wwPDB EM Validation Summary Report (i)

Oct 18, 2021 – 10:54 am BST

PDB ID	:	7OO3
EMDB ID	:	EMD-13004
Title	:	Pol II-CSB-CSA-DDB1-UVSSA (Structure1)
Authors	:	Kokic, G.; Cramer, P.
Deposited on	:	2021-05-26
Resolution	:	2.80 Å(reported)

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

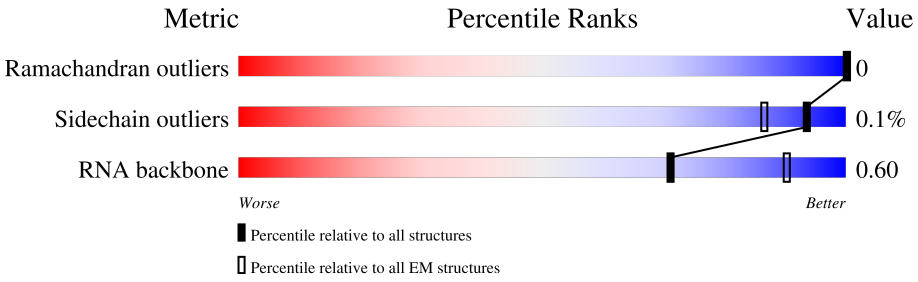
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.80 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1970	71% 28%
2	B	1174	5% 96%
3	C	275	94% 5%
4	D	142	71% 89% 11%
5	E	210	99%
6	F	127	6% 65% 35%
7	G	172	60% 99%
8	H	150	99%

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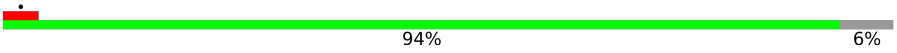
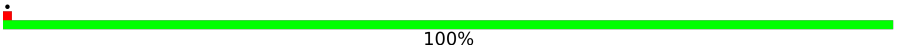
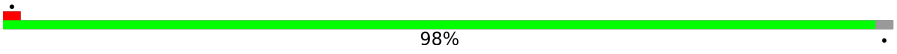
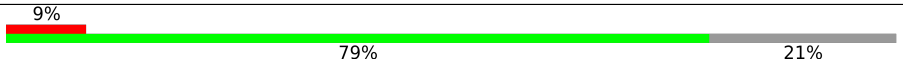
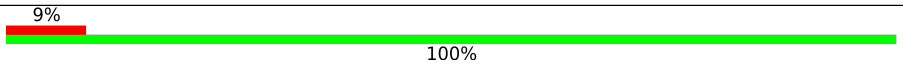
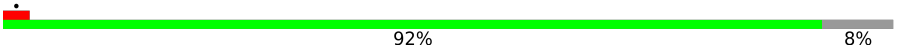
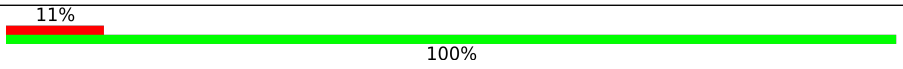
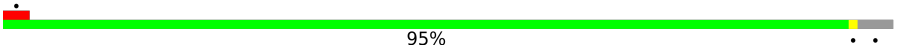
Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	N	47	
14	T	47	
15	P	10	
16	a	396	
17	b	1493	
18	x	35	
19	c	709	
20	d	1143	

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 95988 atoms, of which 46598 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1412	22493	7033	11314	2002	2074	70	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	1131	18140	5727	9088	1592	1669	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	260	4119	1309	2030	359	415	6	0	0

- Molecule 4 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	126	2046	642	1016	175	209	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	209	3457	1089	1737	300	323	8	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	82	1341	418	684	113	121	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2709	875	1358	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	148	Total	C	H	N	O	S	0	0
			2333	750	1147	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	117	Total	C	H	N	O	S	0	0
			1828	587	879	169	182	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	67	Total	C	H	N	O	S	0	0
			1086	345	553	90	92	6		

- Molecule 11 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	115	Total	C	H	N	O	S	0	0
			1862	593	942	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	46	Total	C	H	N	O	S	0	0
			781	241	393	75	66	6		

- Molecule 13 is a DNA chain called NTS.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	35	Total	C	N	O	P	0	0
			727	344	142	206	35		

- Molecule 14 is a DNA chain called TS.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	47	Total	C	N	O	P	0	0
			947	453	159	288	47		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	10	Total	C	H	N	O	P	0	0
			329	98	109	45	67	10		

- Molecule 16 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	a	365	Total	C	H	N	O	S	0	0
			5541	1775	2692	507	548	19		

- Molecule 17 is a protein called DNA excision repair protein ERCC-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	b	534	Total	C	H	N	O	S	0	0
			8744	2803	4390	761	769	21		

- Molecule 18 is a protein called CSB element.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	x	35	Total	C	H	N	O	0	0
			317	105	142	35	35		

- Molecule 19 is a protein called UV-stimulated scaffold protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	141	Total	C	H	N	O	0	0
			707	282	143	141	141		

- Molecule 20 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	d	1096	Total	C	H	N	O	S	0	0
			16472	5397	7981	1423	1625	46		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-2	SER	-	expression tag	UNP Q16531
d	-1	ASN	-	expression tag	UNP Q16531
d	0	ALA	-	expression tag	UNP Q16531

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
21	A	2	Total Zn 2 2	0
21	B	1	Total Zn 1 1	0
21	C	1	Total Zn 1 1	0
21	I	2	Total Zn 2 2	0
21	J	1	Total Zn 1 1	0
21	L	1	Total Zn 1 1	0

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

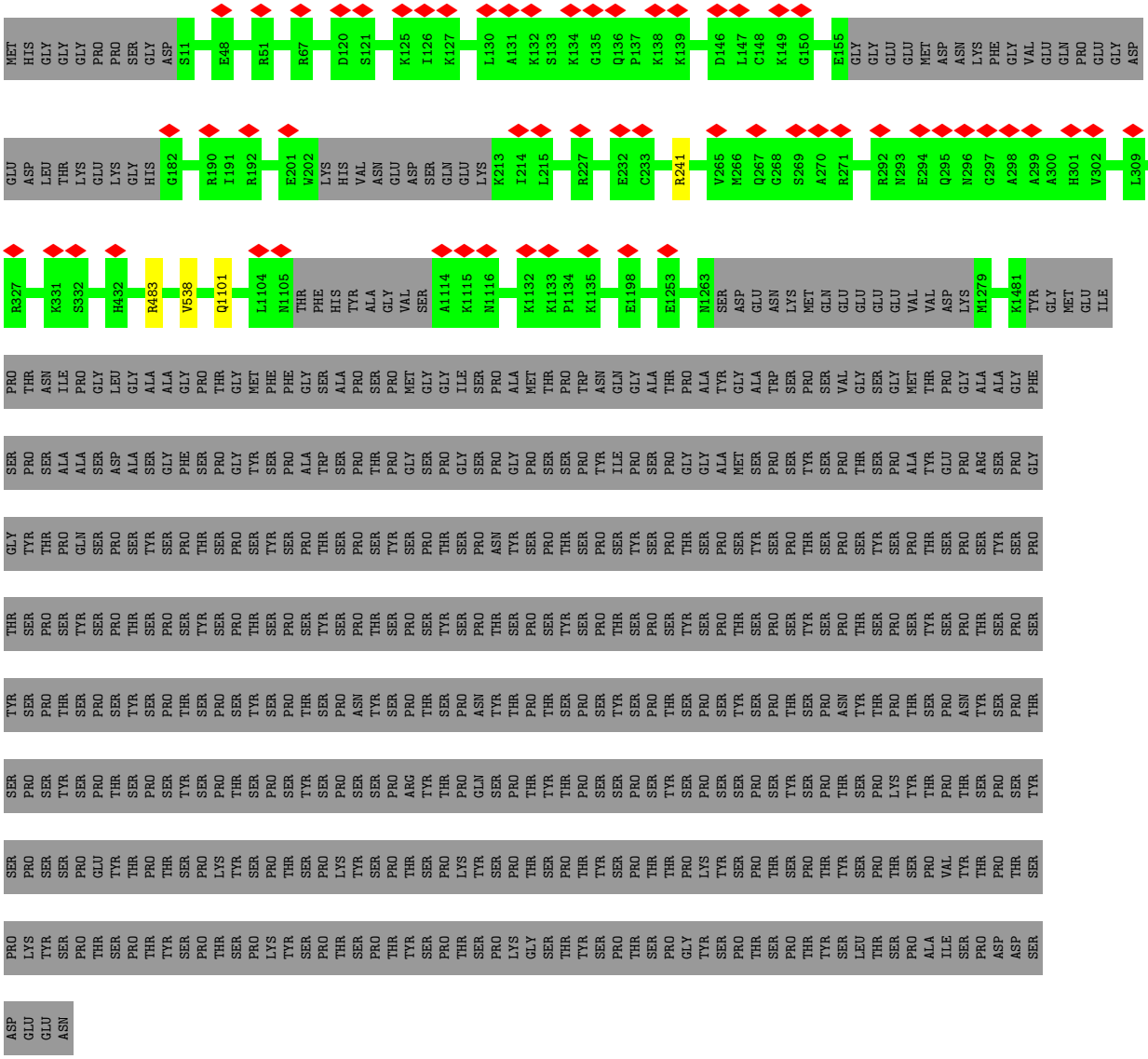
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total Mg 1 1	0

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.

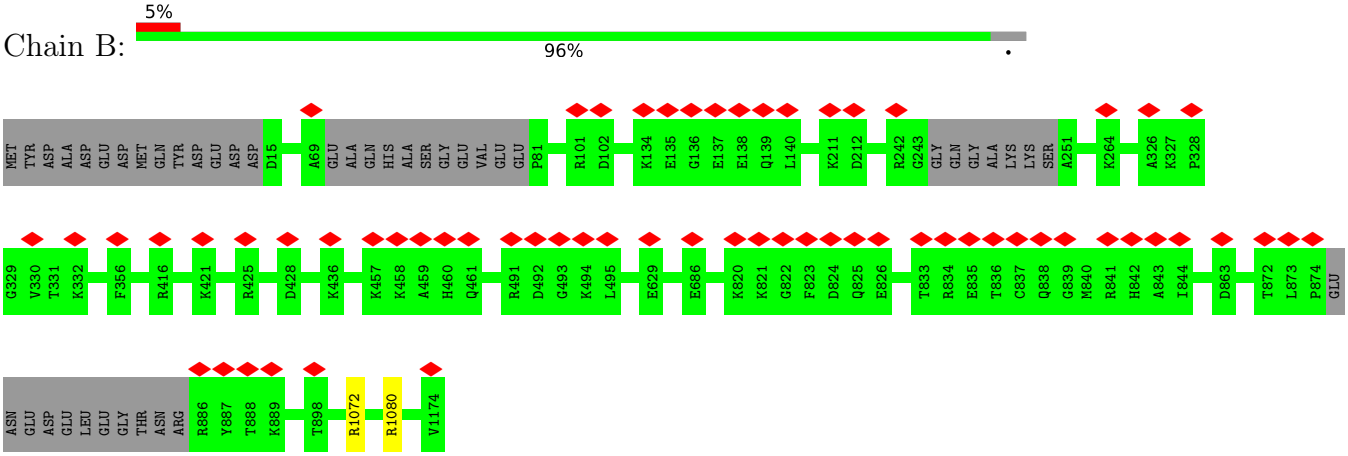
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A:



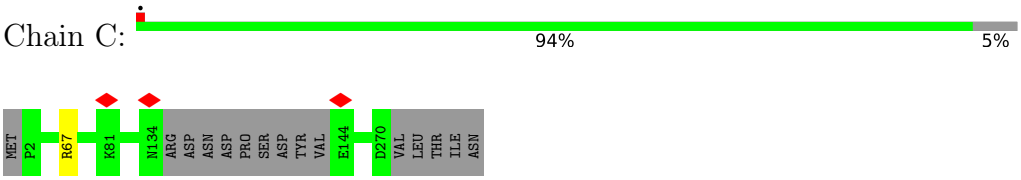
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



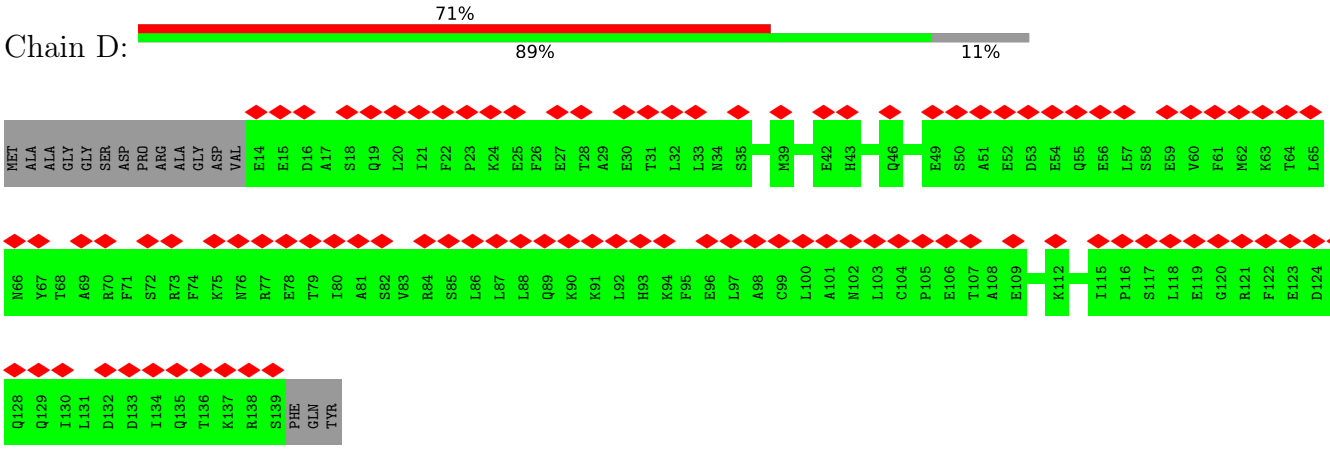
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



• Molecule 4: RPOL4c domain-containing protein

Chain D:

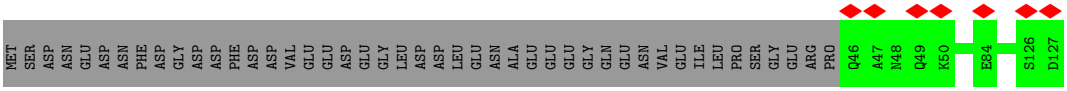


• Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E:

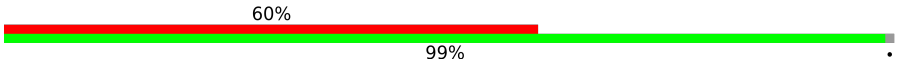
• Molecule 6: DNA-directed RNA polymerase II subunit F

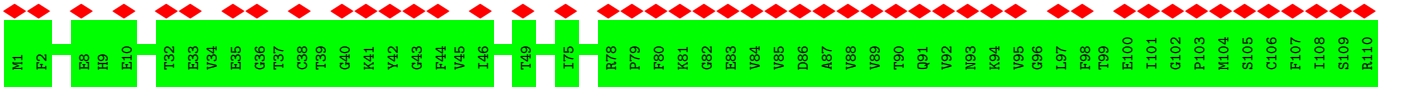
Chain F:

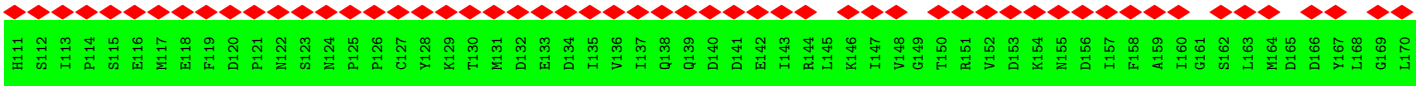


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:

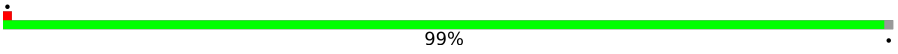


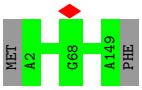




• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

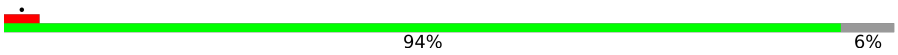
Chain H:

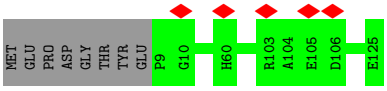




• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

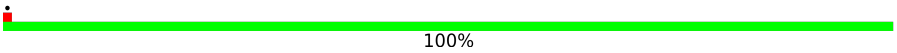
Chain I:





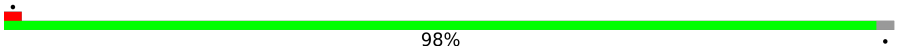
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

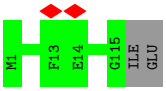
Chain J:



• Molecule 11: RNA_pol_L_2 domain-containing protein

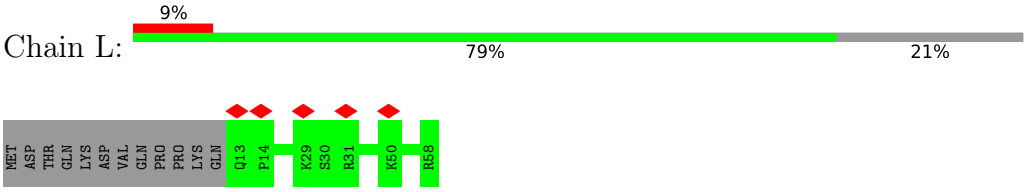
Chain K:





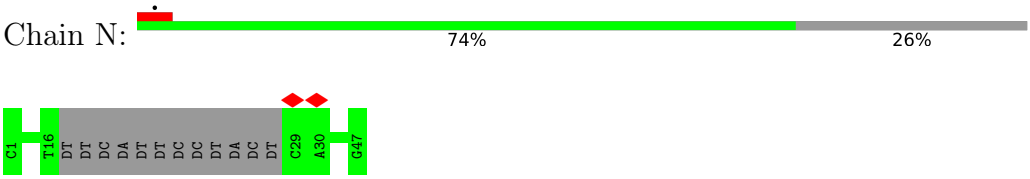
• Molecule 12: RNA polymerase II subunit K

Chain L:



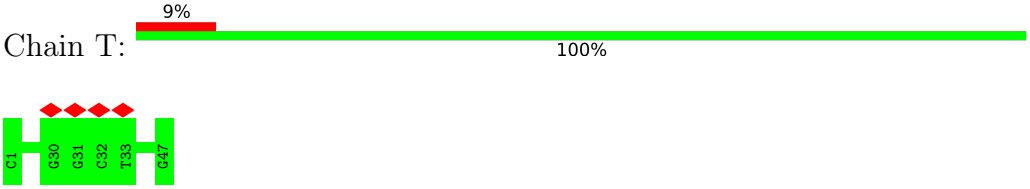
• Molecule 13: NTS

Chain N:



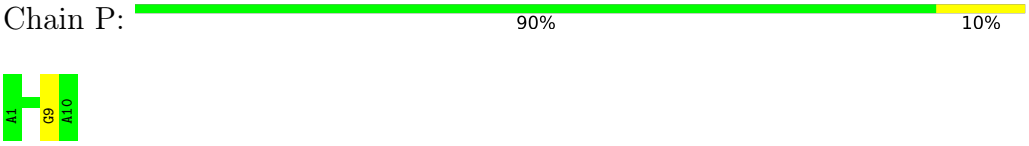
• Molecule 14: TS

Chain T:



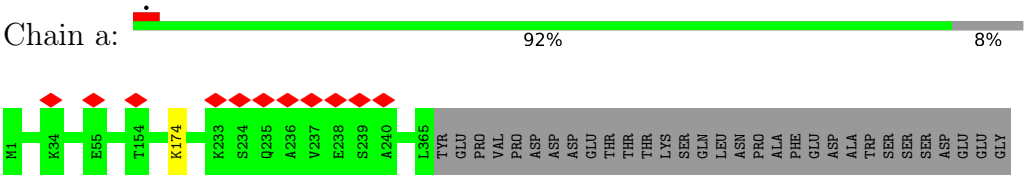
• Molecule 15: RNA

Chain P:



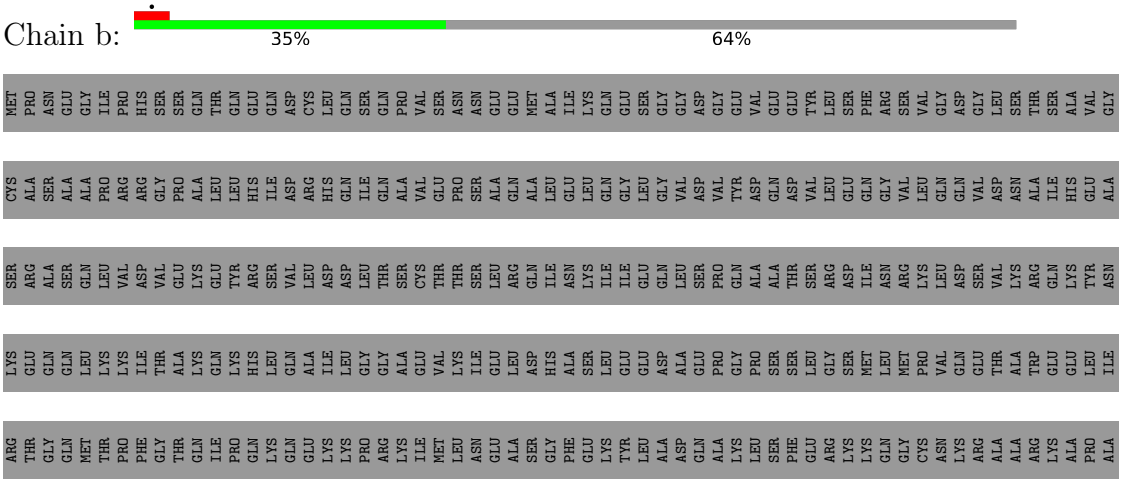
• Molecule 16: DNA excision repair protein ERCC-8

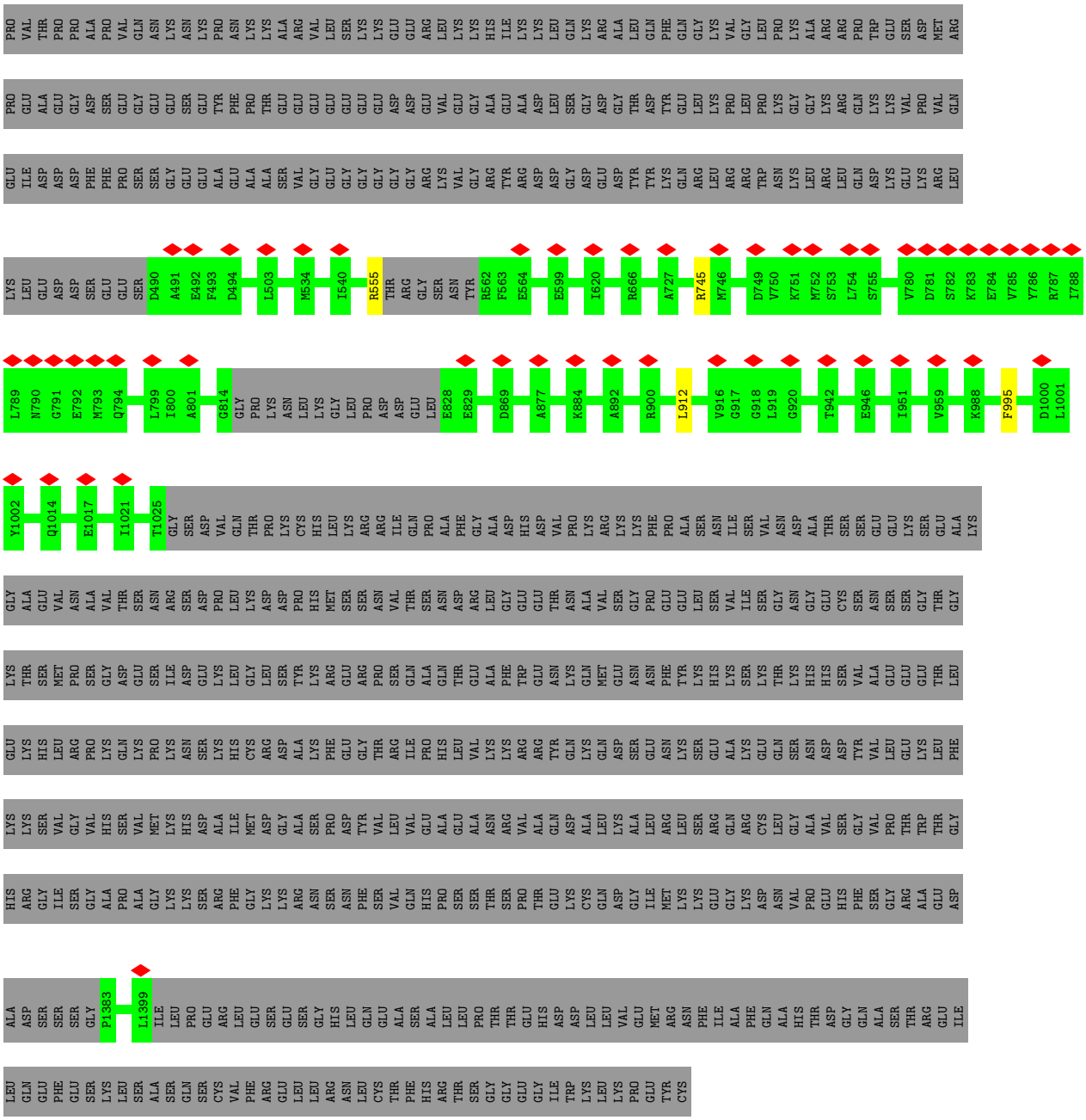
Chain a:



• Molecule 17: DNA excision repair protein ERCC-6

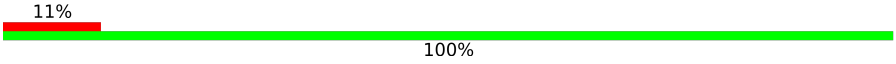
Chain b:

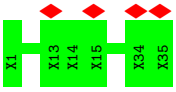




• Molecule 18: CSB element

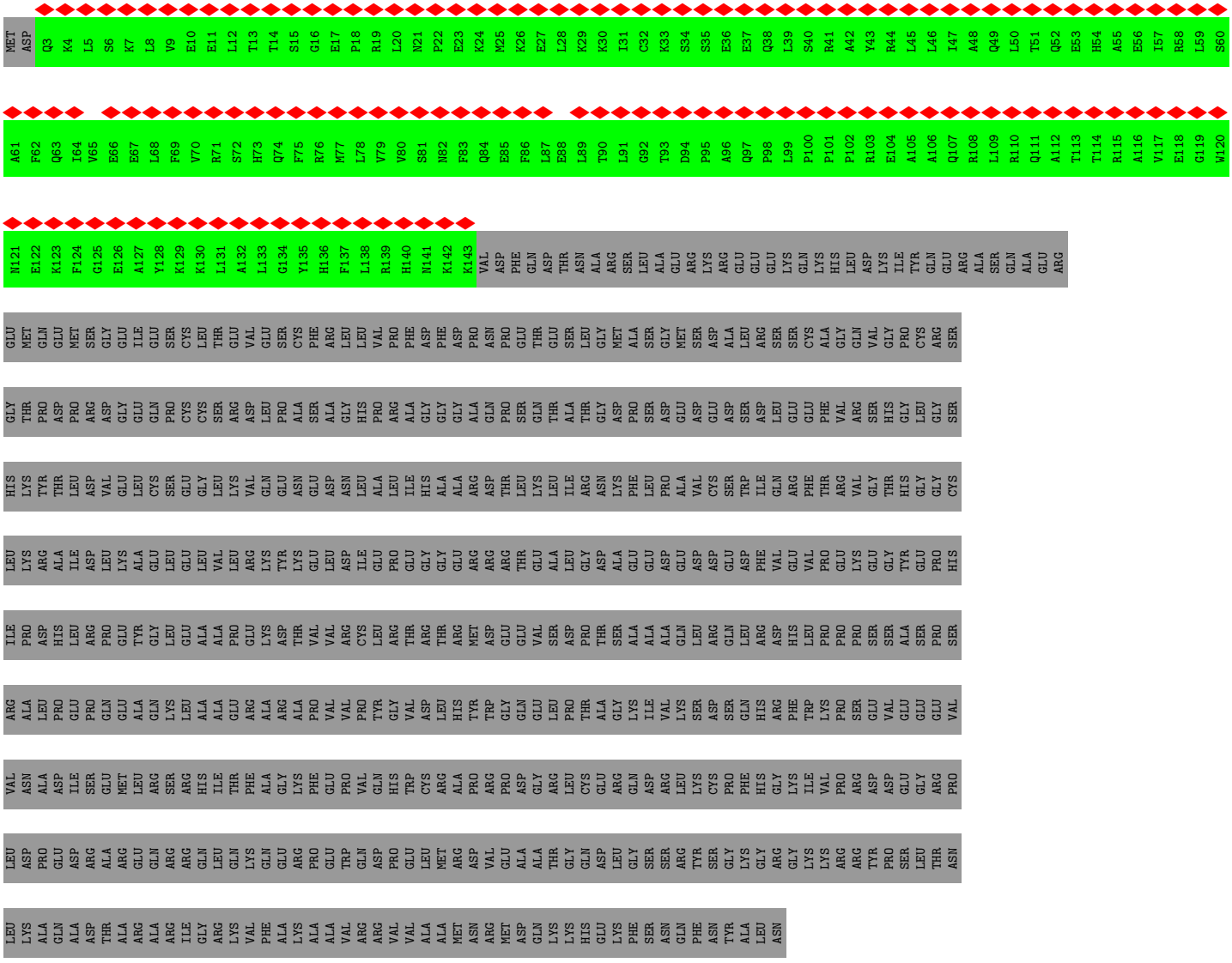
Chain x:





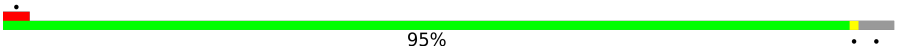
• Molecule 19: UV-stimulated scaffold protein A

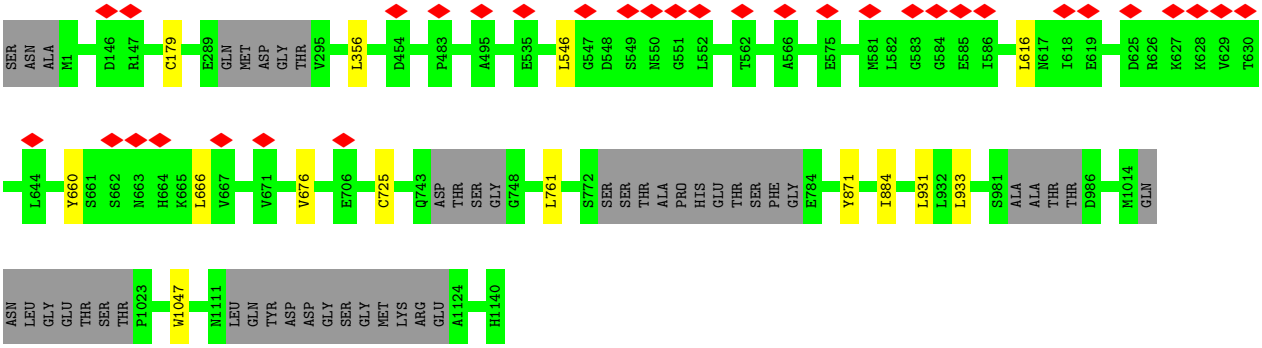
Chain c:



• Molecule 20: DNA damage-binding protein 1

Chain d:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.181	Depositor
Minimum map value	-0.105	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: ZN, 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	0.29	0/11382	0.53	1/15368 (0.0%)
2	B	0.31	0/9233	0.53	0/12463
3	C	0.33	0/2132	0.55	1/2896 (0.0%)
4	D	0.27	0/1043	0.46	0/1400
5	E	0.29	0/1751	0.52	0/2366
6	F	0.31	0/667	0.49	0/901
7	G	0.27	0/1382	0.55	0/1874
8	H	0.32	0/1207	0.52	0/1628
9	I	0.30	0/972	0.54	0/1316
10	J	0.32	0/542	0.50	0/730
11	K	0.30	0/939	0.49	0/1271
12	L	0.32	0/394	0.60	0/524
13	N	0.51	0/817	0.88	0/1258
14	T	0.61	0/1056	0.97	0/1624
15	P	0.49	0/247	0.76	0/384
16	a	0.32	0/2908	0.56	0/3939
17	b	0.29	0/4458	0.55	0/6021
19	c	0.22	0/563	0.42	0/702
20	d	0.94	6/8646 (0.1%)	0.85	7/11725 (0.1%)
All	All	0.49	6/50339 (0.0%)	0.62	9/68390 (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
1	A	0	1
16	a	0	1
17	b	0	2
20	d	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	d	1047	TRP	CB-CG	-6.53	1.38	1.50
20	d	676	VAL	CB-CG2	-6.41	1.39	1.52
20	d	725	CYS	CB-SG	-5.46	1.73	1.81
20	d	179	CYS	CB-SG	-5.32	1.73	1.81
20	d	660	TYR	CD2-CE2	-5.24	1.31	1.39

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	d	761	LEU	CB-CG-CD1	5.81	120.88	111.00
20	d	666	LEU	CA-CB-CG	5.81	128.66	115.30
20	d	933	LEU	CA-CB-CG	5.74	128.49	115.30
3	C	67	ARG	NE-CZ-NH2	-5.64	117.48	120.30
20	d	931	LEU	CA-CB-CG	5.44	127.82	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
16	a	174	LYS	Peptide
17	b	912	LEU	Peptide
17	b	995	PHE	Peptide
20	d	884	ILE	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1402/1970 (71%)	1367 (98%)	35 (2%)	0	100	100
2	B	1123/1174 (96%)	1076 (96%)	47 (4%)	0	100	100
3	C	256/275 (93%)	249 (97%)	7 (3%)	0	100	100
4	D	124/142 (87%)	119 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
6	F	80/127 (63%)	75 (94%)	5 (6%)	0	100	100
7	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
8	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
9	I	115/125 (92%)	111 (96%)	4 (4%)	0	100	100
10	J	65/67 (97%)	65 (100%)	0	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	44/58 (76%)	40 (91%)	4 (9%)	0	100	100
16	a	363/396 (92%)	348 (96%)	15 (4%)	0	100	100
17	b	526/1493 (35%)	507 (96%)	19 (4%)	0	100	100
19	c	139/709 (20%)	136 (98%)	3 (2%)	0	100	100
20	d	1082/1143 (95%)	1010 (93%)	72 (7%)	0	100	100
All	All	5954/8328 (72%)	5725 (96%)	229 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1242/1749 (71%)	1240 (100%)	2 (0%)	93	98
2	B	992/1027 (97%)	990 (100%)	2 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	237/252 (94%)	237 (100%)	0	100 100
4	D	116/126 (92%)	116 (100%)	0	100 100
5	E	191/192 (100%)	190 (100%)	1 (0%)	88 96
6	F	71/111 (64%)	71 (100%)	0	100 100
7	G	152/153 (99%)	152 (100%)	0	100 100
8	H	129/131 (98%)	129 (100%)	0	100 100
9	I	105/112 (94%)	105 (100%)	0	100 100
10	J	56/56 (100%)	56 (100%)	0	100 100
11	K	104/106 (98%)	104 (100%)	0	100 100
12	L	43/55 (78%)	43 (100%)	0	100 100
16	a	320/348 (92%)	320 (100%)	0	100 100
17	b	476/1297 (37%)	474 (100%)	2 (0%)	91 97
20	d	938/1001 (94%)	938 (100%)	0	100 100
All	All	5172/6716 (77%)	5165 (100%)	7 (0%)	93 98

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

Mol	Chain	Res	Type
2	B	1080	ARG
5	E	166	ARG
17	b	745	ARG
17	b	555	ARG
2	B	1072	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
20	d	467	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	9	G

There are no RNA pucker outliers to report.

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 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

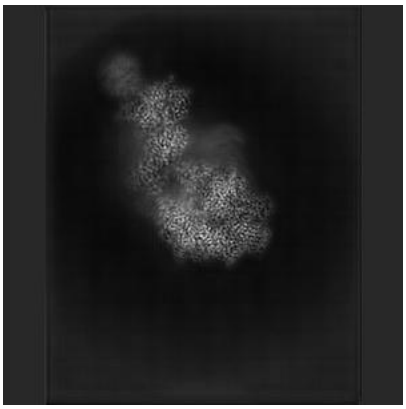
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13004. These allow visual inspection of the internal detail of the map and identification of artifacts.

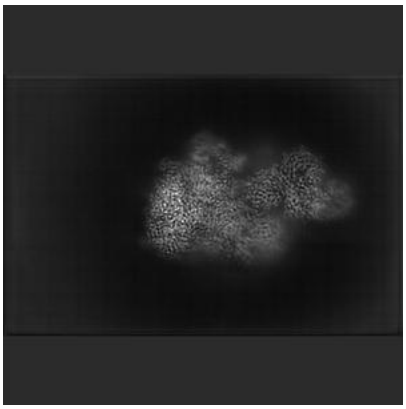
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

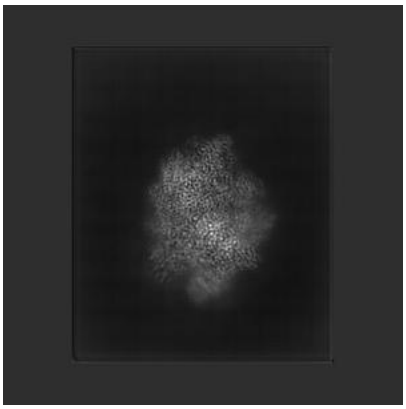
6.1.1 Primary map



X

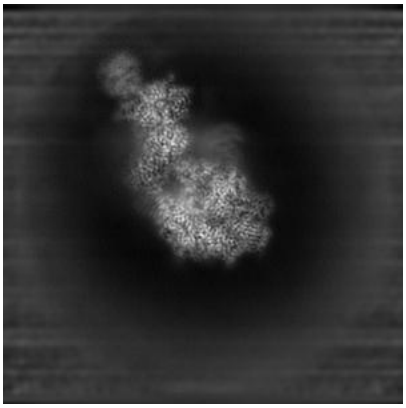


Y

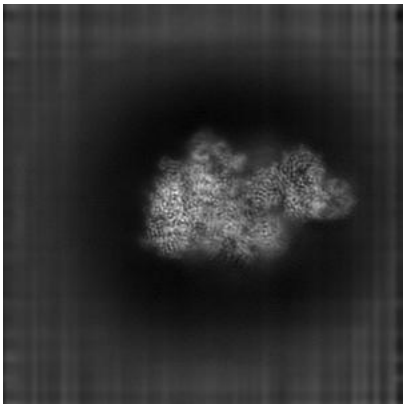


Z

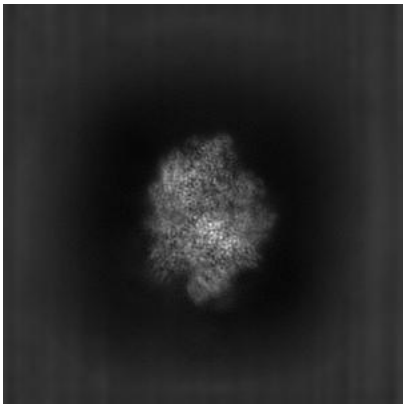
6.1.2 Raw map



X



Y

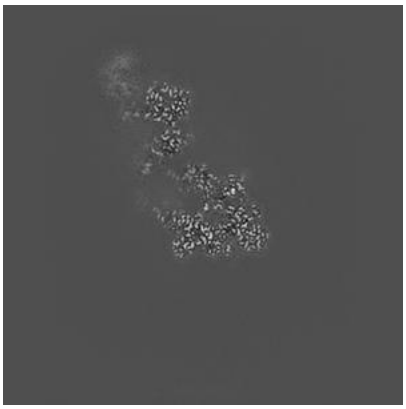


Z

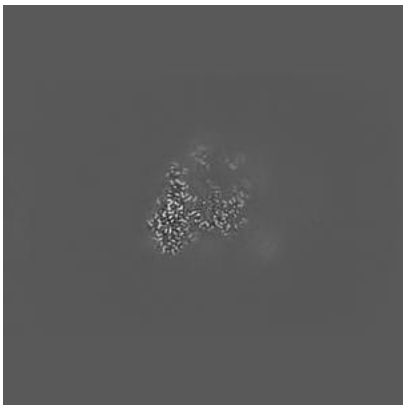
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



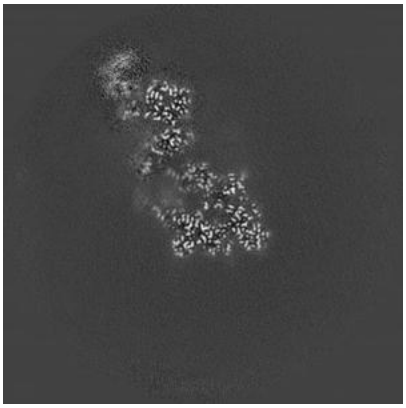
X Index: 200



Y Index: 200

Z Index: 200

6.2.2 Raw map



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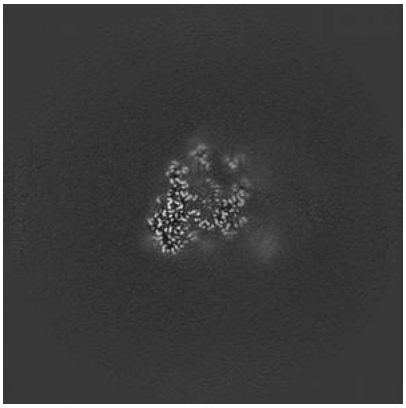
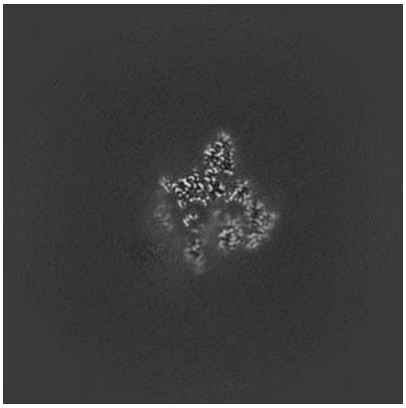


Y Index: 200

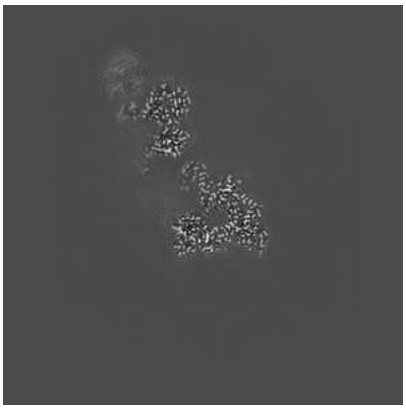


Z Index: 200

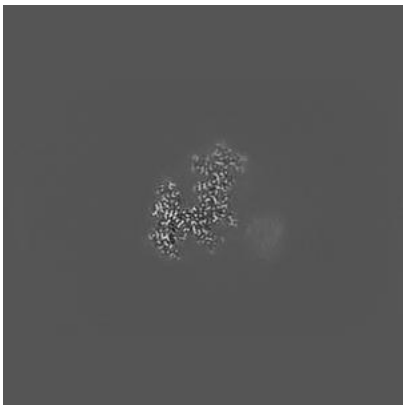
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

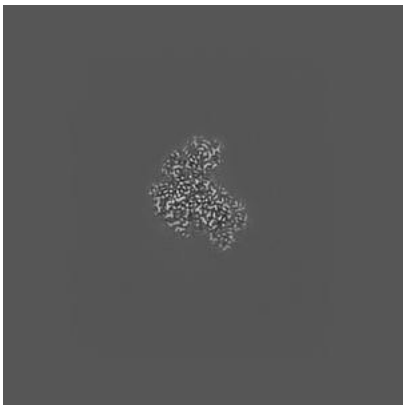
6.3.1 Primary map



X Index: 203

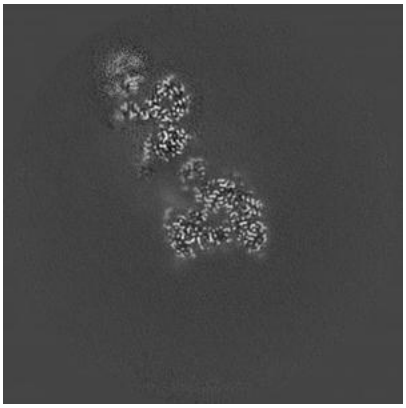


Y Index: 215

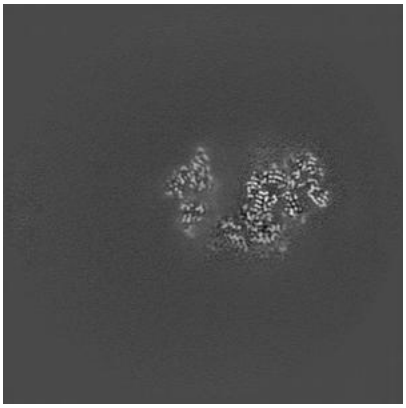


Z Index: 169

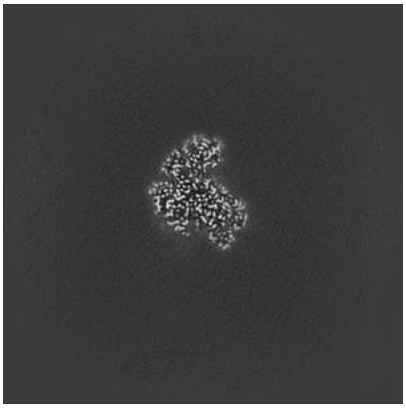
6.3.2 Raw map



X Index: 206



Y Index: 161



Z Index: 169

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

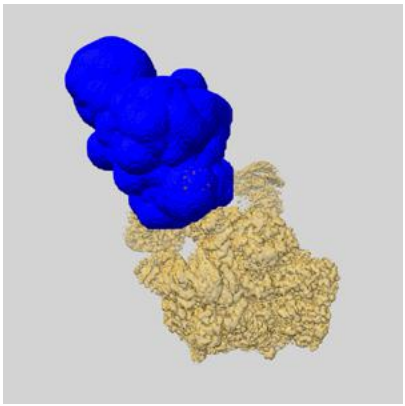
6.5 Mask visualisation (i)

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

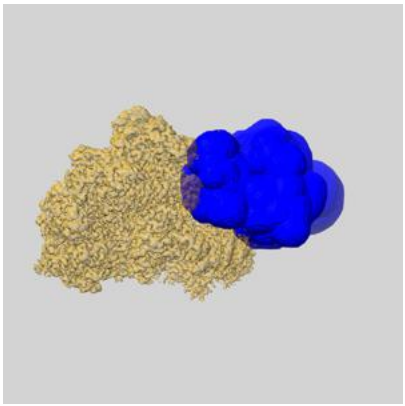
A mask typically either:

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

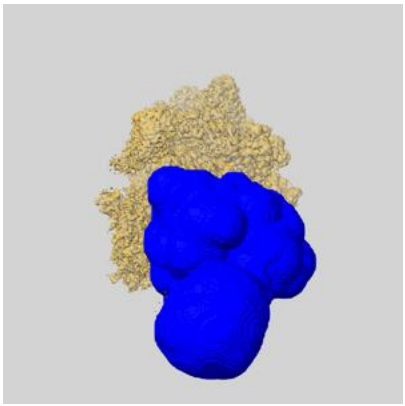
6.5.1 emd_13004_msk_1.map (i)



X

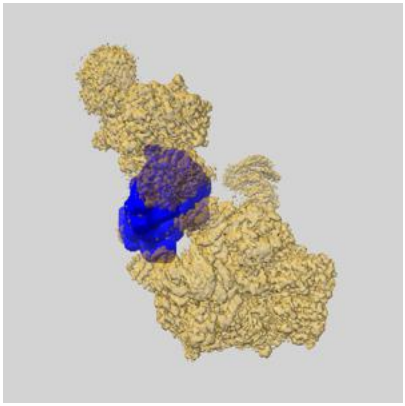


Y

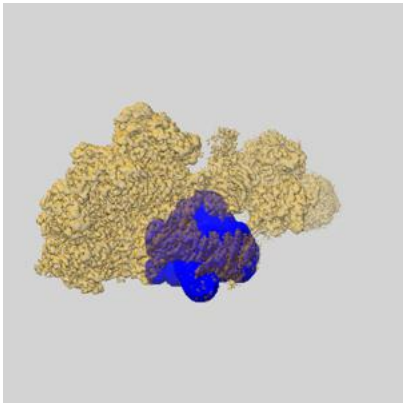


Z

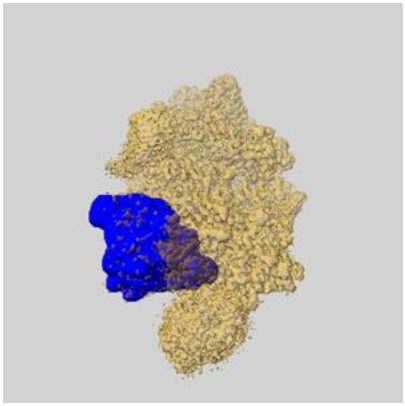
6.5.2 emd_13004_msk_5.map (i)



X

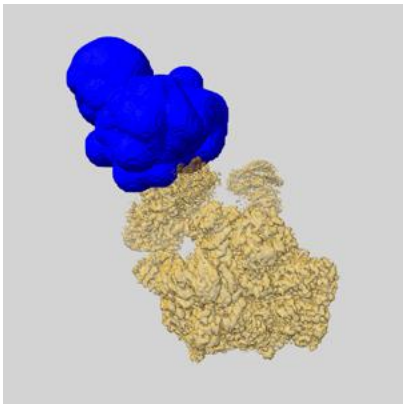


Y

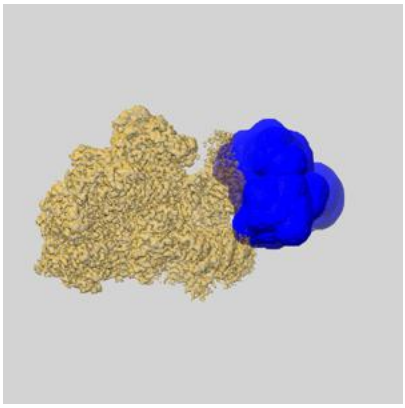


Z

6.5.3 emd_13004_msk_3.map



X



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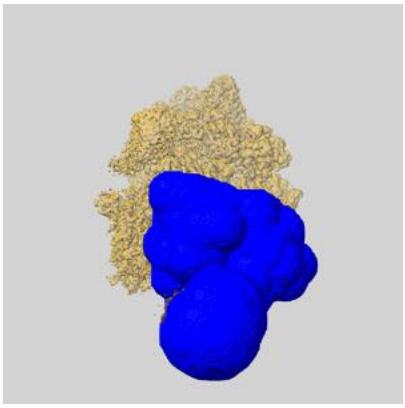
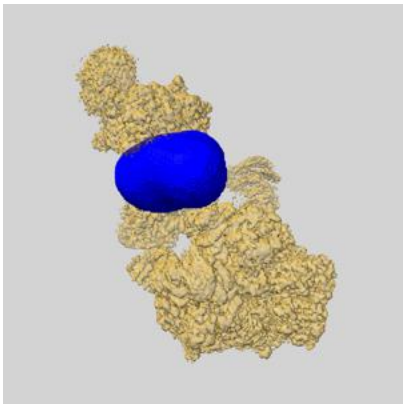
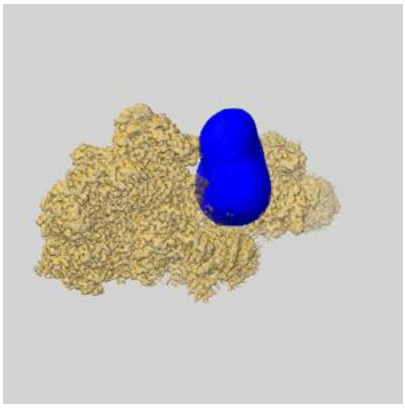


Z

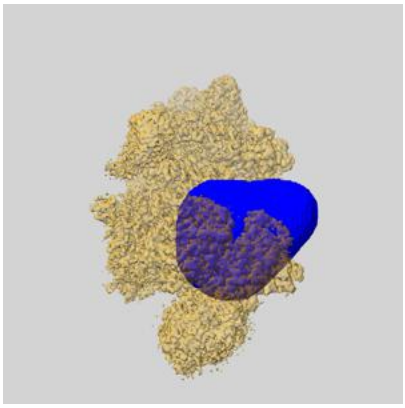
6.5.4 emd_13004_msk_2.map



X

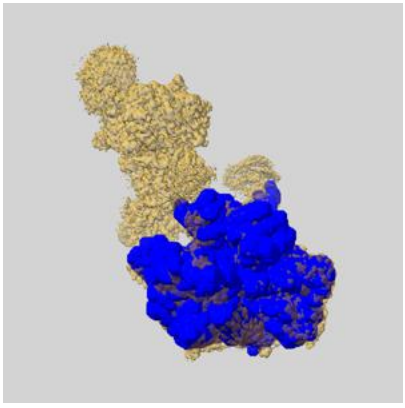


Y

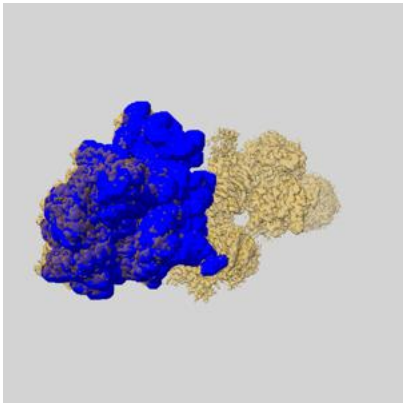


Z

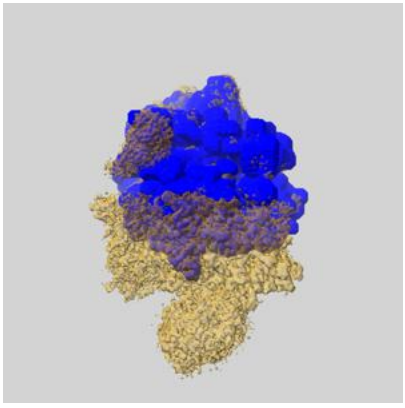
6.5.5 emd_13004_msk_4.map



X



Y

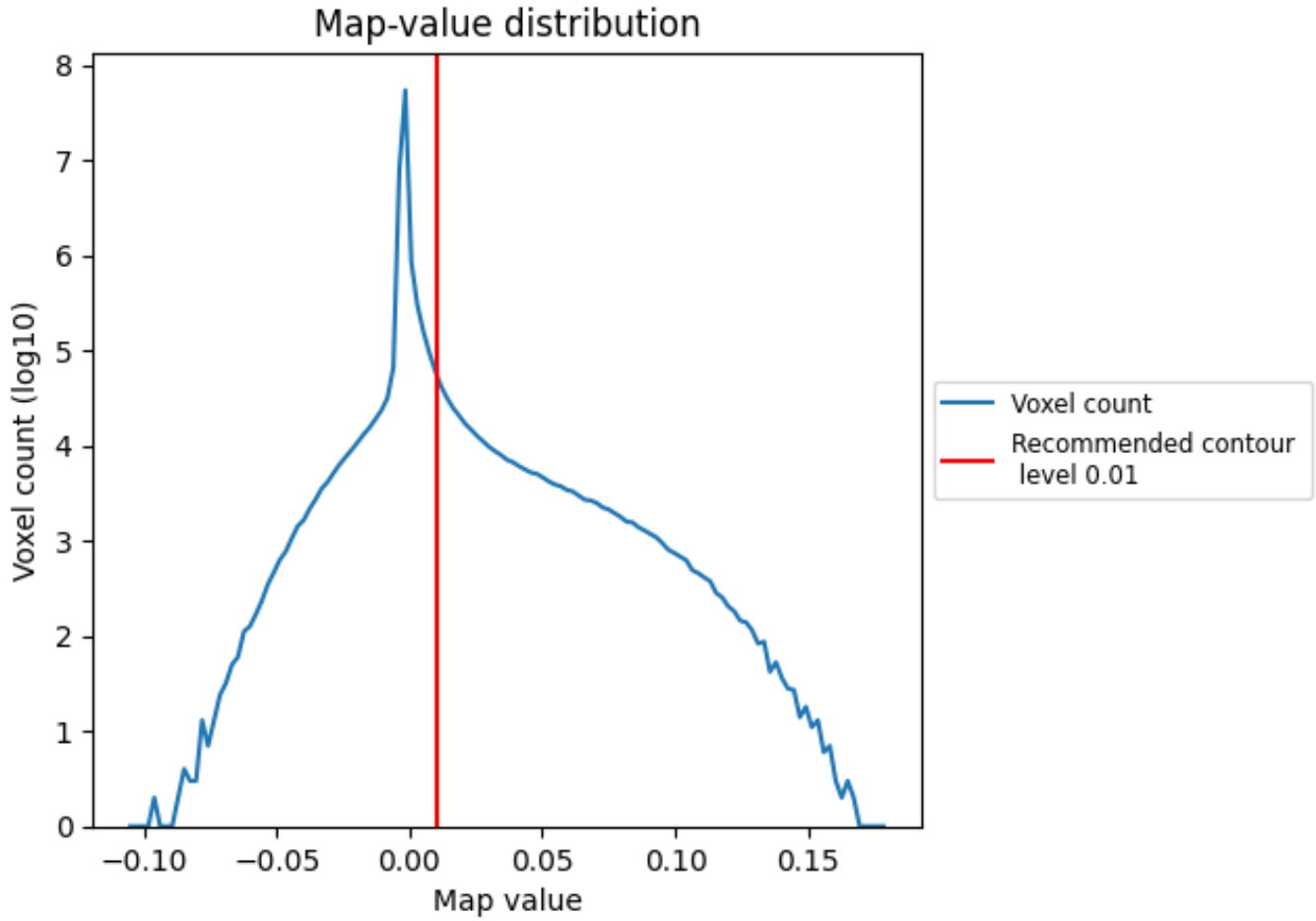


Z

7 Map analysis

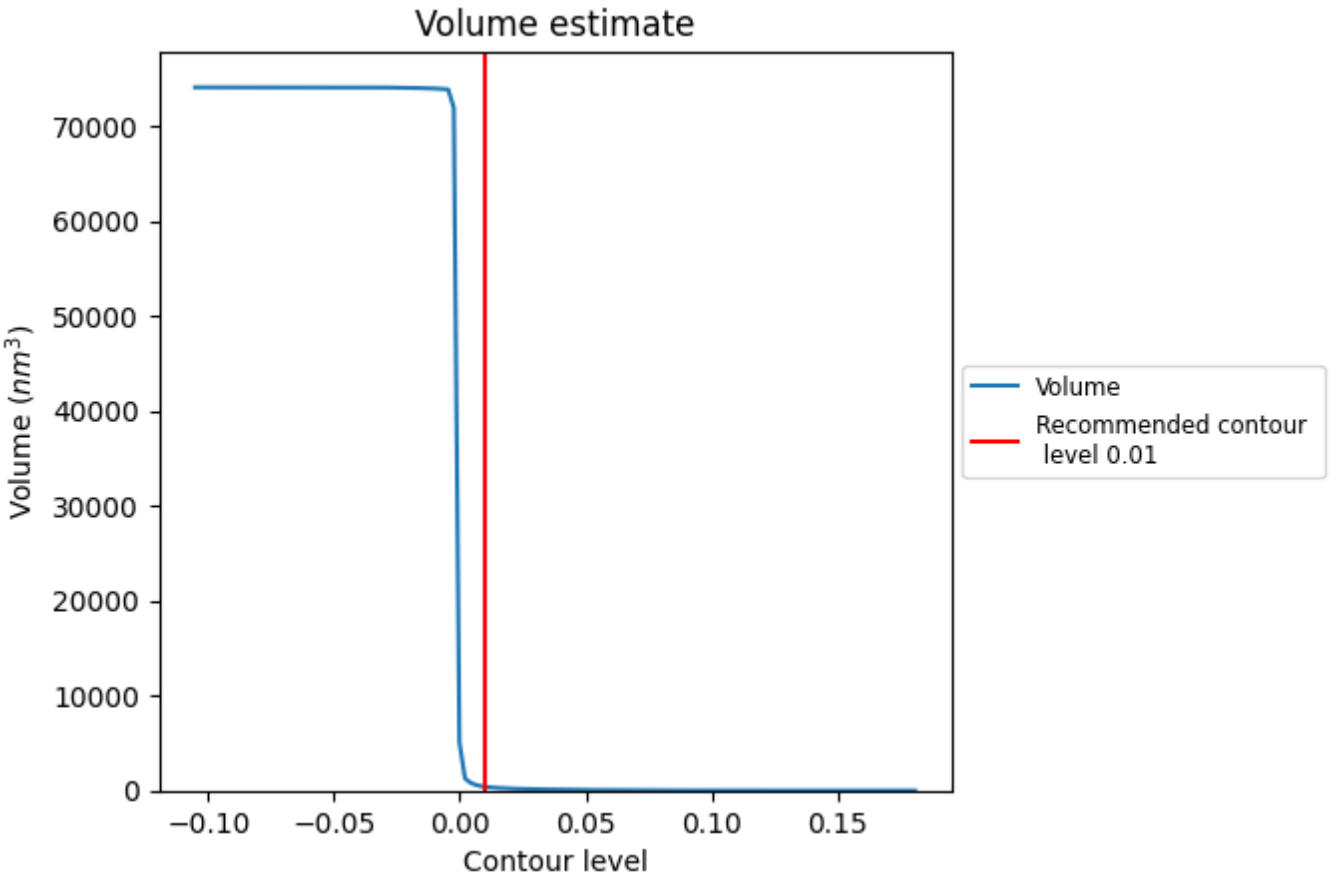
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

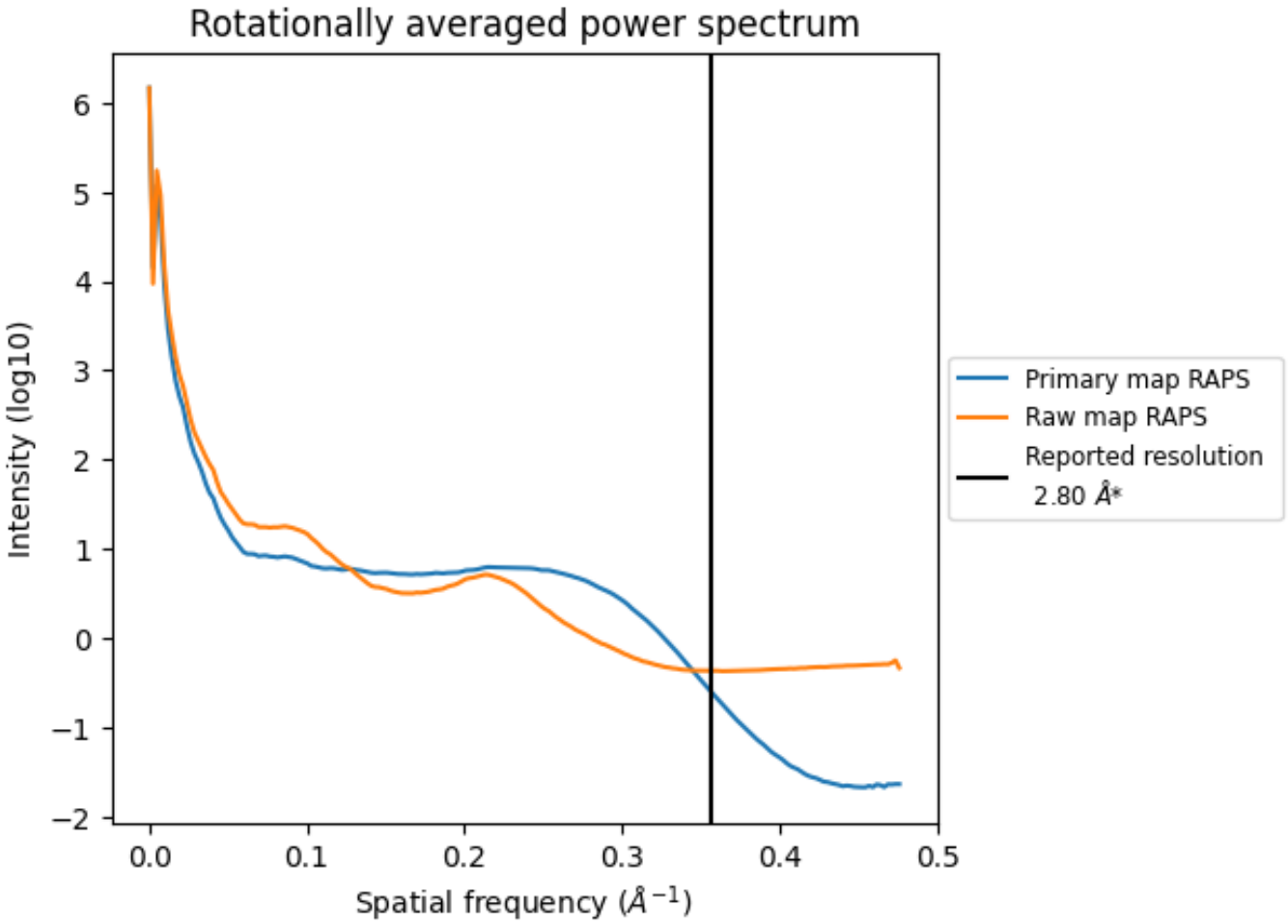
7.2 Volume estimate (i)



The volume at the recommended contour level is 401 nm^3; this corresponds to an approximate mass of 362 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)

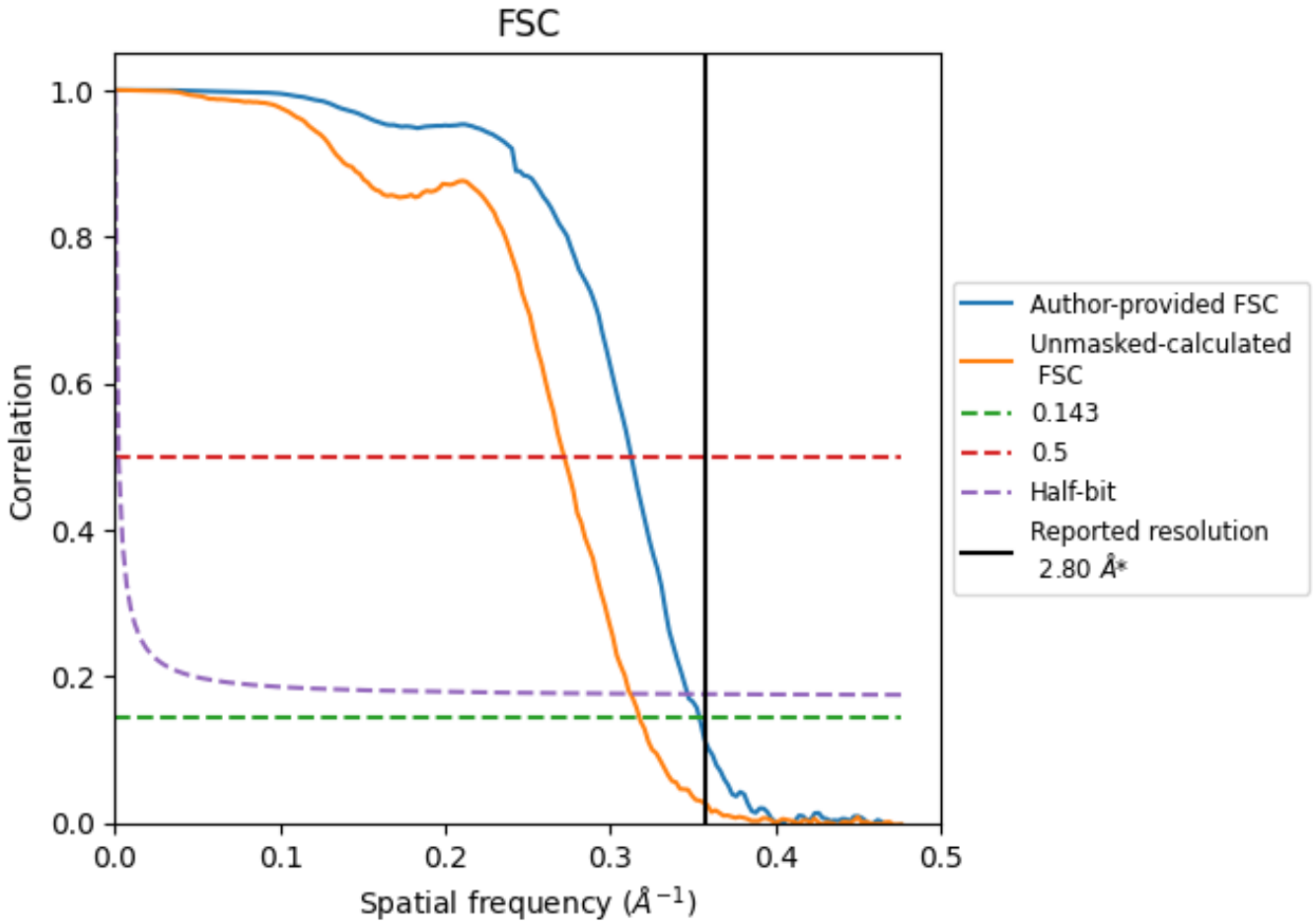


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

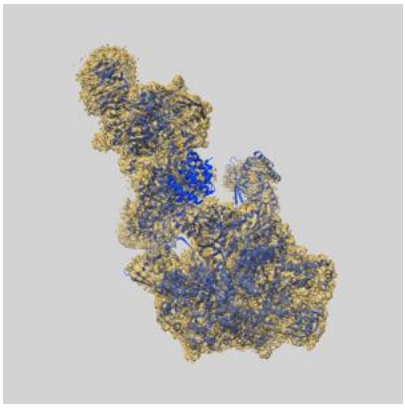
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.83	3.20	2.88
Unmasked-calculated*	3.15	3.68	3.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.15 differs from the reported value 2.8 by more than 10 %

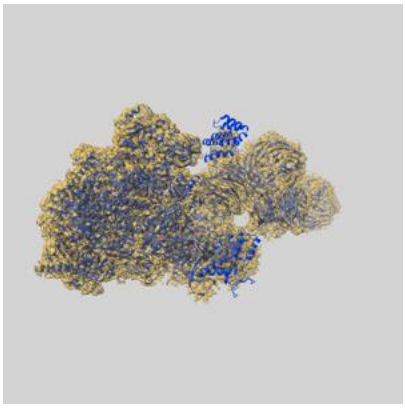
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13004 and PDB model 7OO3. Per-residue inclusion information can be found in section 3 on page 8.

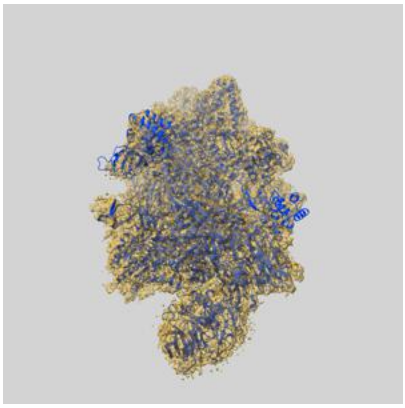
9.1 Map-model overlay



X



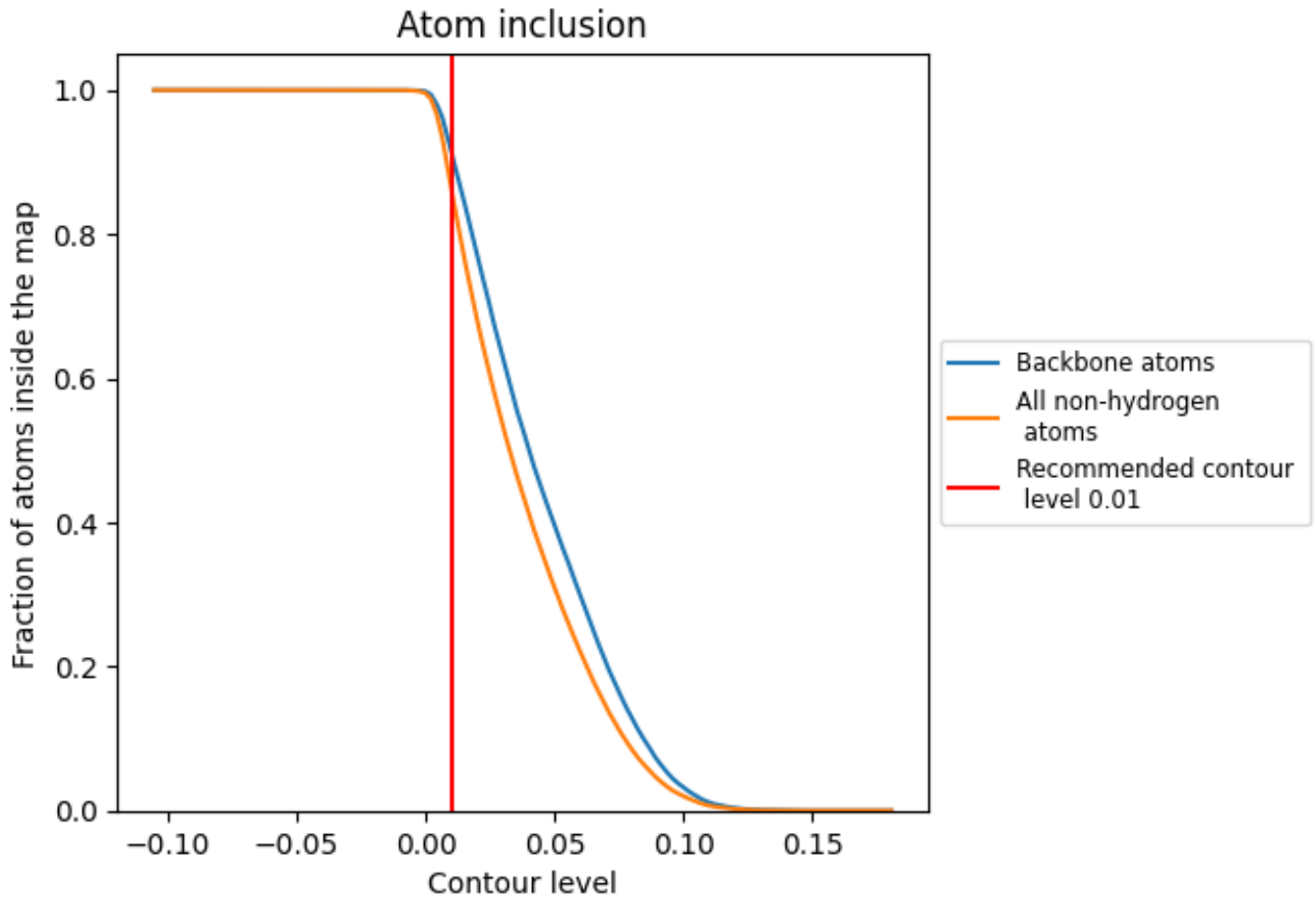
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.