wwPDB EM Validation Summary Report

Oct 18, 2021 – 11:58 am BST

PDB ID	:	7OOB
EMDB ID	:	EMD-13009
Title	:	Pol II-CSB-CSA-DDB1-UVSSA-ADPBeF3 (Structure2)
Authors	:	Kokic, G.; Cramer, P.
Deposited on	:	2021-05-27
Resolution	:	2.70 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 ⓘ symbol.

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

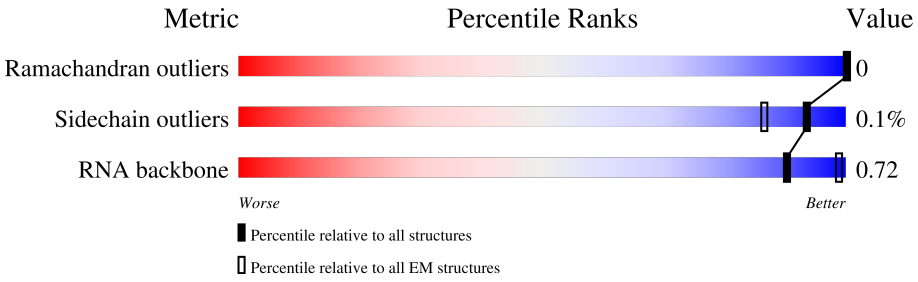
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	15% 71% 28%
2	B	1174	17% 96% .
3	C	275	. 94% 5%
4	D	142	87% 89% 11%
5	E	210	19% 99%
6	F	127	7% 65% 35%
7	G	172	85% 99% .
8	H	150	. 99% .

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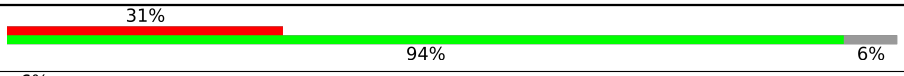
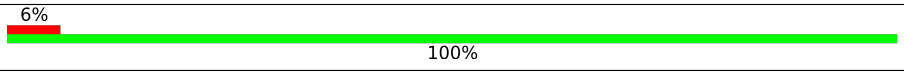
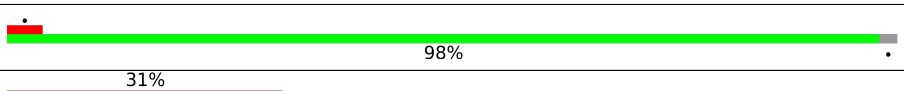
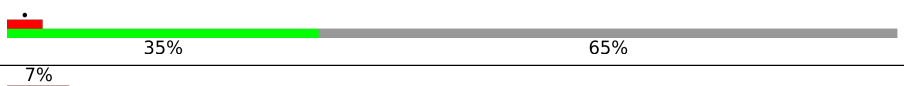
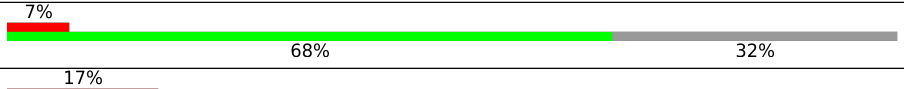
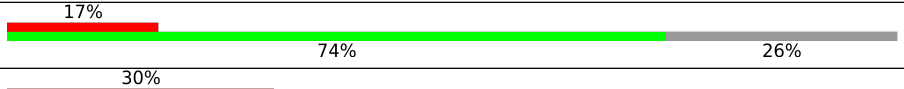
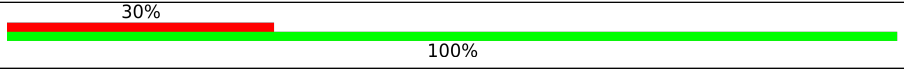
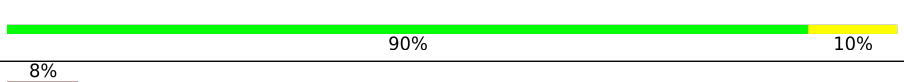
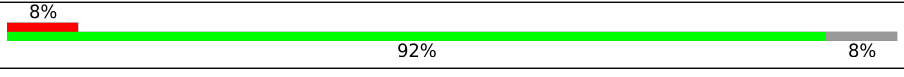
Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	b	1496	
14	d	1143	
15	N	47	
16	T	47	
17	P	10	
18	a	396	

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 90756 atoms, of which 44495 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	22494	7033	11315	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	4120	1309	2031	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 protein called DNA excision repair protein ERCC-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	b	520	Total	C	H	N	O	S	0	0
			8561	2746	4302	746	746	21		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-2	SER	-	expression tag	UNP Q03468
b	-1	ASN	-	expression tag	UNP Q03468
b	0	ALA	-	expression tag	UNP Q03468

- Molecule 14 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	d	781	Total	C	H	N	O	S	0	0
			12317	3919	6153	1038	1173	34		

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 15 is a DNA chain called NTS.

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

- Molecule 16 is a DNA chain called TS.

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

- Molecule 17 is a RNA chain called RNA.

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

- Molecule 18 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	a	365	Total	C	H	N	O	S	0	0
			5626	1775	2777	507	548	19		

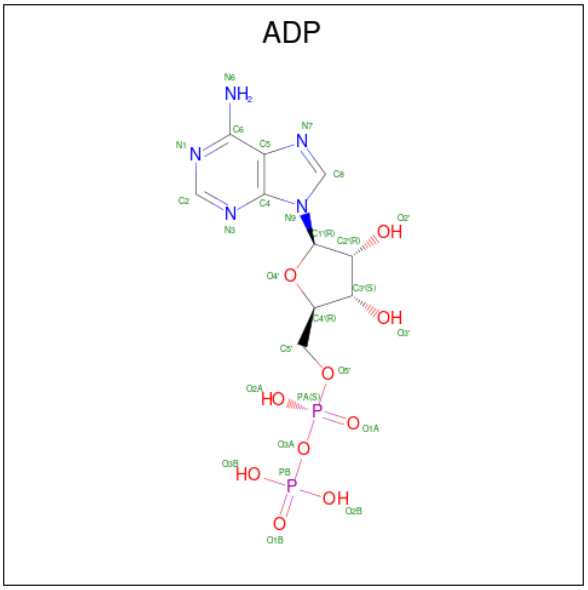
- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

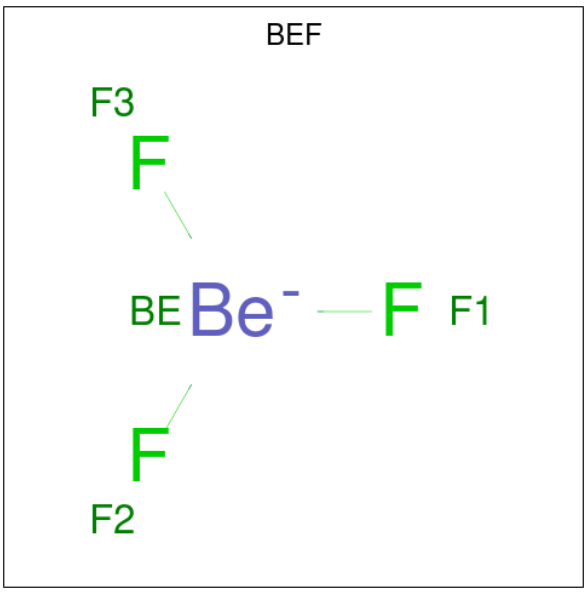
Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total Mg 1 1	0
20	b	1	Total Mg 1 1	0

- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms	AltConf
21	b	1	Total C H N O P 38 10 11 5 10 2	0

- Molecule 22 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



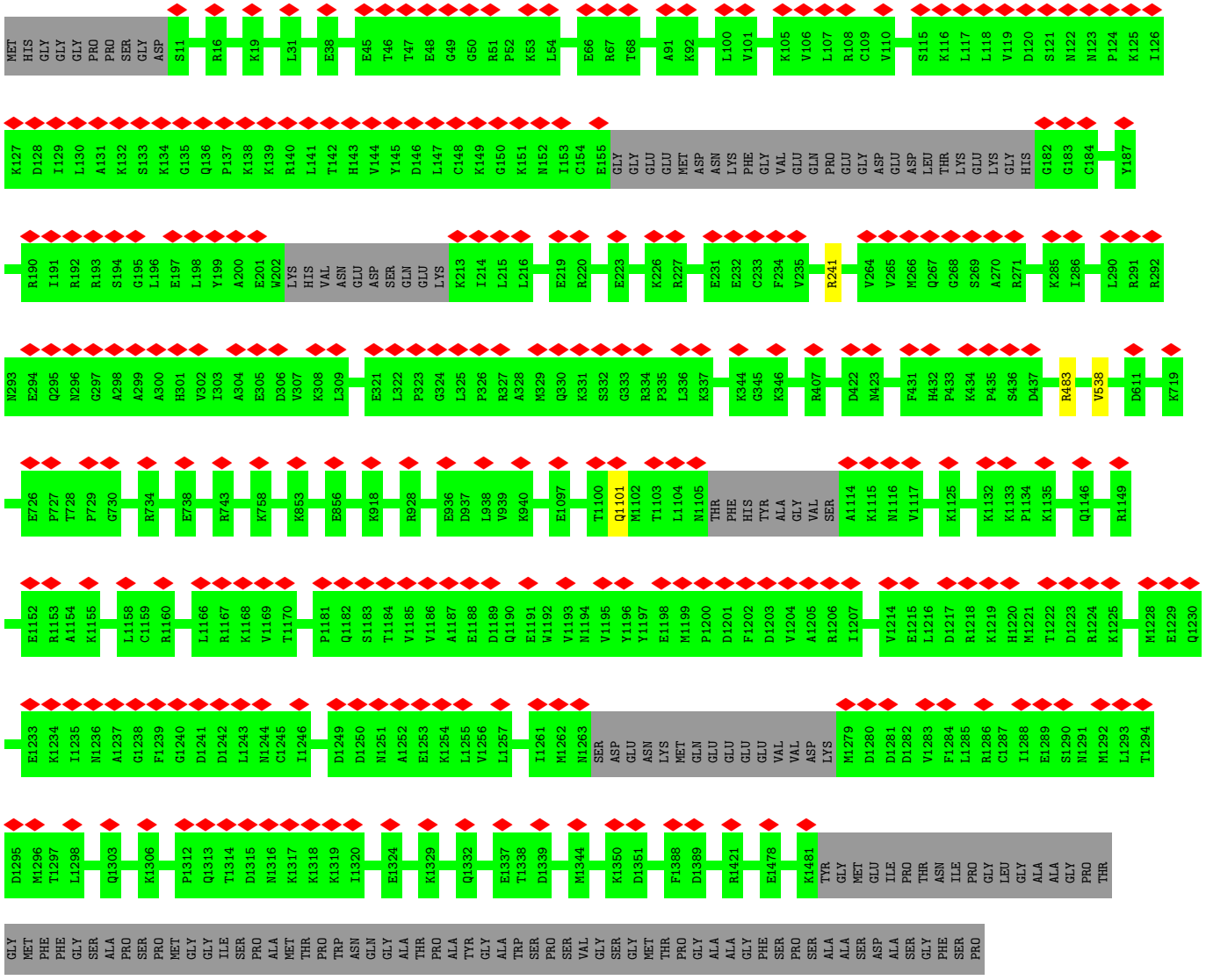
Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
22	b	1	4	1	3	0

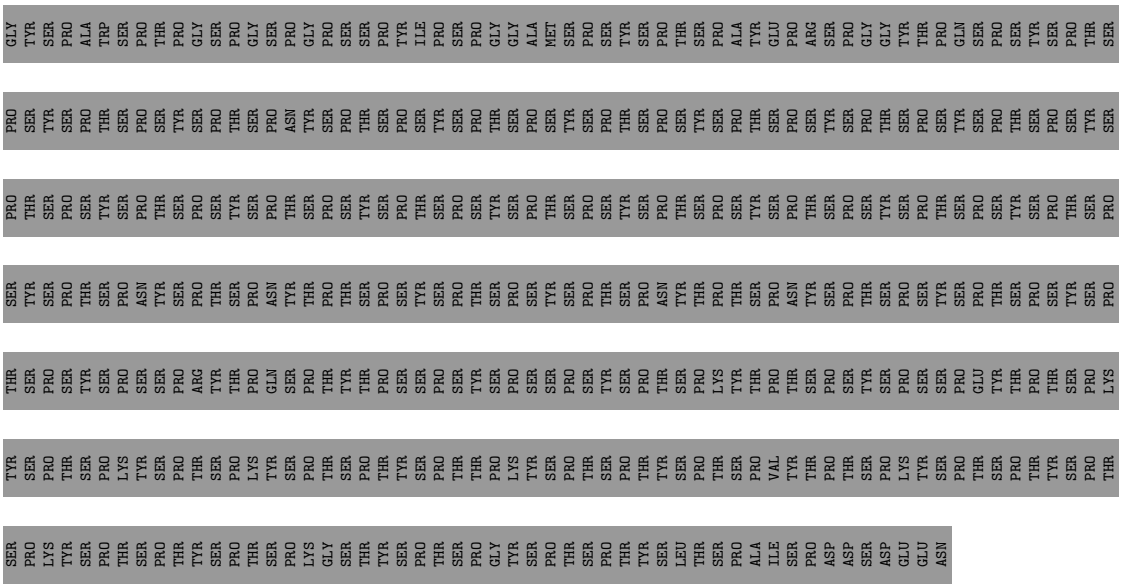
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

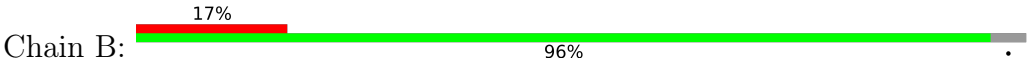
Chain A:

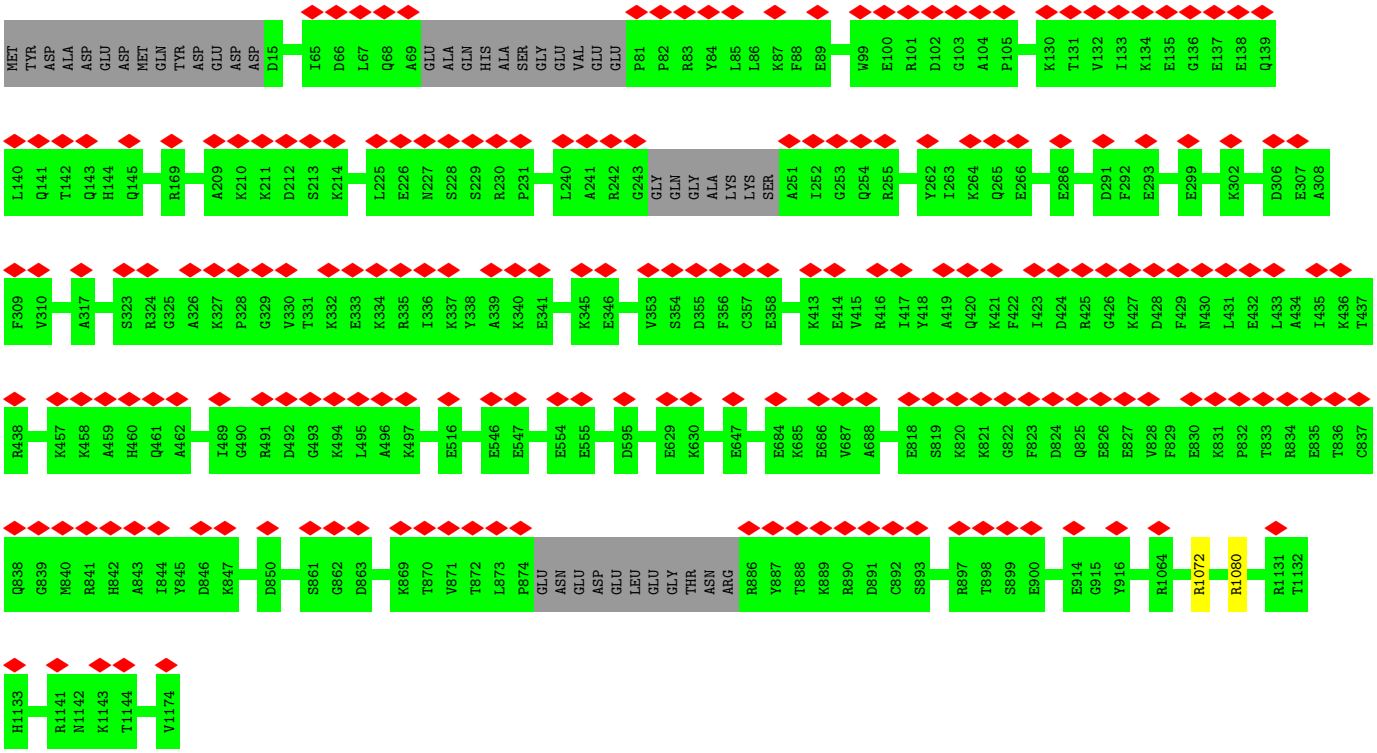




• Molecule 2: DNA-directed RNA polymerase subunit beta

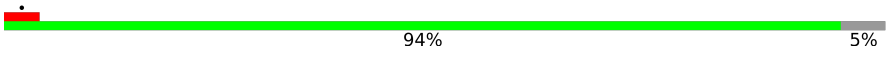
Chain B:

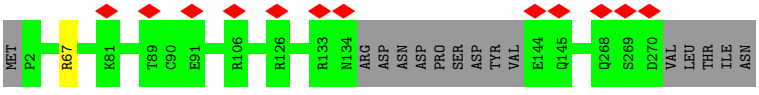




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

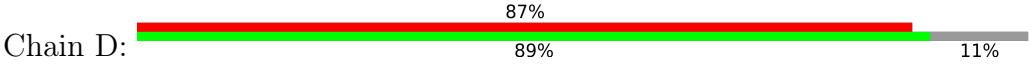
Chain C:





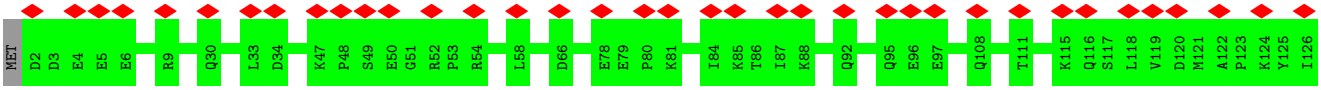
• Molecule 4: RPOL4c domain-containing protein

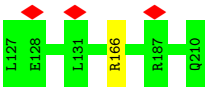
Chain D:



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

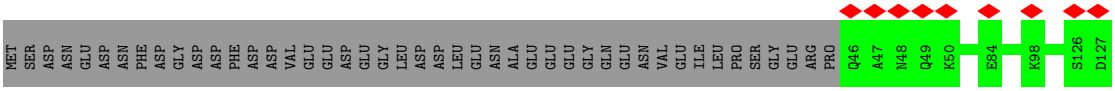
Chain E:





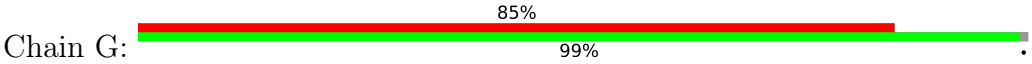
• Molecule 6: DNA-directed RNA polymerase II subunit F

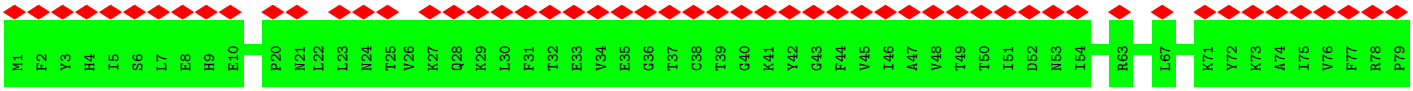
Chain F:

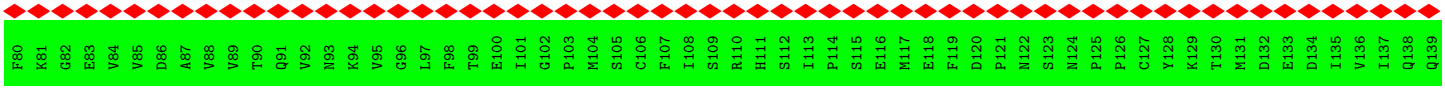


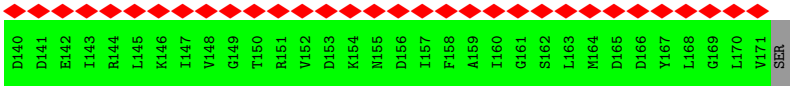
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



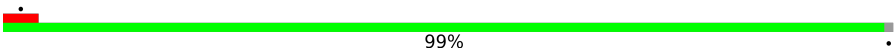


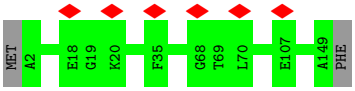




• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

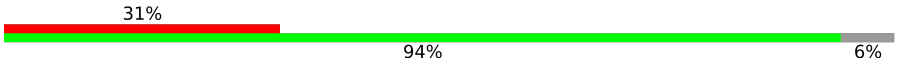
Chain H:

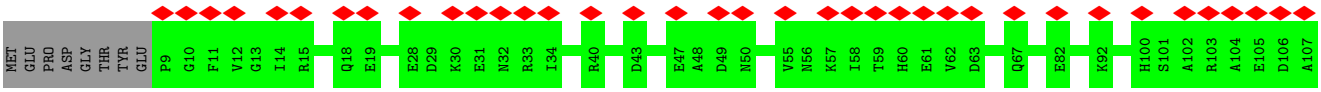




• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

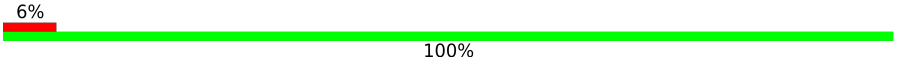
Chain I:

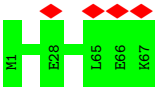




• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

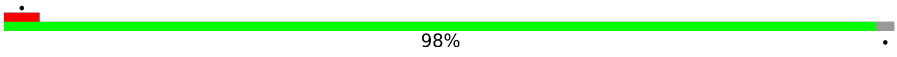
Chain J:

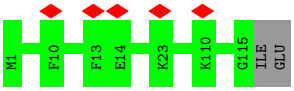




• Molecule 11: RNA_pol_L_2 domain-containing protein

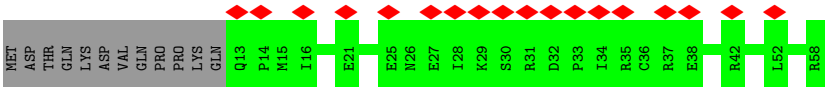
Chain K:





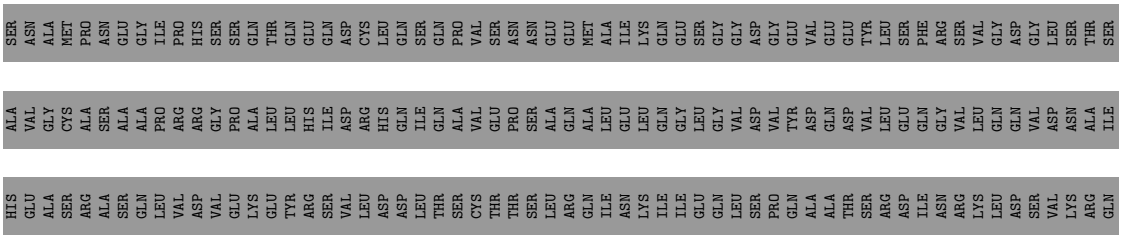
• Molecule 12: RNA polymerase II subunit K

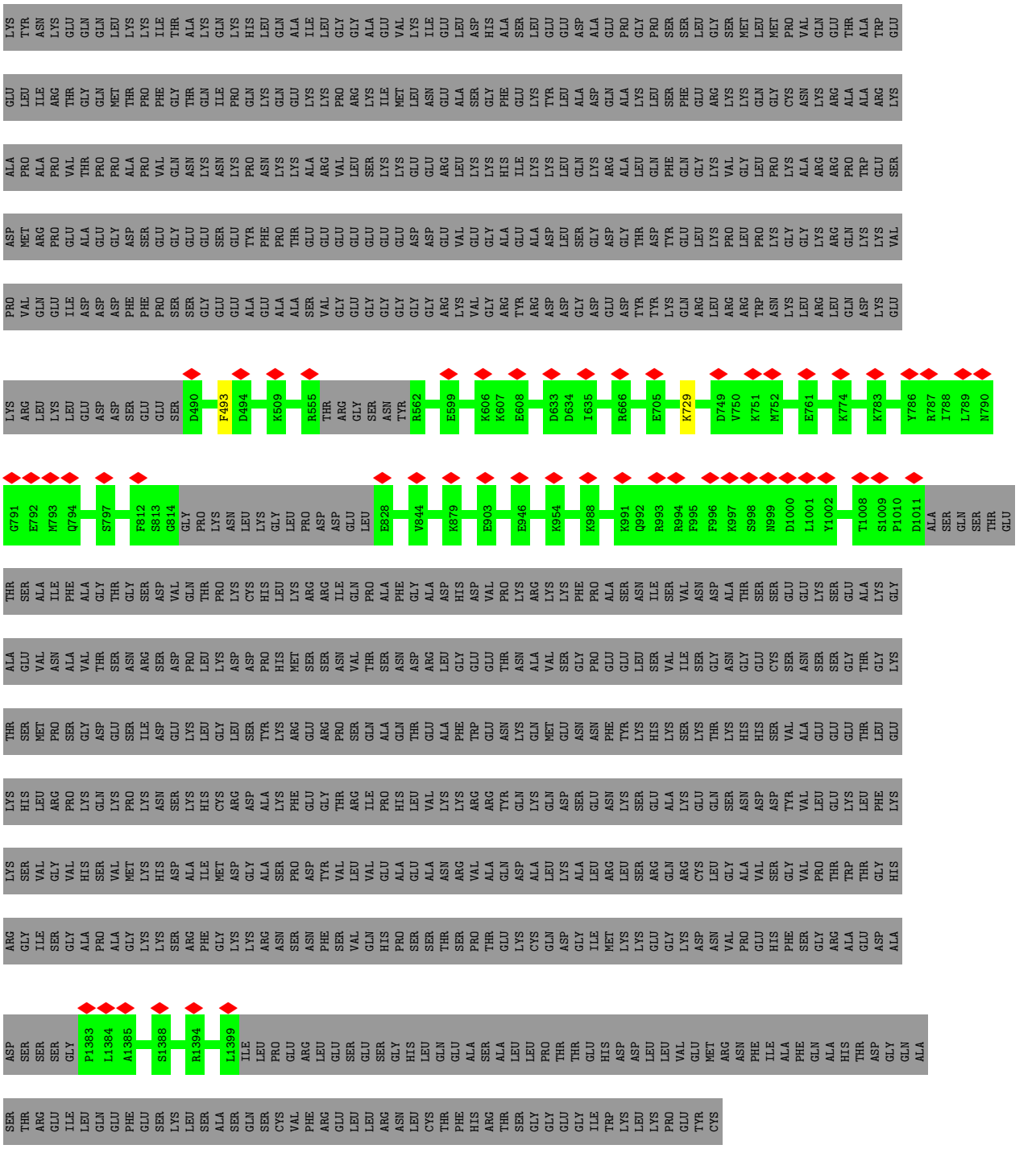
Chain L:



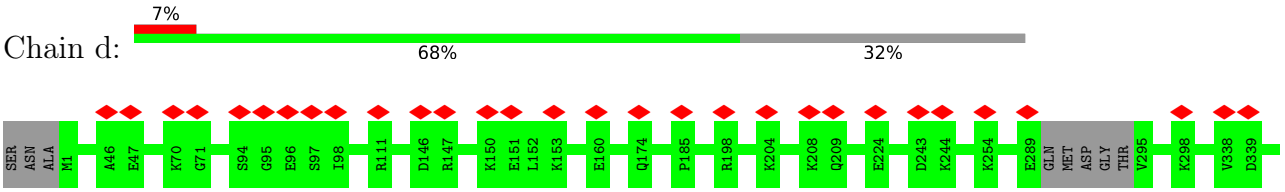
• Molecule 13: DNA excision repair protein ERCC-6

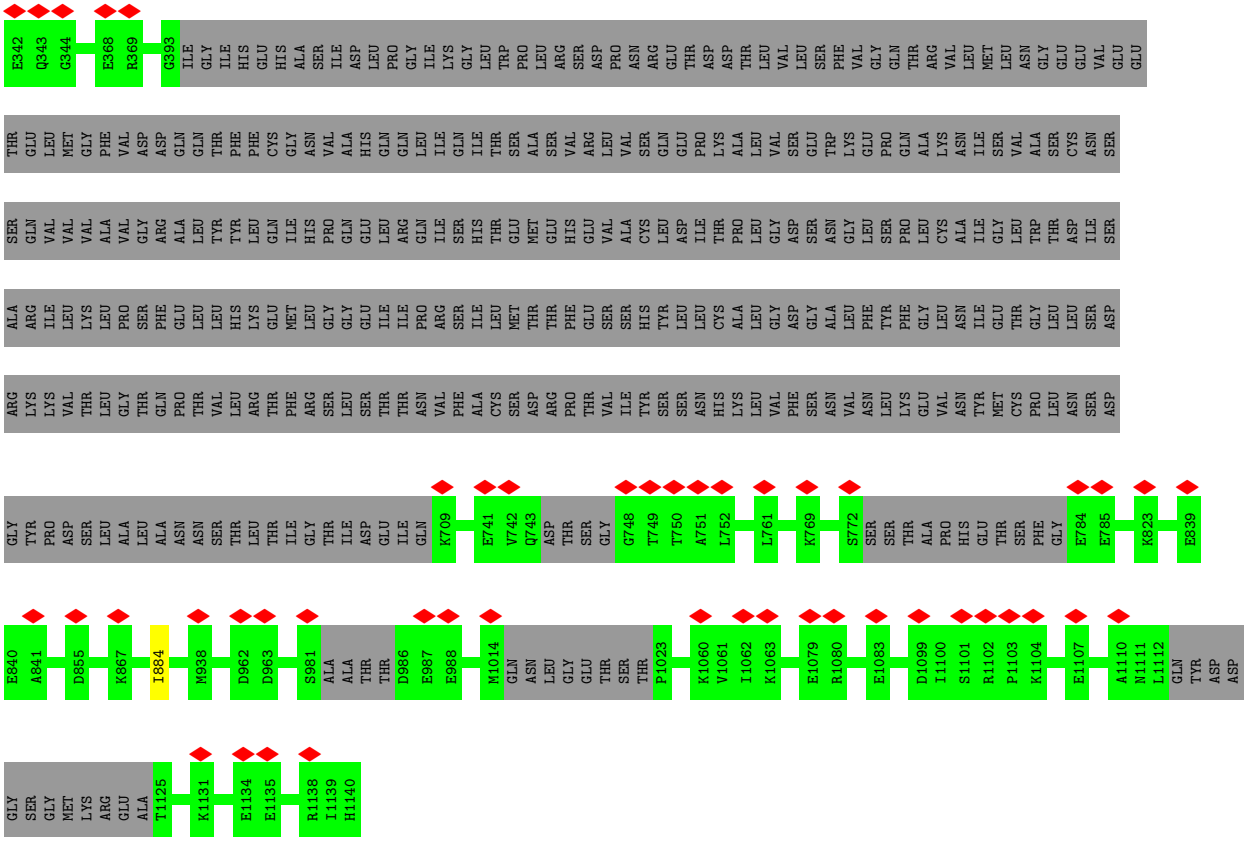
Chain b:





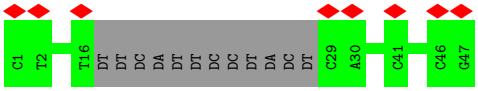
• Molecule 14: DNA damage-binding protein 1





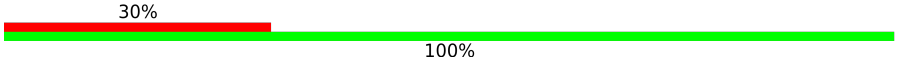
• Molecule 15: NTS

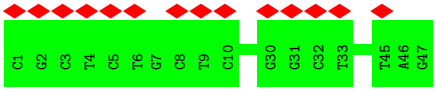
Chain N:



• Molecule 16: TS

Chain T:



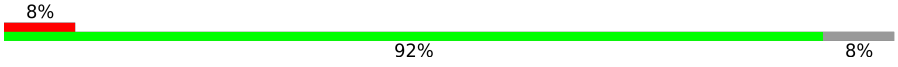


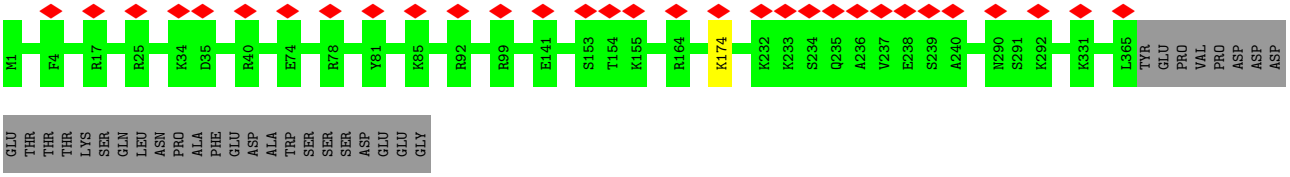
• Molecule 17: RNA

Chain P:

• Molecule 18: DNA excision repair protein ERCC-8

Chain a:




M1
F4
R17
R25
K34
D35
R40
E74
R78
Y81
K85
R92
R99
E141
S153
T154
K155
R164
K174
K232
K233
S234
Q235
A236
V237
E238
S239
A240
N290
S291
K292
K331
L365
TYR
GLU
PRO
VAL
PRO
ASP
ASP
ASP
GLU
THR
THR
THR
LYS
SER
GLN
LEU
ASN
PRO
ALA
PHE
GLU
ASP
ALA
TRP
SER
SER
SER
ASP
GLU
GLU
GLY

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 ($e^-/Å^2$)	41.2	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	0.241	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, BEF, 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	0.30	0/11382	0.53	1/15368 (0.0%)
2	B	0.32	0/9233	0.54	0/12463
3	C	0.34	0/2132	0.56	1/2896 (0.0%)
4	D	0.28	0/1043	0.47	0/1400
5	E	0.29	0/1751	0.53	0/2366
6	F	0.31	0/667	0.49	0/901
7	G	0.27	0/1382	0.56	0/1874
8	H	0.33	0/1207	0.53	0/1628
9	I	0.30	0/972	0.54	0/1316
10	J	0.32	0/542	0.51	0/730
11	K	0.30	0/939	0.49	0/1271
12	L	0.33	0/394	0.59	0/524
13	b	0.36	0/4362	0.60	0/5890
14	d	0.34	0/6271	0.59	0/8470
15	N	0.54	0/817	0.87	0/1258
16	T	0.60	0/1056	0.97	0/1624
17	P	0.50	0/247	0.89	0/384
18	a	0.35	0/2908	0.59	0/3939
All	All	0.34	0/47305	0.58	2/64302 (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
13	b	0	1
14	d	0	1
18	a	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	67	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	483	ARG	CG-CD-NE	5.27	122.87	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
18	a	174	LYS	Peptide
13	b	493	PHE	Peptide
14	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%)	1365 (97%)	37 (3%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
13	b	512/1496 (34%)	477 (93%)	35 (7%)	0	100	100
14	d	765/1143 (67%)	721 (94%)	44 (6%)	0	100	100
18	a	363/396 (92%)	343 (94%)	20 (6%)	0	100	100
All	All	5484/7622 (72%)	5263 (96%)	221 (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
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
13	b	466/1299 (36%)	465 (100%)	1 (0%)	93	98
14	d	686/1001 (68%)	686 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	a	320/348 (92%)	320 (100%)	0	100 100
All	All	4910/6718 (73%)	4904 (100%)	6 (0%)	93 98

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1080	ARG
5	E	166	ARG
13	b	729	LYS
1	A	1101	GLN
1	A	241	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
13	b	616	HIS
18	a	229	HIS

5.3.3 RNA (i)

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

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
17	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 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	ADP	b	1501	20	24,29,29	0.87	0	29,45,45	1.40	4 (13%)
22	BEF	b	1502	-	0,3,3	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	ADP	b	1501	20	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	1501	ADP	N3-C2-N1	-3.88	122.61	128.68
21	b	1501	ADP	PA-O3A-PB	-2.46	124.40	132.83
21	b	1501	ADP	C3'-C2'-C1'	2.35	104.52	100.98
21	b	1501	ADP	N6-C6-N1	2.05	122.83	118.57

There are no chirality outliers.

All (2) torsion outliers are listed below:

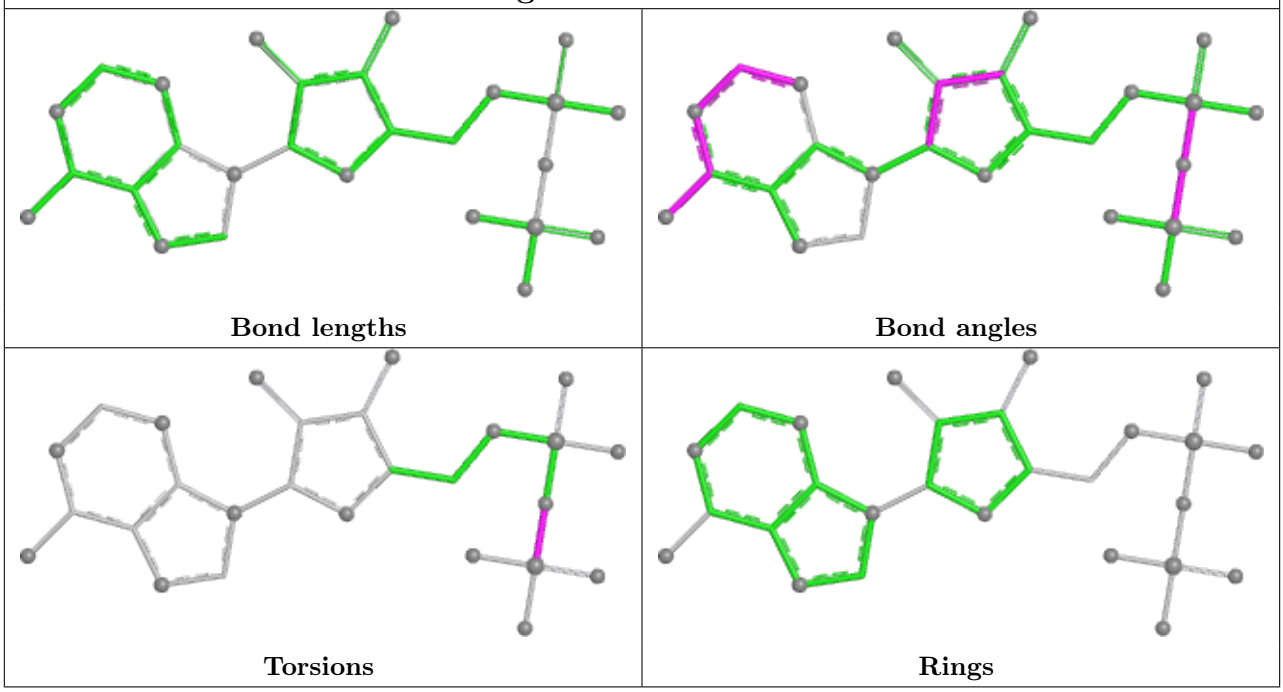
Mol	Chain	Res	Type	Atoms
21	b	1501	ADP	PA-O3A-PB-O1B
21	b	1501	ADP	PA-O3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand ADP b 1501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

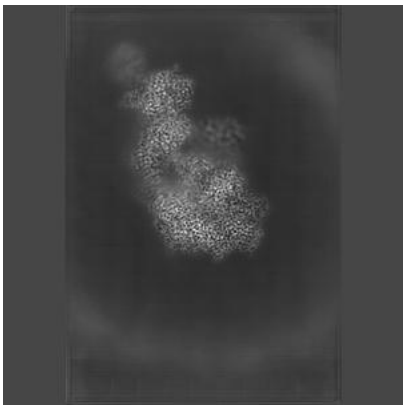
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13009. These allow visual inspection of the internal detail of the map and identification of artifacts.

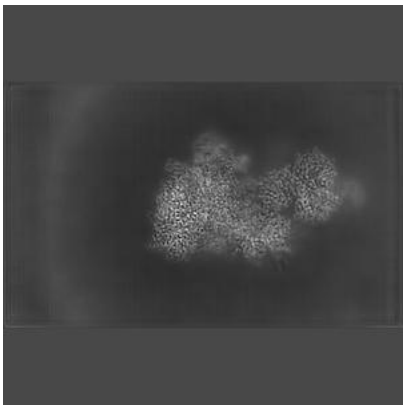
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

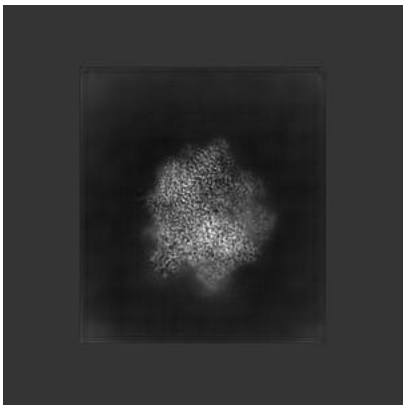
6.1.1 Primary map



X

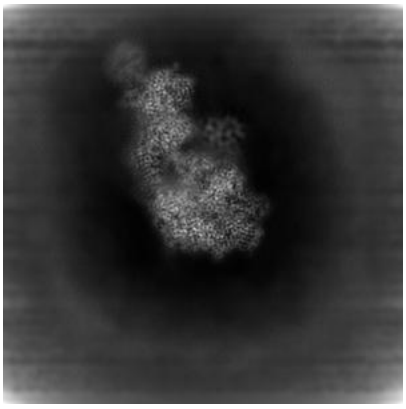


Y

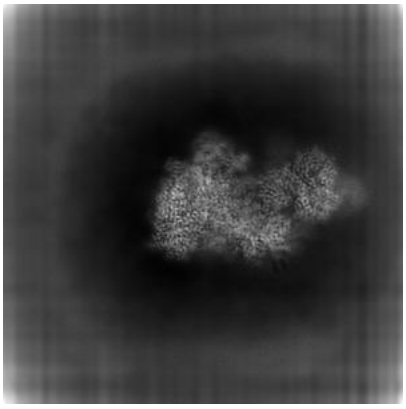


Z

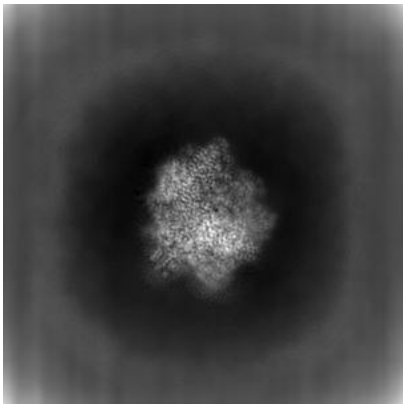
6.1.2 Raw map



X



Y

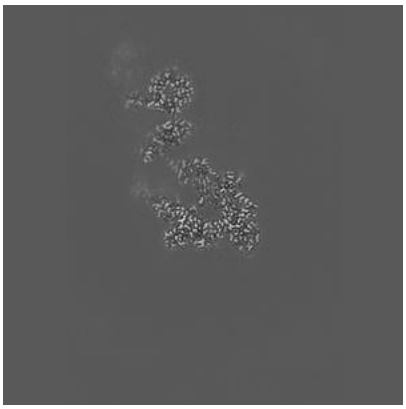


Z

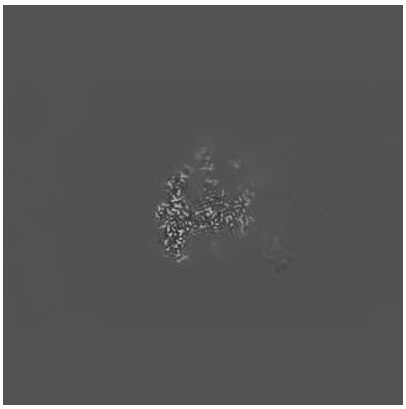
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



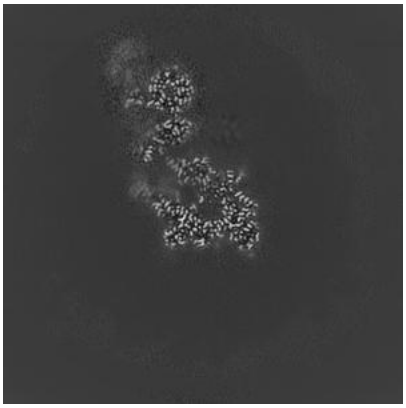
X Index: 200



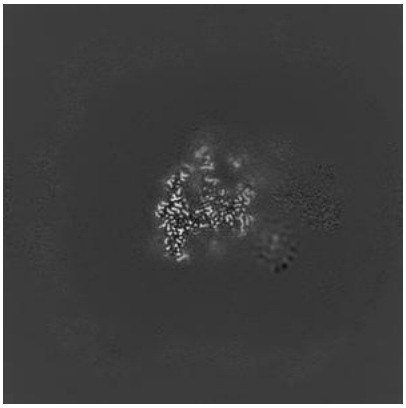
Y Index: 200

Z Index: 200

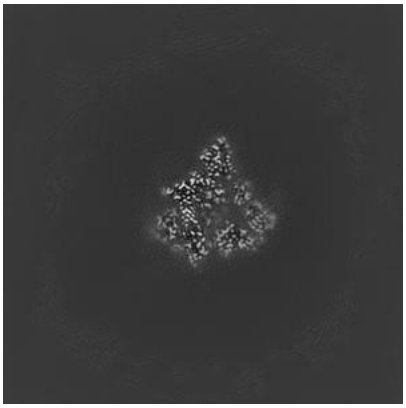
6.2.2 Raw map



X Index: 200



Y Index: 200

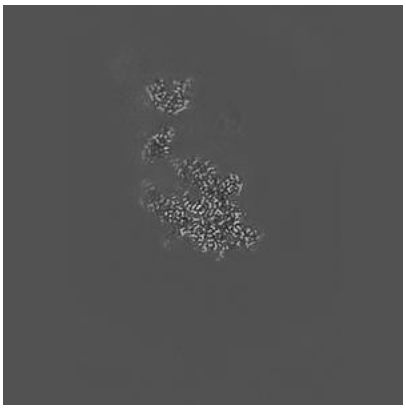


Z Index: 200

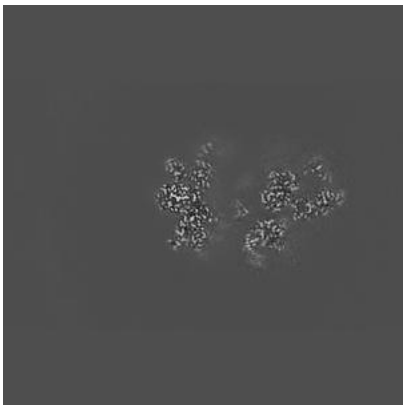
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

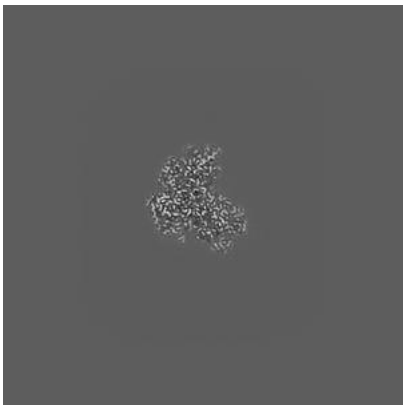
6.3.1 Primary map



X Index: 191

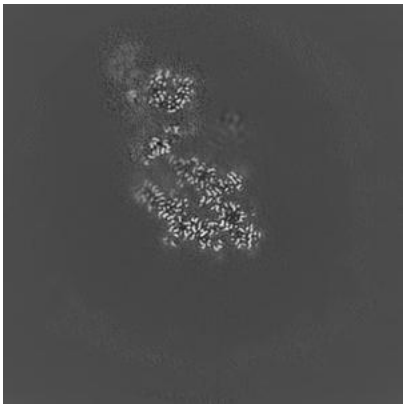


Y Index: 172

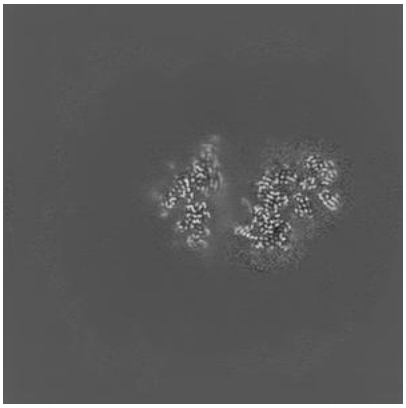


Z Index: 174

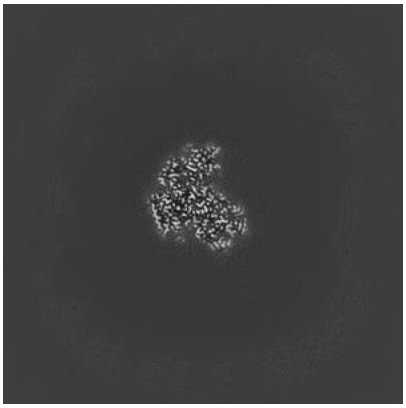
6.3.2 Raw map



X Index: 195



Y Index: 164

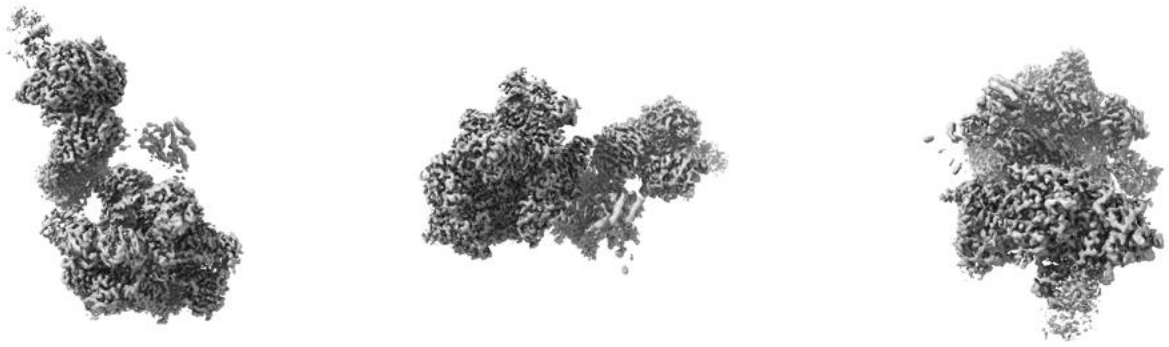


Z Index: 173

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 0.02. 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.

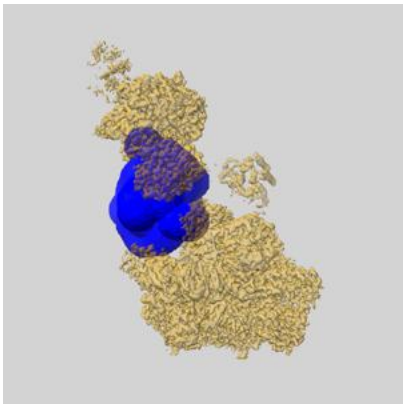
6.5 Mask visualisation

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

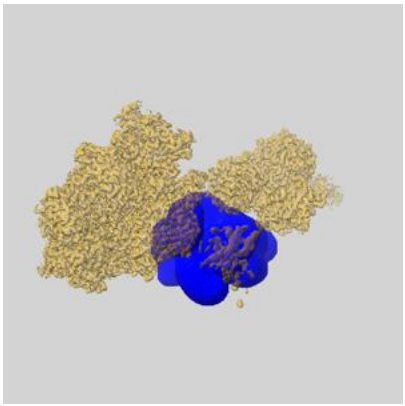
A mask typically either:

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

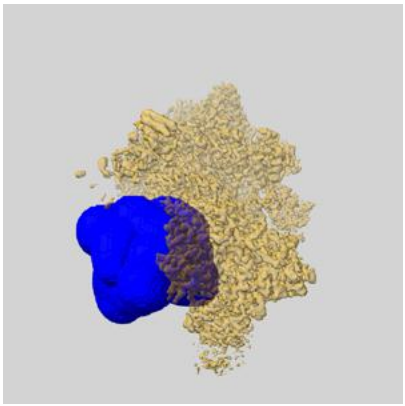
6.5.1 emd_13009_msk_4.map



X

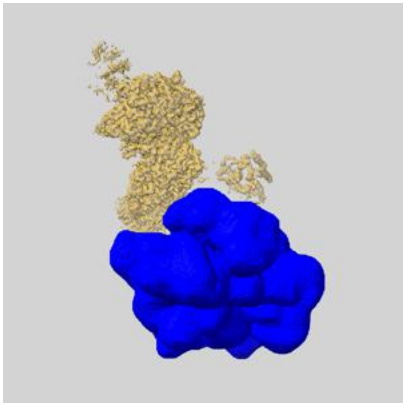


Y

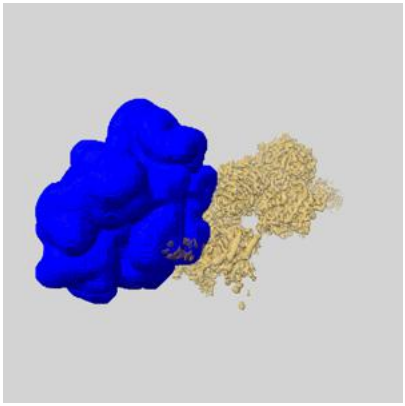


Z

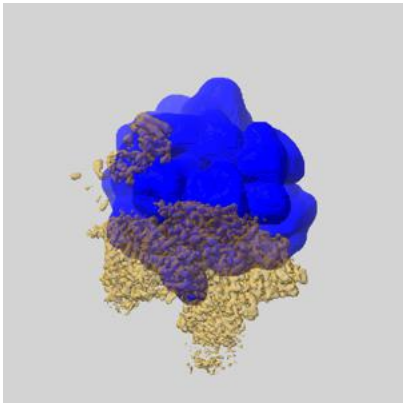
6.5.2 emd_13009_msk_3.map



X

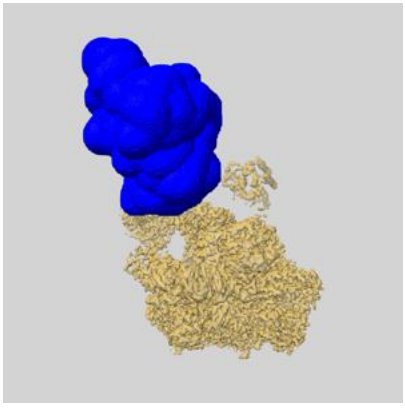


Y

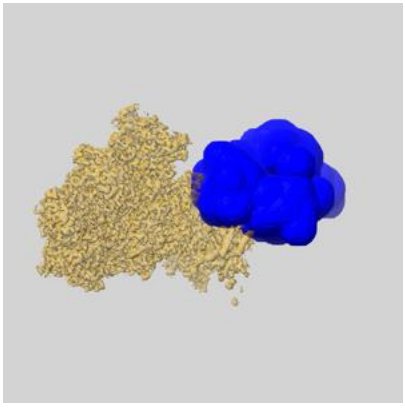


Z

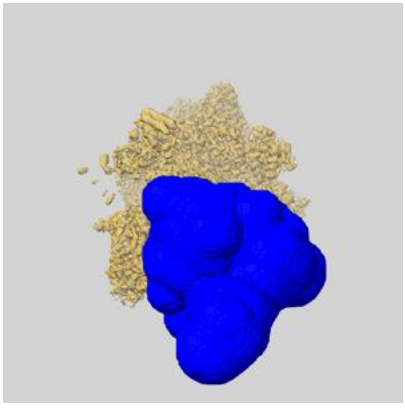
6.5.3 emd_13009_msk_2.map



X

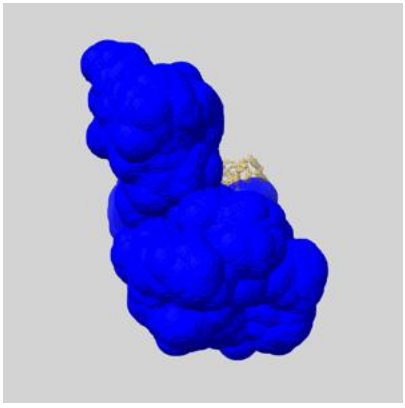


Y



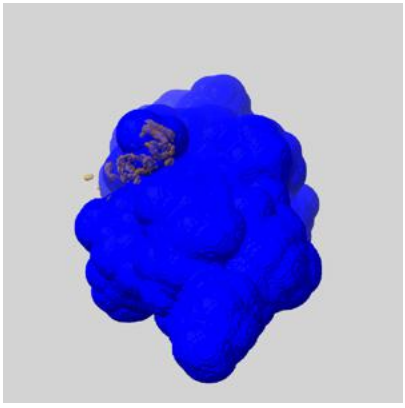
Z

6.5.4 emd_13009_msk_1.map



X

Y

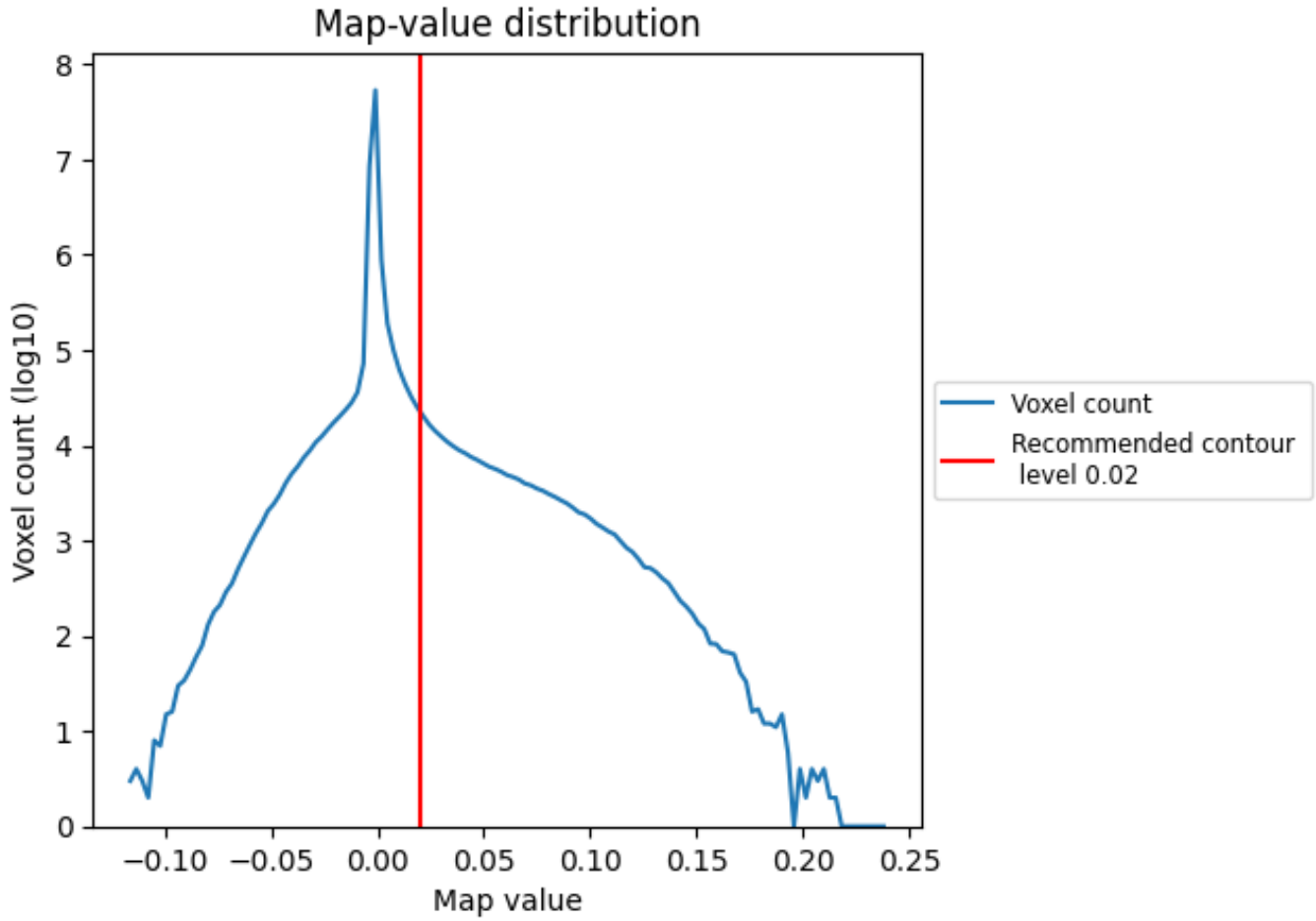


Z

7 Map analysis

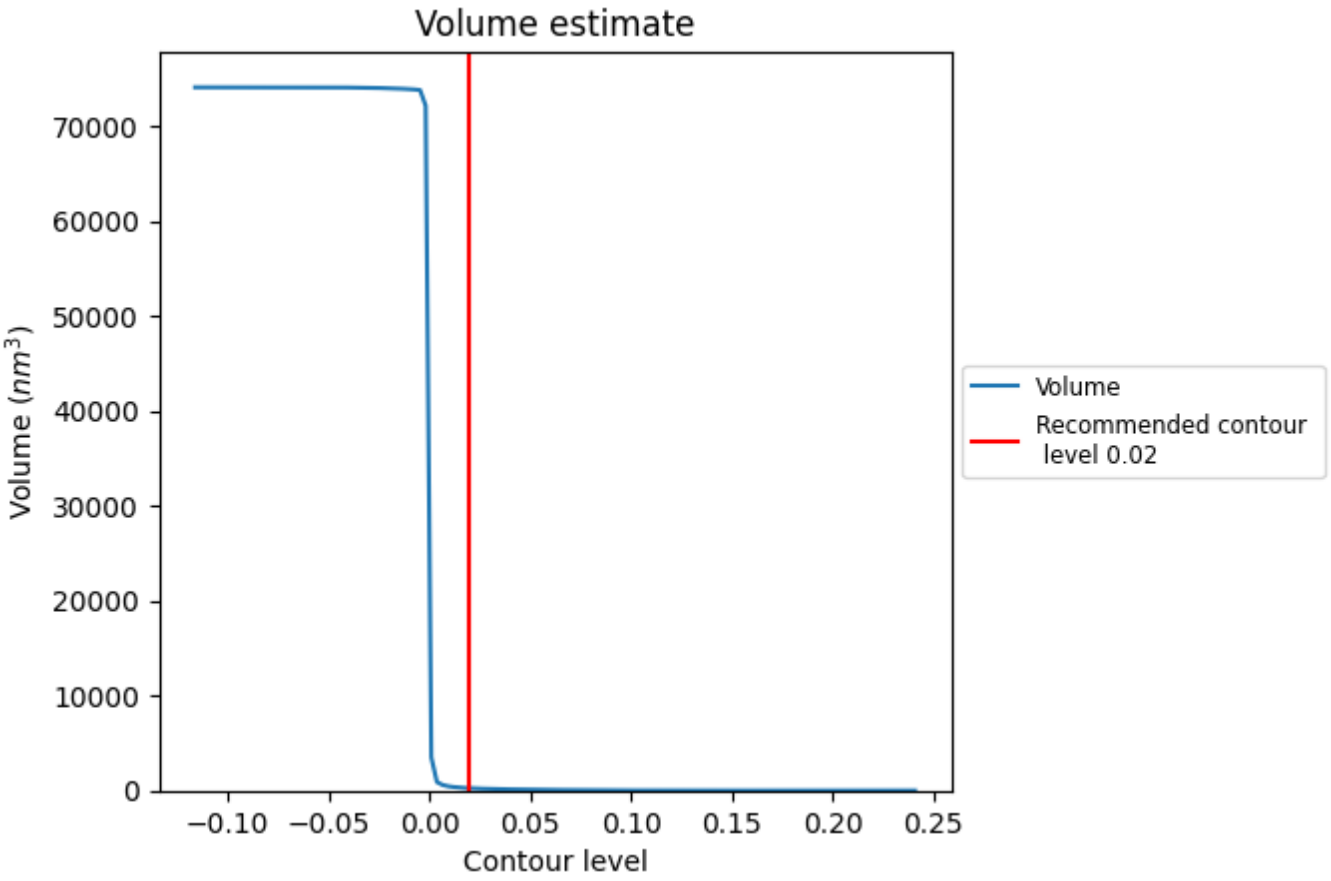
This section contains the results of statistical analysis of the map.

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.

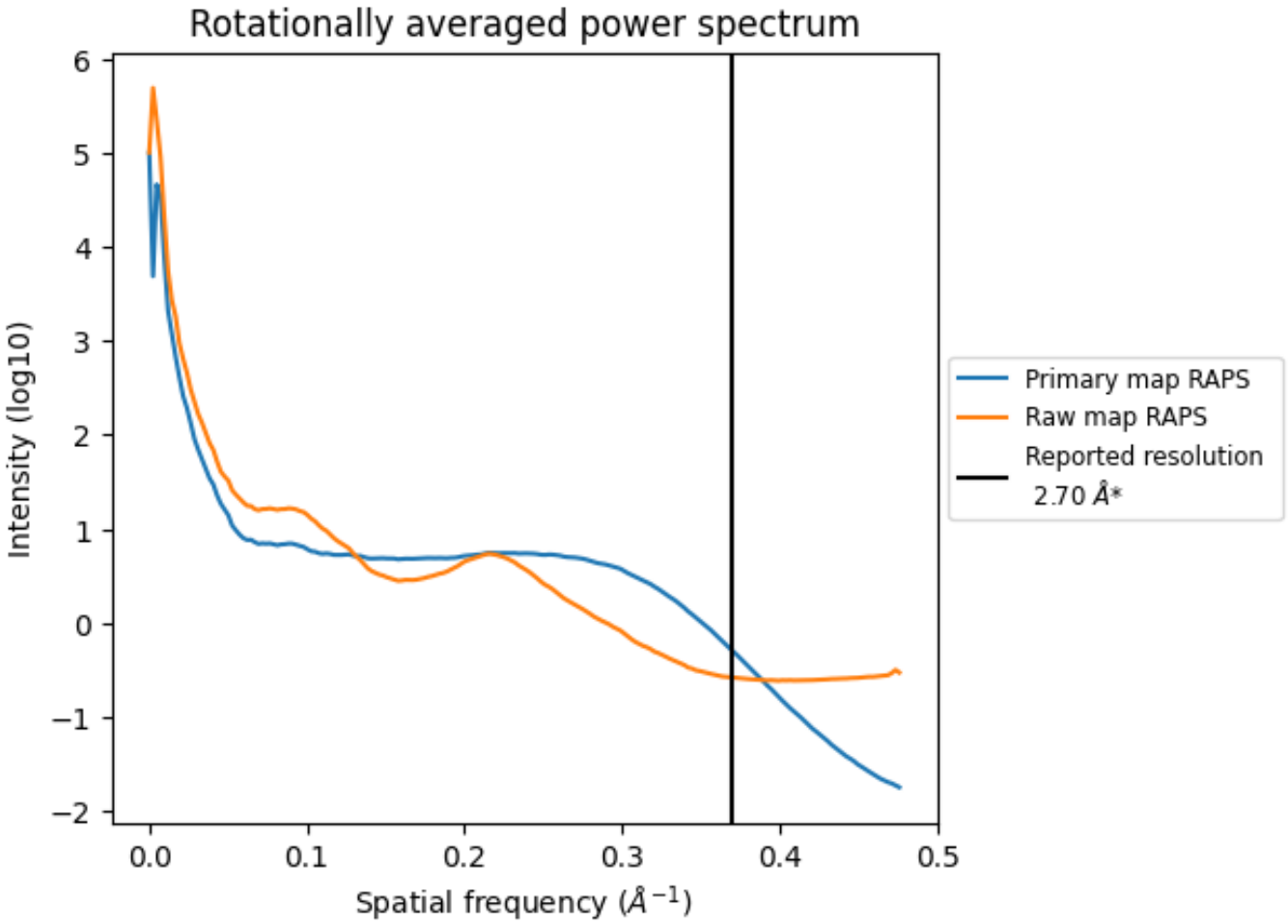
7.2 Volume estimate (i)



The volume at the recommended contour level is 247 nm^3; this corresponds to an approximate mass of 223 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)

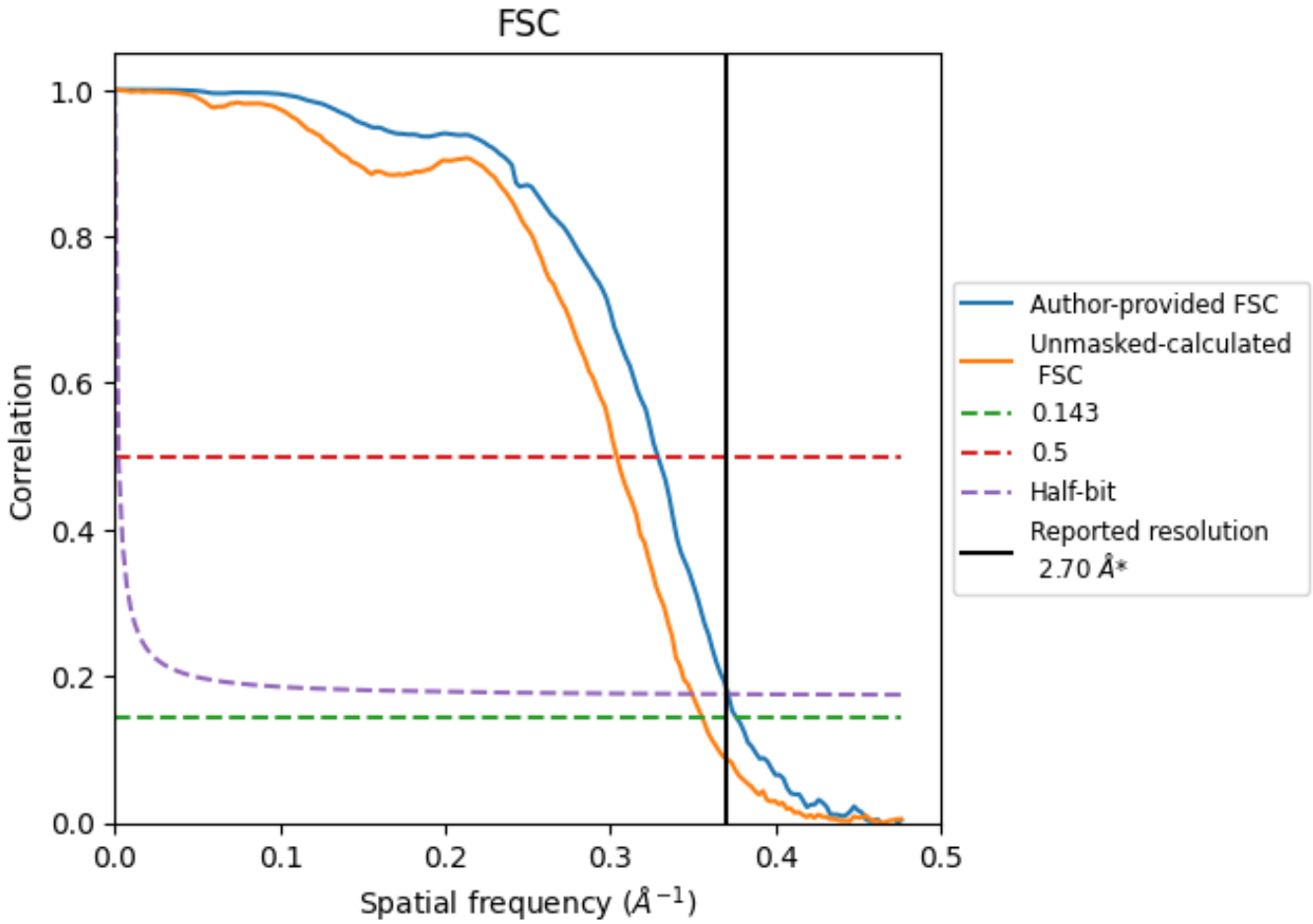


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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 0.370 Å^{-1}

8.2 Resolution estimates (i)

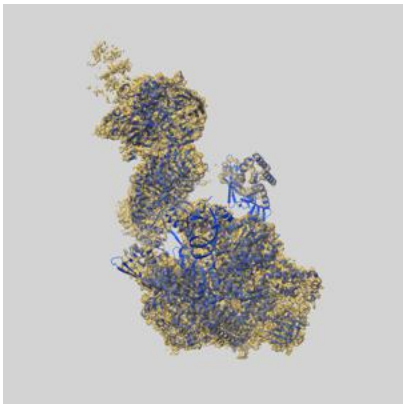
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.66	3.04	2.69
Unmasked-calculated*	2.81	3.29	2.86

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

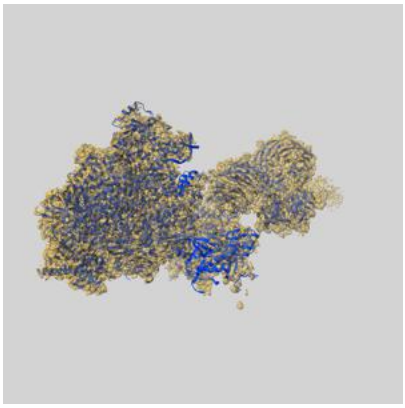
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13009 and PDB model 7OOB. Per-residue inclusion information can be found in section 3 on page 9.

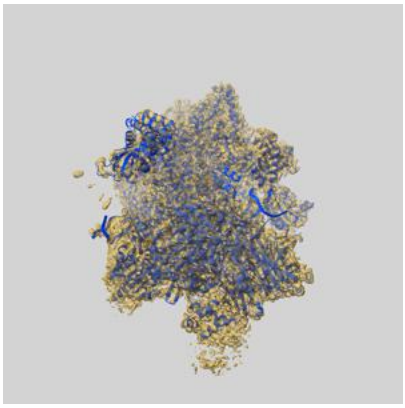
9.1 Map-model overlay



X



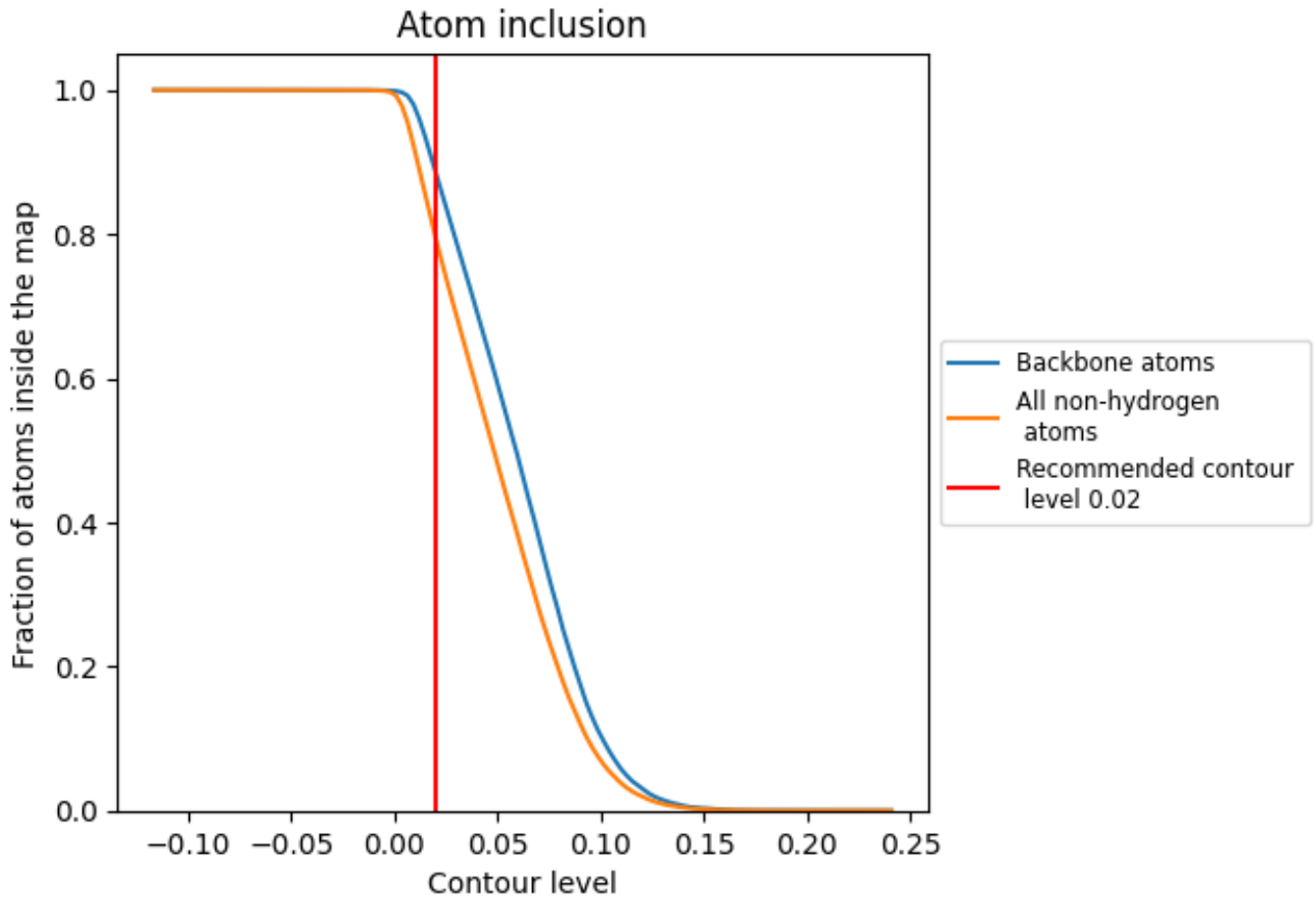
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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, 89% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.