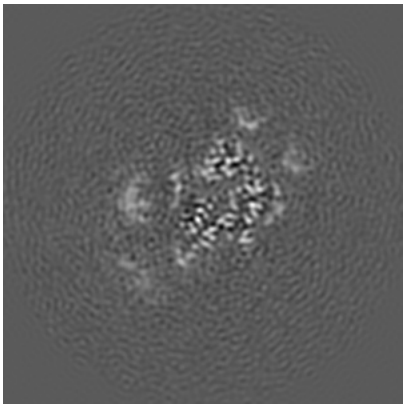
6.2.1 Primary map



X Index: 110



Y Index: 110

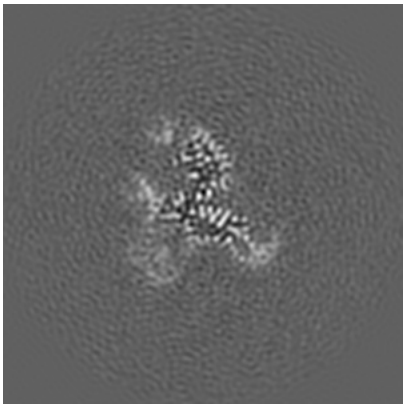


Z Index: 110

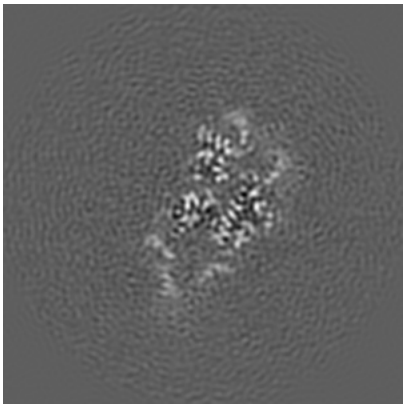
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

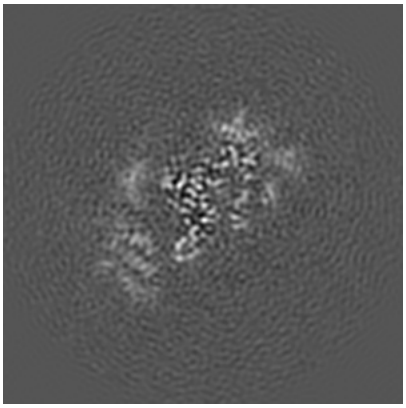
6.3.1 Primary map



X Index: 104



Y Index: 105

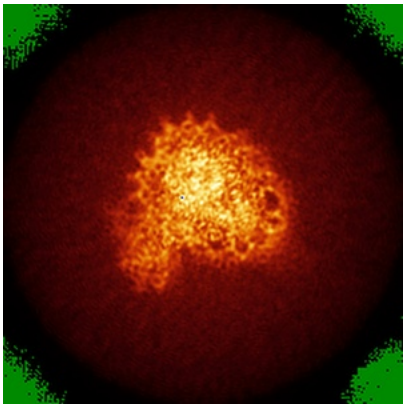


Z Index: 103

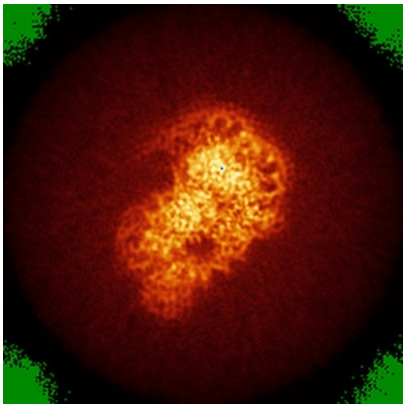
The images above show the largest variance slices of the map in three orthogonal directions.

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

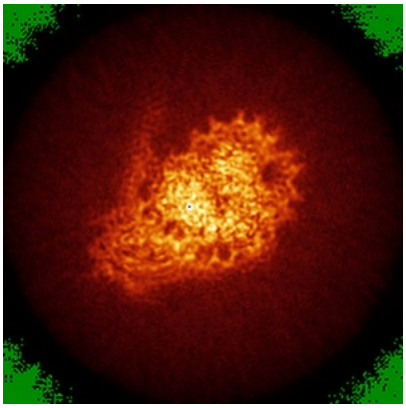
6.4.1 Primary map



X



Y

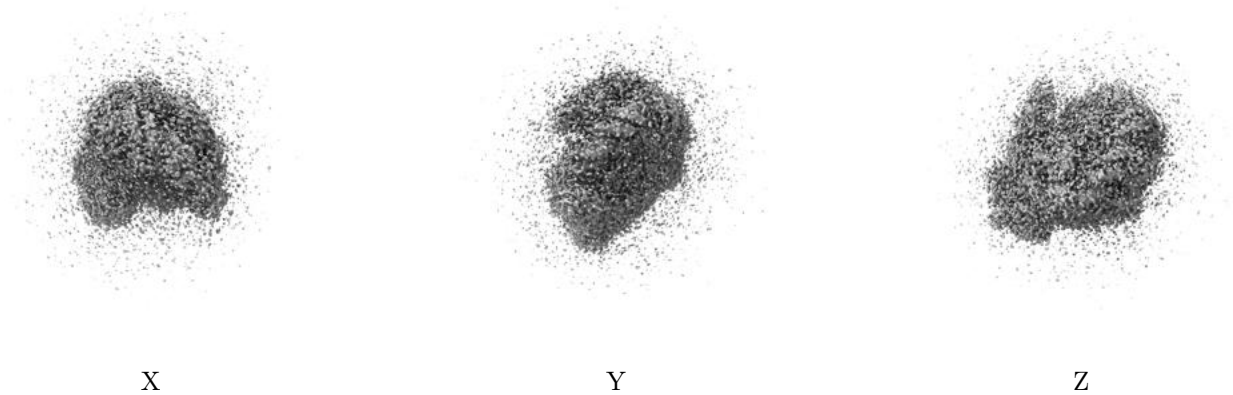


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0253. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

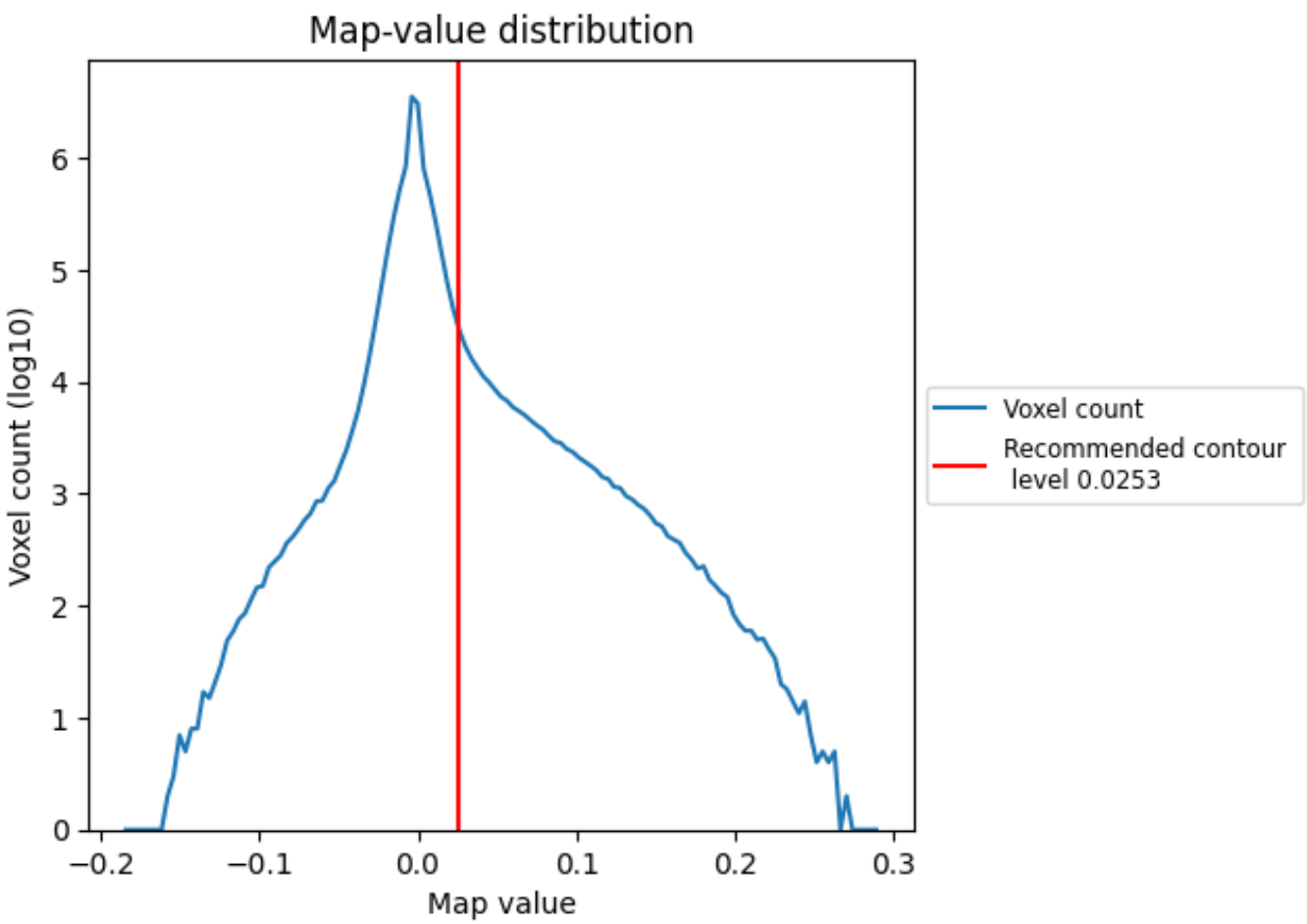
6.6 Mask visualisation (i)

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

7 Map analysis (i)

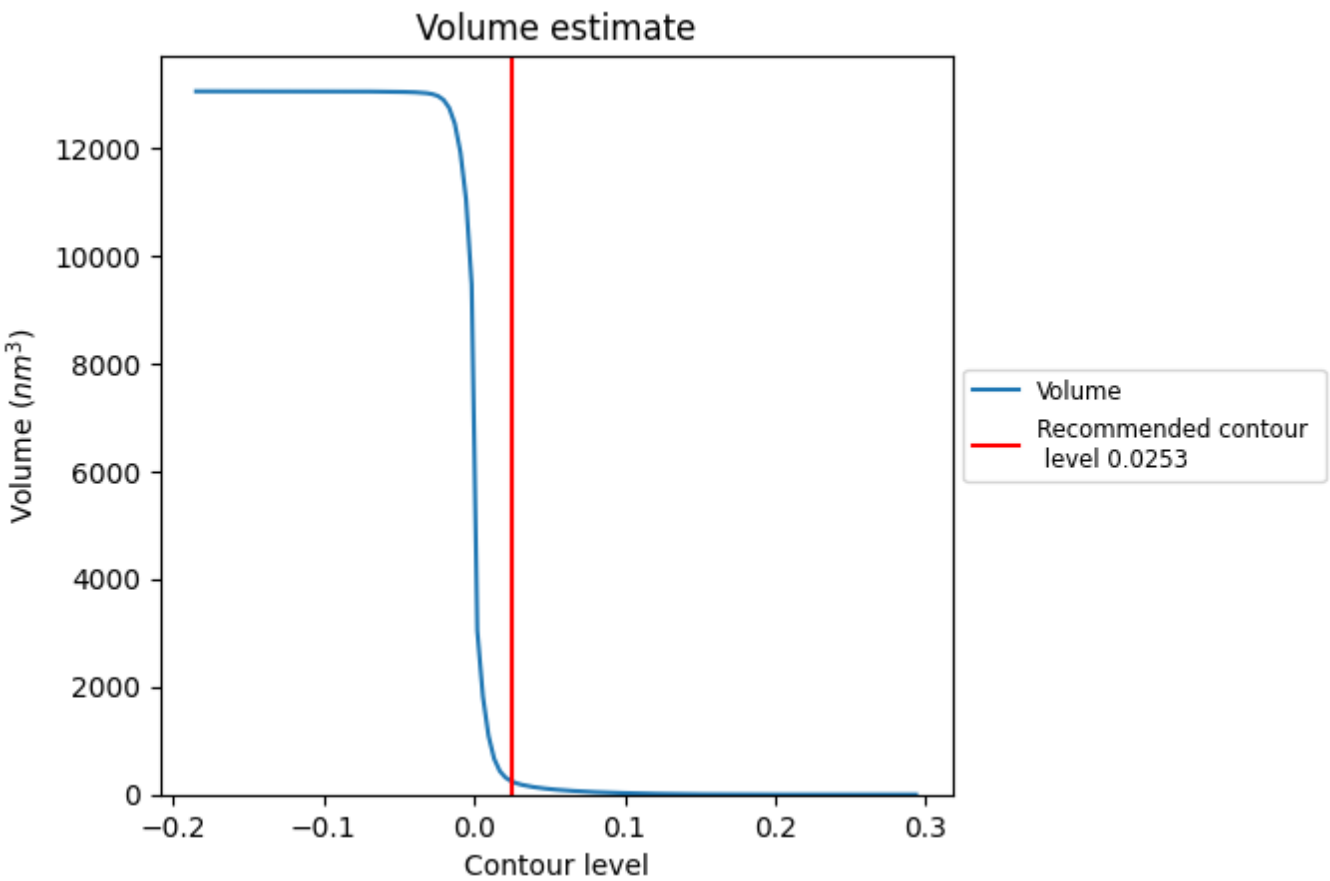
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

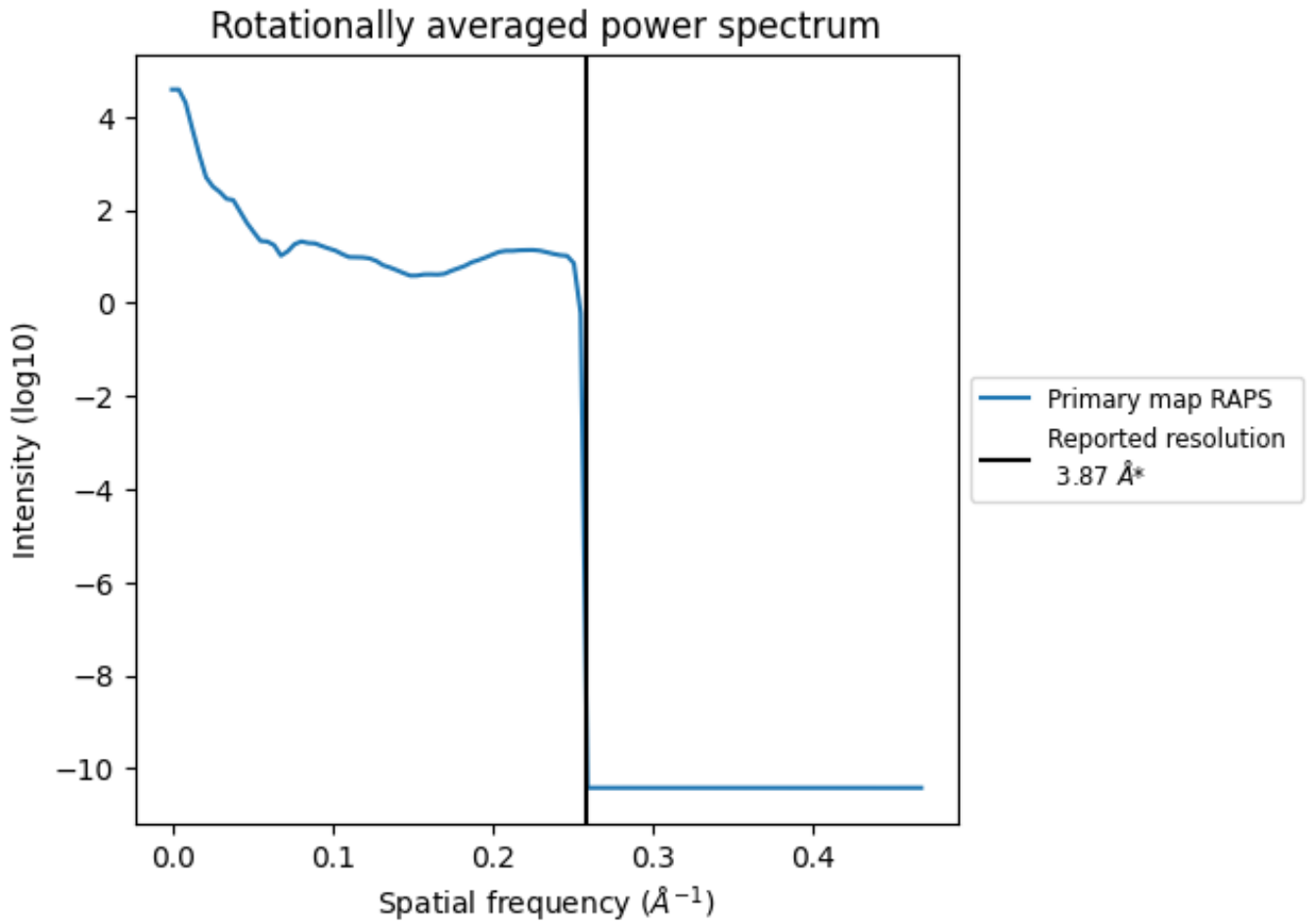
7.2 Volume estimate (i)



The volume at the recommended contour level is 242 nm^3; this corresponds to an approximate mass of 219 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 0.258 Å^{-1}

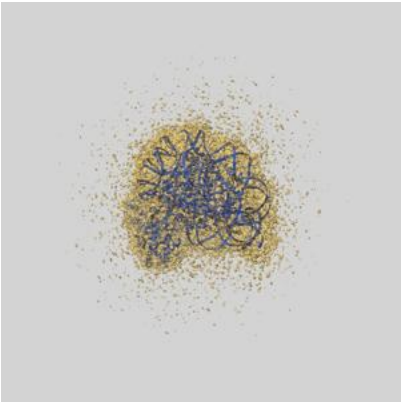
8 Fourier-Shell correlation (i)

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

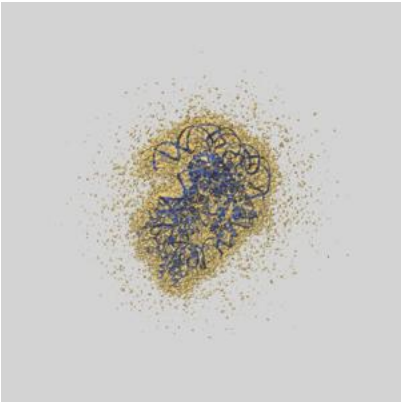
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9719 and PDB model 6K1P. Per-residue inclusion information can be found in section 3 on page 7.

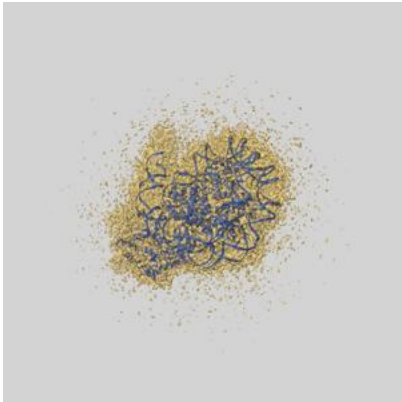
9.1 Map-model overlay (i)



X



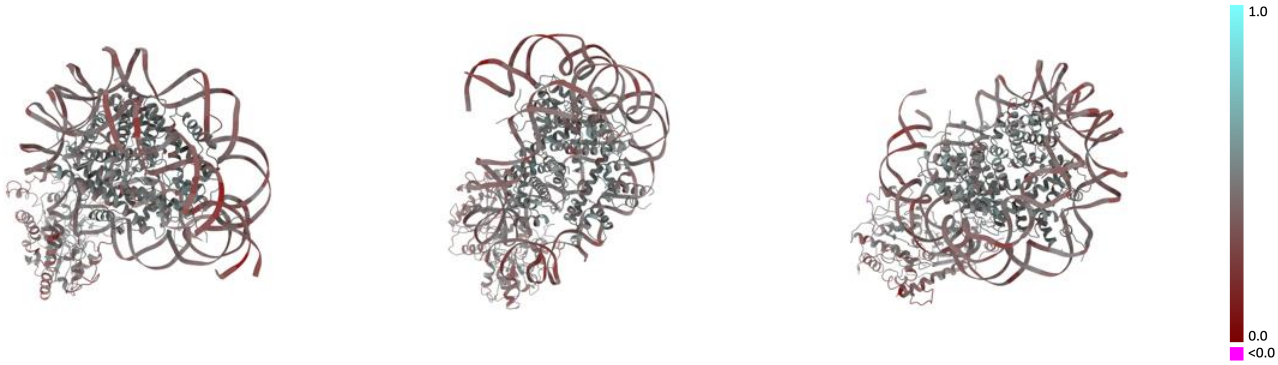
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0253 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.

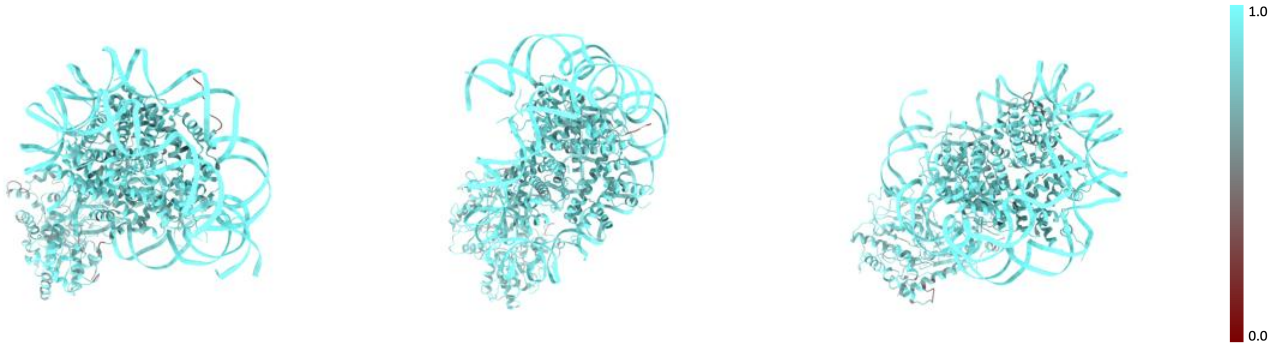
9.2 Q-score mapped to coordinate model (i)



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.

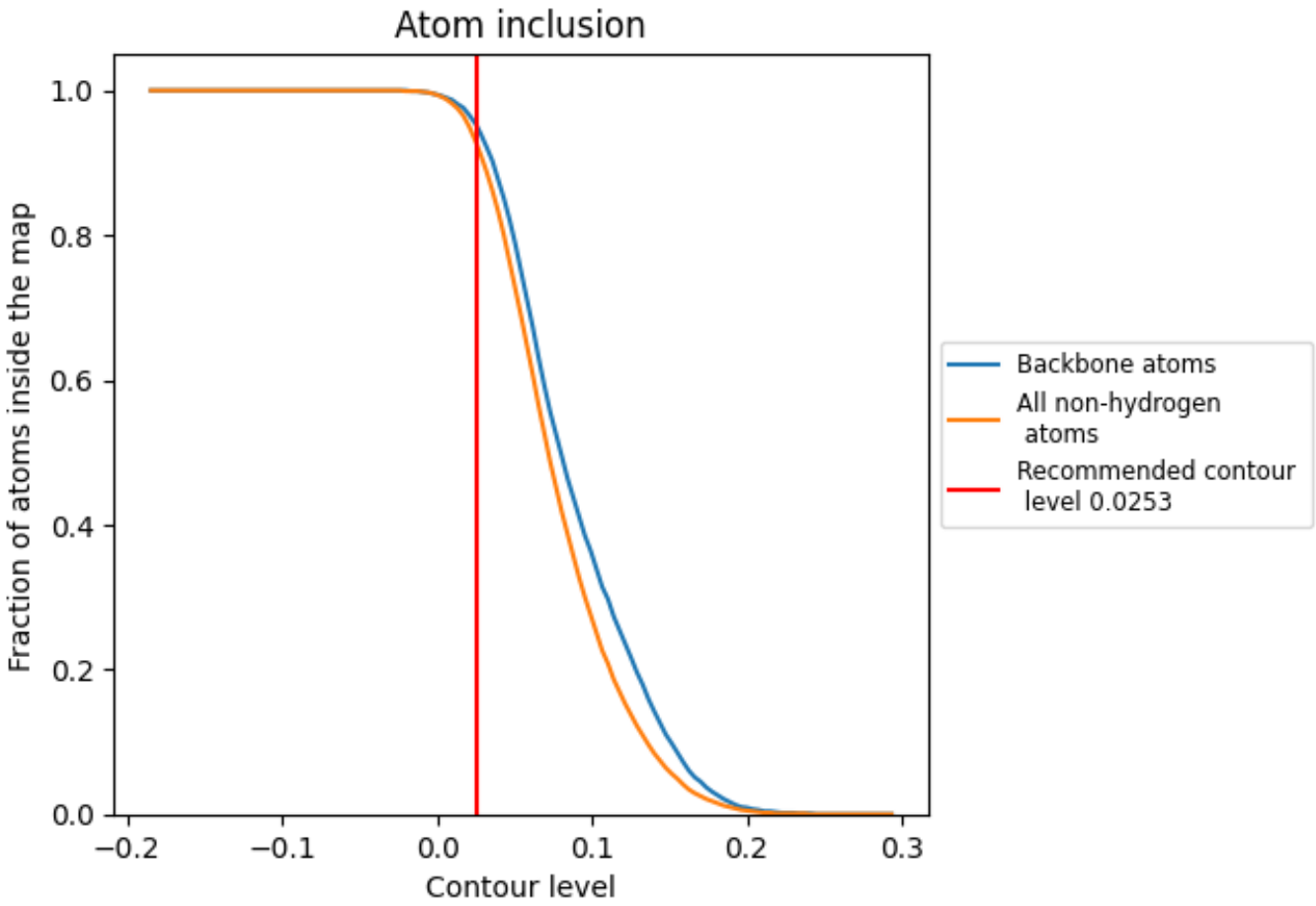
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0253).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.0253) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9280	0.4200
A	0.9110	0.4900
B	0.8980	0.4830
C	0.9240	0.4890
D	0.9270	0.4800
E	0.9210	0.4840
F	0.8810	0.4720
G	0.9350	0.4940
H	0.9200	0.4750
I	0.9770	0.3670
J	0.9730	0.3730
K	0.8720	0.3990