



## wwPDB EM Validation Summary Report ⓘ

Jun 9, 2025 – 10:15 AM EDT

PDB ID : 9CAA / pdb\_00009caa  
EMDB ID : EMD-45384  
Title : Cryo-EM structure of human SRCAP-nucleosome complex in the pre-engaged state (composite structure)  
Authors : Louder, R.K.; Park, G.  
Deposited on : 2024-06-17  
Resolution : 4.04 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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

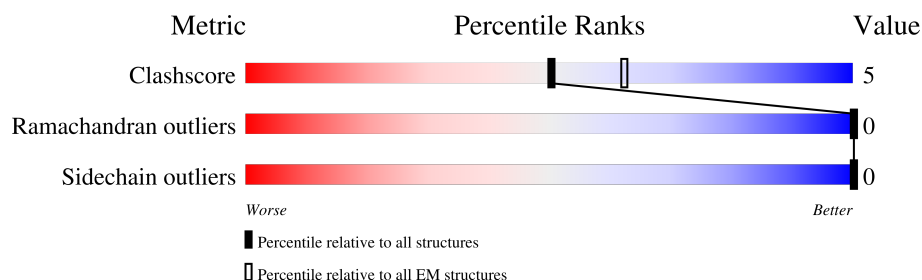
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.04 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.





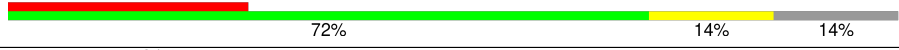



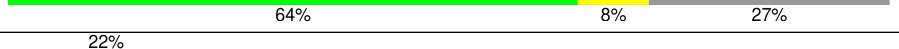
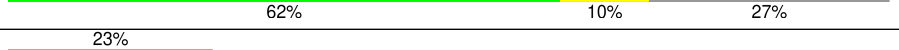
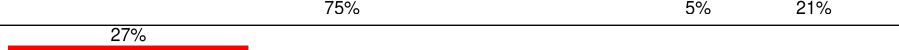
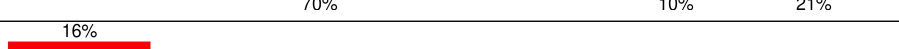
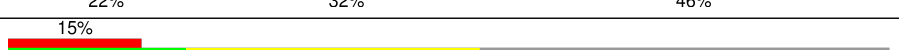
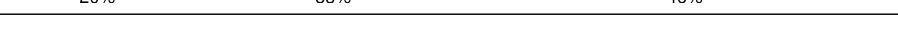
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	3230	
2	B	364	
3	C	396	
4	D	154	
5	E	456	
5	G	456	
5	I	456	
6	F	463	

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Mol	Chain	Length	Quality of chain
6	H	463	
6	J	463	
7	Q	128	
7	S	128	
8	R	125	
8	T	125	
9	U	135	
9	W	135	
10	V	102	
10	X	102	
11	Y	285	
12	Z	285	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 40983 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 Helicase SRCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	414	Total	C	N	O	S	0	0
			3367	2150	613	585	19		

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 72 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	95	Total	C	N	O	S	0	0
			769	494	139	133	3		

- Molecule 3 is a protein called Actin-related protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	396	Total	C	N	O	S	0	0
			3226	2064	528	616	18		

- Molecule 4 is a protein called Zinc finger HIT domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	105	Total	C	N	O	S	0	0
			831	508	164	151	8		

- Molecule 5 is a protein called RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	433	Total	C	N	O	S	0	0
			3344	2107	574	646	17		
5	G	445	Total	C	N	O	S	0	0
			3430	2159	588	665	18		
5	I	436	Total	C	N	O	S	0	0
			3365	2119	577	652	17		

- Molecule 6 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	438	Total	C	N	O	S	0	0
			3395	2121	596	662	16		
6	H	432	Total	C	N	O	S	0	0
			3361	2101	590	654	16		
6	J	418	Total	C	N	O	S	0	0
			3254	2039	568	632	15		

- Molecule 7 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Q	110	Total	C	N	O	0	0
			850	535	168	147		
7	S	110	Total	C	N	O	0	0
			850	535	168	147		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	99	ARG	GLY	conflict	UNP P06897
Q	123	SER	-	expression tag	UNP P06897
Q	124	LYS	-	expression tag	UNP P06897
Q	125	SER	-	expression tag	UNP P06897
Q	126	LYS	-	expression tag	UNP P06897
Q	127	SER	-	expression tag	UNP P06897
Q	128	LYS	-	expression tag	UNP P06897
S	99	ARG	GLY	conflict	UNP P06897
S	123	SER	-	expression tag	UNP P06897
S	124	LYS	-	expression tag	UNP P06897
S	125	SER	-	expression tag	UNP P06897
S	126	LYS	-	expression tag	UNP P06897
S	127	SER	-	expression tag	UNP P06897
S	128	LYS	-	expression tag	UNP P06897

- Molecule 8 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	98	Total	C	N	O	S	0	0
			775	487	144	142	2		
8	T	98	Total	C	N	O	S	0	0
			776	487	144	143	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	32	THR	SER	conflict	UNP P02281
T	32	THR	SER	conflict	UNP P02281

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U	98	Total	C	N	O	S	0	0
			811	512	157	139	3		
9	W	98	Total	C	N	O	S	0	0
			811	512	157	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	102	ALA	GLY	variant	UNP P84233
W	102	ALA	GLY	variant	UNP P84233

- Molecule 10 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	81	Total	C	N	O	S	0	0
			648	410	126	111	1		
10	X	81	Total	C	N	O	S	0	0
			648	410	126	111	1		

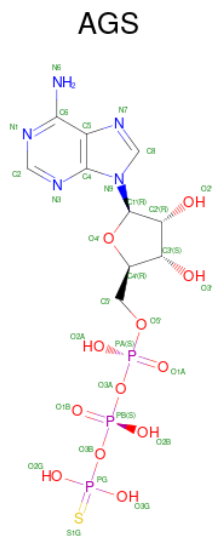
- Molecule 11 is a DNA chain called DNA (285-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	153	Total	C	N	O	P	0	0
			3121	1482	564	922	153		

- Molecule 12 is a DNA chain called DNA (285-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	153	Total	C	N	O	P	0	0
			3152	1491	594	914	153		

- Molecule 13 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					AltConf	
13	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

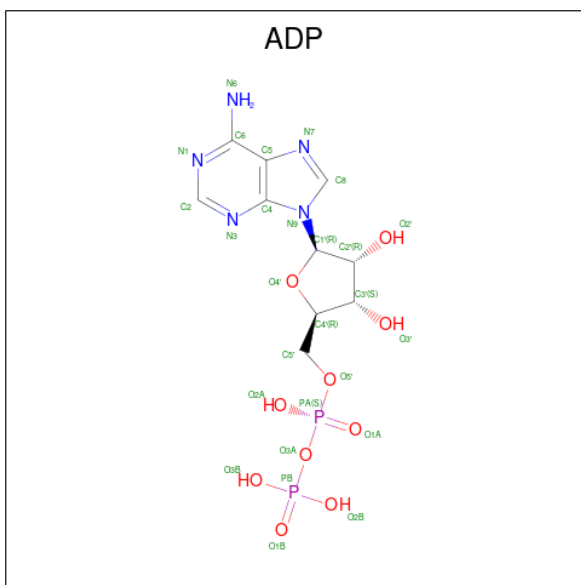
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
14	C	1	Total Mg 1 1	0
14	F	1	Total Mg 1 1	0
14	H	1	Total Mg 1 1	0
14	J	1	Total Mg 1 1	0

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ).

Mol	Chain	Residues	Atoms	AltConf
15	D	2	Total Zn 2 2	0

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



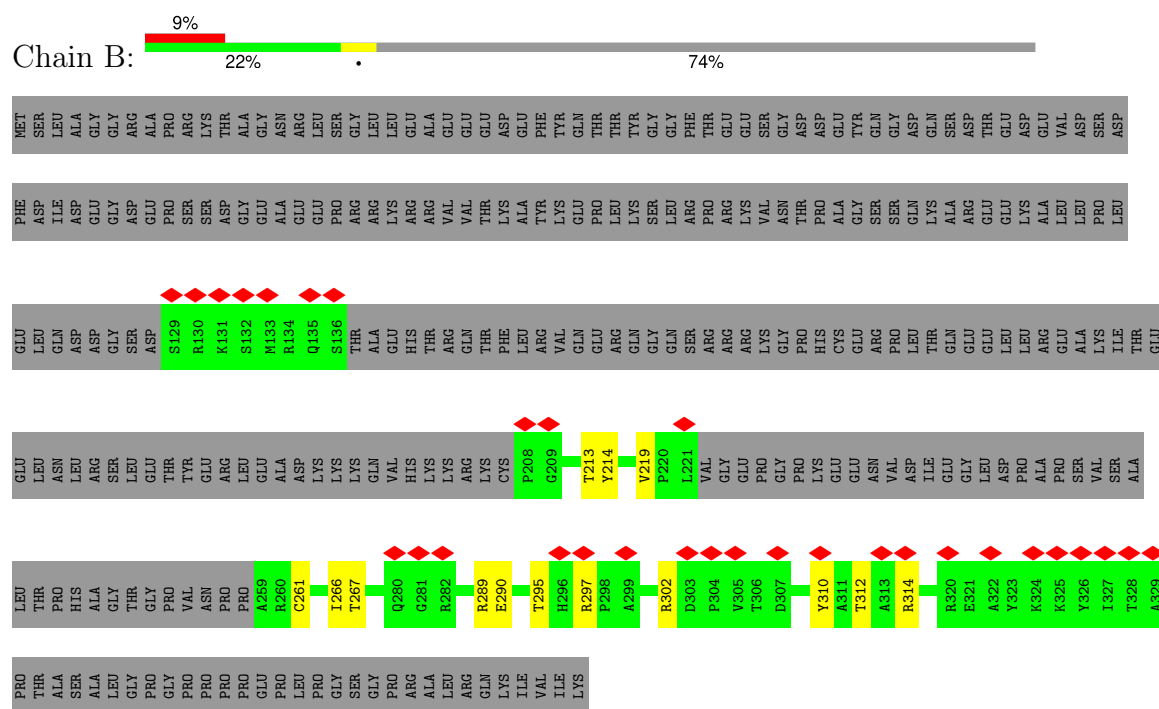
Mol	Chain	Residues	Atoms					AltConf
16	E	1	Total 27	C 10	N 5	O 10	P 2	0
16	F	1	Total 27	C 10	N 5	O 10	P 2	0
16	G	1	Total 27	C 10	N 5	O 10	P 2	0
16	H	1	Total 27	C 10	N 5	O 10	P 2	0
16	I	1	Total 27	C 10	N 5	O 10	P 2	0
16	J	1	Total 27	C 10	N 5	O 10	P 2	0



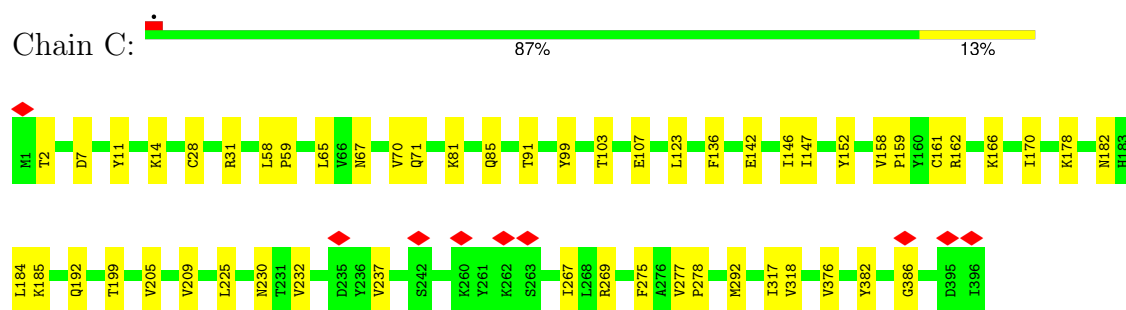




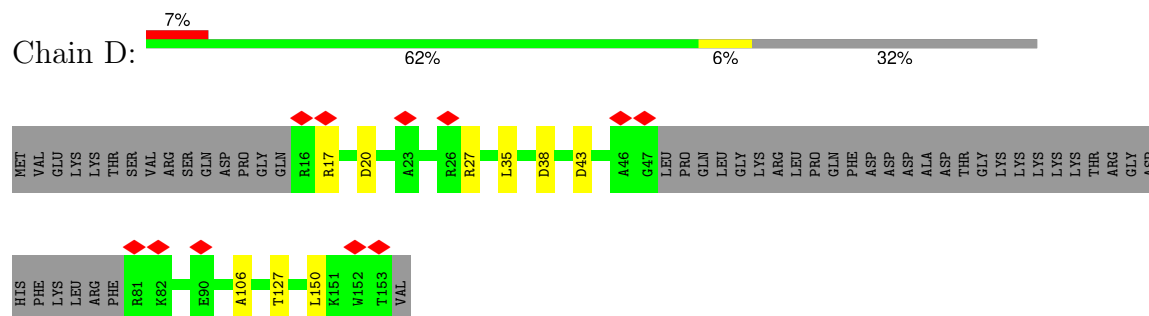
- Molecule 2: Vacuolar protein sorting-associated protein 72 homolog



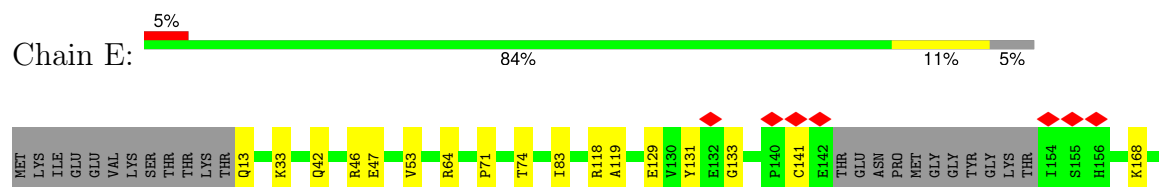
- Molecule 3: Actin-related protein 6

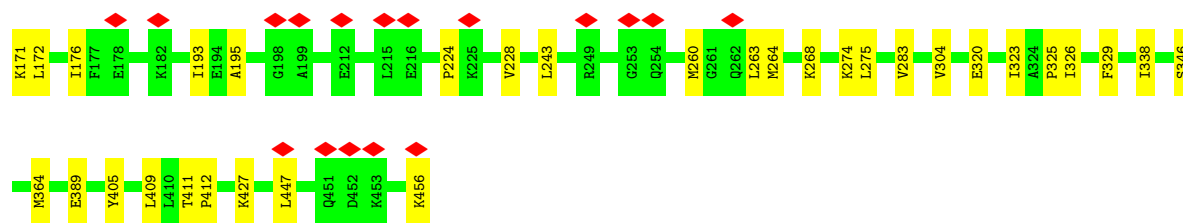


- Molecule 4: Zinc finger HIT domain-containing protein 1



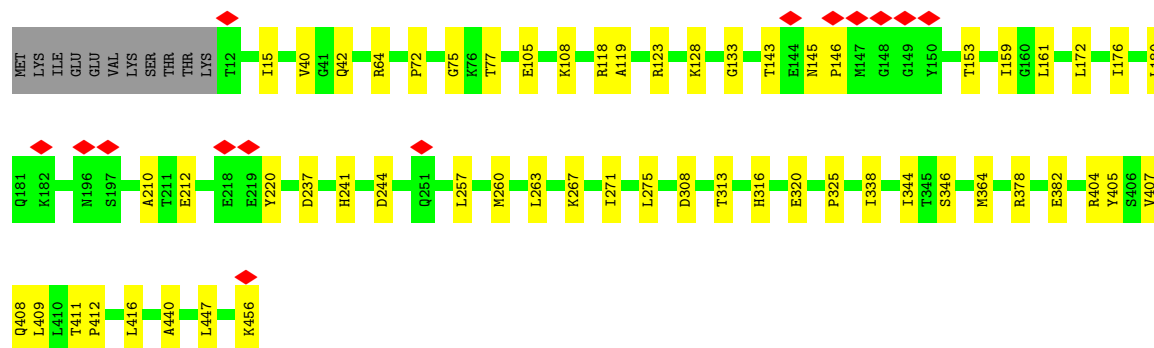
- Molecule 5: RuvB-like 1





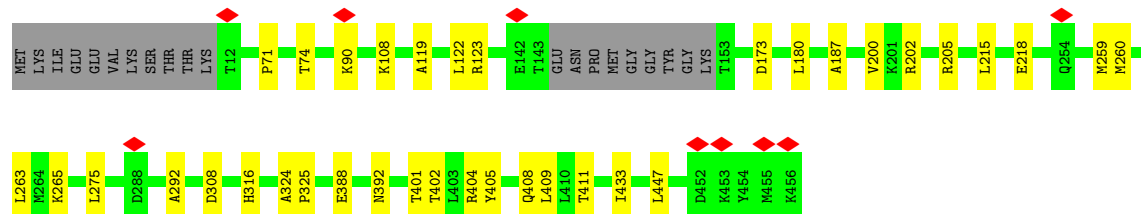
• Molecule 5: RuvB-like 1

Chain G: 85% 12%



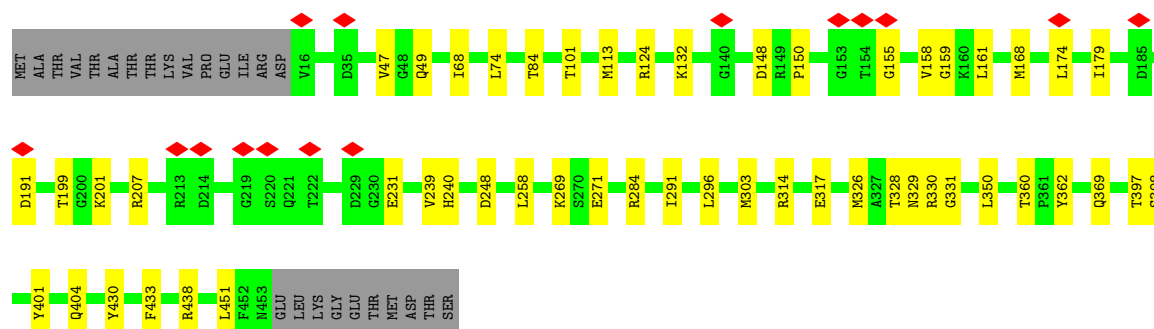
• Molecule 5: RuvB-like 1

Chain I: 88% 8%



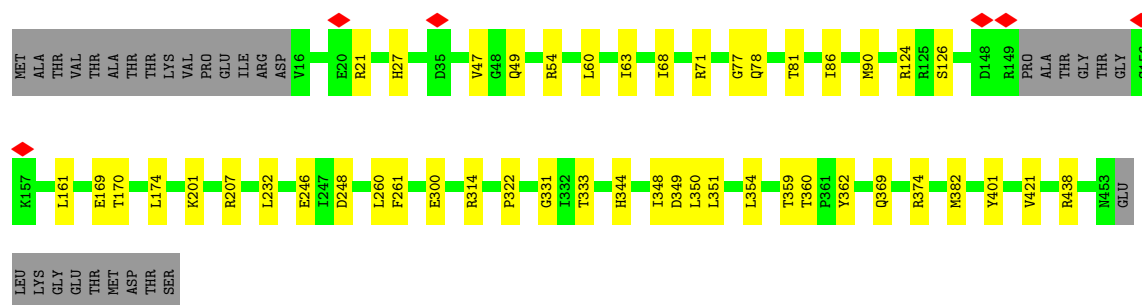
• Molecule 6: RuvB-like 2

Chain F: 83% 11% 5%



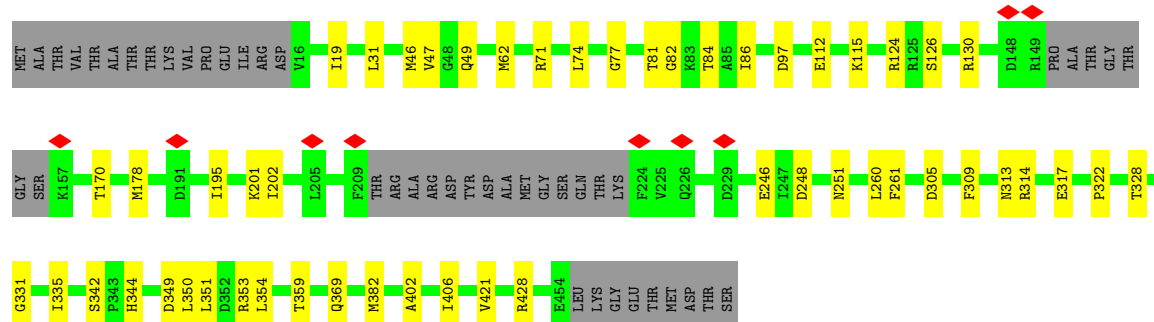
• Molecule 6: RuvB-like 2

Chain H: 83% 10% 7%



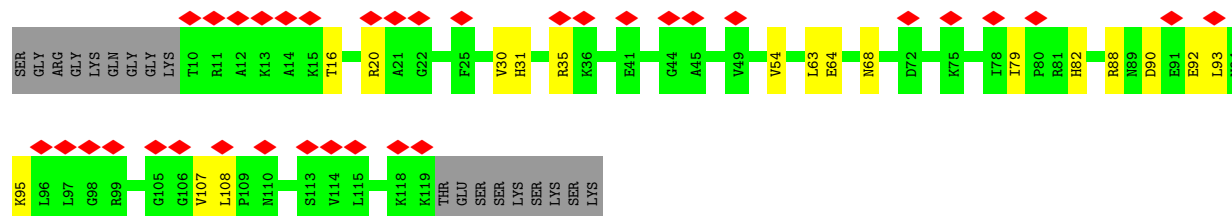
• Molecule 6: RuvB-like 2

Chain J: 79% 11% 10%



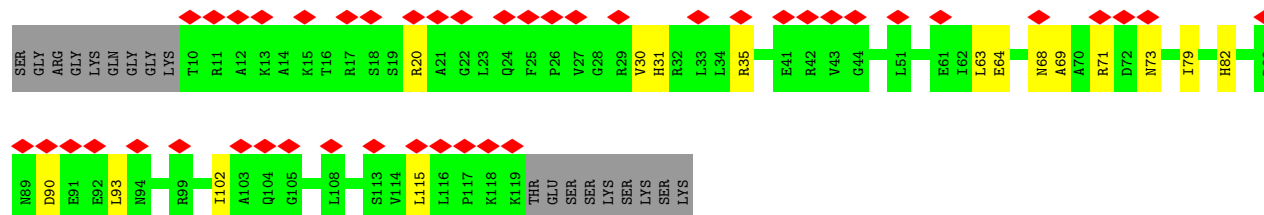
• Molecule 7: Histone H2A type 1

Chain Q: 27% 72% 14% 14%



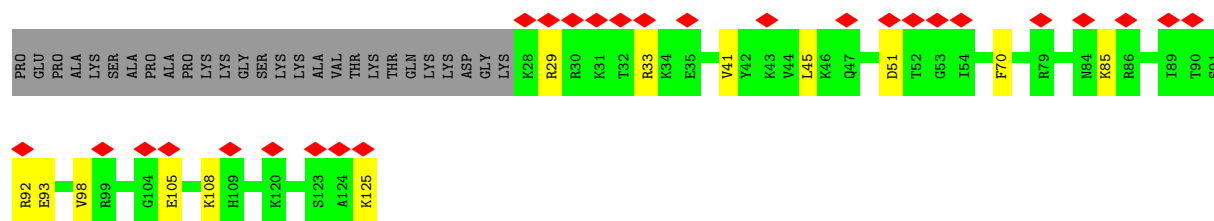
• Molecule 7: Histone H2A type 1

Chain S: 34% 73% 12% 14%



• Molecule 8: Histone H2B 1.1

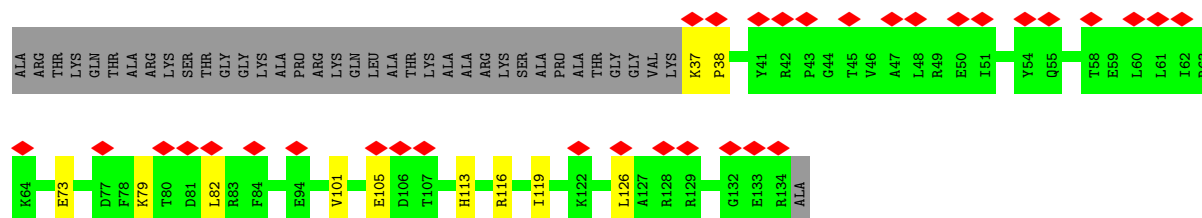
Chain R: 22% 68% 10% 22%



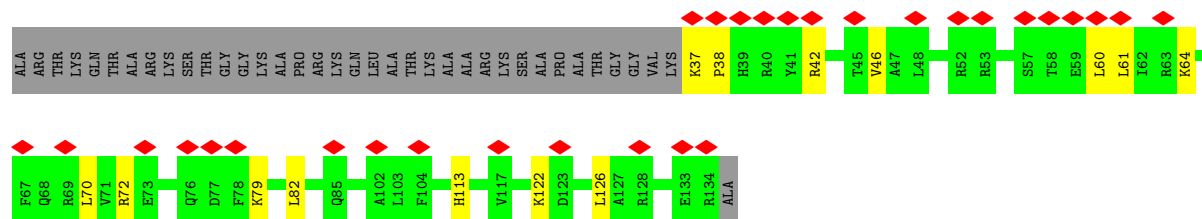
• Molecule 8: Histone H2B 1.1



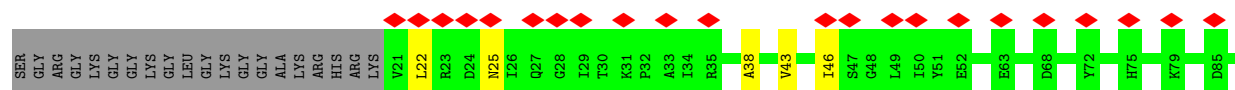
• Molecule 9: Histone H3.2



• Molecule 9: Histone H3.2



• Molecule 10: Histone H4







DC	DC	DA	DC	DC	DC	DC	DC	DC	DT	DT	DA	DT	DA	DT	DA	DA	DA	DG	DG	DC	DG	DC	DC	DC	DT	DT	DC	DG	DA	DT
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28381	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.900	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	393.59998, 393.59998, 393.59998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.025, 1.025, 1.025	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.10	0/3453	0.27	0/4684
2	B	0.10	0/792	0.24	0/1075
3	C	0.09	0/3300	0.23	0/4467
4	D	0.08	0/848	0.22	0/1147
5	E	0.11	0/3387	0.24	0/4561
5	G	0.10	0/3476	0.24	0/4683
5	I	0.11	0/3408	0.24	0/4591
6	F	0.11	0/3435	0.23	0/4625
6	H	0.11	0/3399	0.24	0/4573
6	J	0.11	0/3290	0.23	0/4426
7	Q	0.09	0/860	0.20	0/1159
7	S	0.08	0/860	0.19	0/1159
8	R	0.07	0/786	0.21	0/1054
8	T	0.08	0/787	0.22	0/1054
9	U	0.07	0/823	0.19	0/1104
9	W	0.09	0/823	0.20	0/1104
10	V	0.09	0/655	0.21	0/878
10	X	0.09	0/655	0.21	0/878
11	Y	0.17	0/3496	0.40	0/5390
12	Z	0.18	0/3540	0.40	0/5465
All	All	0.12	0/42073	0.27	0/58077

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3367	0	3401	23	0
2	B	769	0	770	9	0
3	C	3226	0	3147	35	0
4	D	831	0	798	9	0
5	E	3344	0	3449	35	0
5	G	3430	0	3530	42	0
5	I	3365	0	3470	28	0
6	F	3395	0	3467	35	0
6	H	3361	0	3434	34	0
6	J	3254	0	3330	41	0
7	Q	850	0	915	15	0
7	S	850	0	915	13	0
8	R	775	0	812	13	0
8	T	776	0	812	13	0
9	U	811	0	853	11	0
9	W	811	0	853	13	0
10	V	648	0	693	5	0
10	X	648	0	693	9	0
11	Y	3121	0	1719	66	0
12	Z	3152	0	1715	72	0
13	C	31	0	12	0	0
14	C	1	0	0	0	0
14	F	1	0	0	0	0
14	H	1	0	0	0	0
14	J	1	0	0	0	0
15	D	2	0	0	0	0
16	E	27	0	12	0	0
16	F	27	0	12	1	0
16	G	27	0	12	2	0
16	H	27	0	12	1	0
16	I	27	0	12	0	0
16	J	27	0	12	1	0
All	All	40983	0	38860	429	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 429 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)
5:E:411:THR:HG21	6:F:68:ILE:HG13	1.64	0.78
3:C:65:LEU:HD11	3:C:71:GLN:HG2	1.67	0.74
6:H:207:ARG:NH1	5:I:173:ASP:OD1	2.27	0.68
6:F:451:LEU:HD21	5:G:72:PRO:HG3	1.74	0.67
12:Z:15:DT:H2"	12:Z:16:DA:C8	2.30	0.66

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	406/3230 (13%)	397 (98%)	9 (2%)	0	100	100
2	B	89/364 (24%)	87 (98%)	2 (2%)	0	100	100
3	C	394/396 (100%)	379 (96%)	15 (4%)	0	100	100
4	D	101/154 (66%)	98 (97%)	3 (3%)	0	100	100
5	E	429/456 (94%)	425 (99%)	4 (1%)	0	100	100
5	G	443/456 (97%)	440 (99%)	3 (1%)	0	100	100
5	I	432/456 (95%)	424 (98%)	8 (2%)	0	100	100
6	F	436/463 (94%)	428 (98%)	8 (2%)	0	100	100
6	H	428/463 (92%)	417 (97%)	11 (3%)	0	100	100
6	J	412/463 (89%)	404 (98%)	8 (2%)	0	100	100
7	Q	108/128 (84%)	106 (98%)	2 (2%)	0	100	100
7	S	108/128 (84%)	108 (100%)	0	0	100	100
8	R	96/125 (77%)	95 (99%)	1 (1%)	0	100	100
8	T	96/125 (77%)	93 (97%)	3 (3%)	0	100	100
9	U	96/135 (71%)	94 (98%)	2 (2%)	0	100	100

*Continued on next page...*

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	W	96/135 (71%)	94 (98%)	2 (2%)	0	100	100
10	V	79/102 (78%)	78 (99%)	1 (1%)	0	100	100
10	X	79/102 (78%)	79 (100%)	0	0	100	100
All	All	4328/7881 (55%)	4246 (98%)	82 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	372/2721 (14%)	372 (100%)	0	100	100
2	B	84/312 (27%)	84 (100%)	0	100	100
3	C	361/361 (100%)	361 (100%)	0	100	100
4	D	89/133 (67%)	89 (100%)	0	100	100
5	E	367/387 (95%)	367 (100%)	0	100	100
5	G	376/387 (97%)	376 (100%)	0	100	100
5	I	370/387 (96%)	370 (100%)	0	100	100
6	F	368/390 (94%)	368 (100%)	0	100	100
6	H	365/390 (94%)	365 (100%)	0	100	100
6	J	354/390 (91%)	354 (100%)	0	100	100
7	Q	87/101 (86%)	87 (100%)	0	100	100
7	S	87/101 (86%)	87 (100%)	0	100	100
8	R	84/105 (80%)	84 (100%)	0	100	100
8	T	84/105 (80%)	84 (100%)	0	100	100
9	U	86/110 (78%)	86 (100%)	0	100	100
9	W	86/110 (78%)	86 (100%)	0	100	100
10	V	67/78 (86%)	67 (100%)	0	100	100
10	X	67/78 (86%)	67 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3754/6646 (56%)	3754 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
7	Q	110	ASN
10	V	93	GLN
8	R	84	ASN
7	S	84	GLN
6	F	275	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	$\# Z  > 2$
16	ADP	G	501	-	24,29,29	0.86	0	29,45,45	1.24	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	ADP	H	501	14	24,29,29	0.93	1 (4%)	29,45,45	1.23	2 (6%)
13	AGS	C	401	14	28,33,33	0.82	1 (3%)	31,52,52	1.02	2 (6%)
16	ADP	J	501	14	24,29,29	0.89	0	29,45,45	1.21	2 (6%)
16	ADP	F	501	14	24,29,29	0.86	0	29,45,45	1.23	2 (6%)
16	ADP	E	501	-	24,29,29	0.85	0	29,45,45	1.18	2 (6%)
16	ADP	I	501	-	24,29,29	0.85	0	29,45,45	1.22	2 (6%)

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
16	ADP	G	501	-	-	5/12/32/32	0/3/3/3
16	ADP	H	501	14	-	4/12/32/32	0/3/3/3
13	AGS	C	401	14	-	4/17/38/38	0/3/3/3
16	ADP	J	501	14	-	5/12/32/32	0/3/3/3
16	ADP	F	501	14	-	3/12/32/32	0/3/3/3
16	ADP	E	501	-	-	3/12/32/32	0/3/3/3
16	ADP	I	501	-	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	401	AGS	PG-S1G	2.14	1.95	1.90
16	H	501	ADP	PA-O3A	2.11	1.61	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	401	AGS	PB-O3B-PG	-3.68	119.70	133.17
16	F	501	ADP	N3-C2-N1	-3.68	123.68	128.67
16	E	501	ADP	N3-C2-N1	-3.67	123.69	128.67
16	I	501	ADP	N3-C2-N1	-3.63	123.74	128.67
16	G	501	ADP	N3-C2-N1	-3.63	123.75	128.67

There are no chirality outliers.

5 of 27 torsion outliers are listed below:



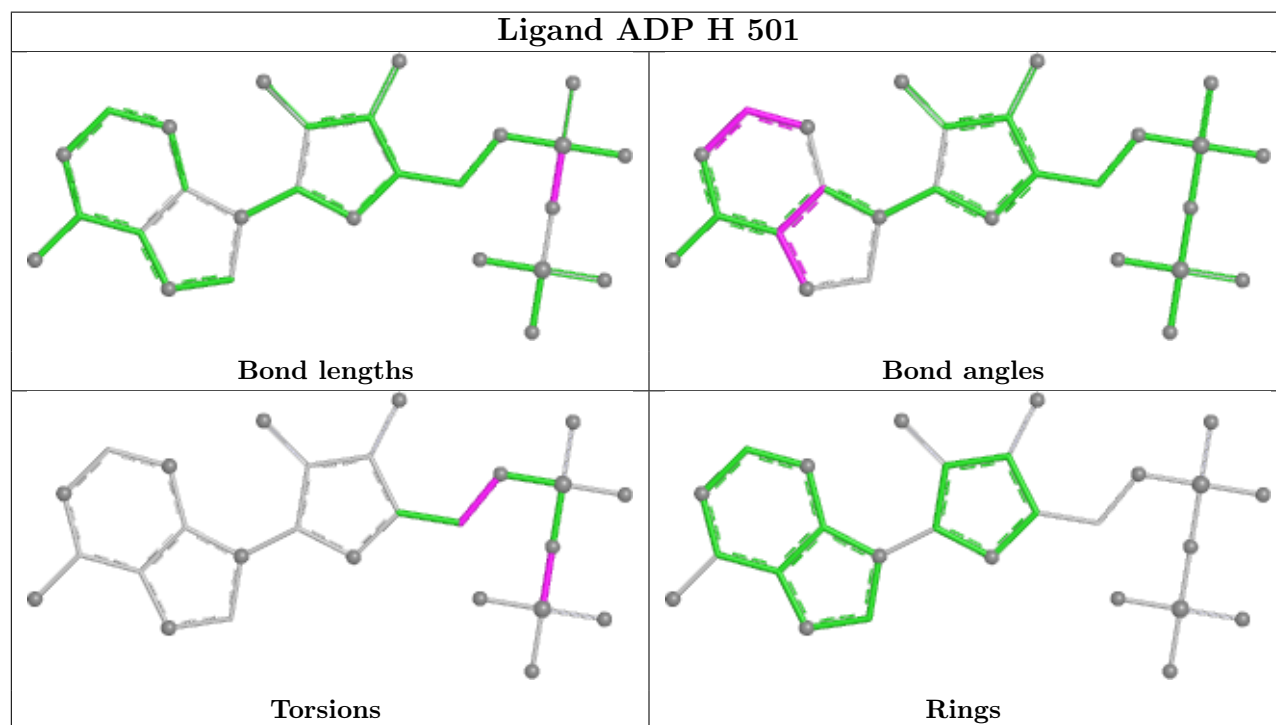
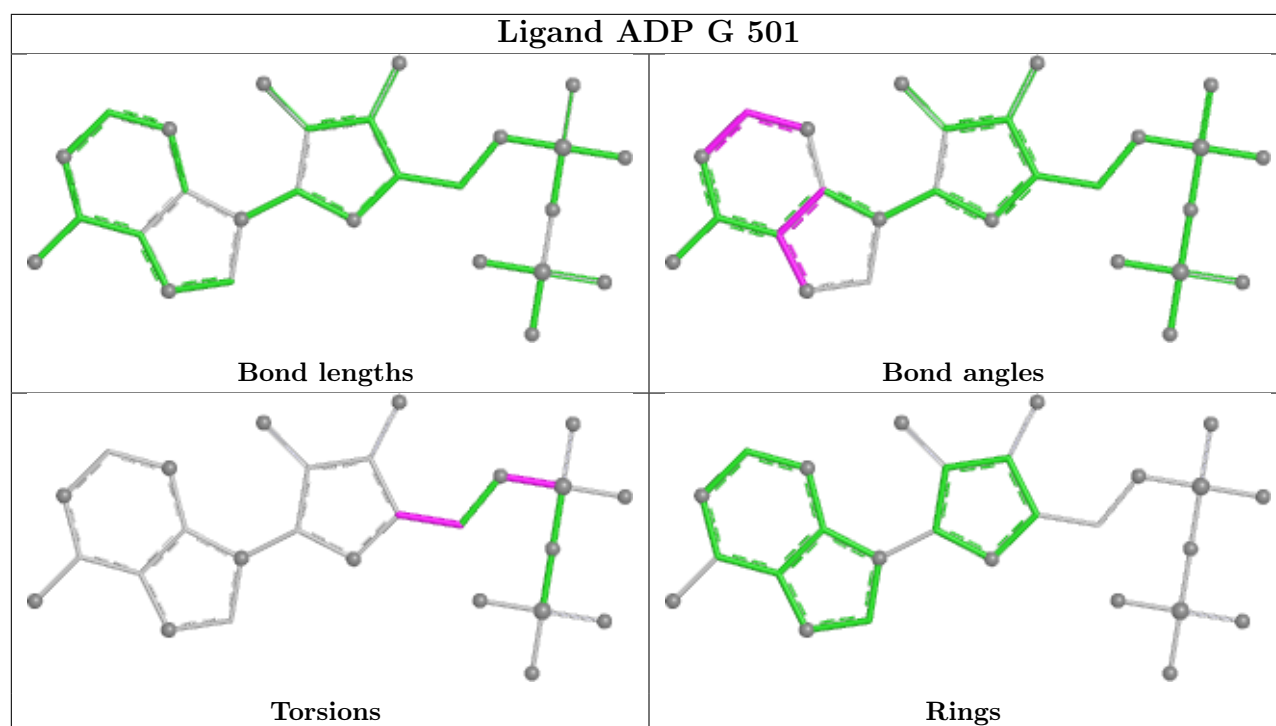
Mol	Chain	Res	Type	Atoms
13	C	401	AGS	C5'-O5'-PA-O1A
16	E	501	ADP	PA-O3A-PB-O2B
16	F	501	ADP	C5'-O5'-PA-O2A
16	F	501	ADP	C5'-O5'-PA-O3A
16	G	501	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

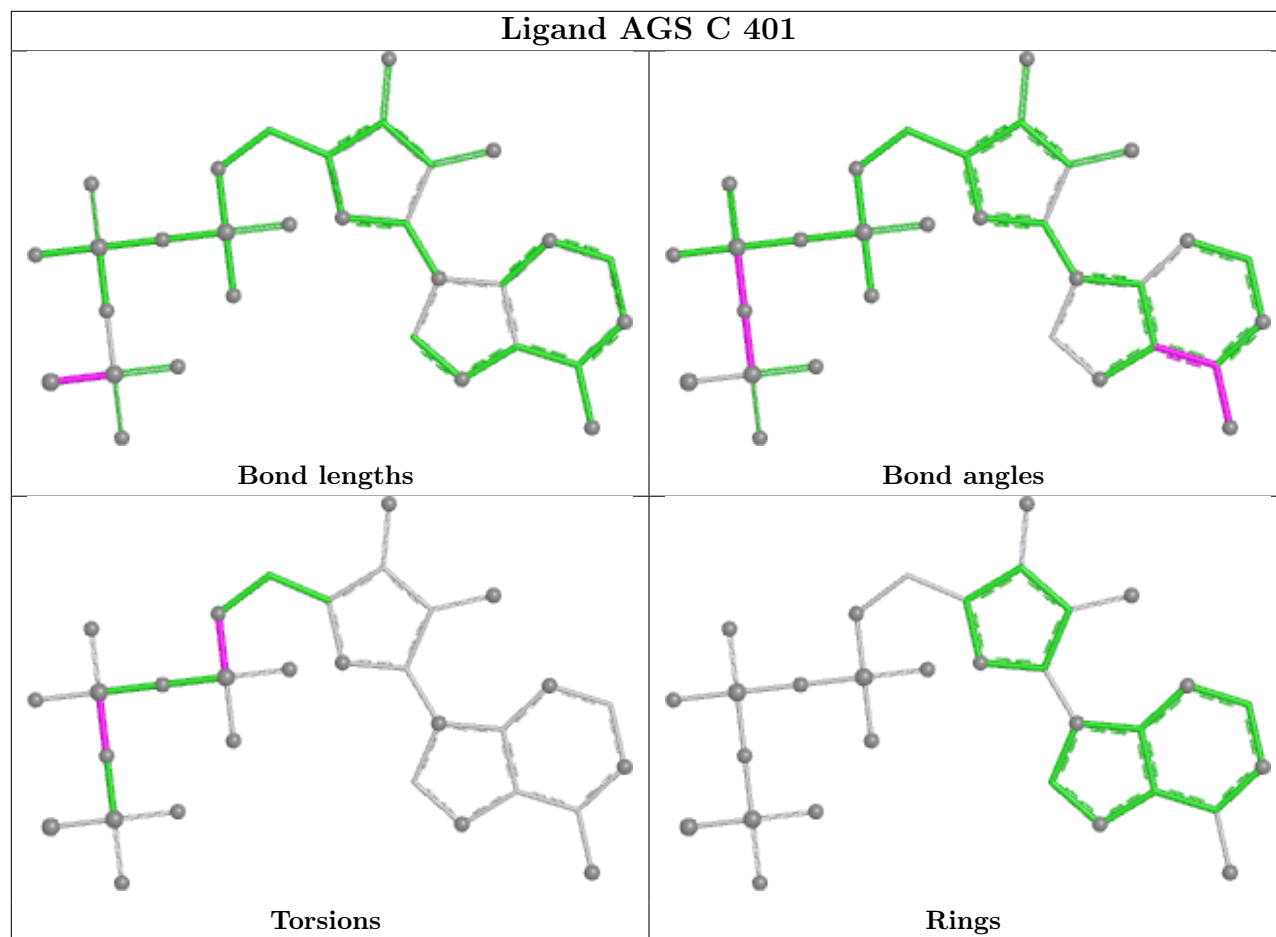
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	501	ADP	2	0
16	H	501	ADP	1	0
16	J	501	ADP	1	0
16	F	501	ADP	1	0

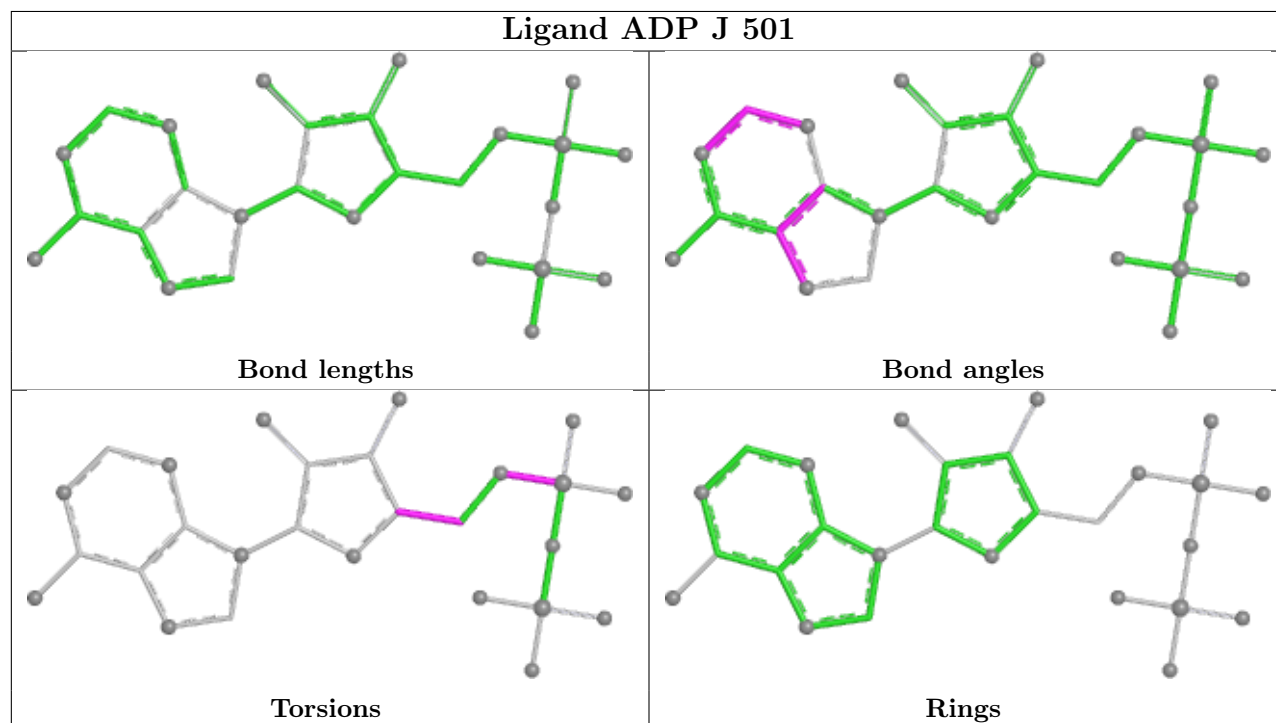
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

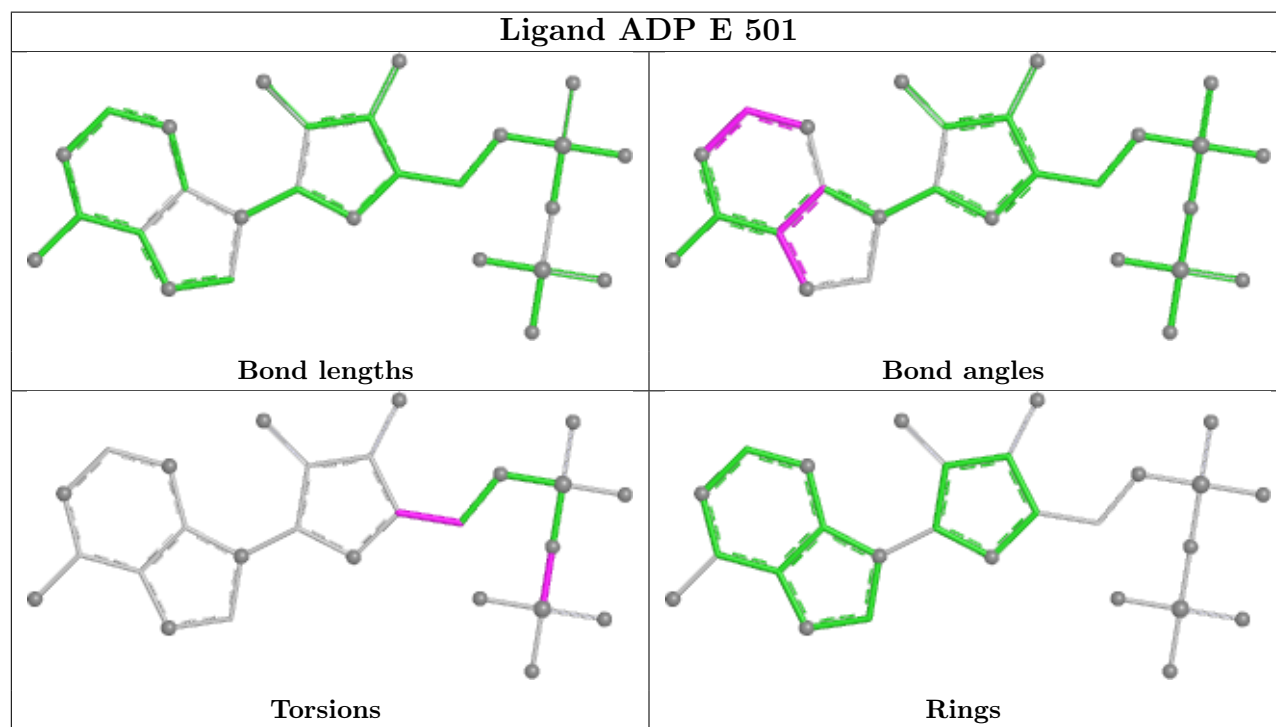
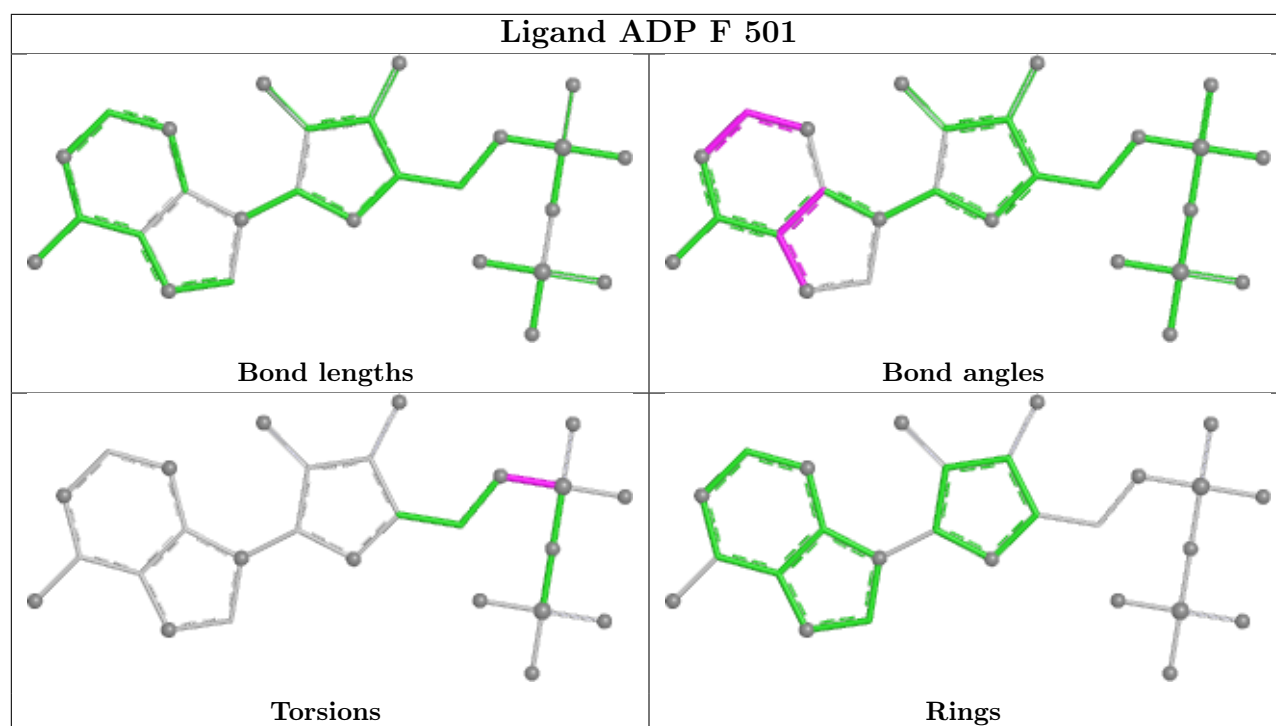


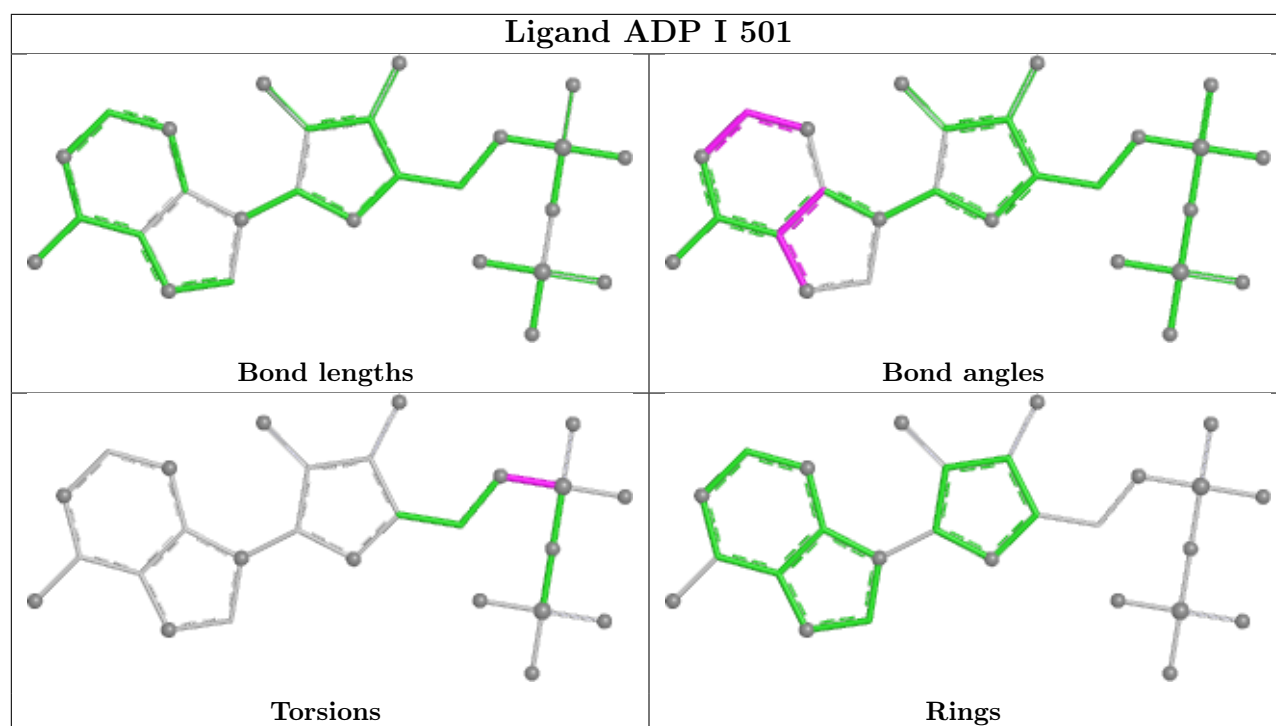
## Ligand AGS C 401



## Ligand ADP J 501







## 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.

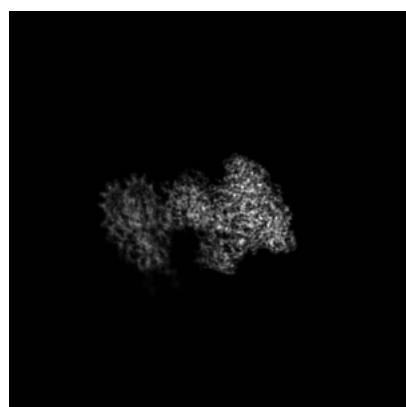
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45384. These allow visual inspection of the internal detail of the map and identification of artifacts.

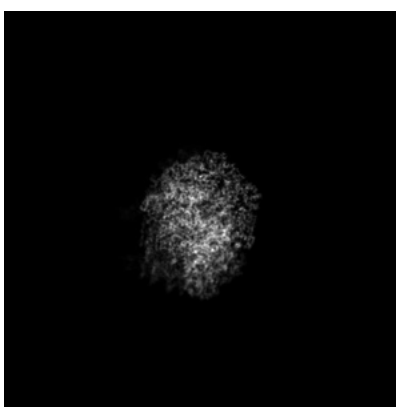
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

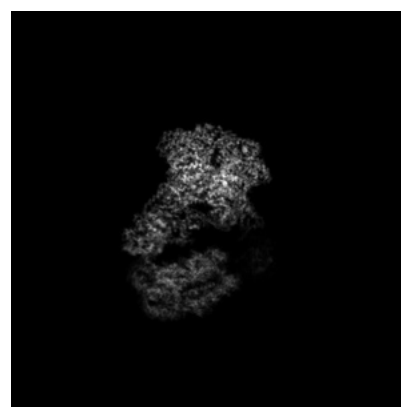
#### 6.1.1 Primary map



X



Y

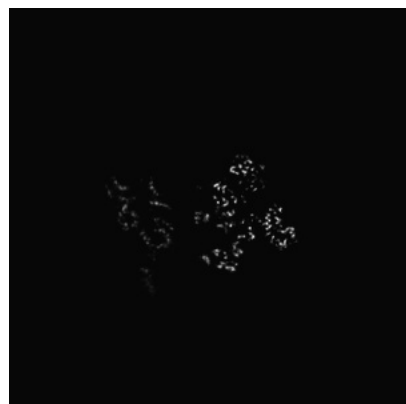


Z

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

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

#### 6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

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

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

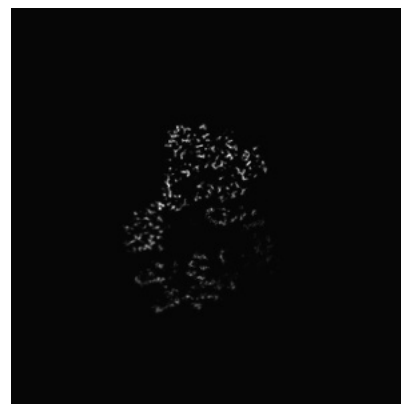
### 6.3.1 Primary map



X Index: 204



Y Index: 224

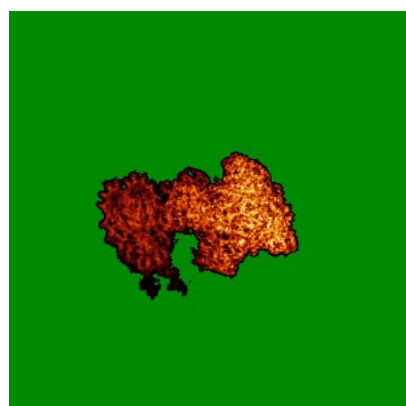


Z Index: 184

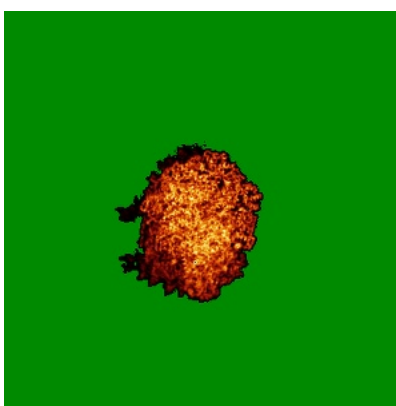
The images above show the largest variance slices of the map in three orthogonal directions.

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

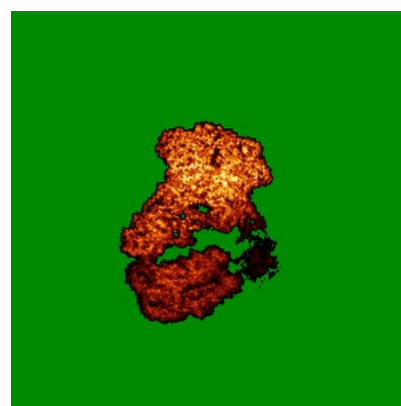
### 6.4.1 Primary map



X



Y

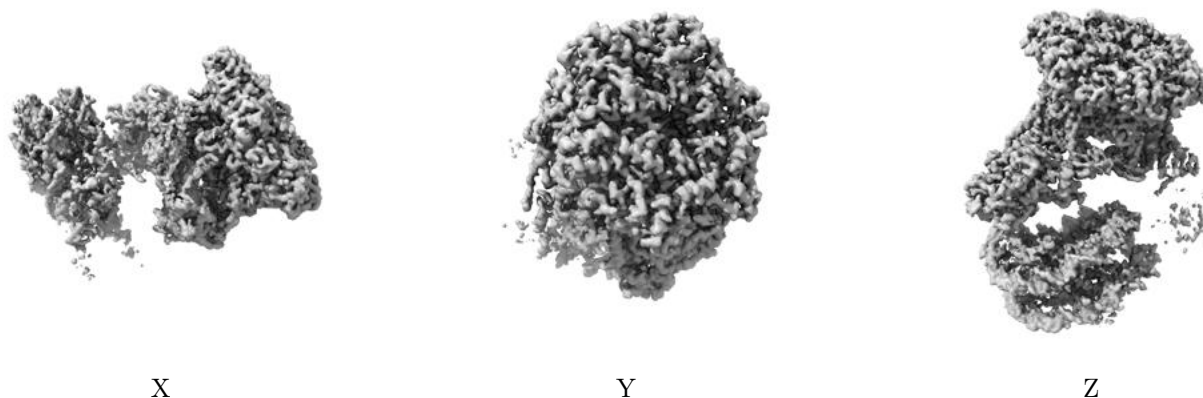


Z

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 0.1. 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](#)

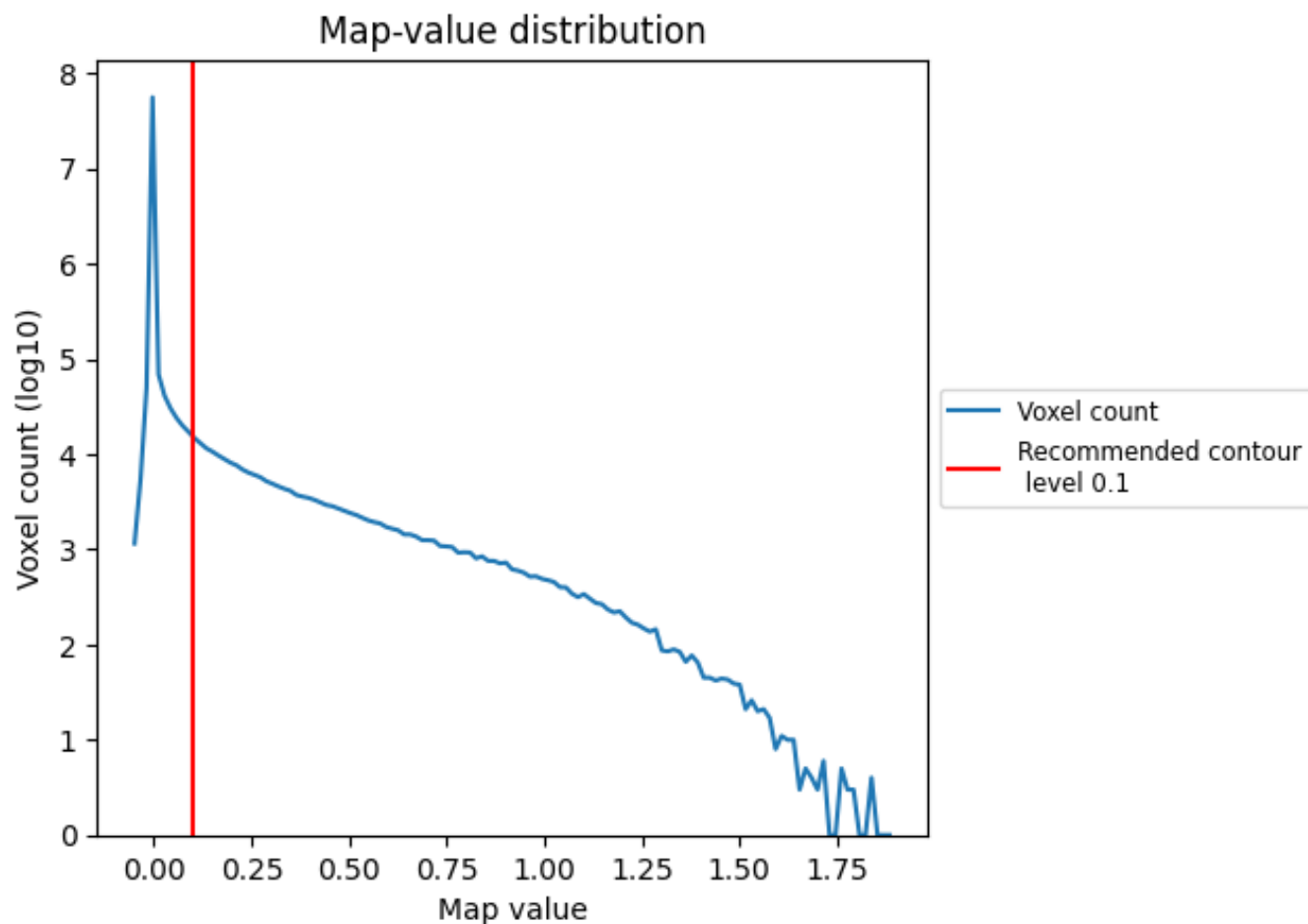
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

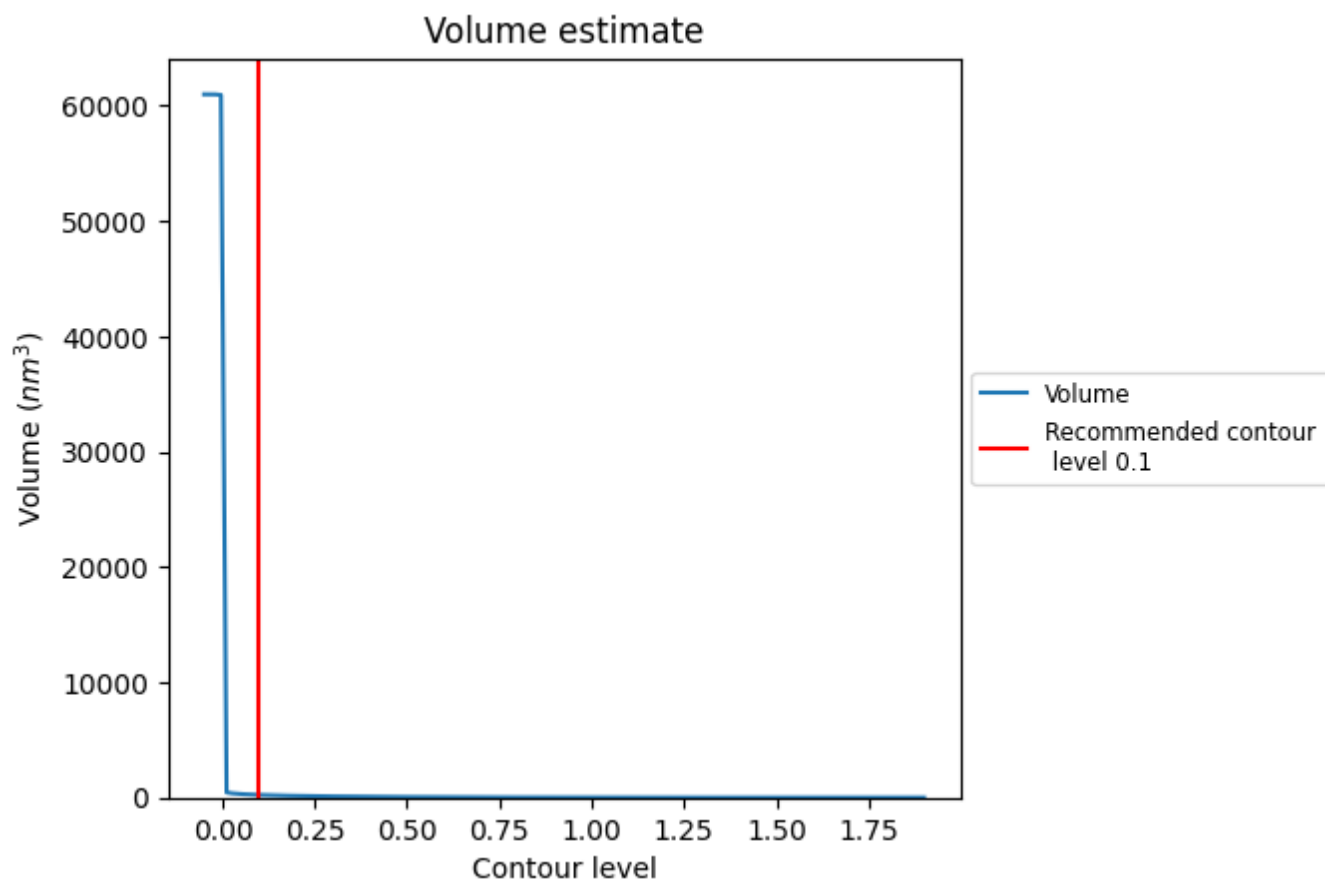
This section contains the results of statistical analysis of the map.

### 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.

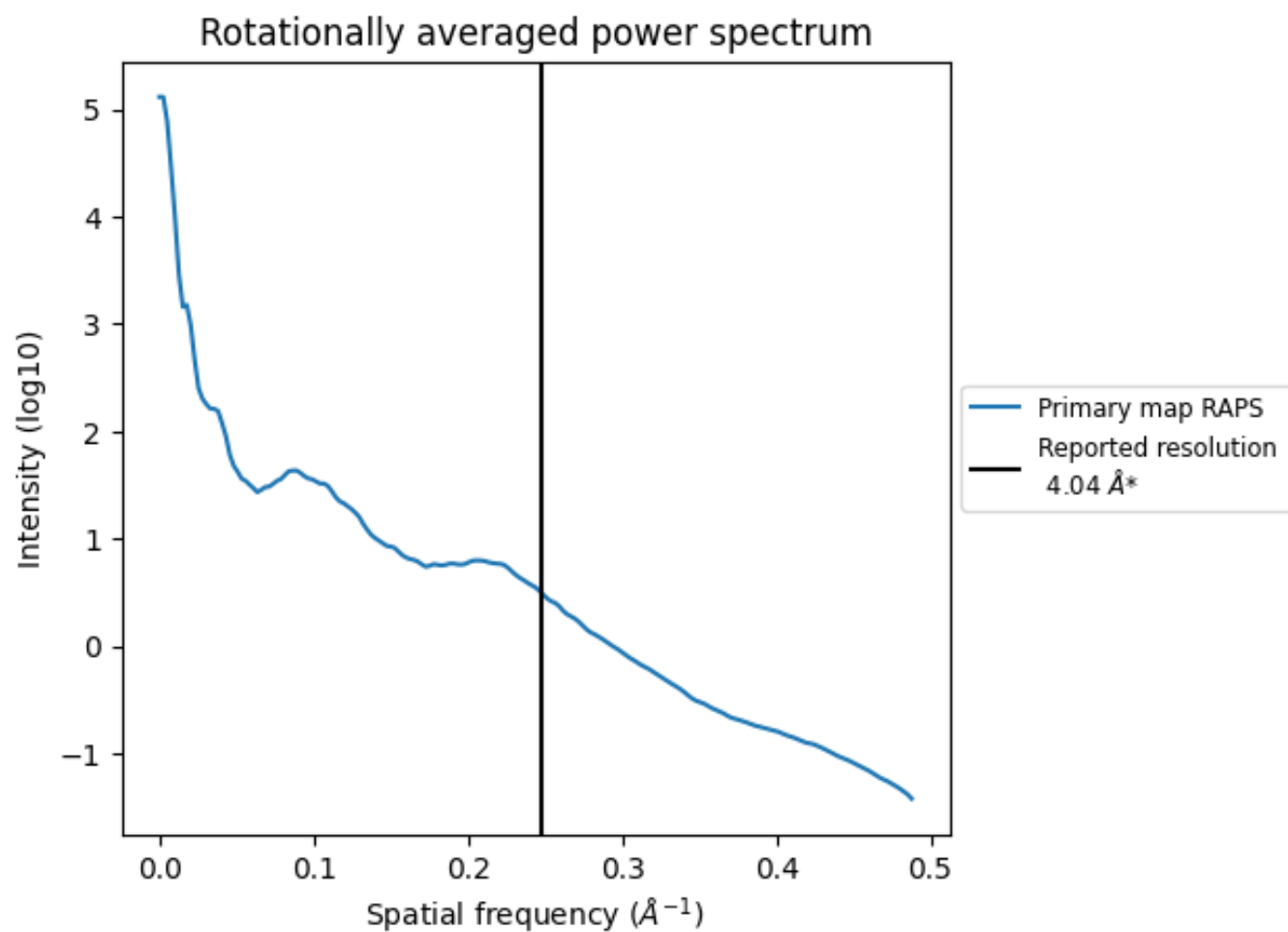
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 227  $\text{nm}^3$ ; this corresponds to an approximate mass of 205 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.248 Å<sup>-1</sup>

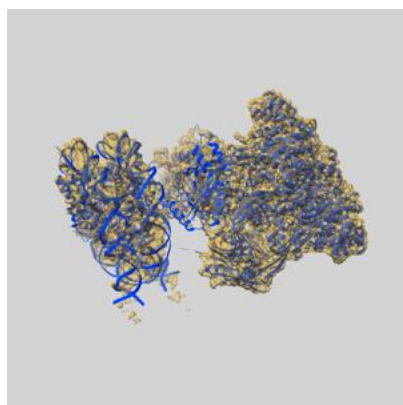
## 8 Fourier-Shell correlation

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

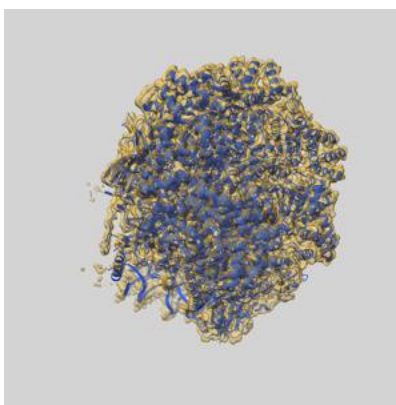
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45384 and PDB model 9CAA. Per-residue inclusion information can be found in section [3](#) on page [9](#).

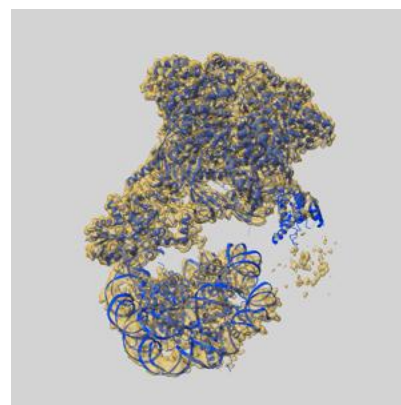
### 9.1 Map-model overlay [i](#)



X



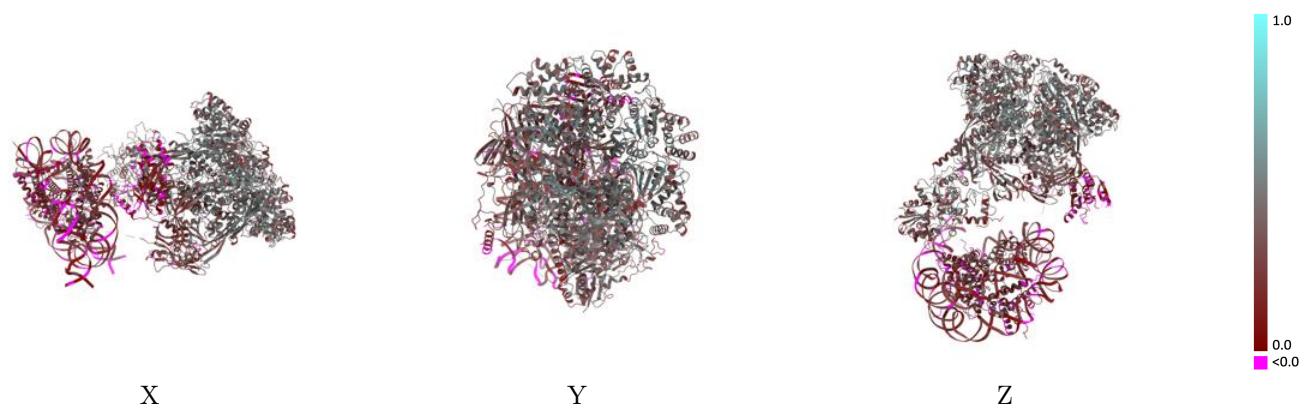
Y



Z

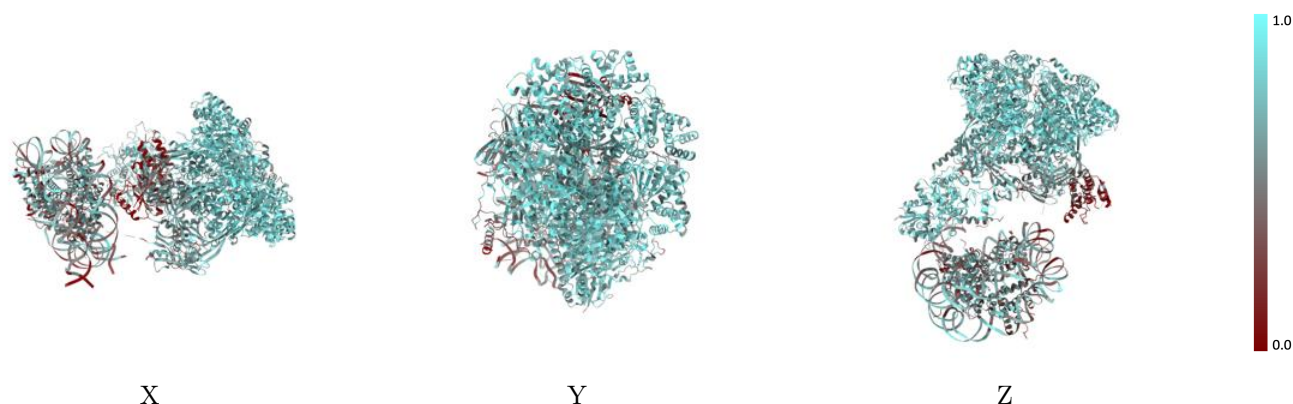
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



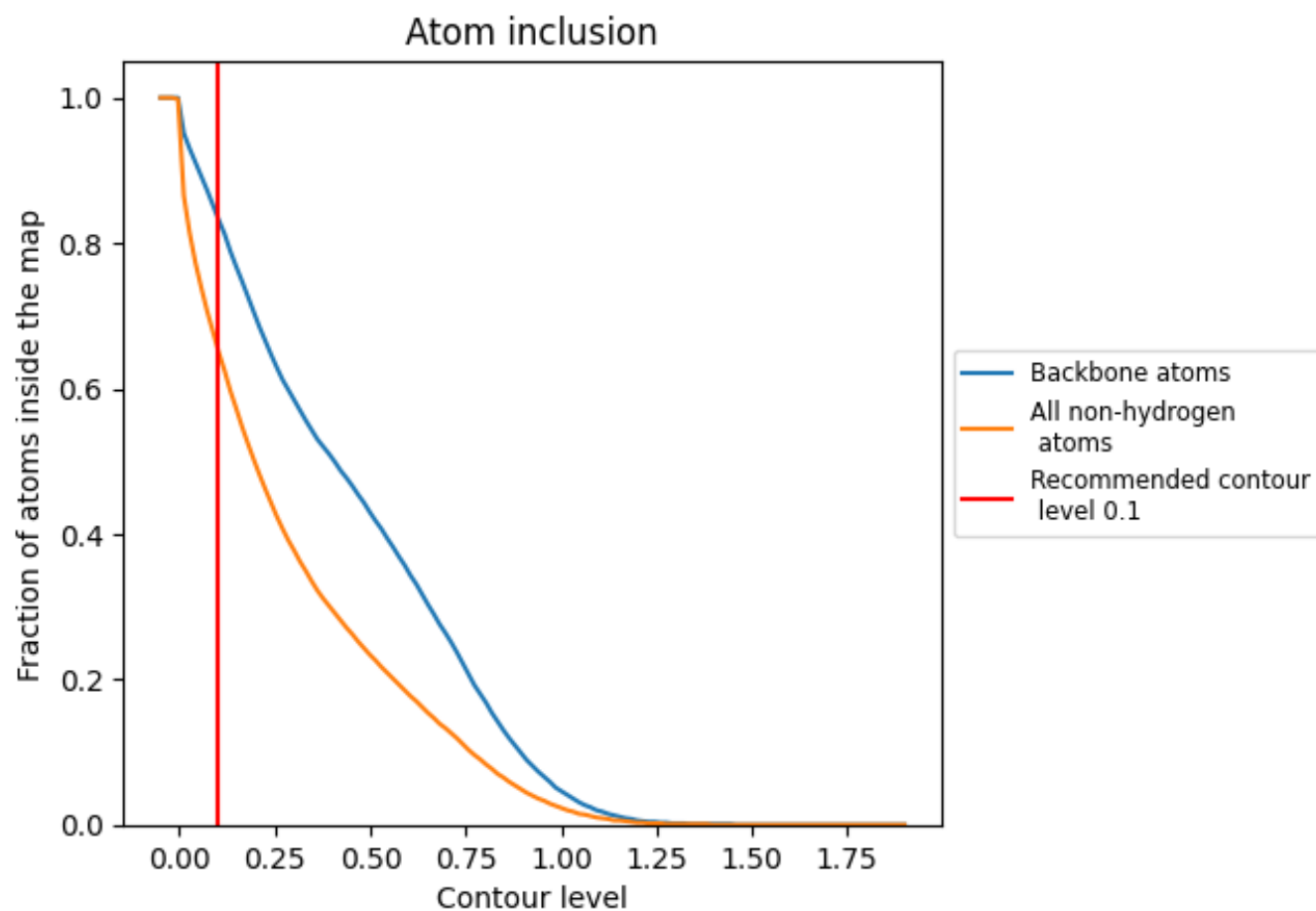
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 66% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6560	 0.3030
A	 0.4900	 0.2310
B	 0.4710	 0.2060
C	 0.7550	 0.3590
D	 0.7250	 0.3250
E	 0.7270	 0.3920
F	 0.7570	 0.3860
G	 0.7590	 0.3900
H	 0.7690	 0.4130
I	 0.7630	 0.4100
J	 0.7610	 0.4120
Q	 0.5040	 0.1760
R	 0.5290	 0.1880
S	 0.4640	 0.1650
T	 0.5030	 0.1440
U	 0.5040	 0.1650
V	 0.5550	 0.2070
W	 0.5000	 0.2010
X	 0.5260	 0.2120
Y	 0.5260	 0.1340
Z	 0.5220	 0.1210

