



## wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 09:43 AM UTC

PDB ID : 6FML / pdb\_00006fml  
EMDB ID : EMD-4277  
Title : CryoEM Structure INO80core Nucleosome complex  
Authors : Eustermann, S.; Schall, K.; Kostrewa, D.; Strauss, M.; Hopfner, K.  
Deposited on : 2018-01-31  
Resolution : 4.34 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

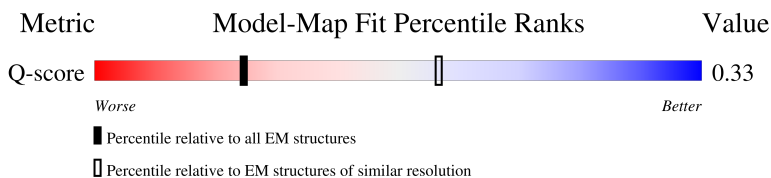
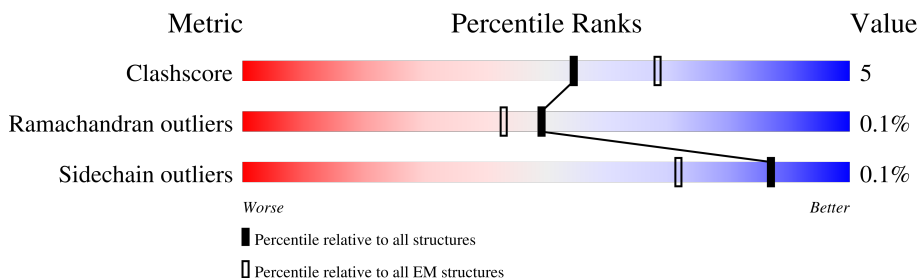
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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) : 2.49

# 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 4.34 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	3836 ( 3.84 - 4.84 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	462	6% 88% 10% .
1	B	462	5% 83% 11% 5%
1	C	462	7% 86% 13% .
2	D	488	6% 81% 9% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	488	
2	F	488	
3	G	1856	
4	H	491	
5	I	219	
6	J	770	
7	K	196	
8	L	196	
9	M	135	
9	Q	135	
10	N	102	
10	R	102	
11	O	129	
11	S	129	
12	P	125	
12	T	125	

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 43460 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 RuvB-like helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	449	Total	C	N	O	S	0	0
			3432	2154	610	653	15		
1	B	438	Total	C	N	O	S	0	0
			3352	2103	597	637	15		
1	C	459	Total	C	N	O	S	0	0
			3511	2199	627	670	15		

- Molecule 2 is a protein called RuvB-like helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	439	Total	C	N	O	S	0	0
			3383	2117	595	656	15		
2	E	441	Total	C	N	O	S	0	0
			3396	2124	598	659	15		
2	F	437	Total	C	N	O	S	0	0
			3376	2113	594	654	15		

- Molecule 3 is a protein called Ino80.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	731	Total	C	N	O	S	0	0
			5964	3797	1057	1075	35		

- Molecule 4 is a protein called Ies2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	66	Total	C	N	O	S	0	0
			413	259	75	76	3		

- Molecule 5 is a protein called Ies6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	109	Total	C	N	O	S	0	0
			875	550	167	154	4		

- Molecule 6 is a protein called Actin related protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	503	Total	C	N	O	S	0	0
			3843	2443	682	702	16		

- Molecule 7 is a DNA chain called Nucleosomal DNA Strand 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	144	Total	C	N	O	P	0	0
			2969	1405	557	863	144		

- Molecule 8 is a DNA chain called Nucleosomal DNA Strand 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	144	Total	C	N	O	P	0	0
			2935	1394	532	865	144		

- Molecule 9 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	95	Total	C	N	O	S	0	0
			766	485	142	136	3		
9	Q	97	Total	C	N	O	S	0	0
			787	497	151	136	3		

- Molecule 10 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	79	Total	C	N	O	S	0	0
			623	392	120	110	1		
10	R	82	Total	C	N	O	S	0	0
			635	400	121	113	1		

- Molecule 11 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	O	104	Total	C	N	O	0	0
			764	484	141	139		

*Continued on next page...*

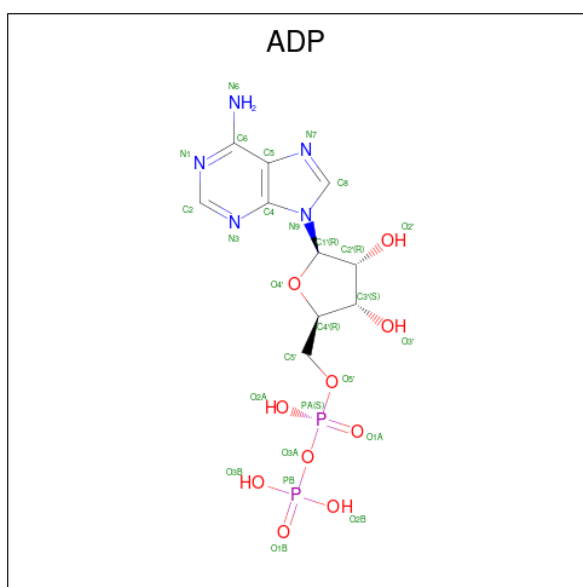
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	S	107	791	499	150	142	0	0

- Molecule 12 is a protein called Histone H2B type 1-C/E/F/G/I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	P	95	728	455	130	141	2	0	0
12	T	95	724	452	129	141	2	0	0

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



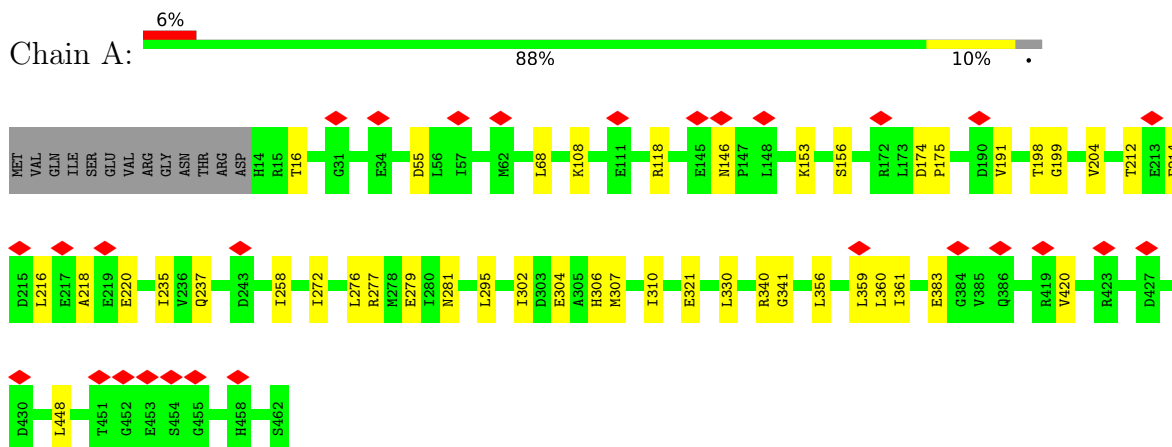
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	A	1	27	10	5	10	2	0
13	B	1	27	10	5	10	2	0
13	C	1	27	10	5	10	2	0
13	D	1	27	10	5	10	2	0
13	E	1	27	10	5	10	2	0
13	F	1	27	10	5	10	2	0



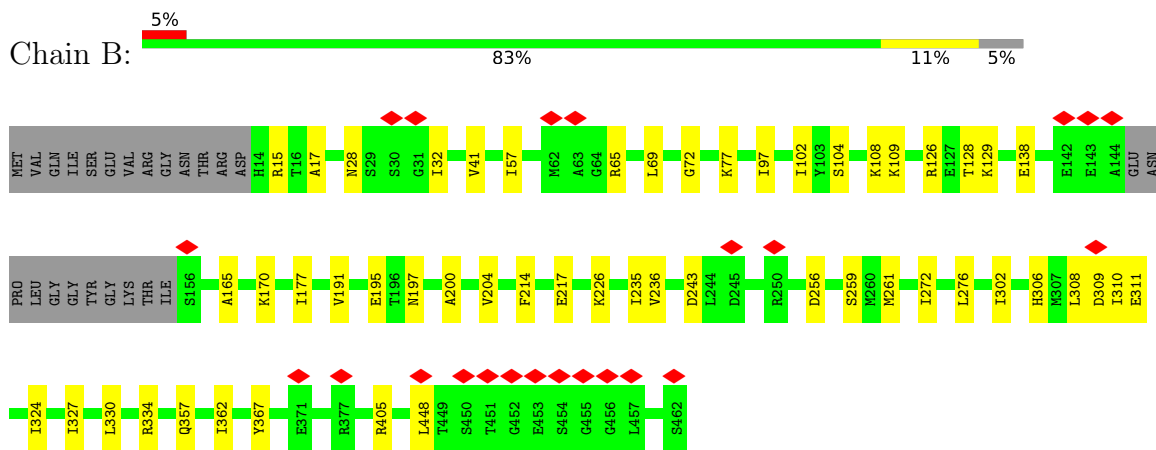
### 3 Residue-property plots

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.

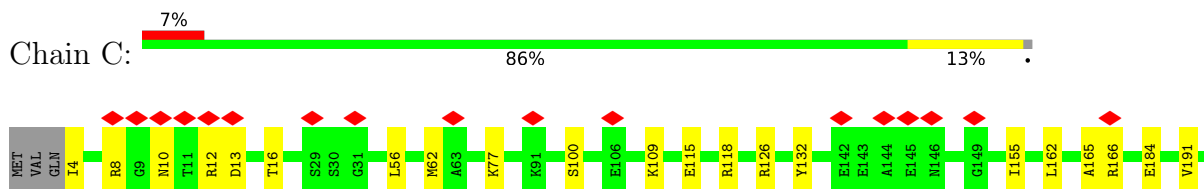
- Molecule 1: RuvB-like helicase

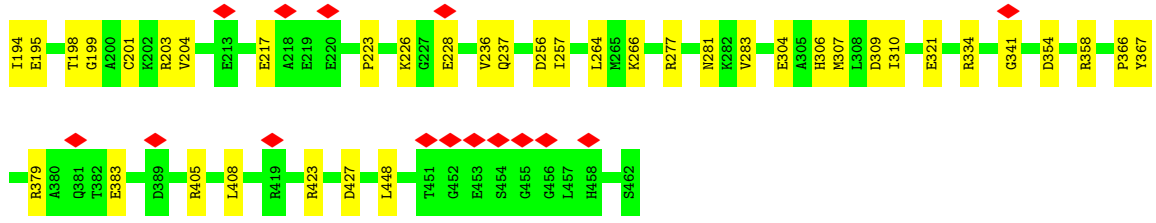


- Molecule 1: RuvB-like helicase

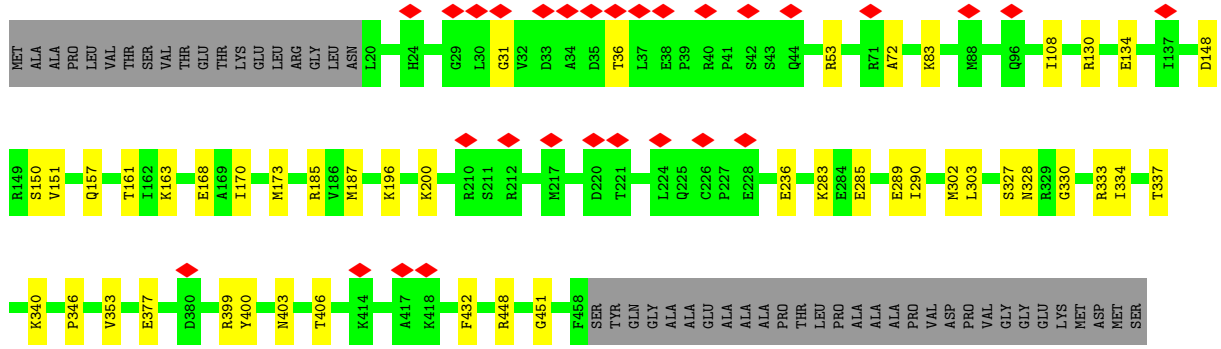
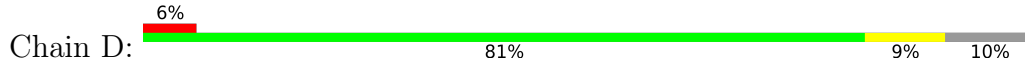


- Molecule 1: RuvB-like helicase

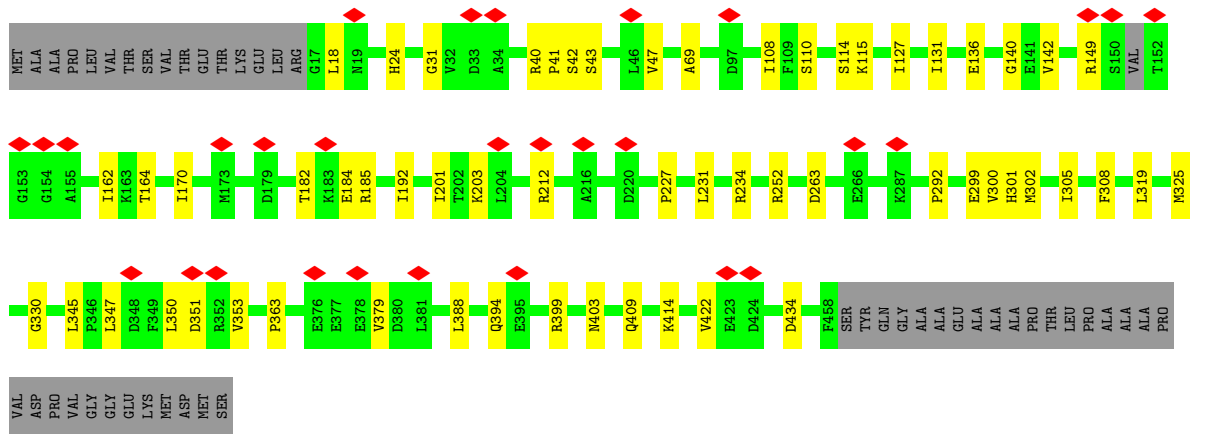
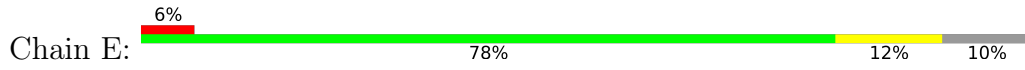




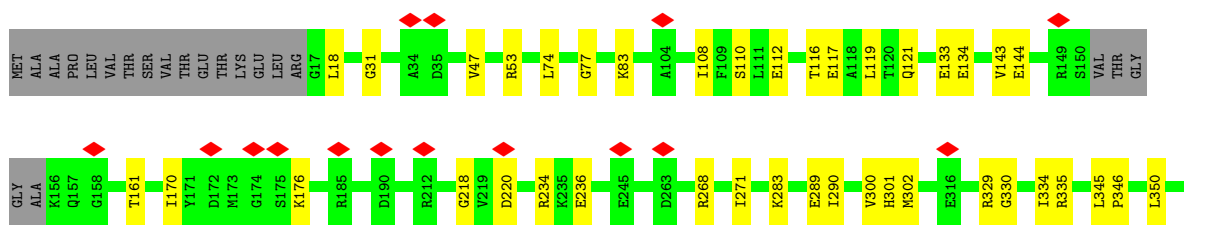
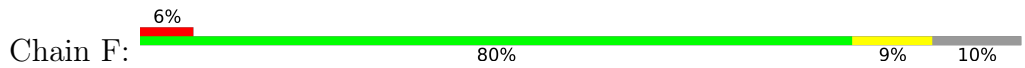
• Molecule 2: RuvB-like helicase



• Molecule 2: RuvB-like helicase



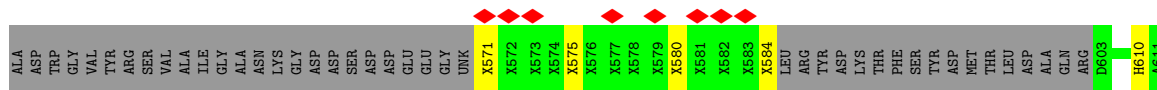
• Molecule 2: RuvB-like helicase



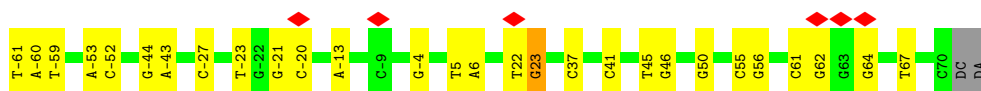
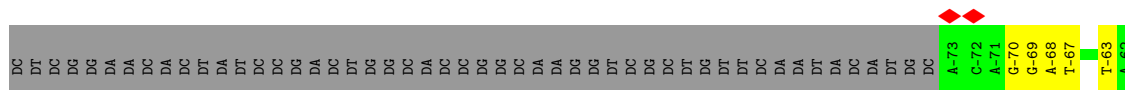




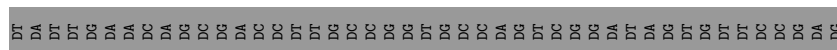




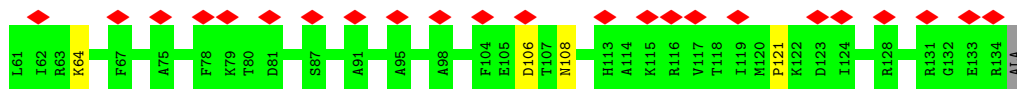
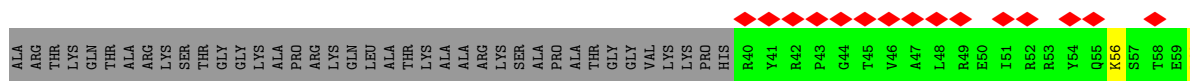
• Molecule 7: Nucleosomal DNA Strand 1



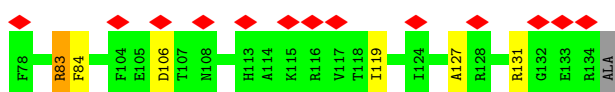
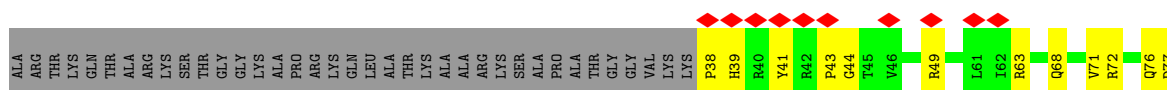
• Molecule 8: Nucleosomal DNA Strand 2



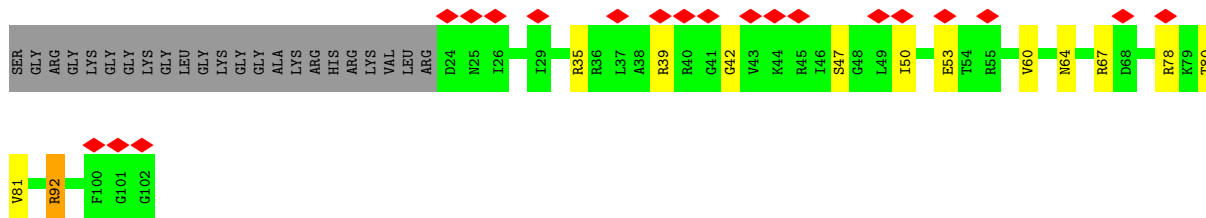
• Molecule 9: Histone H3.2



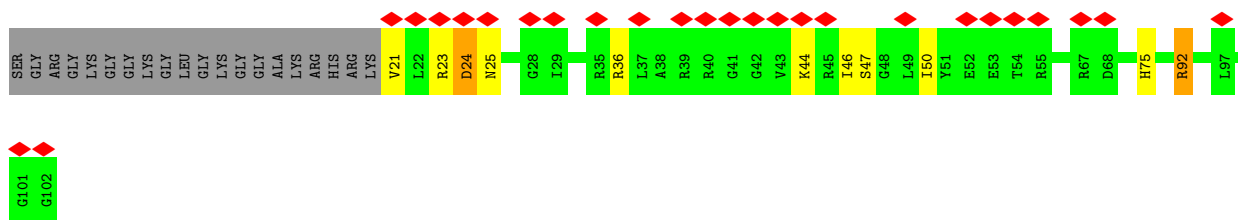
• Molecule 9: Histone H3.2



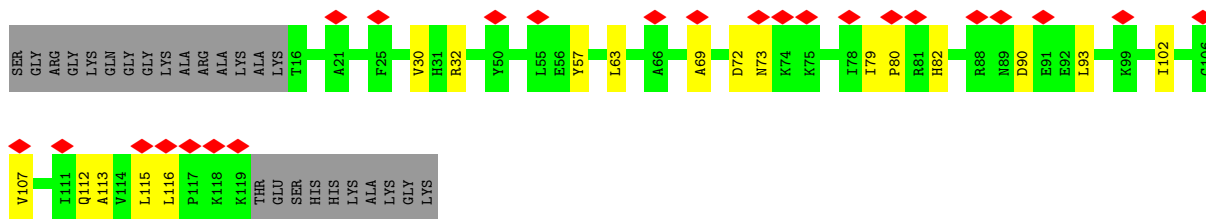
• Molecule 10: Histone H4



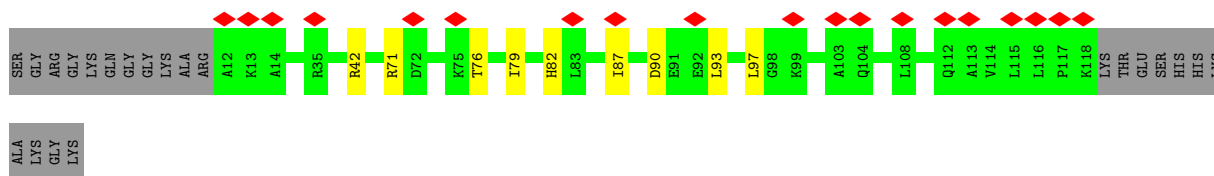
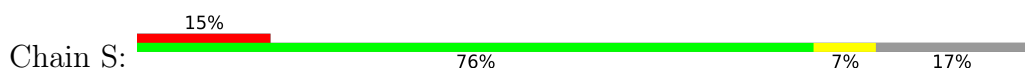
• Molecule 10: Histone H4



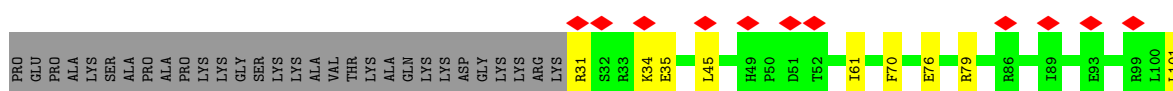
• Molecule 11: Histone H2A type 1

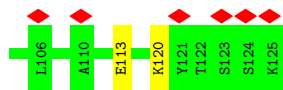


• Molecule 11: Histone H2A type 1

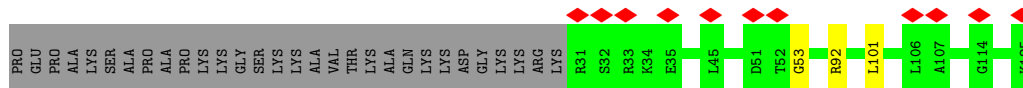
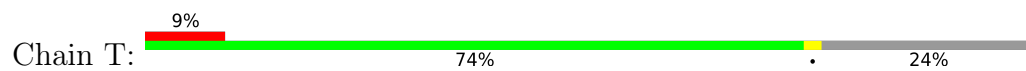


• Molecule 12: Histone H2B type 1-C/E/F/G/I





- Molecule 12: Histone H2B type 1-C/E/F/G/I



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33937	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	59.6	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.140	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.034	Depositor
Map size (Å)	360.4, 360.4, 360.4	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: ADP, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.45	0/3481	0.56	0/4703
1	B	0.46	0/3398	0.56	0/4589
1	C	0.43	0/3560	0.53	0/4809
2	D	0.43	0/3426	0.56	0/4614
2	E	0.46	0/3438	0.57	0/4628
2	F	0.44	0/3418	0.56	0/4601
3	G	0.44	0/6101	0.74	8/8246 (0.1%)
4	H	0.37	0/270	0.47	0/367
5	I	0.40	0/895	0.59	0/1209
6	J	0.40	2/3647 (0.1%)	0.53	0/4944
7	K	0.35	0/3334	0.45	1/5148 (0.0%)
8	L	0.34	0/3288	0.45	2/5068 (0.0%)
9	M	0.32	0/776	0.61	0/1043
9	Q	0.39	0/799	0.74	1/1074 (0.1%)
10	N	0.29	0/630	0.66	0/844
10	R	0.35	0/642	0.79	2/864 (0.2%)
11	O	0.36	0/774	0.68	0/1055
11	S	0.37	0/801	0.64	0/1090
12	P	0.37	0/739	0.70	0/996
12	T	0.37	0/735	0.61	0/992
All	All	0.41	2/44152 (0.0%)	0.59	14/60884 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	G	0	10
9	Q	0	1
11	O	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	112	ARG	CZ-NH1	6.26	1.41	1.32
6	J	112	ARG	CG-CD	-5.66	1.35	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	63	DA	O3'-P-O5'	7.38	115.07	104.00
7	K	23	DG	OP1-P-OP2	-6.88	99.36	120.00
9	Q	83	ARG	CA-CB-CG	6.49	127.07	114.10
3	G	1649	ASP	CA-C-N	6.21	131.07	121.19
3	G	1649	ASP	C-N-CA	6.21	131.07	121.19

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	1021	TRP	Peptide
3	G	1066	TRP	Peptide
3	G	1073	TYR	Peptide
3	G	1274	PHE	Peptide
3	G	1548	PHE	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3432	0	3518	33	0
1	B	3352	0	3438	36	0
1	C	3511	0	3595	44	0
2	D	3383	0	3458	34	0
2	E	3396	0	3468	42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3376	0	3450	36	0
3	G	5964	0	5972	123	0
4	H	413	0	296	4	0
5	I	875	0	879	14	0
6	J	3843	0	3541	42	0
7	K	2969	0	1616	27	0
8	L	2935	0	1617	22	0
9	M	766	0	791	5	0
9	Q	787	0	813	15	0
10	N	623	0	652	8	0
10	R	635	0	652	9	0
11	O	764	0	773	11	0
11	S	791	0	807	7	0
12	P	728	0	725	11	0
12	T	724	0	714	3	0
13	A	27	0	12	0	0
13	B	27	0	12	2	0
13	C	27	0	12	3	0
13	D	27	0	12	2	0
13	E	27	0	12	1	0
13	F	27	0	12	4	0
14	J	31	0	12	0	0
All	All	43460	0	40859	425	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 425 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1259:ASN:O	3:G:1263:GLN:HB3	1.84	0.76
3:G:1571:ARG:HH22	3:G:1639:THR:HB	1.55	0.70
7:K:41:DC:H42	8:L:-41:DG:H1	1.38	0.70
7:K:64:DG:H1	8:L:-64:DC:H42	1.40	0.69
3:G:1155:PRO:HA	3:G:1158:PHE:HB2	1.74	0.69

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	447/462 (97%)	420 (94%)	27 (6%)	0	100	100
1	B	434/462 (94%)	404 (93%)	30 (7%)	0	100	100
1	C	457/462 (99%)	428 (94%)	29 (6%)	0	100	100
2	D	437/488 (90%)	409 (94%)	28 (6%)	0	100	100
2	E	437/488 (90%)	410 (94%)	27 (6%)	0	100	100
2	F	433/488 (89%)	402 (93%)	31 (7%)	0	100	100
3	G	727/1856 (39%)	647 (89%)	75 (10%)	5 (1%)	18	55
4	H	34/491 (7%)	32 (94%)	2 (6%)	0	100	100
5	I	105/219 (48%)	99 (94%)	6 (6%)	0	100	100
6	J	437/770 (57%)	411 (94%)	26 (6%)	0	100	100
9	M	93/135 (69%)	90 (97%)	3 (3%)	0	100	100
9	Q	95/135 (70%)	90 (95%)	5 (5%)	0	100	100
10	N	77/102 (76%)	74 (96%)	3 (4%)	0	100	100
10	R	80/102 (78%)	74 (92%)	5 (6%)	1 (1%)	9	41
11	O	102/129 (79%)	99 (97%)	3 (3%)	0	100	100
11	S	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
12	P	93/125 (74%)	86 (92%)	7 (8%)	0	100	100
12	T	93/125 (74%)	90 (97%)	3 (3%)	0	100	100
All	All	4686/7168 (65%)	4367 (93%)	313 (7%)	6 (0%)	49	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	1069	LYS
3	G	1549	VAL
10	R	24	ASP
3	G	1551	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	G	1573	LEU

### 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	365/377 (97%)	365 (100%)	0	100	100
1	B	357/377 (95%)	357 (100%)	0	100	100
1	C	374/377 (99%)	374 (100%)	0	100	100
2	D	367/402 (91%)	367 (100%)	0	100	100
2	E	368/402 (92%)	368 (100%)	0	100	100
2	F	367/402 (91%)	367 (100%)	0	100	100
3	G	651/1604 (41%)	650 (100%)	1 (0%)	87	85
4	H	28/369 (8%)	28 (100%)	0	100	100
5	I	93/171 (54%)	93 (100%)	0	100	100
6	J	371/593 (63%)	371 (100%)	0	100	100
9	M	80/110 (73%)	80 (100%)	0	100	100
9	Q	82/110 (74%)	82 (100%)	0	100	100
10	N	63/78 (81%)	61 (97%)	2 (3%)	34	55
10	R	63/78 (81%)	62 (98%)	1 (2%)	55	69
11	O	74/98 (76%)	73 (99%)	1 (1%)	59	71
11	S	76/98 (78%)	76 (100%)	0	100	100
12	P	78/105 (74%)	78 (100%)	0	100	100
12	T	77/105 (73%)	77 (100%)	0	100	100
All	All	3934/5856 (67%)	3929 (100%)	5 (0%)	87	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	1681	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	N	81	VAL
10	N	92	ARG
11	O	107	VAL
10	R	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	1287	HIS
9	M	85	GLN
3	G	1570	HIS
3	G	1697	GLN
10	N	25	ASN

### 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](#)

7 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
13	ADP	B	501	-	28,29,29	1.48	5 (17%)	43,45,45	1.73	7 (16%)
14	ATP	J	801	-	32,33,33	1.33	5 (15%)	48,52,52	1.74	10 (20%)
13	ADP	E	501	-	28,29,29	1.38	5 (17%)	43,45,45	1.84	11 (25%)
13	ADP	F	501	-	28,29,29	1.37	5 (17%)	43,45,45	1.82	8 (18%)
13	ADP	A	501	-	28,29,29	1.37	6 (21%)	43,45,45	1.76	8 (18%)
13	ADP	C	501	-	28,29,29	1.40	5 (17%)	43,45,45	1.81	9 (20%)
13	ADP	D	501	-	28,29,29	1.39	5 (17%)	43,45,45	1.90	12 (27%)

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
13	ADP	B	501	-	-	1/16/32/32	0/3/3/3
14	ATP	J	801	-	-	3/22/38/38	0/3/3/3
13	ADP	E	501	-	-	0/16/32/32	0/3/3/3
13	ADP	F	501	-	-	0/16/32/32	0/3/3/3
13	ADP	A	501	-	-	0/16/32/32	0/3/3/3
13	ADP	C	501	-	-	3/16/32/32	0/3/3/3
13	ADP	D	501	-	-	0/16/32/32	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	501	ADP	C5-C4	4.32	1.46	1.39
14	J	801	ATP	C5-C4	4.32	1.46	1.39
13	B	501	ADP	C5-C4	4.27	1.46	1.39
13	F	501	ADP	C5-C4	4.13	1.46	1.39
13	C	501	ADP	C5-C4	3.98	1.46	1.39

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	501	ADP	C5-C4-N3	-6.11	118.30	126.72
13	A	501	ADP	C5-C4-N3	-5.59	119.02	126.72
13	B	501	ADP	C5-C4-N3	-5.57	119.05	126.72
13	C	501	ADP	C5-C4-N3	-5.52	119.11	126.72
13	D	501	ADP	C5-C4-N3	-5.50	119.15	126.72

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

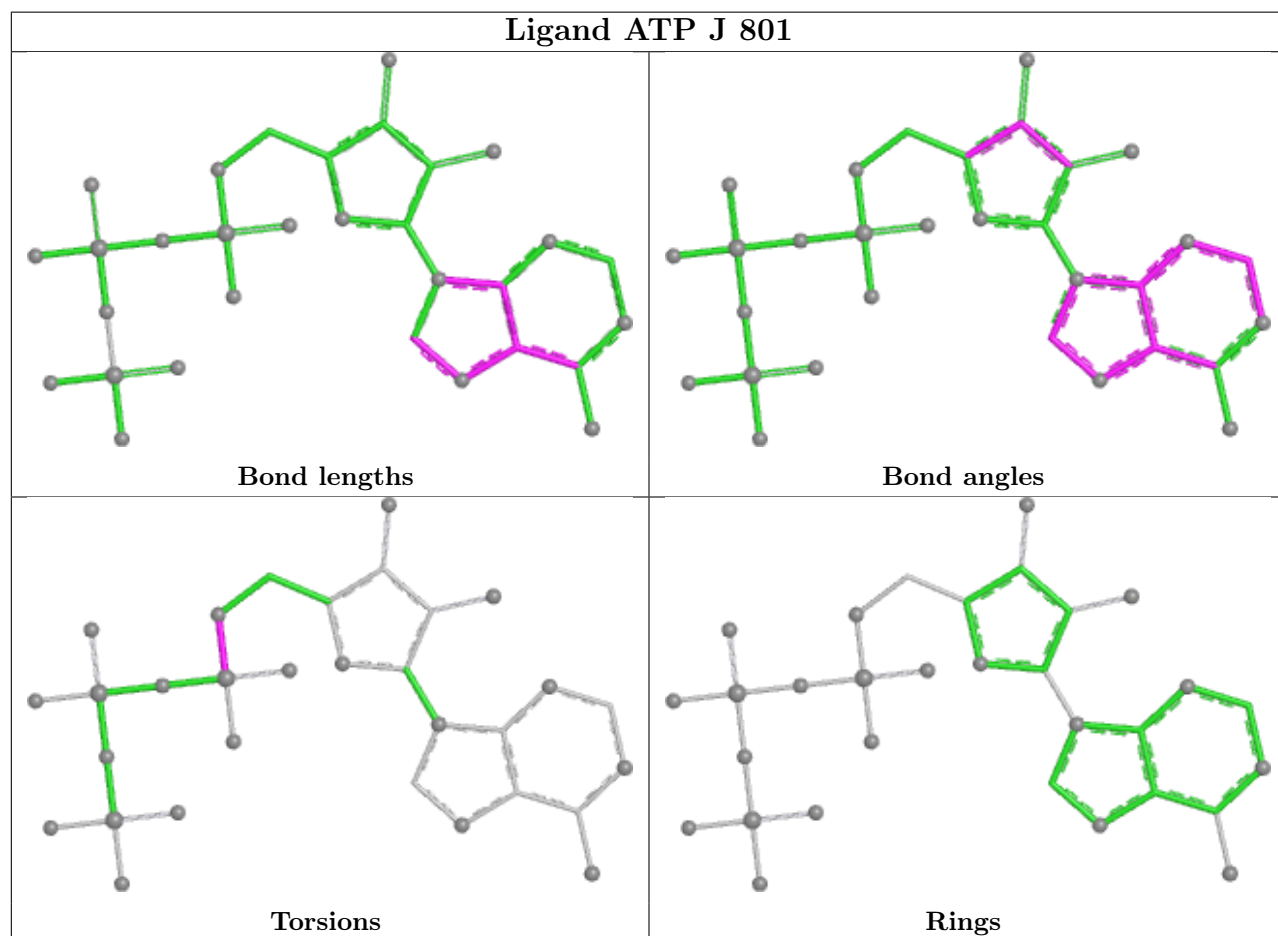
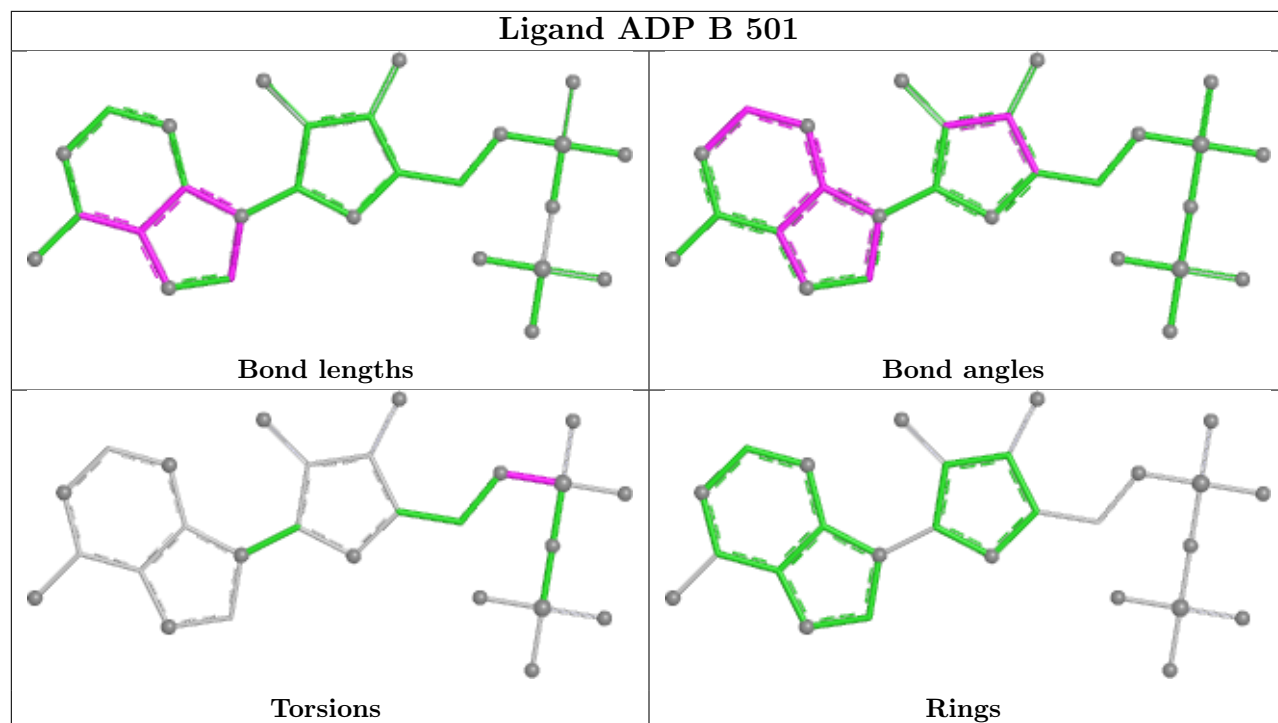
Mol	Chain	Res	Type	Atoms
13	B	501	ADP	C5'-O5'-PA-O1A
13	C	501	ADP	C5'-O5'-PA-O1A
13	C	501	ADP	C5'-O5'-PA-O2A
13	C	501	ADP	C5'-O5'-PA-O3A
14	J	801	ATP	C5'-O5'-PA-O1A

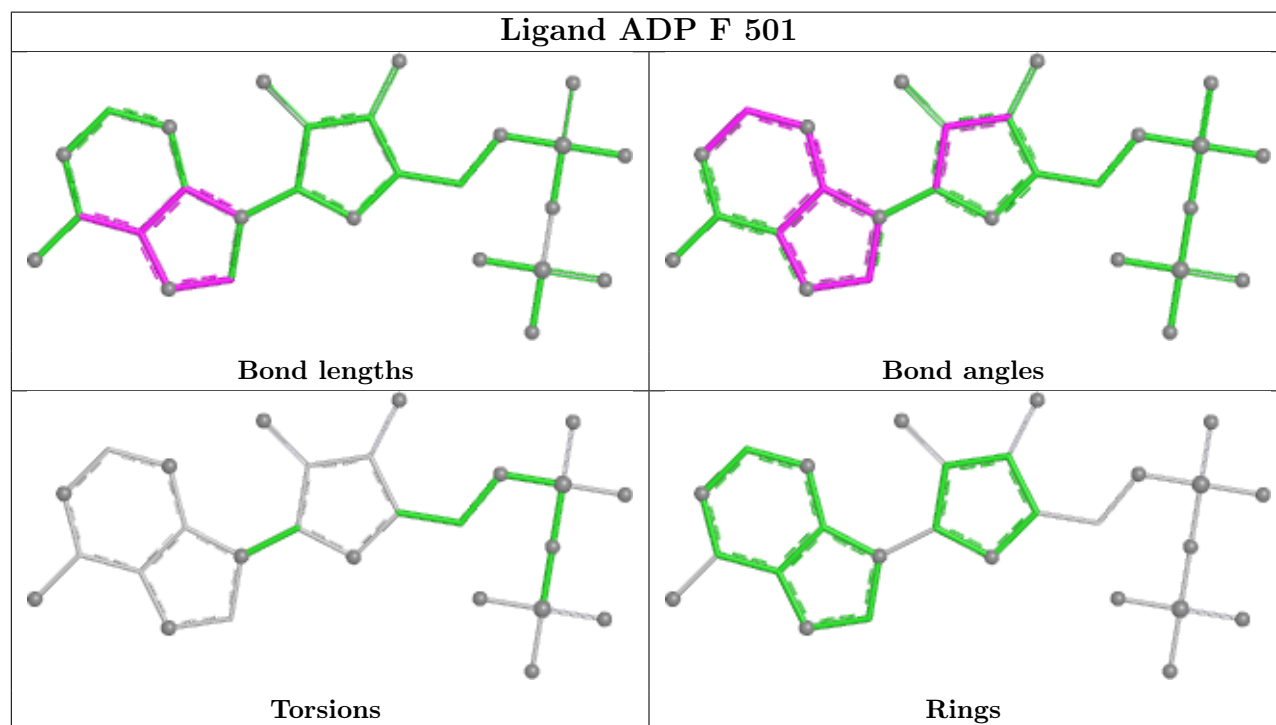
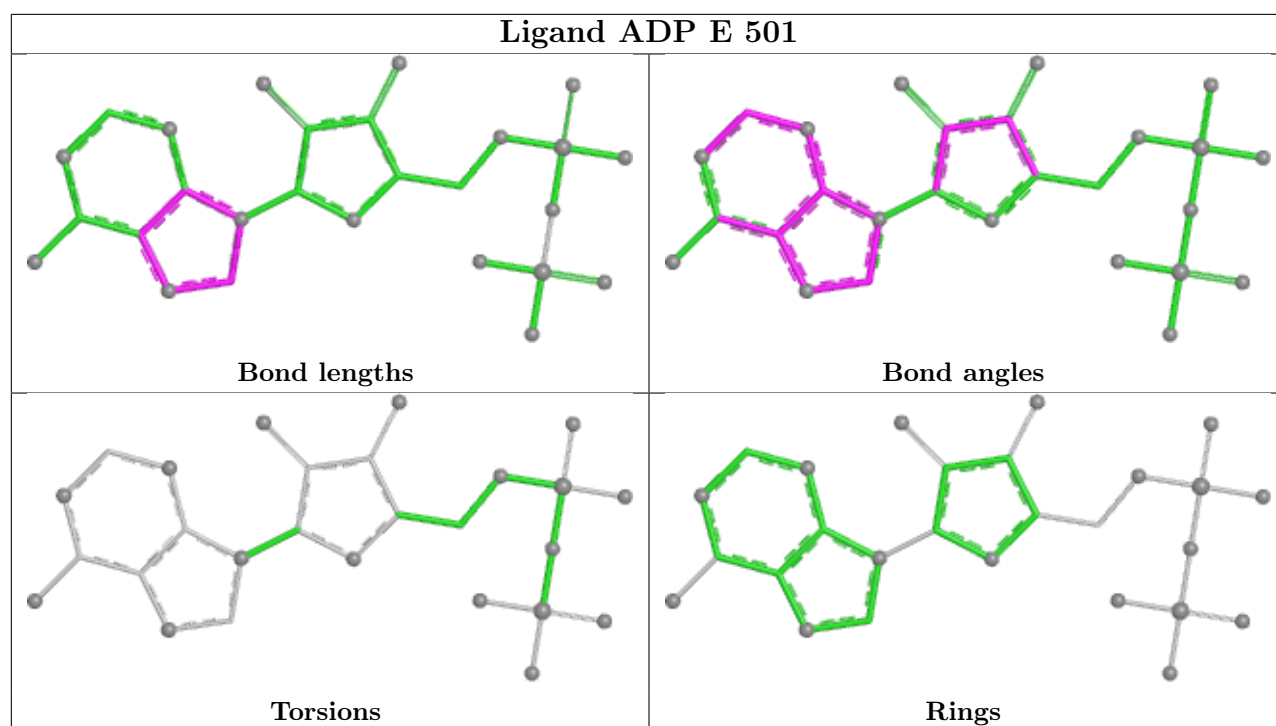
There are no ring outliers.

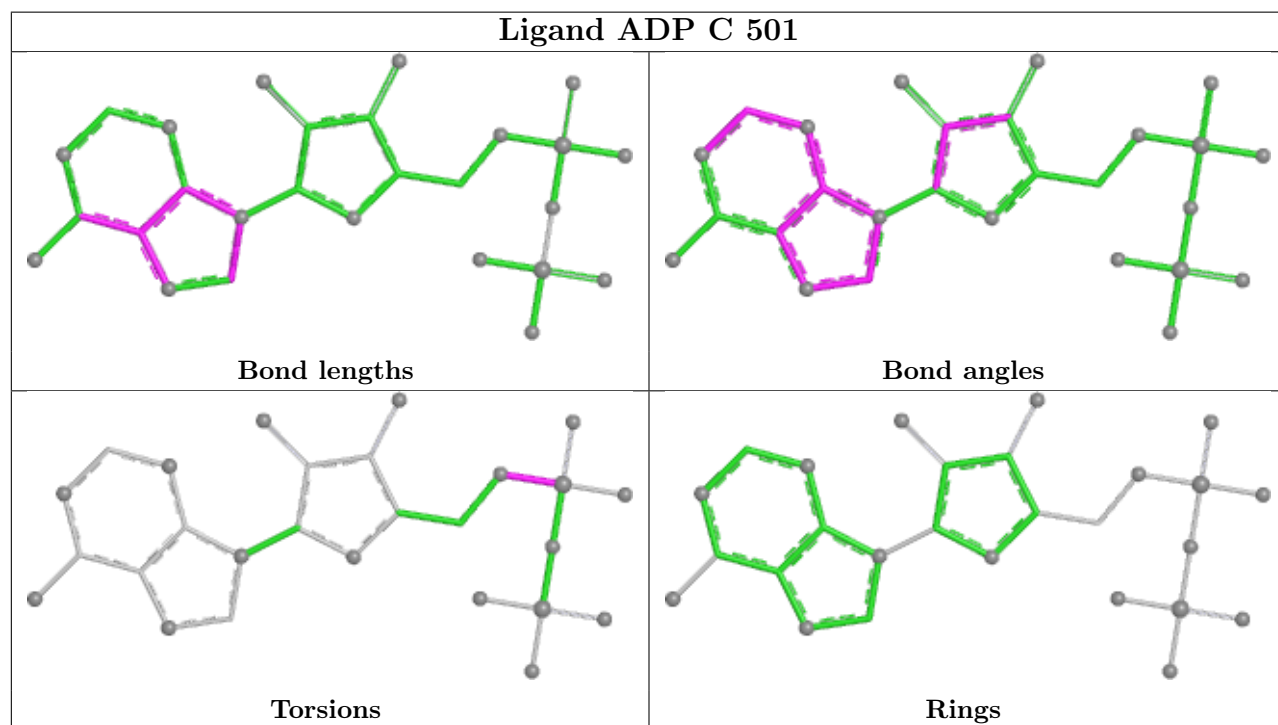
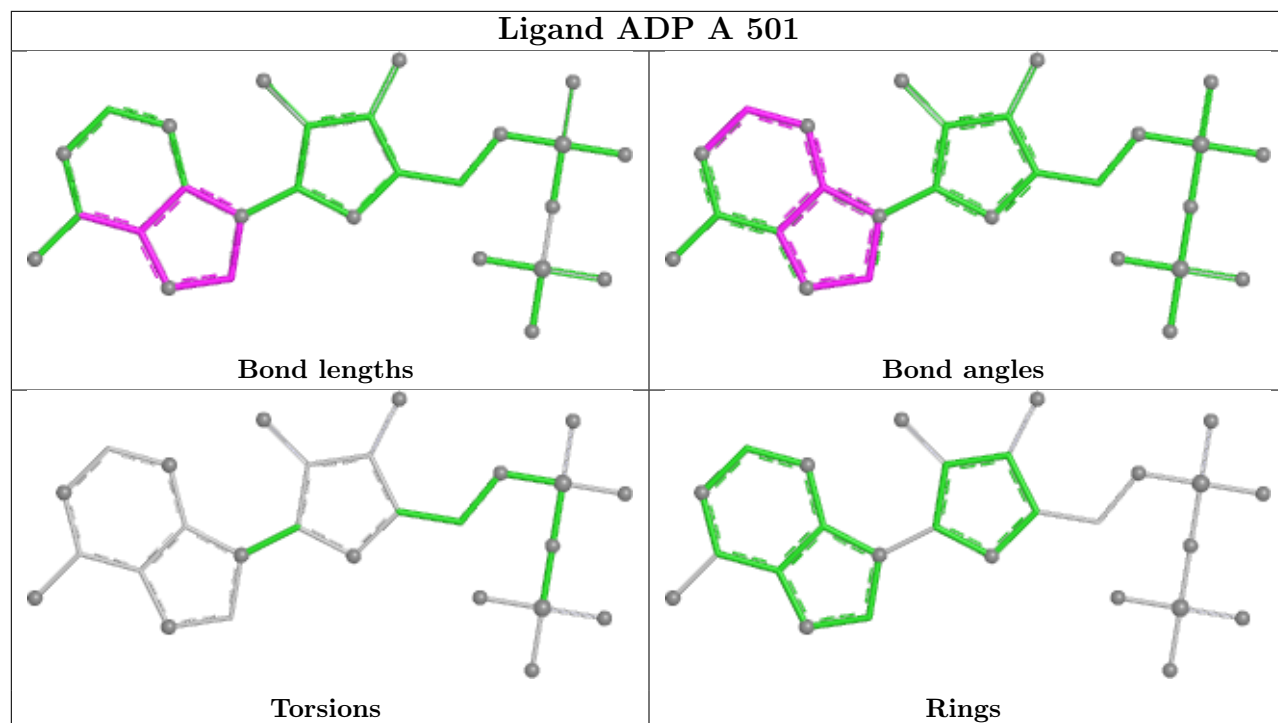
5 monomers are involved in 12 short contacts:

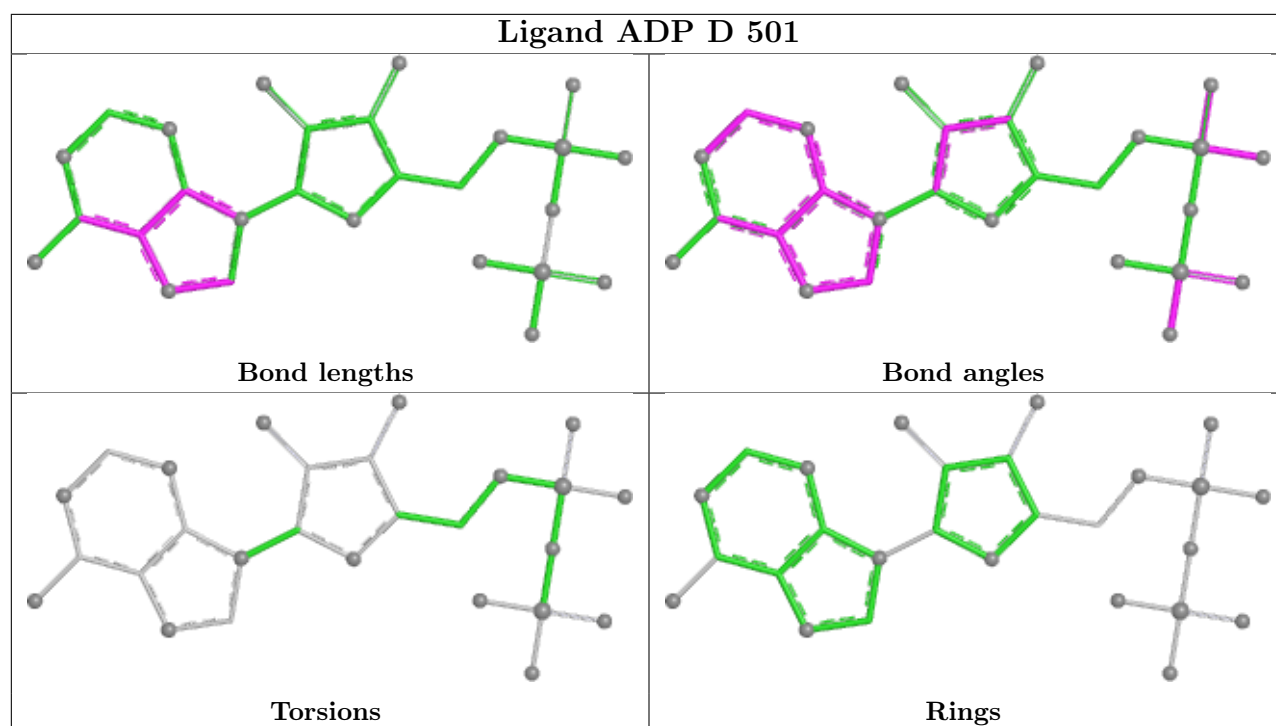
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	501	ADP	2	0
13	E	501	ADP	1	0
13	F	501	ADP	4	0
13	C	501	ADP	3	0
13	D	501	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

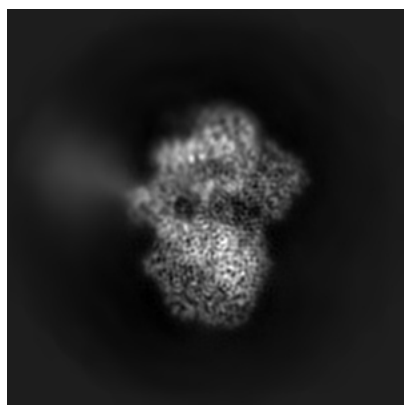
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4277. These allow visual inspection of the internal detail of the map and identification of artifacts.

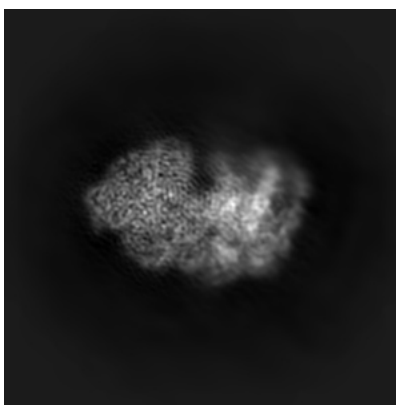
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

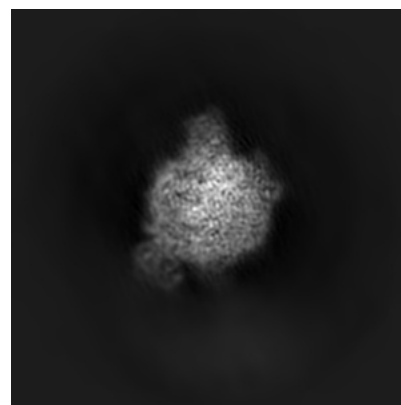
#### 6.1.1 Primary map



X



Y

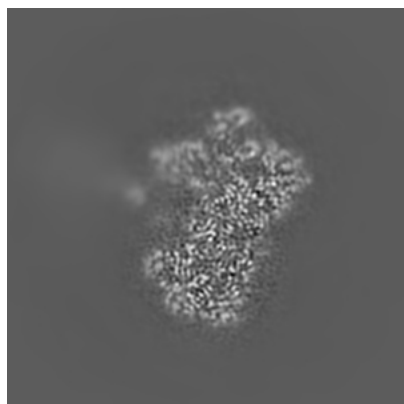


Z

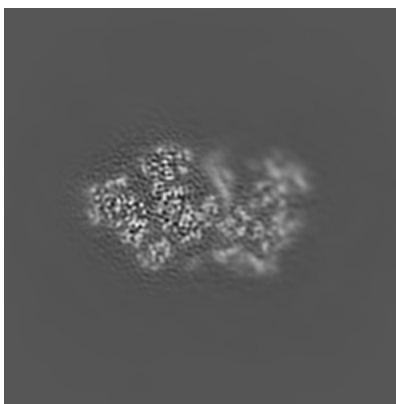
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

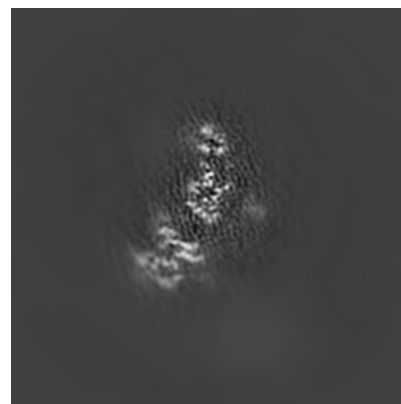
#### 6.2.1 Primary map



X Index: 170



Y Index: 170

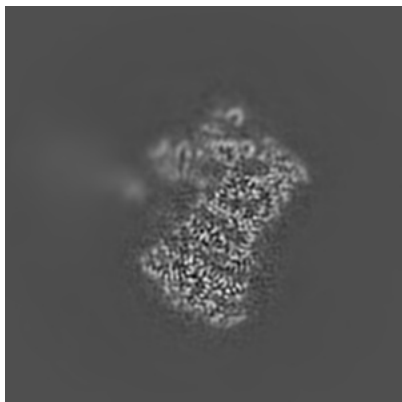


Z Index: 170

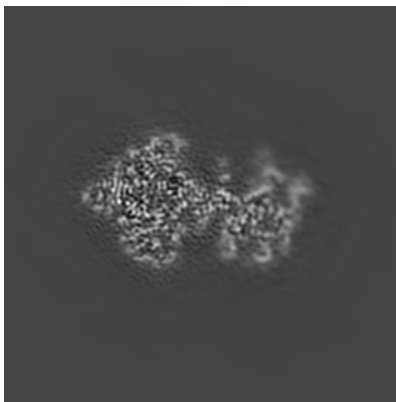
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

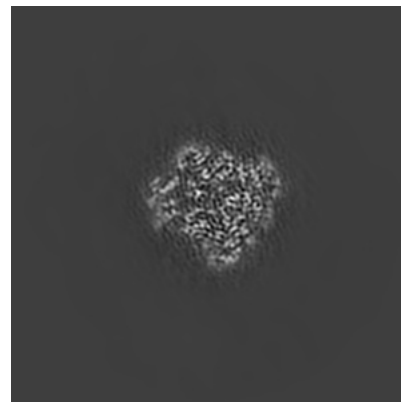
### 6.3.1 Primary map



X Index: 174



Y Index: 189

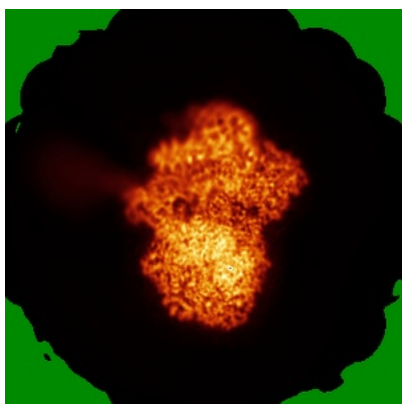


Z Index: 128

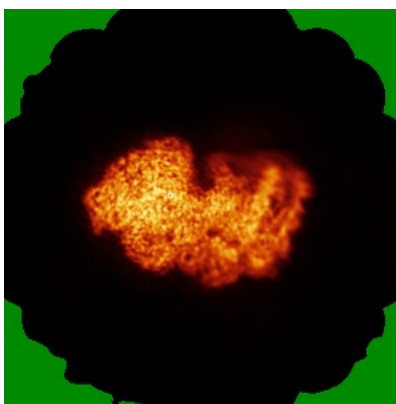
The images above show the largest variance slices of the map in three orthogonal directions.

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

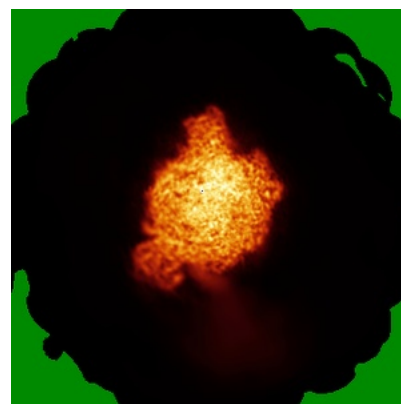
### 6.4.1 Primary map



X



Y

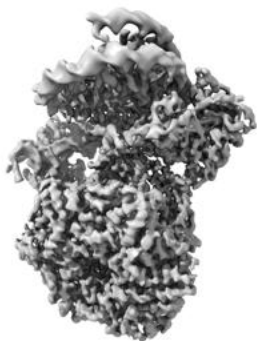


Z

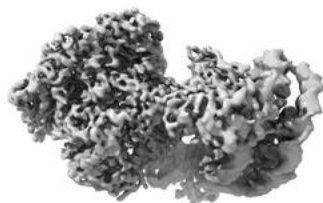
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

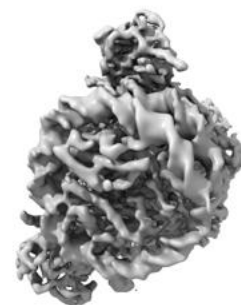
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

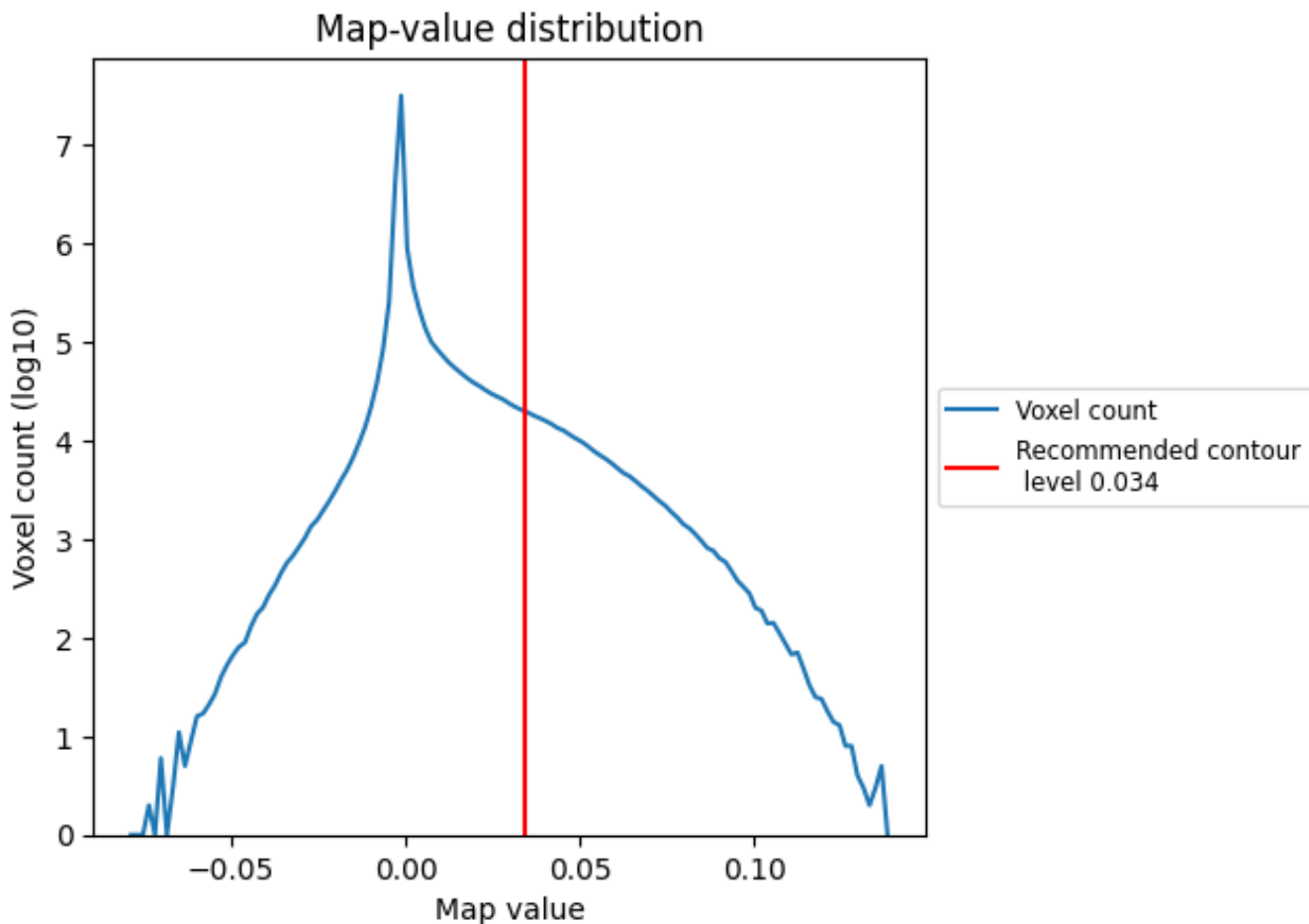
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

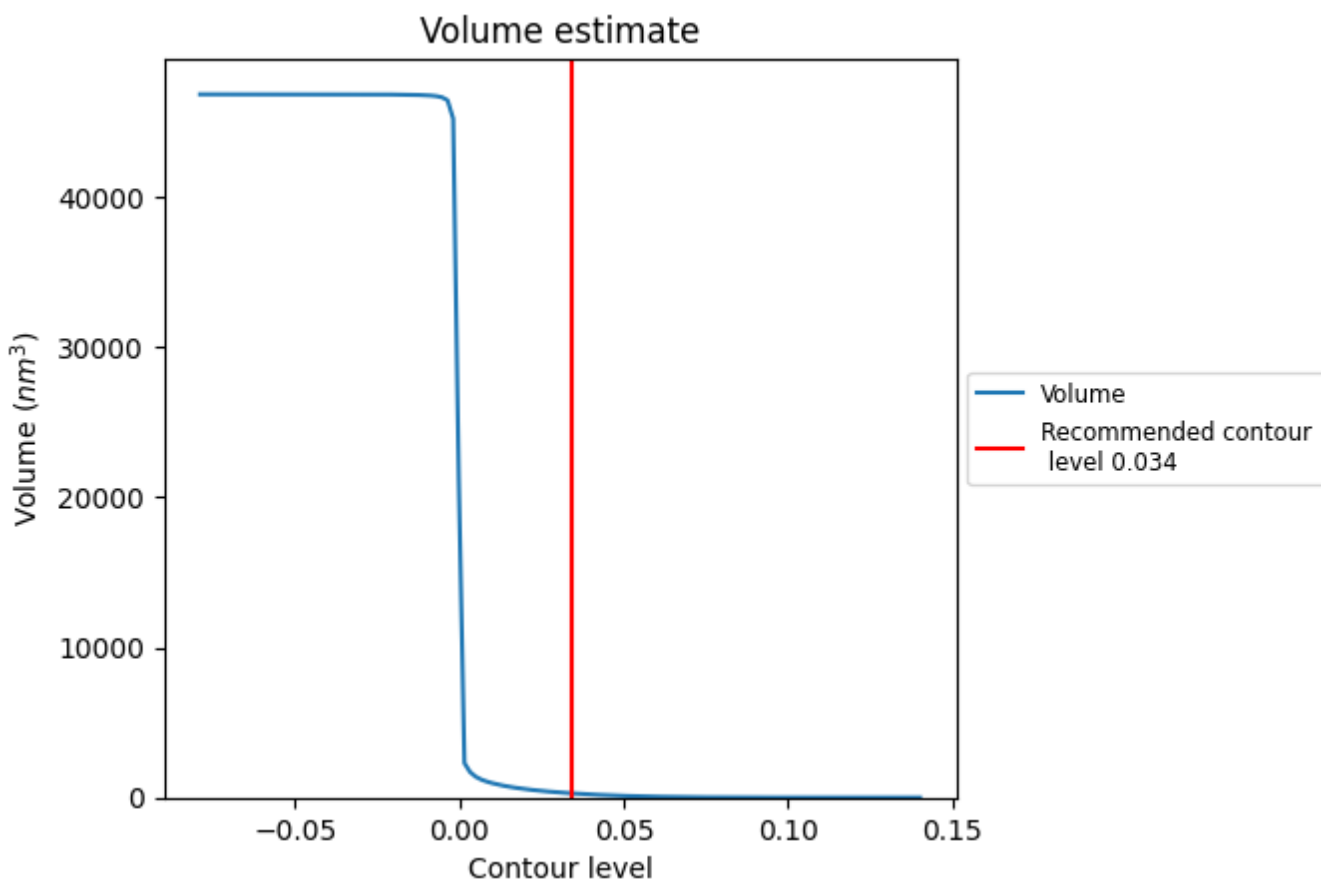
This section contains the results of statistical analysis of the map.

### 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.

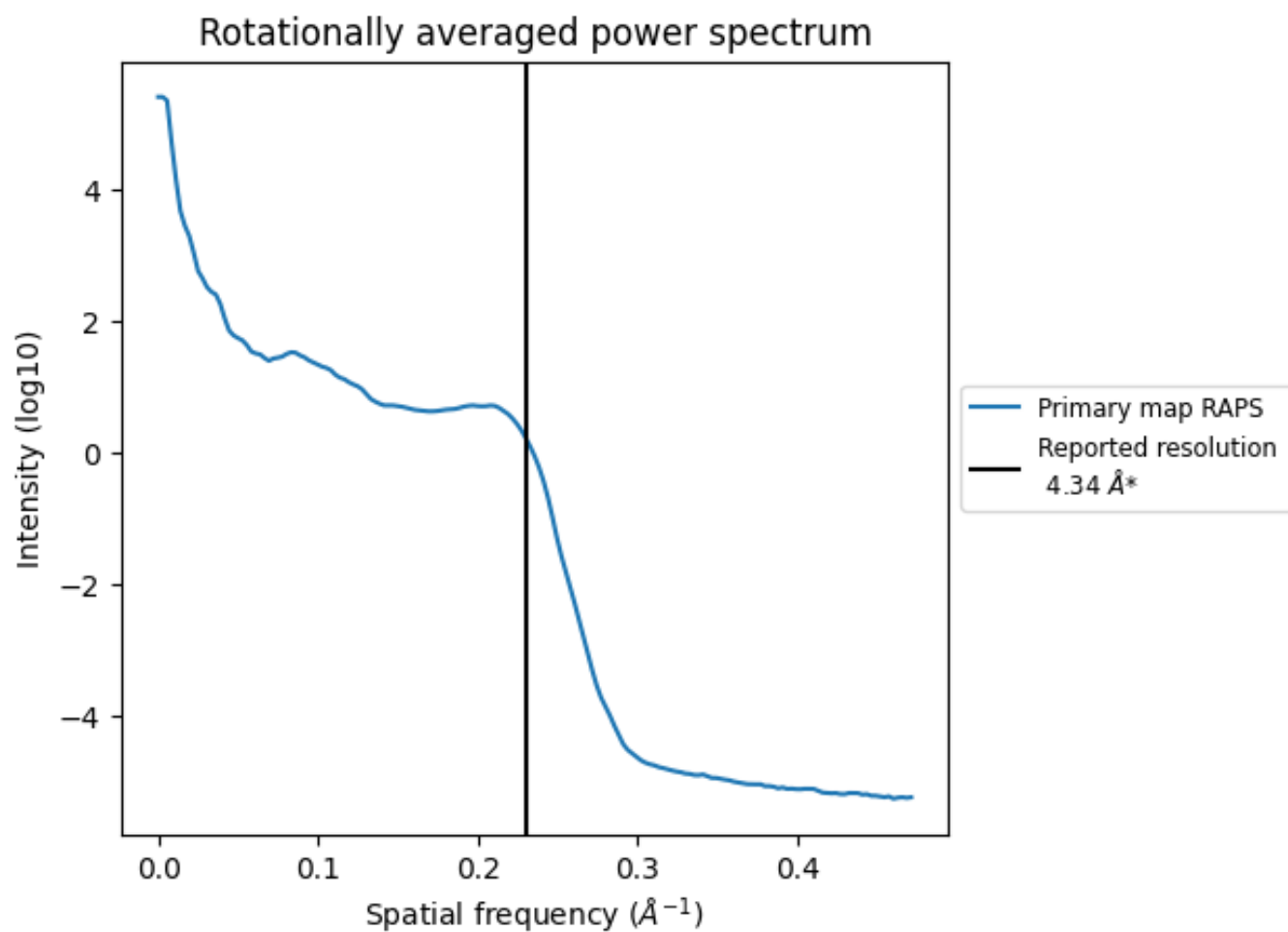
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 284 nm<sup>3</sup>; this corresponds to an approximate mass of 257 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](#)

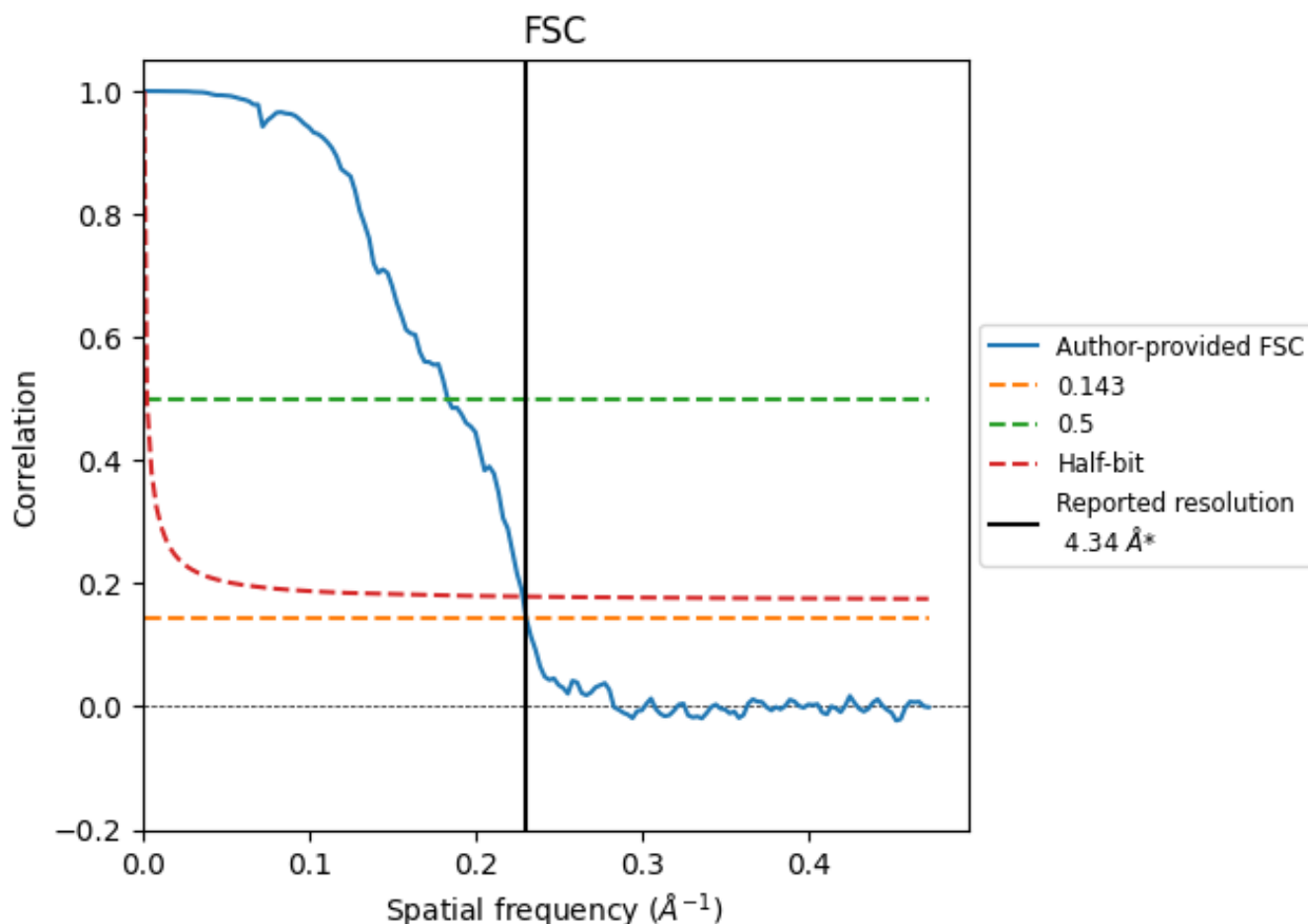


\*Reported resolution corresponds to spatial frequency of  $0.230 \text{\AA}^{-1}$

## 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 0.230 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

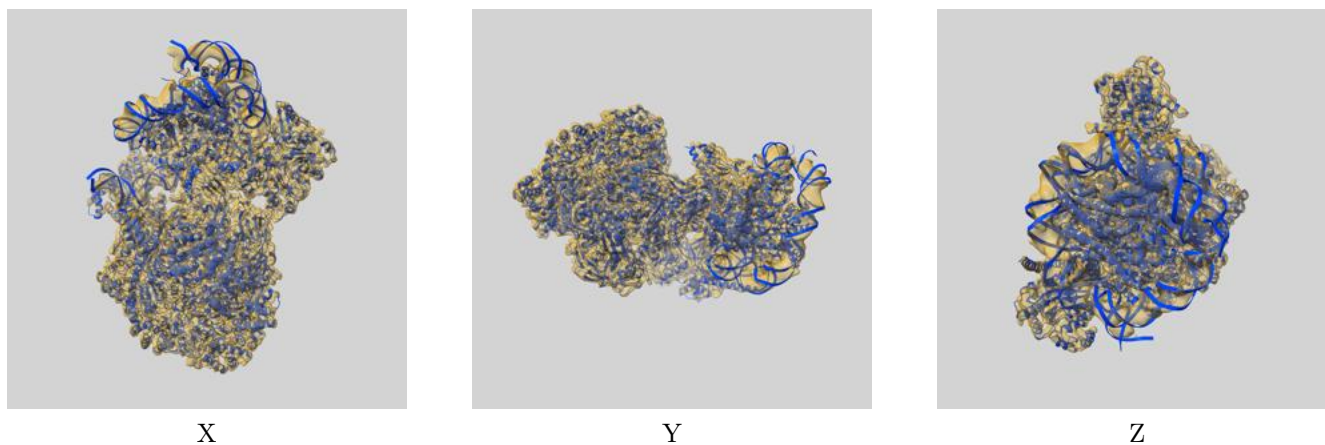
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.34	-	-
Author-provided FSC curve	4.34	5.46	4.38
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

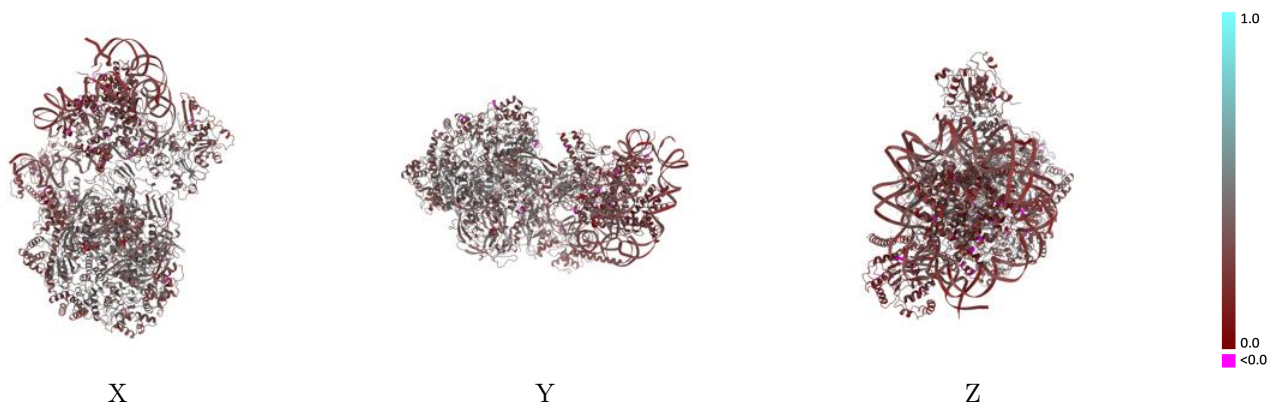
This section contains information regarding the fit between EMDB map EMD-4277 and PDB model 6FML. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



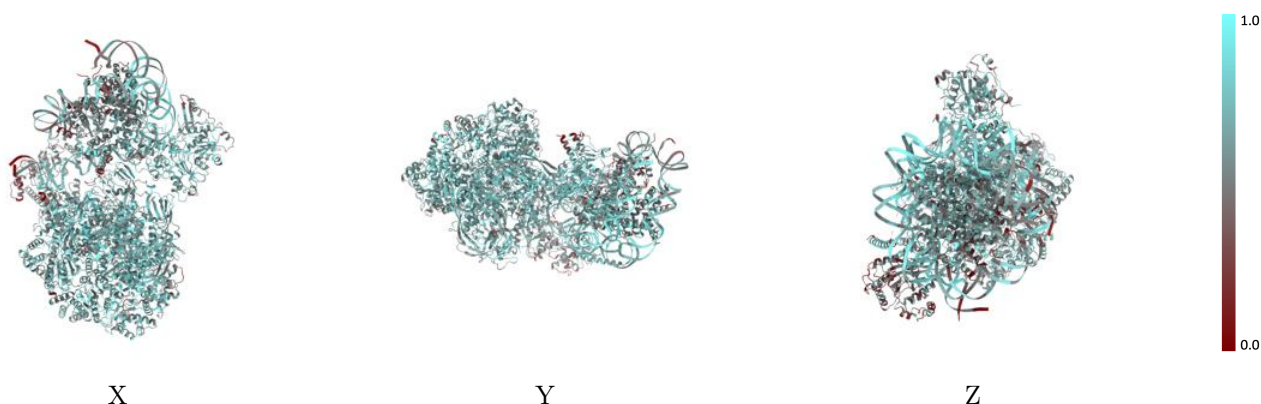
The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



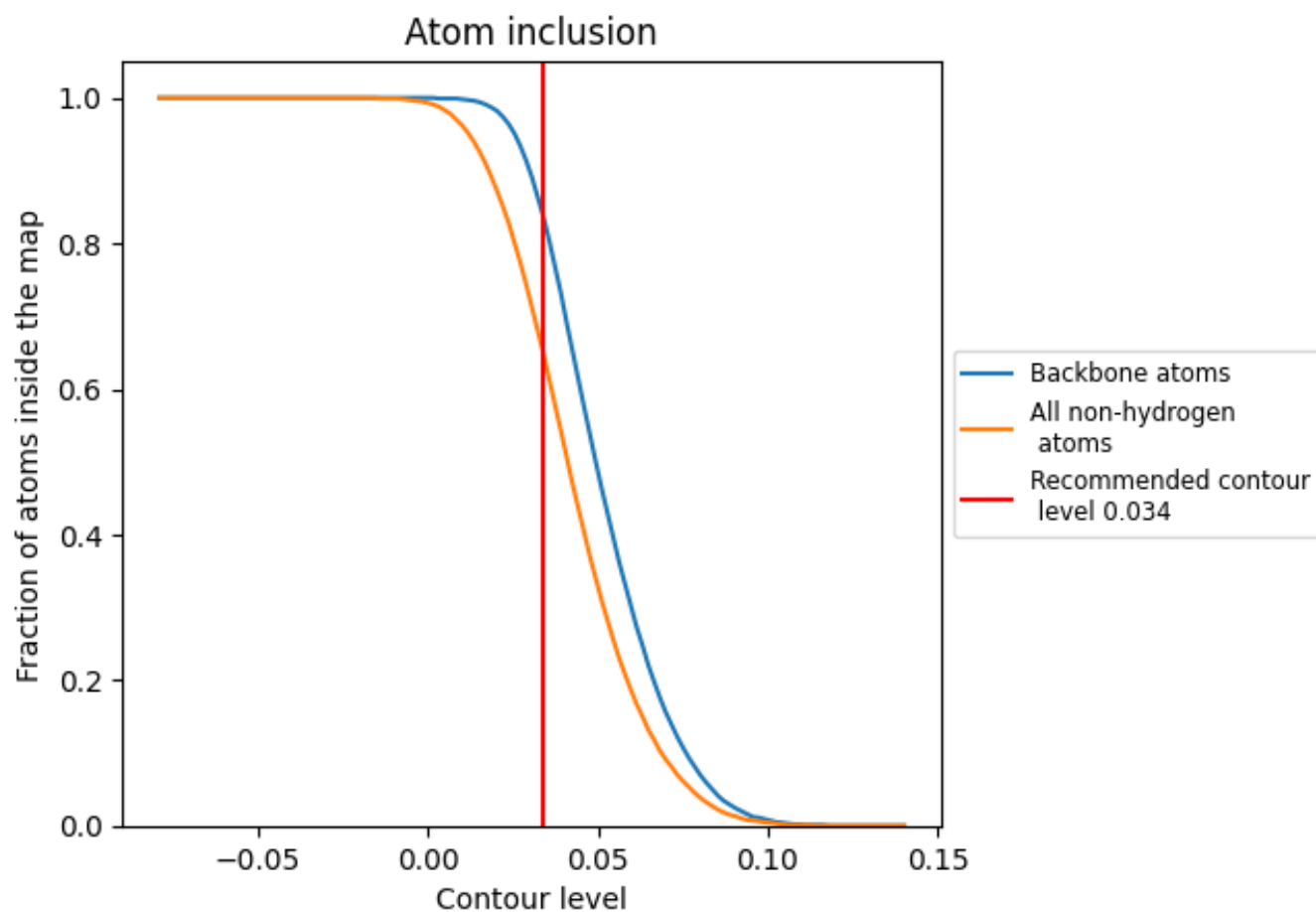
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.034).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 65% 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 (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6500	 0.3300
A	 0.6970	 0.3810
B	 0.6900	 0.3800
C	 0.6700	 0.3750
D	 0.6570	 0.3620
E	 0.6890	 0.3770
F	 0.6830	 0.3830
G	 0.5870	 0.3130
H	 0.6850	 0.3420
I	 0.6430	 0.3260
J	 0.6540	 0.3320
K	 0.6980	 0.2630
L	 0.6940	 0.2610
M	 0.4740	 0.2100
N	 0.5410	 0.2300
O	 0.5370	 0.2340
P	 0.5640	 0.2460
Q	 0.4840	 0.2200
R	 0.5430	 0.2660
S	 0.6000	 0.2910
T	 0.6480	 0.2900

