wwPDB EM Validation Summary Report (i)

Aug 26, 2026 – 10:21 am BST

PDB ID	:	7OOB / pdb_00007oob
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

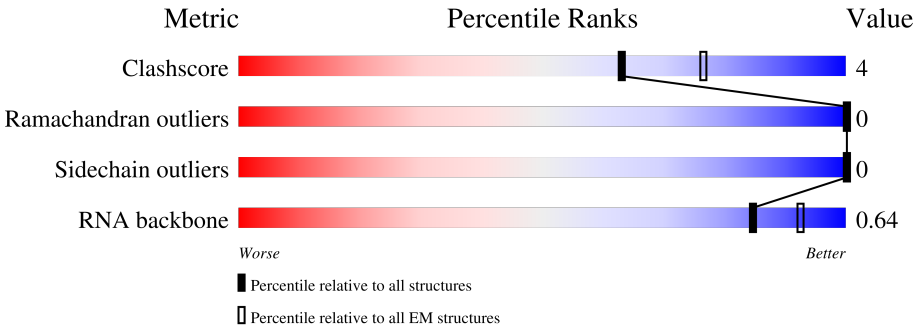
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

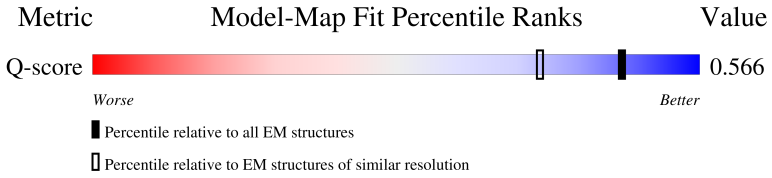
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	8% 65% 6% 28%
2	B	1174	11% 89% 7% .
3	C	275	. 87% 8% 5%

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Mol	Chain	Length	Quality of chain
4	D	142	66% 80% 8% 11%
5	E	210	6% 92% 7%
6	F	127	6% 59% 6% 35%
7	G	172	74% 92% 8%
8	H	150	87% 11%
9	I	125	20% 85% 9% 6%
10	J	67	93% 7%
11	K	117	91% 8%
12	L	58	10% 74% 5% 21%
13	b	1496	30% 5% 65%
14	d	1143	62% 6% 32%
15	N	47	17% 23% 51% 26%
16	T	47	30% 19% 81%
17	P	10	80% 20%
18	a	396	85% 8% 8%

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		

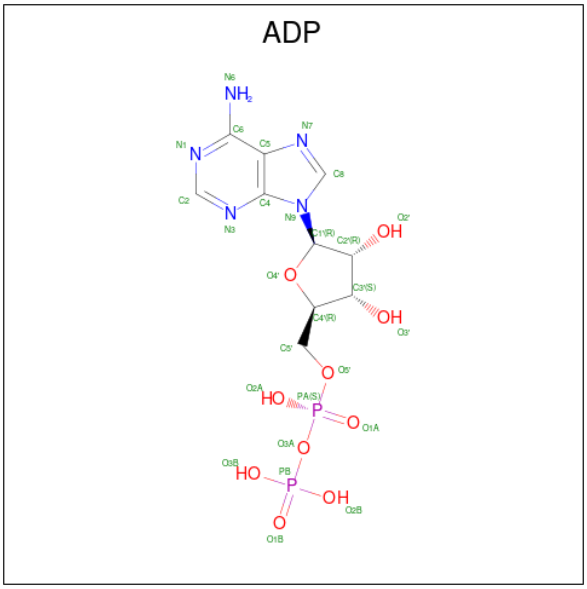
- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 (CCD ID: MG) (formula: Mg).

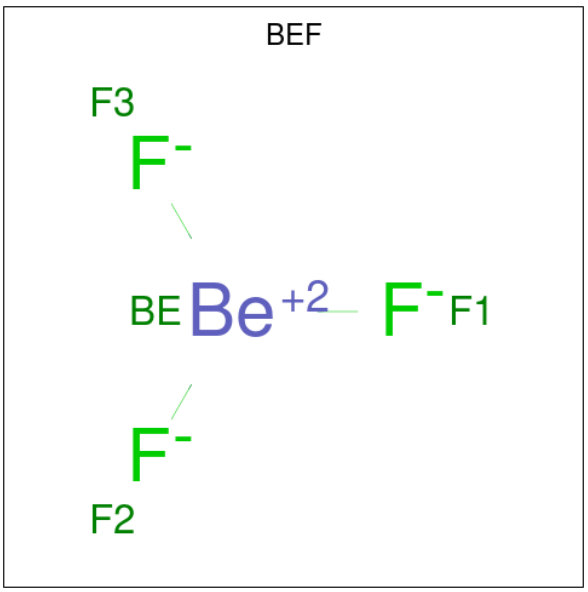
Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total Mg 1 1	0
20	b	1	Total Mg 1 1	0

- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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 (CCD ID: BEF) (formula: BeF_3).



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

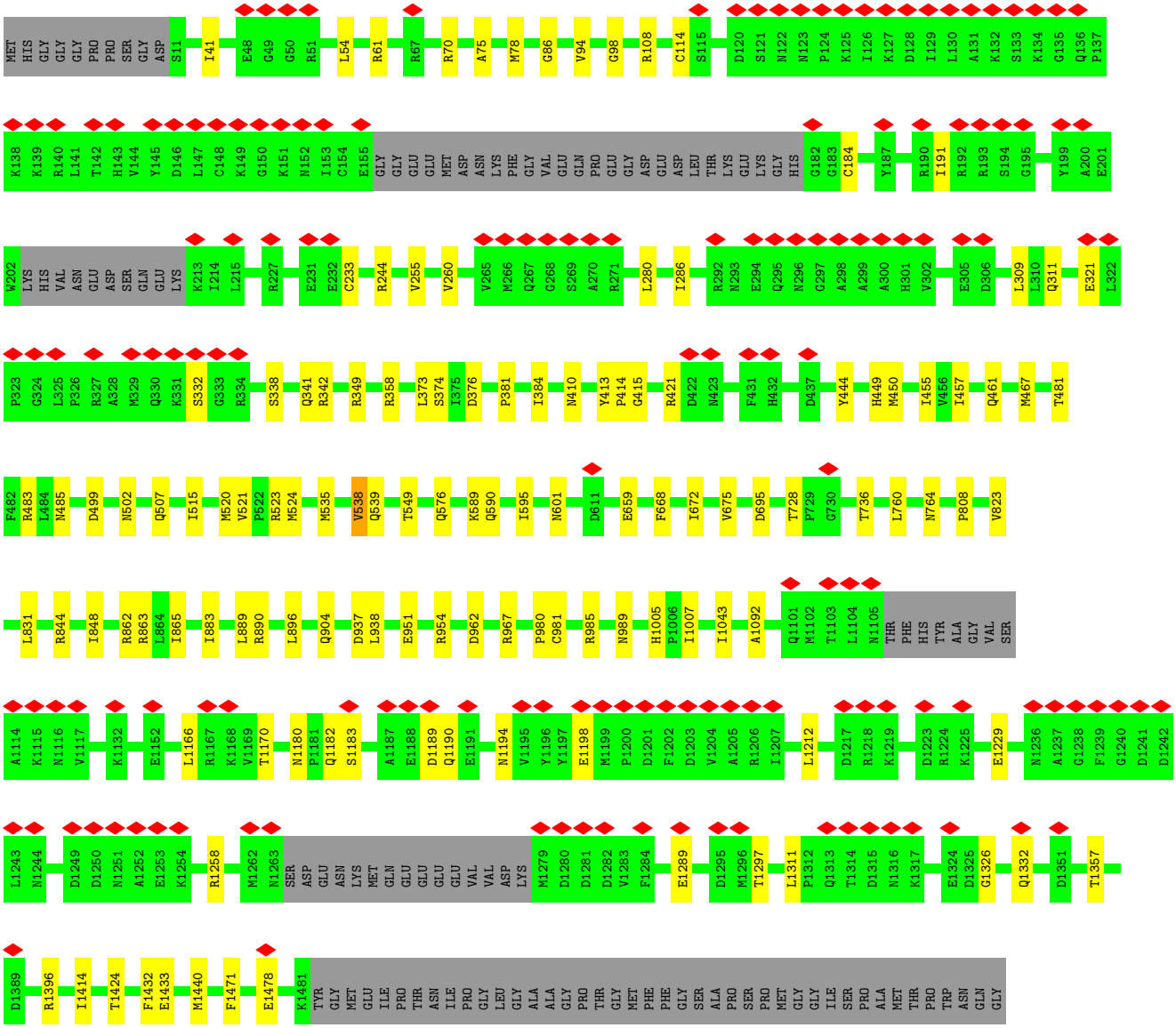
3 Residue-property plots (i)

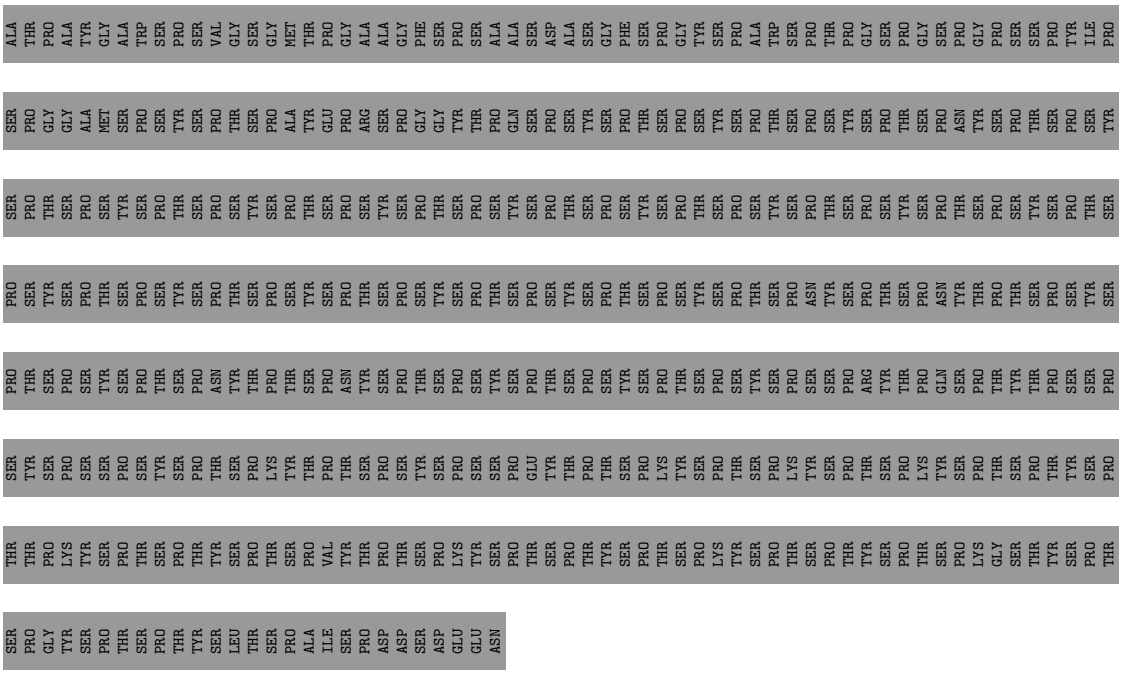
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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:



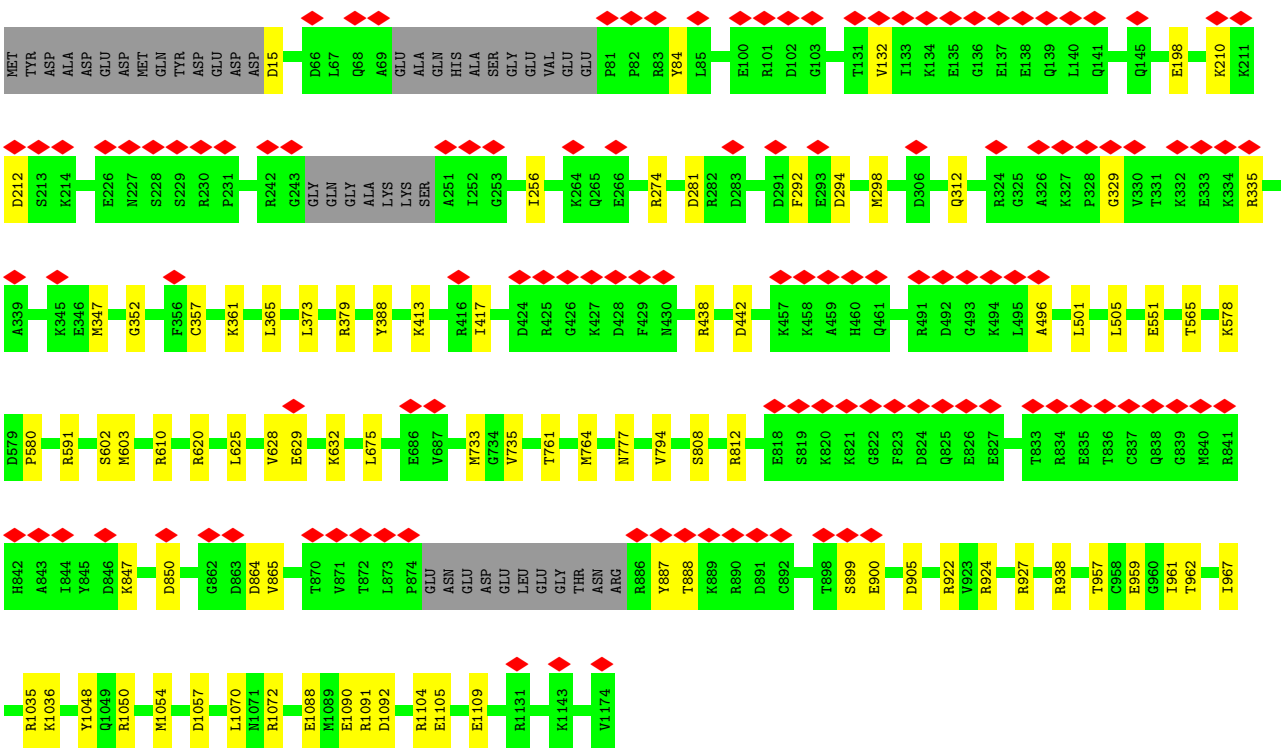




• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:

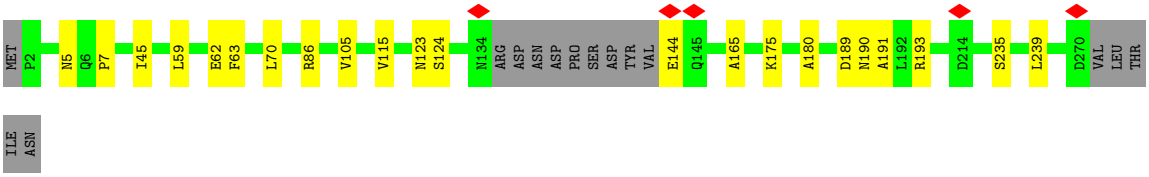




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:

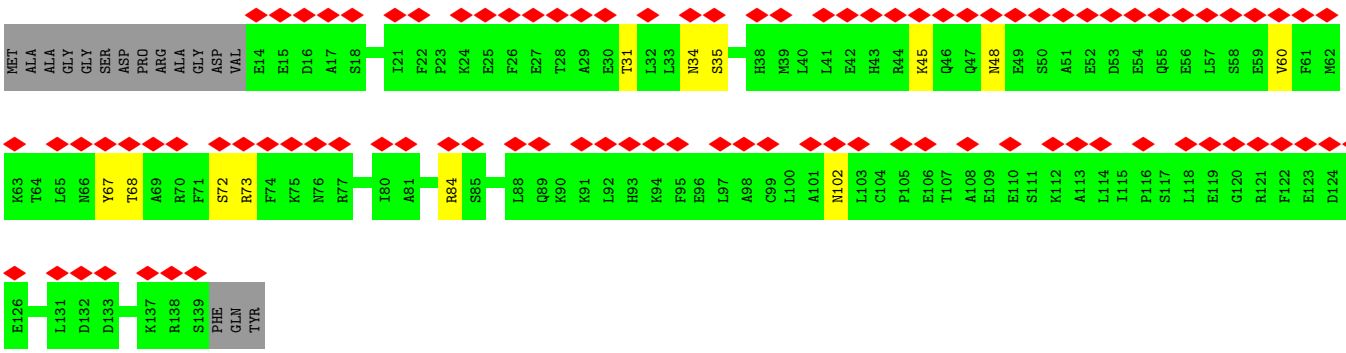




• Molecule 4: RPOL4c domain-containing protein

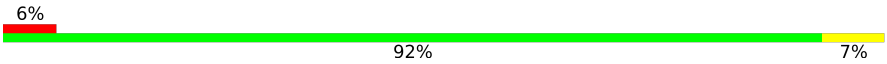
Chain D:





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

Chain E:

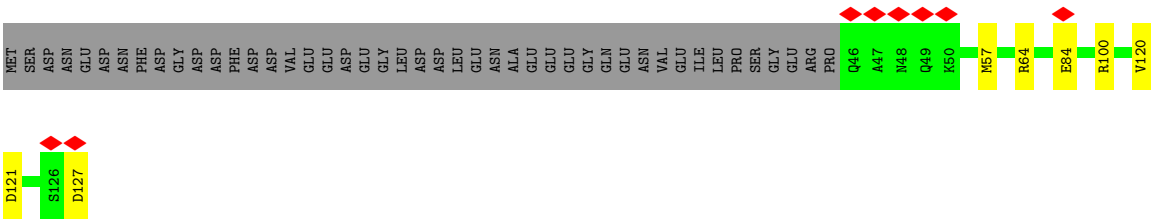




• Molecule 6: DNA-directed RNA polymerase II subunit F

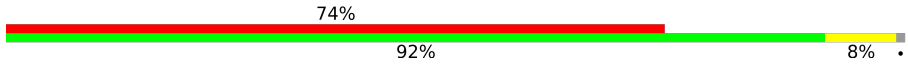
Chain F:



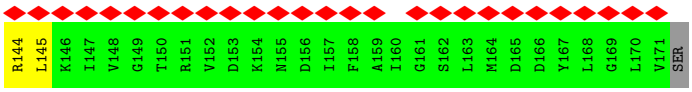


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

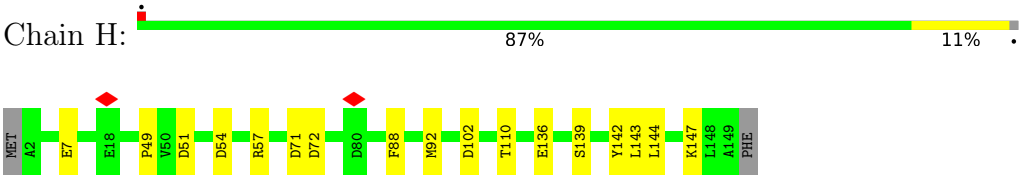
Chain G:



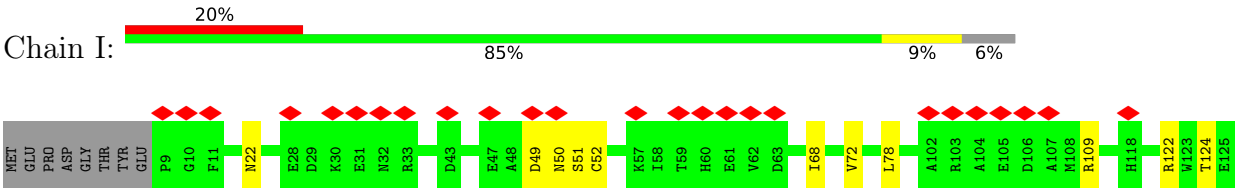




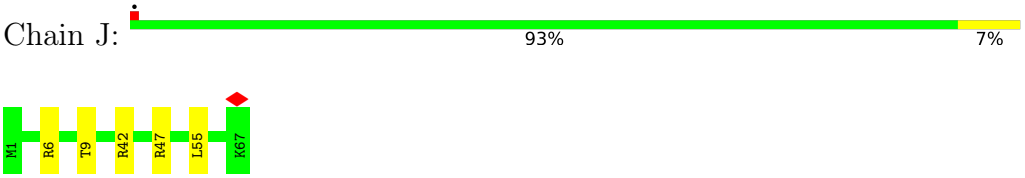
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



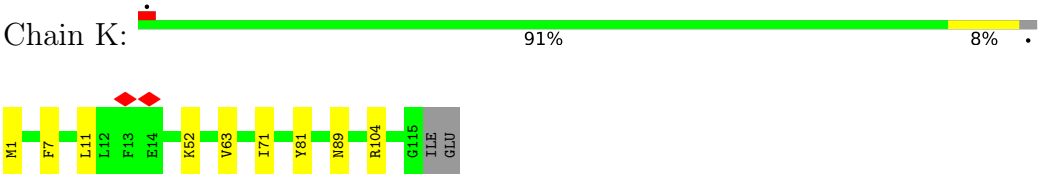
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



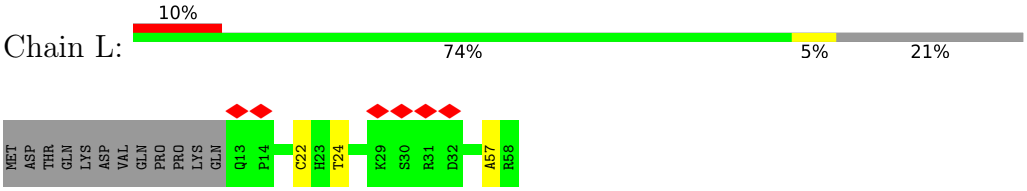
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



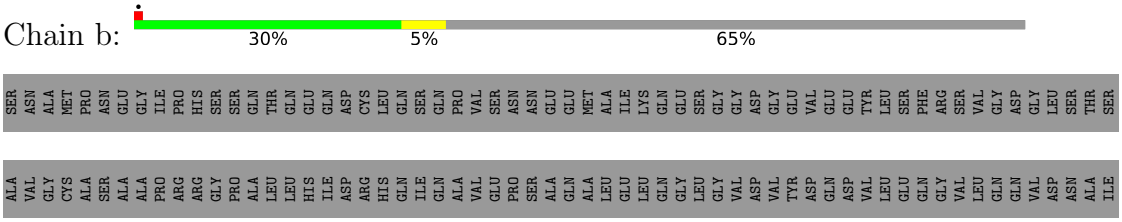
• Molecule 11: RNA_pol_L_2 domain-containing protein

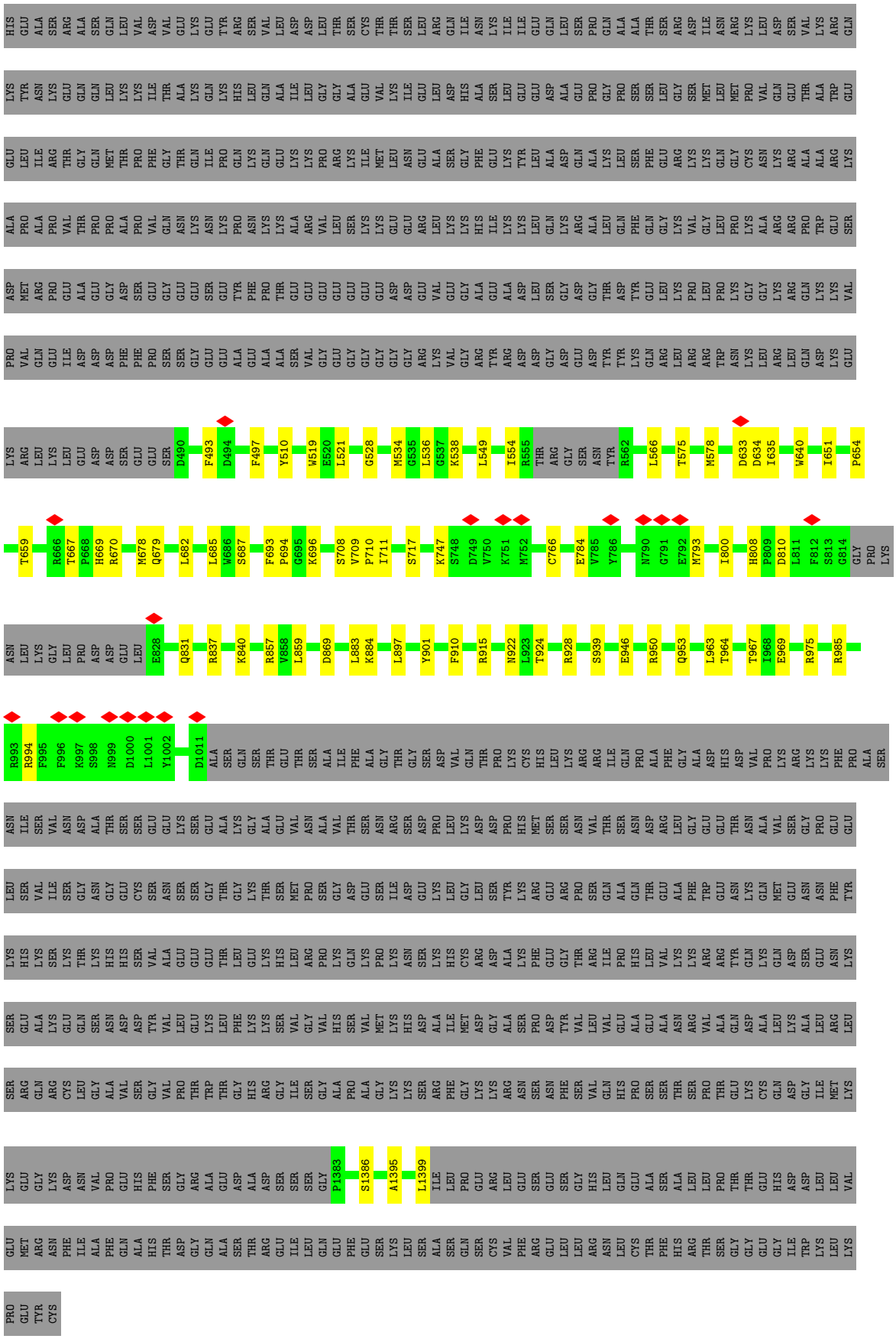


• Molecule 12: RNA polymerase II subunit K



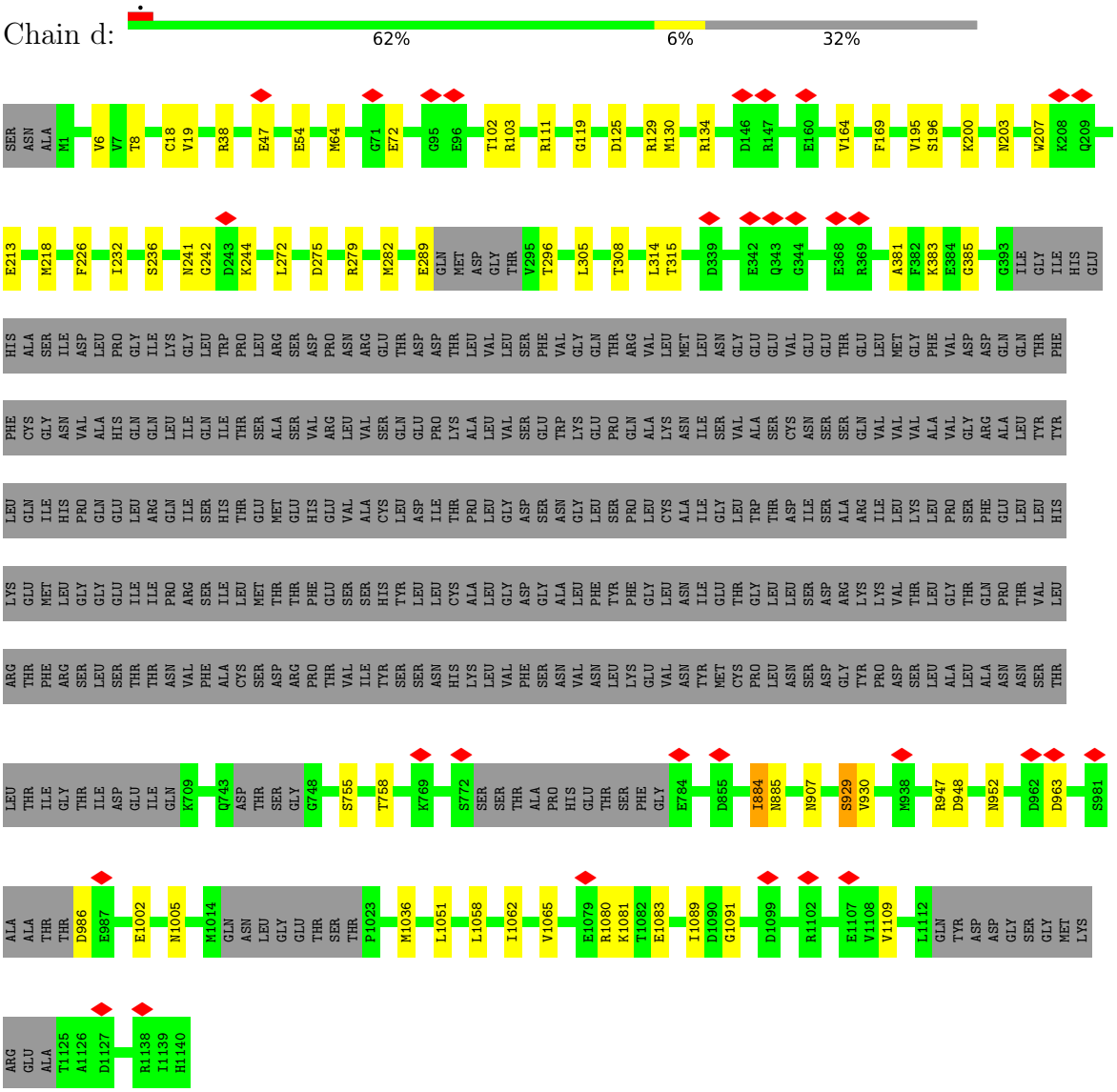
• Molecule 13: DNA excision repair protein ERCC-6




HIS GLU ALA SER ARG ALA SER GLN LEU VAL ASP VAL GLU LYS GLU TYR ARG SER VAL LEU ASP ASP LEU THR SER CYS THR THR SER LEU ARG ASP ILE ASN ARG GLN ILE GLU GLN LEU SER PRO GLN ALA ALA THR SER ARG ASP ILE ASN ARG LYS LEU ASP SER VAL LYS ARG GLN
LYS TYR ASN LYS GLU GLN GLN LEU LYS LYS ILE THR ALA LYS GLN LYS HIS LEU GLN ALA ILE LEU LEU GLY GLY ALA GLU VAL LYS ILE GLU LEU GLU ASP ALA GLU PRO GLY PRO SER SER LEU GLY SER MET LEU MET PRO VAL GLN GLU THR ALA TRP GLU
GLU LEU ILE ARG THR GLY GLN MET THR PRO PHE GLY THR GLN ILE PRO GLN LYS GLN LEU GLN LYS HIS LEU GLN ALA GLU LYS LYS PRO ARG LYS ILE MET LEU ASN GLU GLU ALA SER GLY PHE GLU LYS TYR LEU ALA ASP GLN ALA LYS LEU GLN GLY PHE GLU ARG LYS LYS GLN ASN LYS ARG ALA ALA ARG LYS
ALA PRO ALA PRO VAL THR PRO PRO ALA PRO VAL GLN ASN LYS ASN LYS LYS PRO ASN LYS LYS ALA ARG VAL LEU SER LYS LYS GLU GLN ARG LEU LYS LYS HIS ILE LYS LYS LEU GLN LEU GLY GLY LYS VAL GLY LEU PRO LYS GLY GLY LYS ALA ARG ARG PRO TRP GLU SER
ASP MET ARG PRO GLU ALA GLU GLY ASP SER GLU GLY GLU GLU SER GLU TYR PHE PRO THR GLU GLU GLU GLU GLU GLU GLU GLU GLY ASP GLU VAL GLY ALA ASP LEU SER LEU GLY ASP GLU ASP GLY THR ASP TYR LEU GLU LEU LYS PRO LEU PRO LYS GLY GLY LYS ASP ARG GLN LYS VAL
PRO VAL GLN GLU ILE ASP ASP ASP PHE PHE PRO SER SER GLY GLU GLU ALA ALA GLU ASP GLY GLY GLY GLY ARG LYS VAL GLY ARG TYR ARG ASP ASP GLY GLY ASP GLU ASP TYR TYR LYS GLN ARG LEU ARG ARG TRP ASN LYS LEU ARG LEU GLN ASP LYS LYS GLU
LYS ARG LEU LYS LEU GLU D490 F493 D494 F497 Y510 W519 E520 L521 G528 M534 Q535 L536 G537 K538 L549 I554 R555 THR ARG GLY SER ASN TYR R562 L566 T575 M578 D633 D634 I635 W640 I651 P654
T659 R666 T667 P668 H669 R670 M678 Q679 L682 L685 W686 S687 F693 P694 G695 K696 S708 V709 P710 I711 S717 K747 S748 D749 V750 K751 M752 C766 E784 V785 Y786 N790 G791 E792 M793 I800 H808 P809 D810 L811 F812 S813 G814 GLY PRO LYS
ASN LEU LYS GLY LEU PRO ASP ASP GLU LEU E828 Q831 R837 K840 R857 V858 L859 D869 L883 K884 L897 Y901 F910 R915 N922 L923 T924 R928 S939 E946 R950 Q953 L963 T964 T967 I968 E969 R975 R985
R993 R994 F995 F996 K997 S998 N999 D1000 L1001 Y1002 D1011 ALA SER GLN SER THR GLU THR SER ALA ALA ILE PHE ALA GLY THR GLY SER ASP VAL GLN THR PRO LYS CYS HIS LEU LYS ARG ARG ILE GLN PRO ALA PHE GLY ALA ASP HIS ASP VAL PRO LYS ARG LYS LYS PHE PRO ALA SER
ASN ILE SER VAL ASN ASP ALA THR SER SER GLU GLU GLU LYS SER GLU ALA LYS GLY ALA GLU VAL ASN ASP ALA VAL THR SER ASN ARG SER ASP PRO LEU LYS ASP PRO HIS MET SER SER ASN VAL THR SER ASN ASP ARG LEU GLY GLU GLU THR ASN ALA VAL SER GLY PRO GLU GLU
LEU SER VAL ILE SER GLY CYS SER ASN GLY GLU CYS SER ASN GLY GLY LYS THR SER MET PRO SER GLY THR GLY LYS LEU GLY LEU SER TYR LYS ARG GLU ARG PRO SER GLN ALA GLN THR GLU GLU ALA PHE TRP GLU ASN LYS GLN MET GLU ASN ASN PHE TYR
LYS HIS LYS SER LYS THR LYS HIS HIS SER VAL ALA GLU GLU GLU THR LEU GLU LYS HIS LEU ARG PRO LYS ASN SER LYS HIS CYS ARG ASP ALA LYS PHE GLU GLY THR ARG ILE PRO HIS LEU VAL LYS LYS ARG ARG TYR GLN LYS GLN ASP SER GLU ASN LYS
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SER SER ARG GLN ARG CYS LEU GLY ALA VAL SER GLY VAL PRO THR TRP THR GLY HIS ARG GLY ILE SER GLY ALA PRO ALA GLY LYS LYS SER ARG PHE GLY LYS LYS ARG ASN SER ASN PHE SER VAL GLN HIS PRO SER SER THR SER PRO THR GLU LYS CYS GLN ASP GLY ILE MET LYS
LYS GLU GLY LYS ASP PHE GLU HIS PHE SER GLY ARG ALA GLU ASP ALA ASP SER SER SER GLY P1383 S1386 A1395 L1399 ILE LEU PRO GLU ARG LEU GLU SER GLU SER GLY HIS LEU GLN GLU ALA SER ALA LEU LEU LEU PRO THR THR GLU HIS ASP ASP LEU LEU VAL
GLU MET ARG ASN PHE ILE ALA PHE GLN ALA HIS THR ASP GLY GLN ALA SER THR ARG GLU ILE LEU GLU GLU SER LYS LEU SER ALA SER GLN SER CYS VAL PHE ARG GLU LEU LEU ARG ASN LEU CYS THR PHE HIS ARG THR SER GLY GLY GLU GLY ILE TRP LYS LEU LEU LYS
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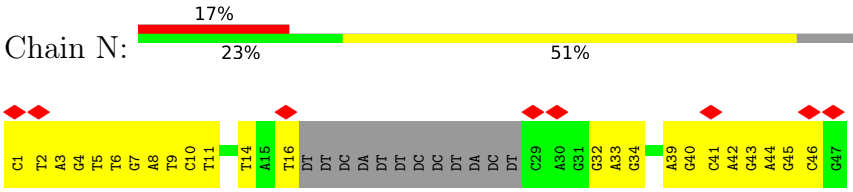
• Molecule 14: DNA damage-binding protein 1

Chain d:



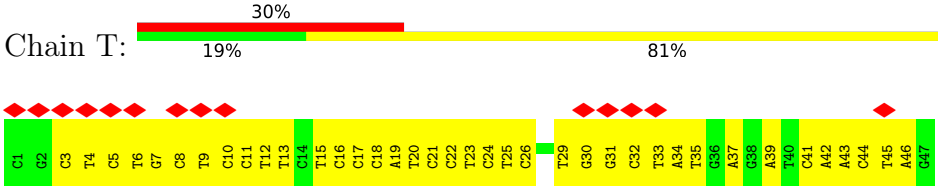
• Molecule 15: NTS

Chain N:



• Molecule 16: TS

Chain T:



• Molecule 17: RNA

Chain P:



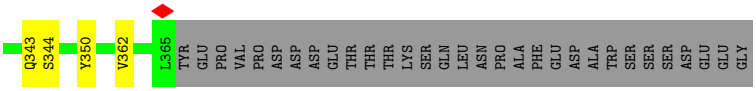


• Molecule 18: DNA excision repair protein ERCC-8

Chain a:







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: BEF, ADP, 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	0.23	0/11382	0.41	0/15368
2	B	0.23	0/9233	0.39	0/12463
3	C	0.26	0/2132	0.41	0/2896
4	D	0.18	0/1043	0.32	0/1400
5	E	0.20	0/1751	0.35	0/2366
6	F	0.22	0/667	0.35	0/901
7	G	0.19	0/1382	0.39	0/1874
8	H	0.22	0/1207	0.37	0/1628
9	I	0.18	0/972	0.40	0/1316
10	J	0.23	0/542	0.37	0/730
11	K	0.21	0/939	0.34	0/1271
12	L	0.23	0/394	0.42	0/524
13	b	0.28	0/4362	0.49	0/5890
14	d	0.26	0/6271	0.46	1/8470 (0.0%)
15	N	0.20	0/817	0.34	0/1258
16	T	0.25	0/1056	0.44	0/1624
17	P	0.24	0/247	0.31	0/384
18	a	0.26	0/2908	0.46	0/3939
All	All	0.24	0/47305	0.41	1/64302 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	d	929	SER	N-CA-C	5.22	121.91	110.80

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)

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	11179	11315	11313	87	0
2	B	9052	9088	9087	57	0
3	C	2089	2031	2031	15	0
4	D	1030	1016	1016	9	0
5	E	1720	1737	1737	11	0
6	F	657	684	684	5	0
7	G	1351	1358	1358	10	0
8	H	1186	1147	1147	9	0
9	I	949	879	879	8	0
10	J	533	553	553	5	0
11	K	920	942	942	7	0
12	L	388	393	393	2	0
13	b	4259	4302	4302	46	0
14	d	6164	6153	6165	43	0
15	N	727	0	394	30	0
16	T	947	0	532	65	0
17	P	220	109	109	1	0
18	a	2849	2777	2778	18	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	C	1	0	0	0	0
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
20	A	1	0	0	0	0
20	b	1	0	0	0	0
21	b	27	11	12	2	0
22	b	4	0	0	1	0
All	All	46261	44495	45432	387	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 4.

The worst 5 of 387 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)
1:A:114:CYS:SG	1:A:184:CYS:HB3	1.83	1.17
16:T:12:DT:H2"	16:T:13:DT:H5"	1.48	0.92
13:b:964:THR:HG1	13:b:967:THR:HG1	1.16	0.89
16:T:8:DC:H2'	16:T:9:DT:H71	1.56	0.87
1:A:338:SER:OG	1:A:341:GLN:OE1	1.92	0.87

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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	1242 (100%)	0	100	100
2	B	992/1027 (97%)	992 (100%)	0	100	100
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%)	191 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	466 (100%)	0	100	100
14	d	686/1001 (68%)	686 (100%)	0	100	100
18	a	320/348 (92%)	320 (100%)	0	100	100
All	All	4910/6718 (73%)	4910 (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 22 such sidechains are listed below:

Mol	Chain	Res	Type
13	b	723	GLN
14	d	163	HIS
13	b	852	HIS
18	a	169	GLN
2	B	319	ASN

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 oligosaccharides 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	$\#\|Z\| > 2$
22	BEF	b	1502	-	0,3,3	-	-	-		
21	ADP	b	1501	20	27,29,29	1.26	4 (14%)	42,45,45	1.96	12 (28%)

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	-	2/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	1501	ADP	C5-C4	3.76	1.46	1.39
21	b	1501	ADP	C5-N7	-2.37	1.34	1.39
21	b	1501	ADP	C4-N9	-2.36	1.32	1.37
21	b	1501	ADP	C8-N7	2.11	1.35	1.31

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	1501	ADP	C5-C4-N3	-5.38	119.73	126.75
21	b	1501	ADP	N3-C4-N9	4.87	135.11	127.08
21	b	1501	ADP	C4-N9-C8	3.88	109.93	105.73
21	b	1501	ADP	C2-N3-C4	3.86	120.86	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	1501	ADP	N3-C2-N1	-3.83	122.61	128.60

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

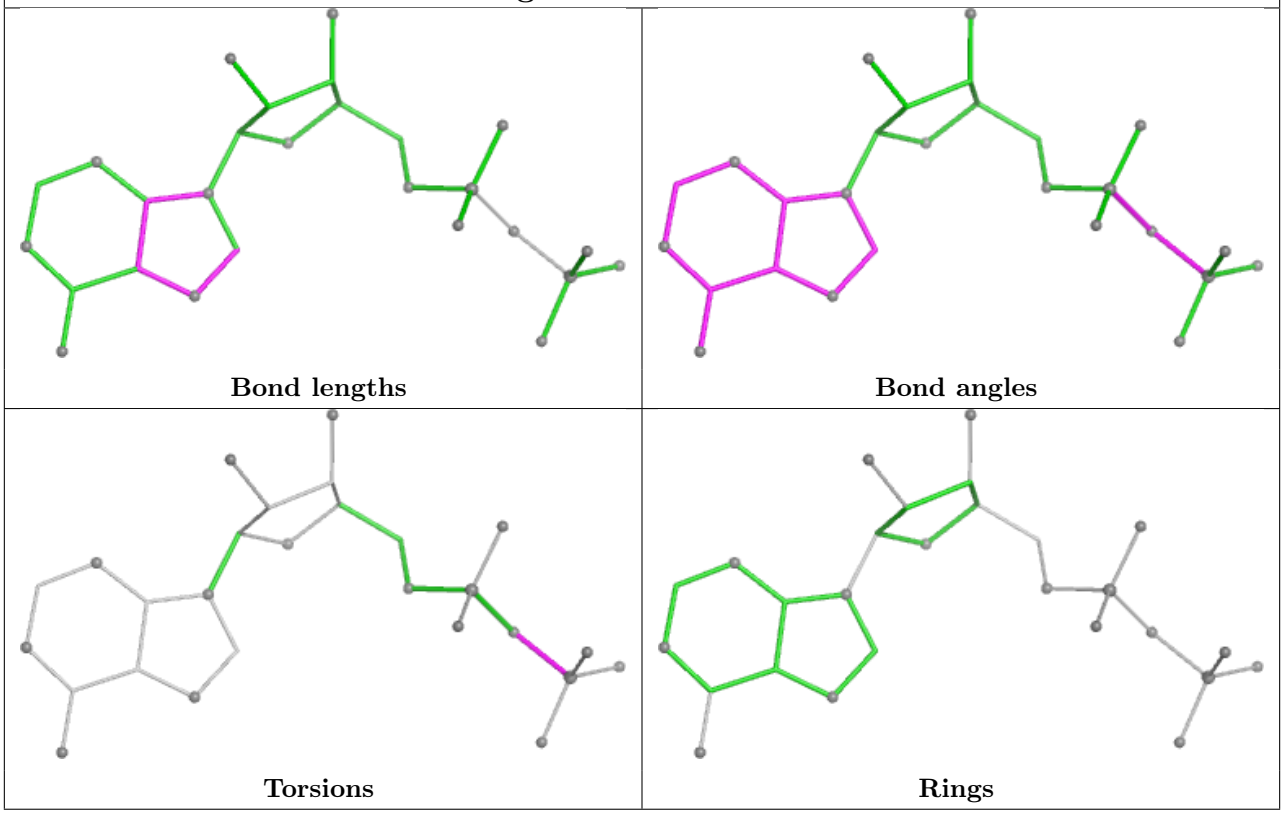
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	1502	BEF	1	0
21	b	1501	ADP	2	0

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

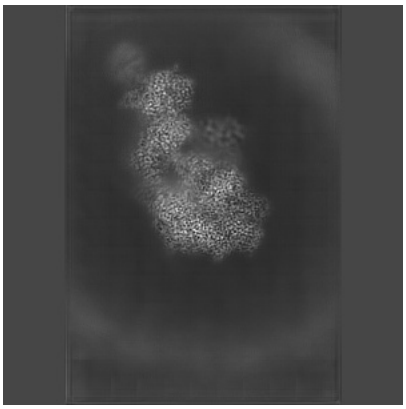
6 Map visualisation

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.

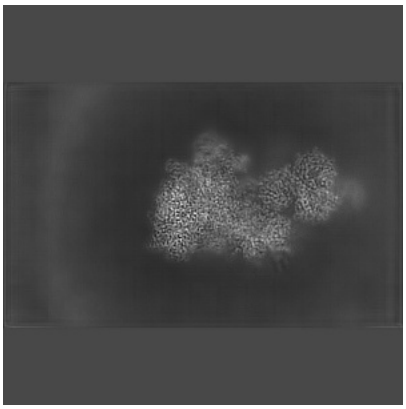
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

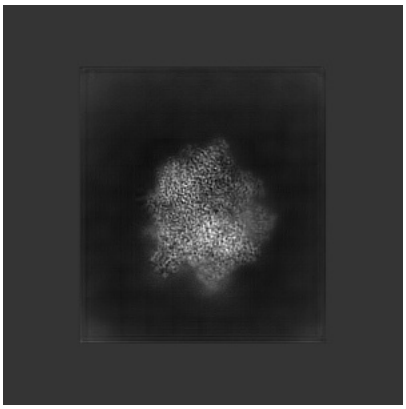
6.1.1 Primary map



X

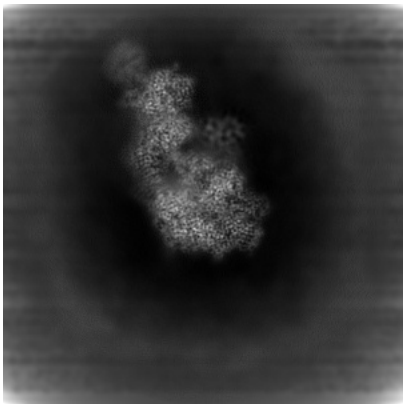


Y

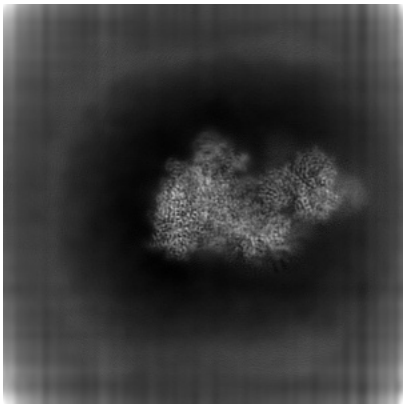


Z

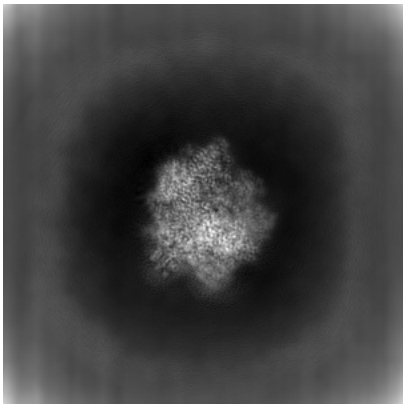
6.1.2 Raw map



X



Y

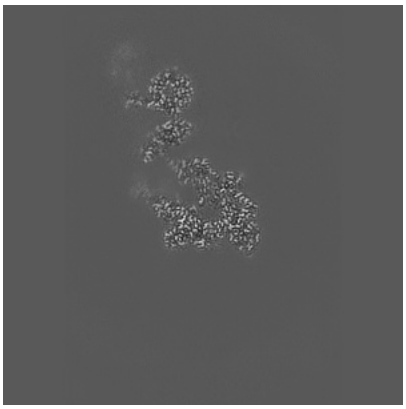


Z

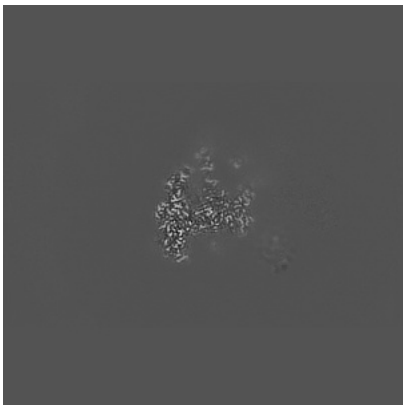
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 200

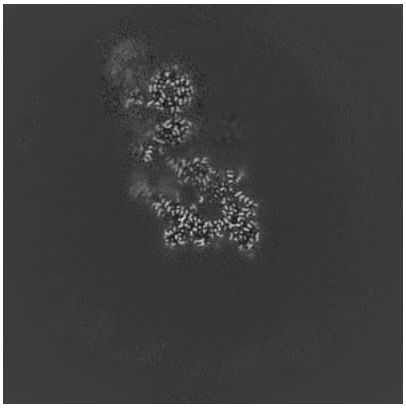


Y Index: 200

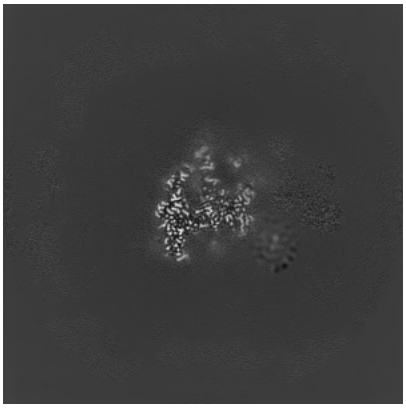


Z Index: 200

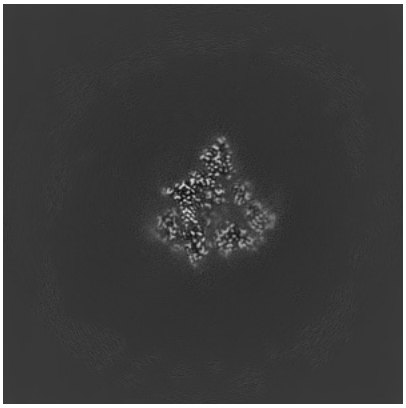
6.2.2 Raw map



X Index: 200



Y Index: 200

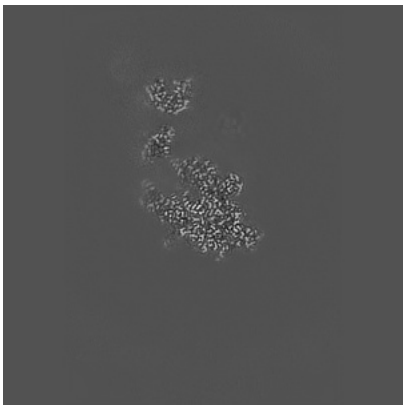


Z Index: 200

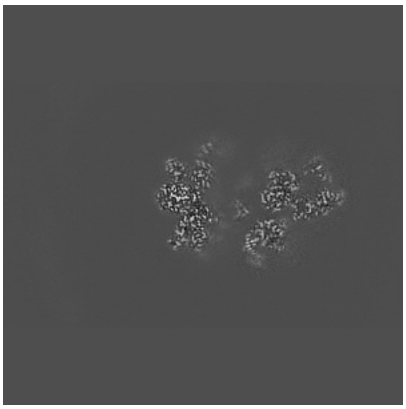
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

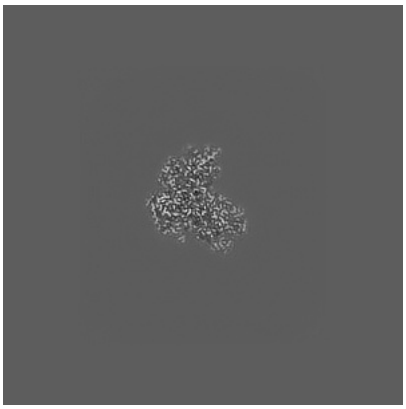
6.3.1 Primary map



X Index: 191

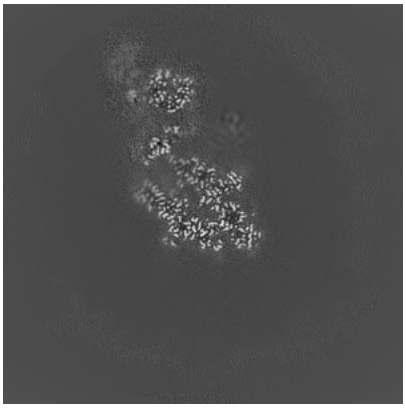


Y Index: 172

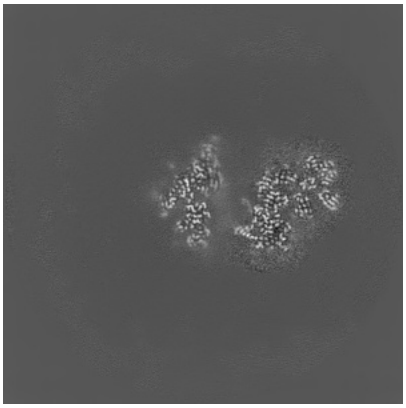


Z Index: 174

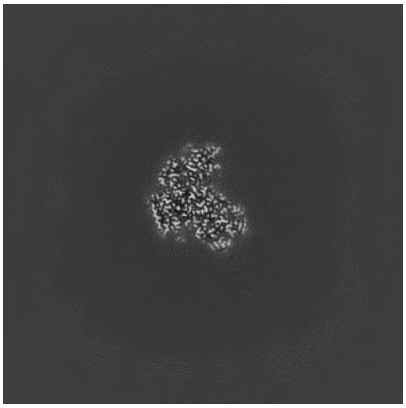
6.3.2 Raw map



X Index: 195



Y Index: 164

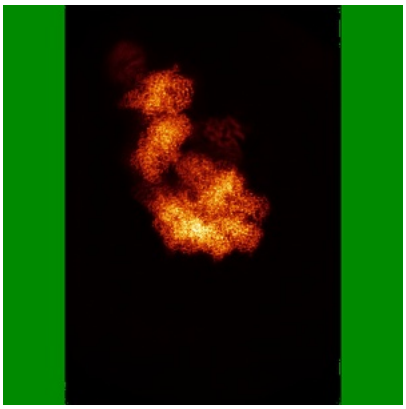


Z Index: 173

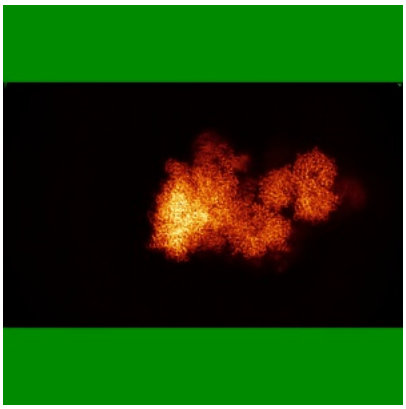
The images above show the largest variance slices of the map in three orthogonal directions.

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

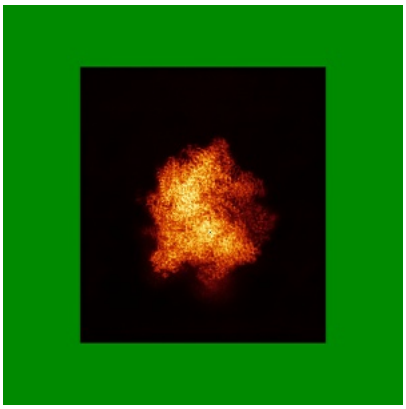
6.4.1 Primary map



X

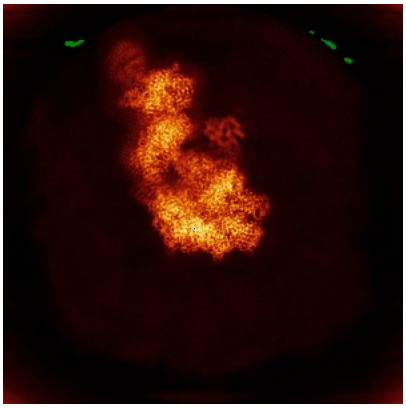


Y

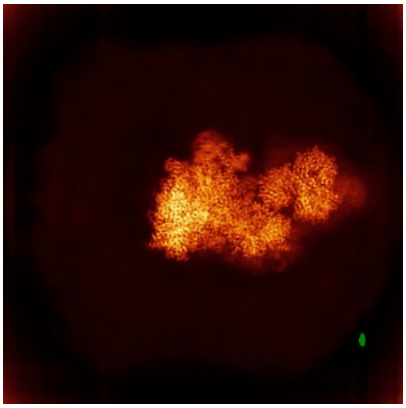


Z

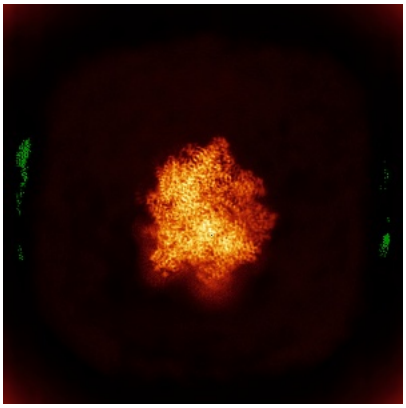
6.4.2 Raw map



X



Y

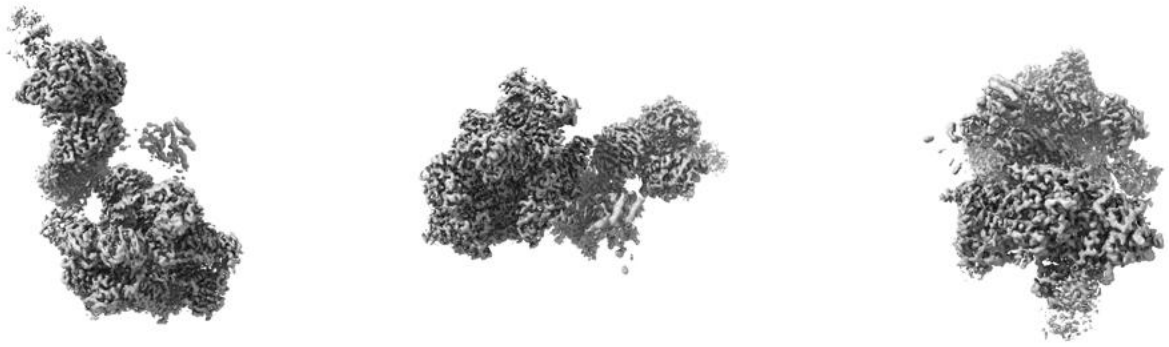


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

6.6 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

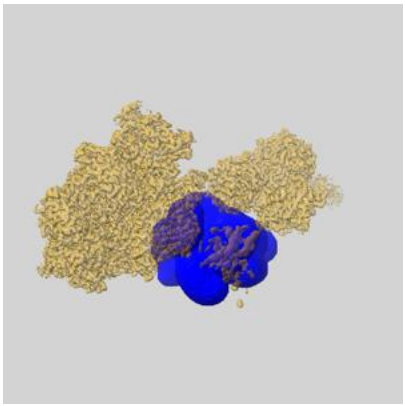
A mask typically either:

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

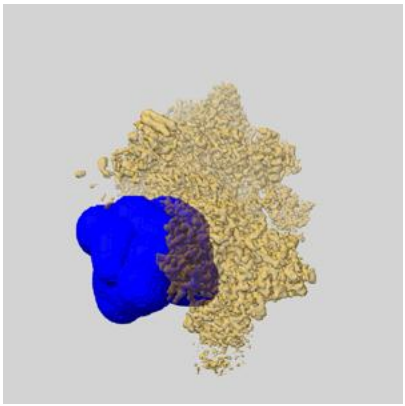
6.6.1 emd_13009_msk_4.map (i)



X

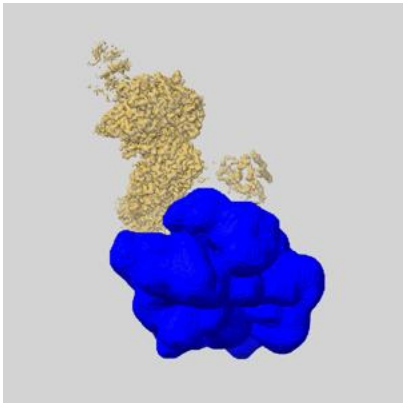


Y

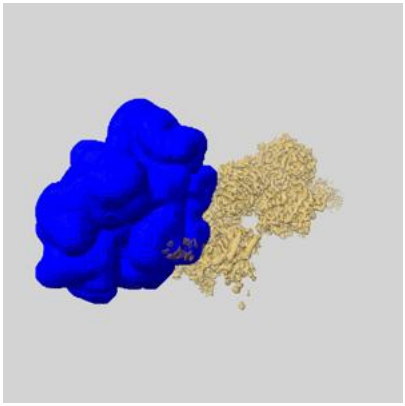


Z

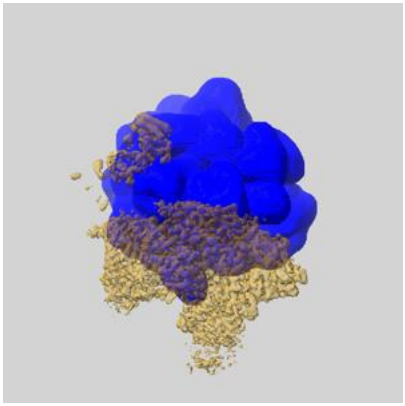
6.6.2 emd_13009_msk_3.map (i)



X

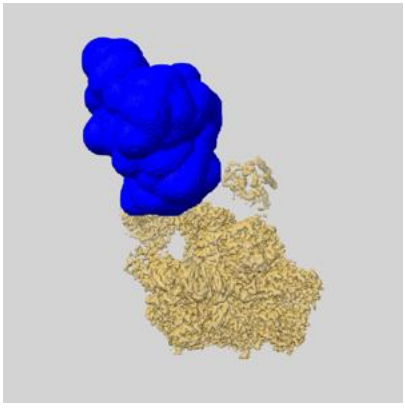


Y

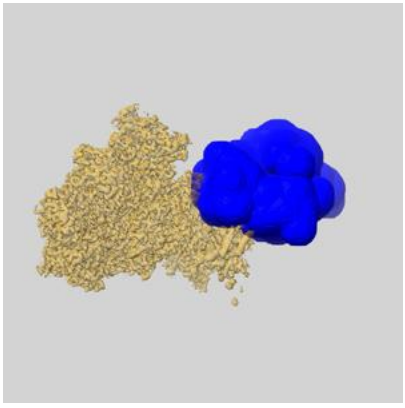


Z

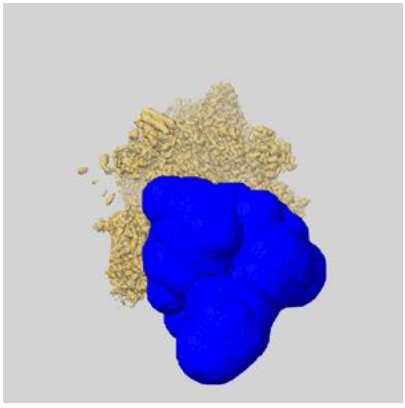
6.6.3 emd_13009_msk_2.map



X

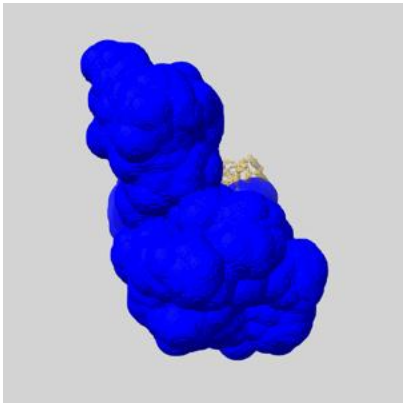


Y



Z

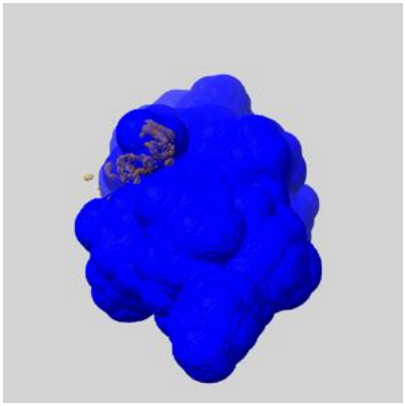
6.6.4 emd_13009_msk_1.map



X



Y

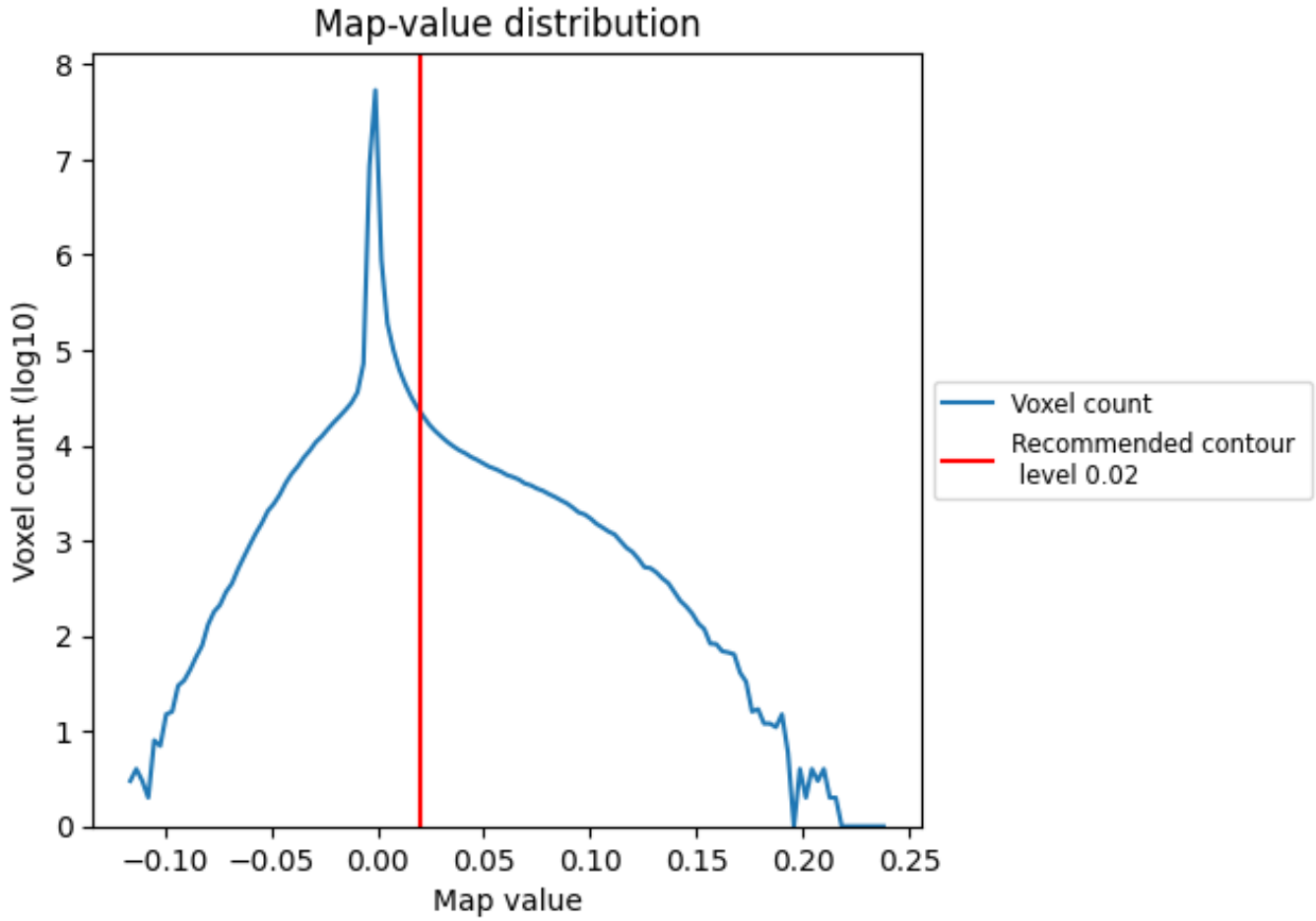


Z

7 Map analysis

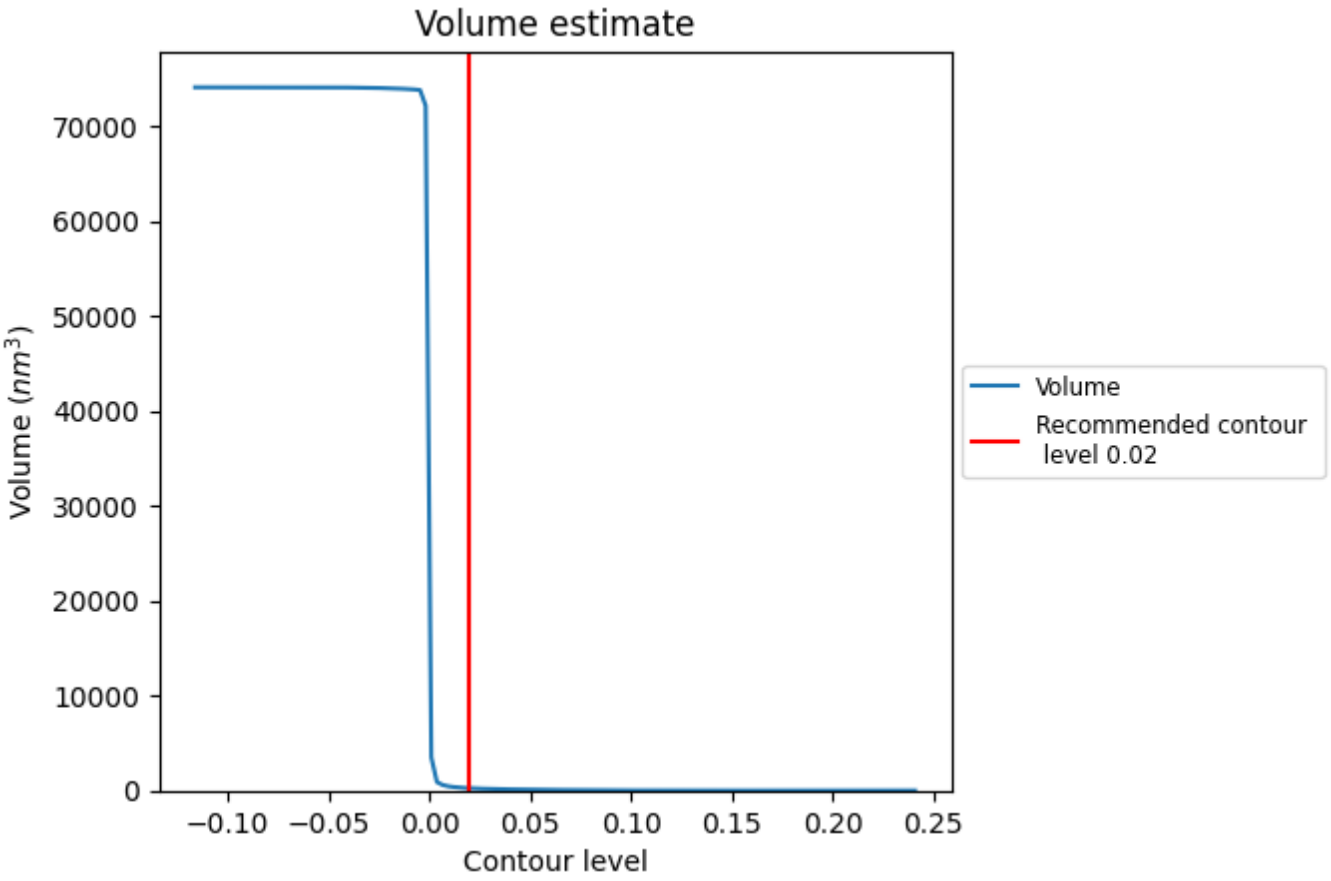
This section contains the results of statistical analysis of the map.

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.

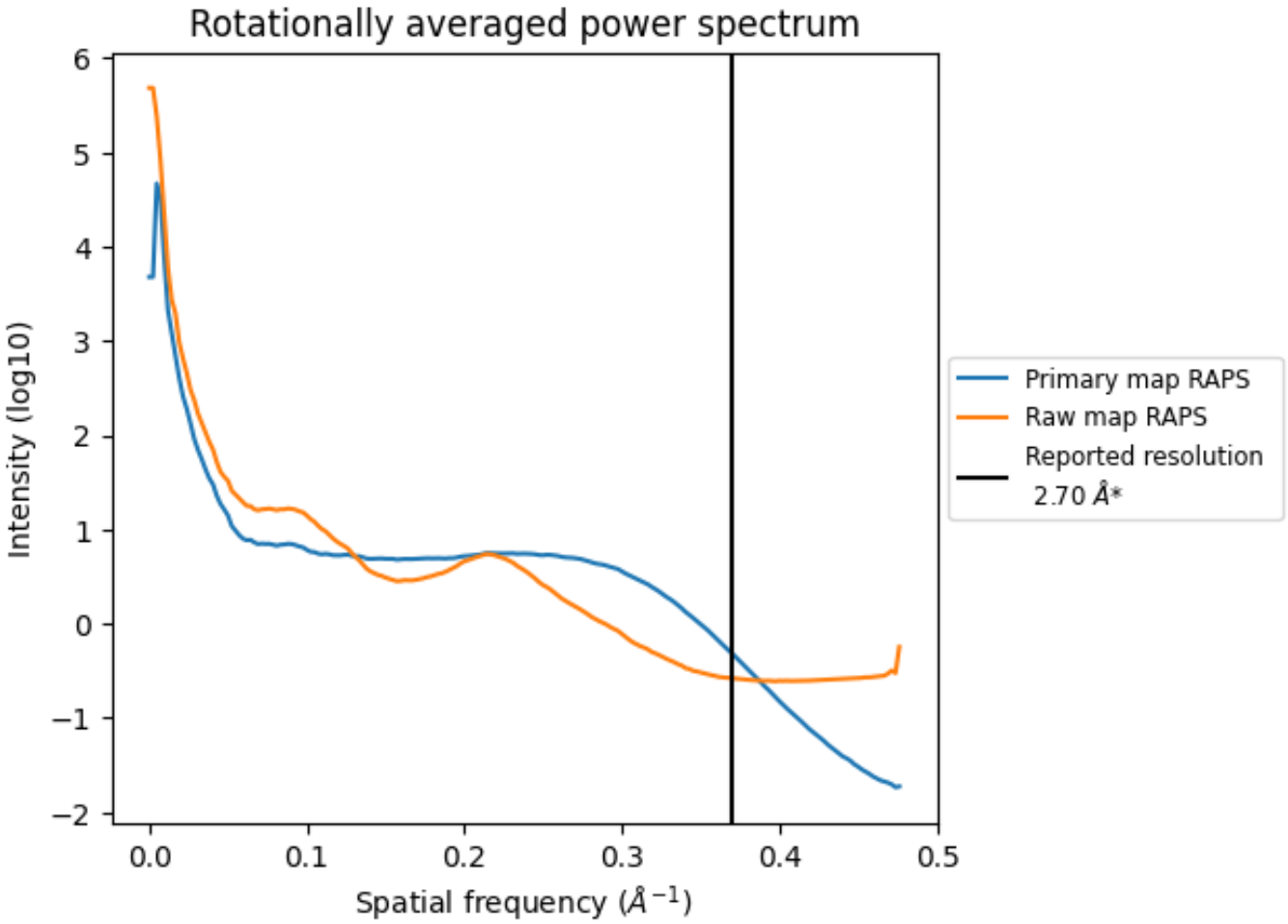
7.2 Volume estimate (i)



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)

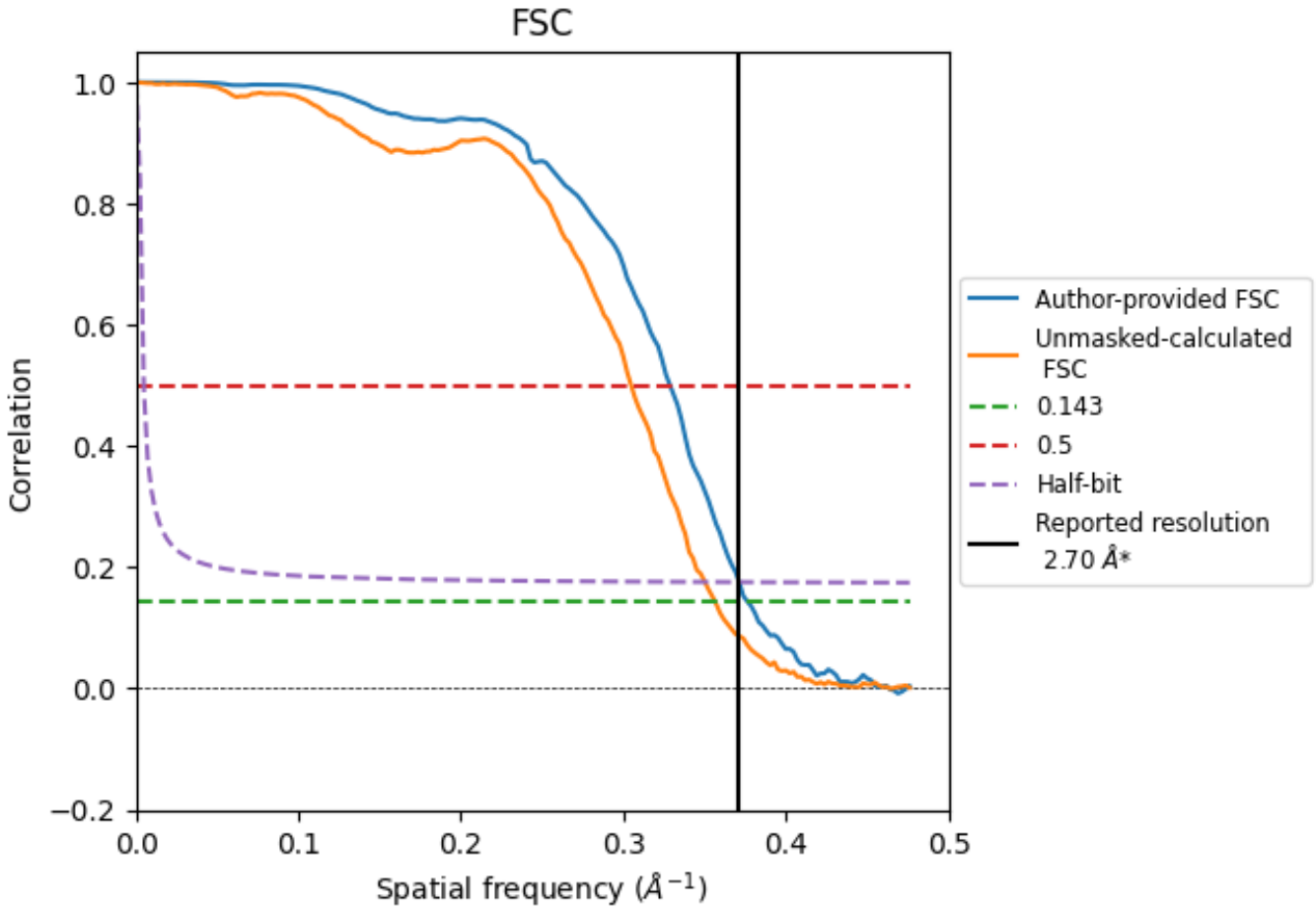


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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)

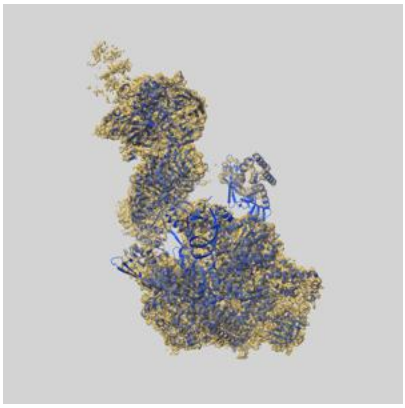
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.66	3.04	2.69
Unmasked-calculated*	2.81	3.28	2.86

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

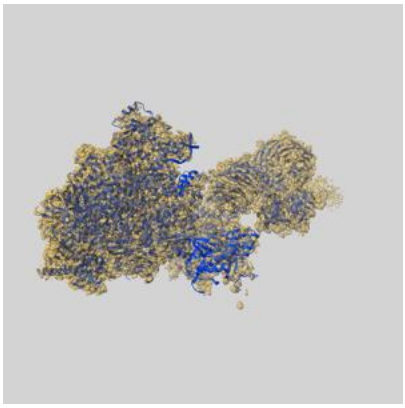
9 Map-model fit

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.

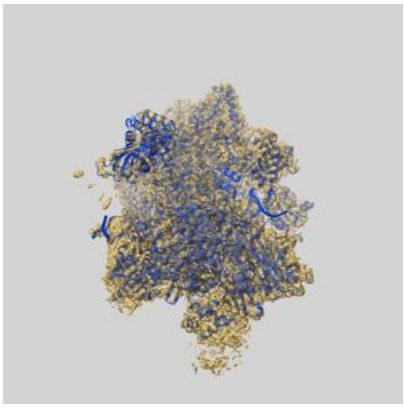
9.1 Map-model overlay



X



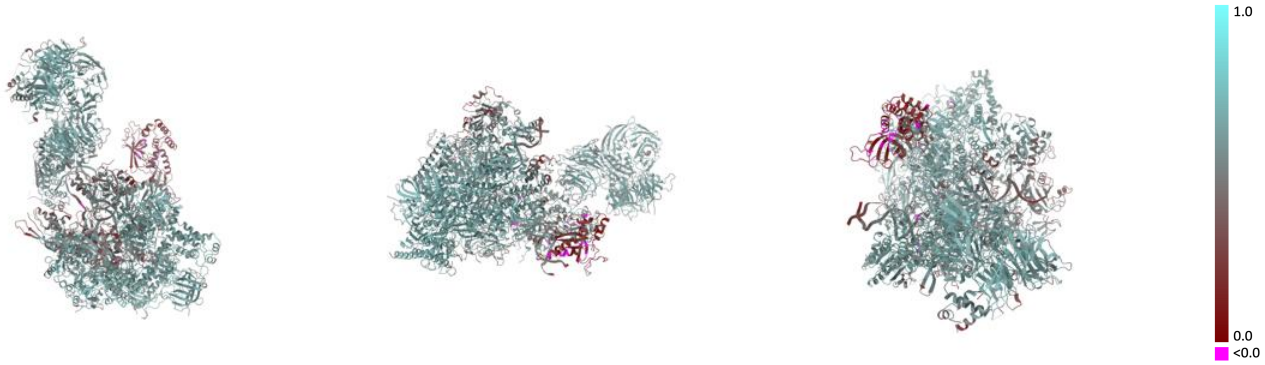
Y



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.

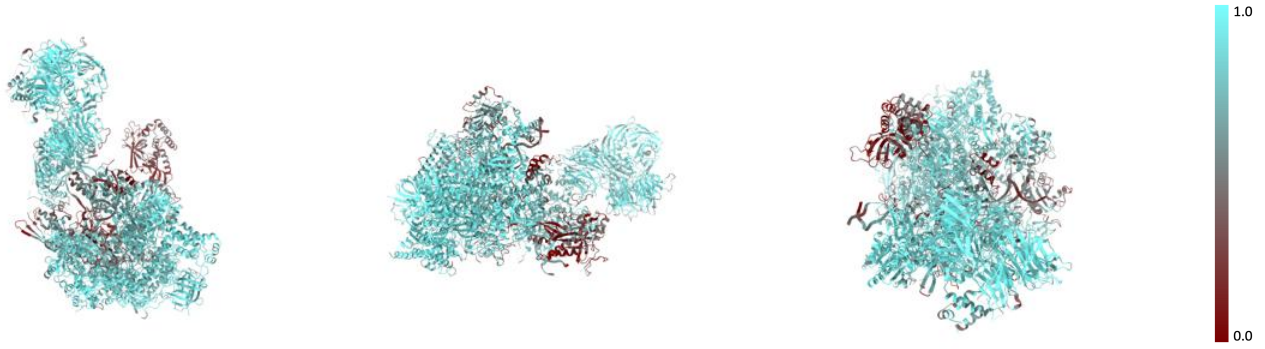
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

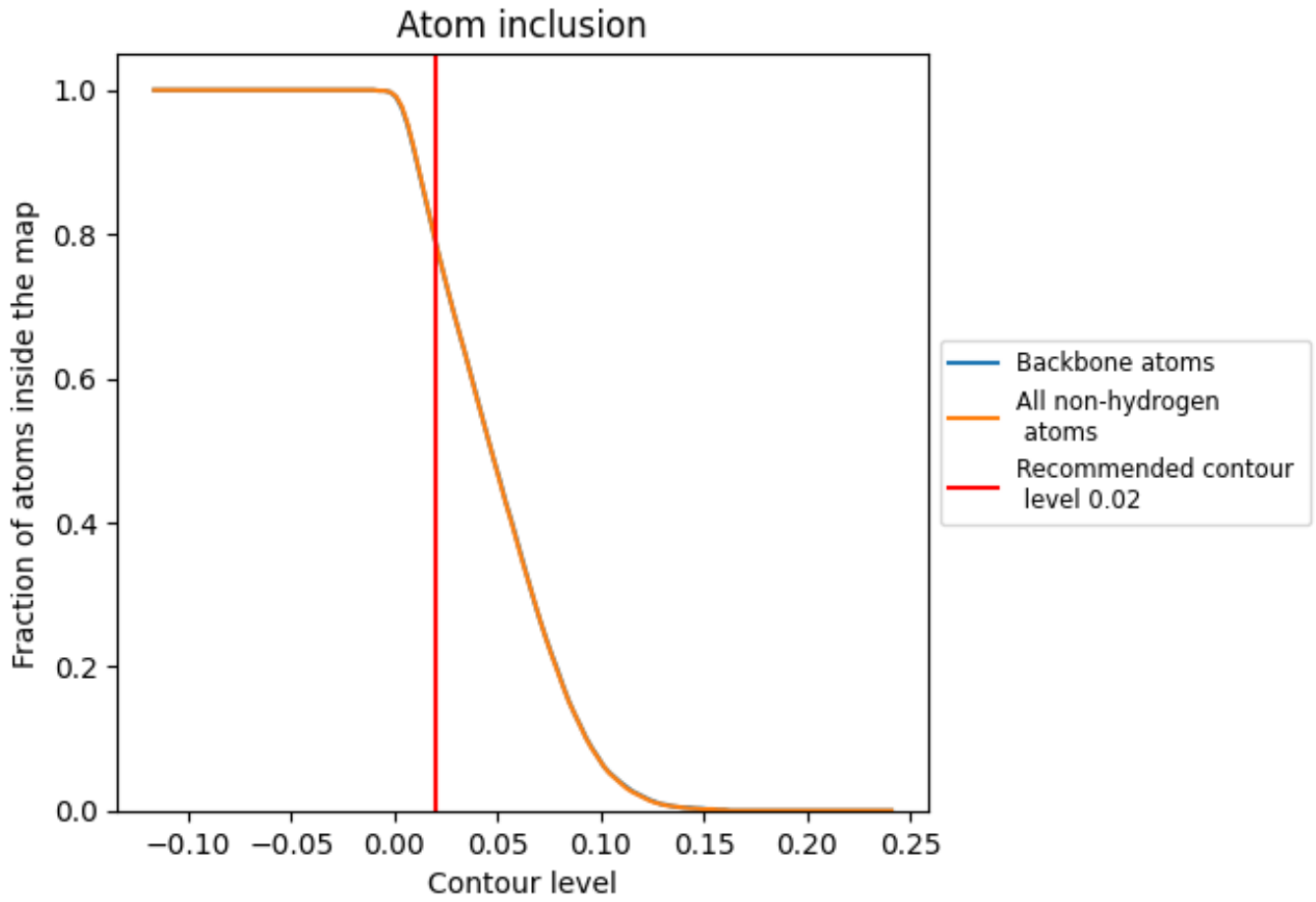
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7900	0.5660
A	0.7980	0.5810
B	0.8190	0.5900
C	0.8980	0.6280
D	0.2350	0.1820
E	0.7920	0.5690
F	0.8510	0.6030
G	0.2930	0.2910
H	0.8820	0.6130
I	0.6810	0.5050
J	0.9230	0.6540
K	0.9060	0.6290
L	0.7180	0.5180
N	0.5750	0.4840
P	0.9500	0.6530
T	0.6470	0.4900
a	0.8700	0.5970
b	0.8640	0.5760
d	0.8650	0.5880

