Full wwPDB EM Validation Report (i)

Jun 20, 2024 – 07:16 AM JST

PDB ID	:	7X75
EMDB ID	:	EMD-33032
Title	:	Cryo-EM structure of Streptomyces coelicolor RNAP-promoter open complex with three Zur dimers
Authors	:	Yang, X.; Zheng, J.
Deposited on	:	2022-03-09
Resolution	:	3.45 Å(reported)

This is a Full wwPDB EM Validation 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:

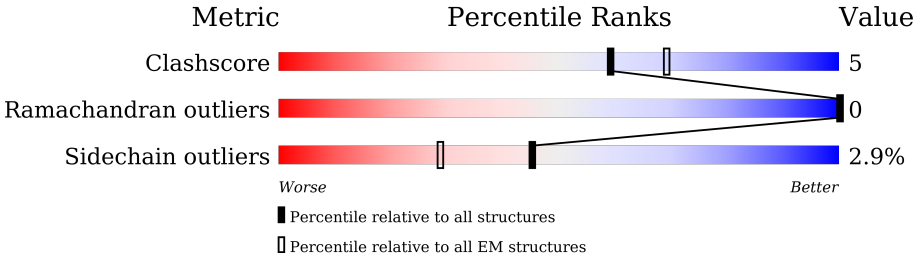
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	340	54% 12% • 34%
1	B	340	60% 7% • 31%
1	S	340	9% 16% 83%
2	C	1161	83% 13% •
3	D	1307	85% 11% •
4	E	90	70% 14% • 14%
5	F	531	46% 11% 43%
6	G	159	• 73% 9% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	H	159	71% 10% 18%
6	K	159	74% 9% 18%
6	L	159	75% 7% 18%
6	M	159	70% 11% 18%
6	N	159	70% 13% 18%
7	O	84	86% 14%
8	P	84	81% 19%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 34872 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	226	1742	1102	302	334	4	0	0
1	B	233	1792	1131	309	347	5	0	0
1	S	57	438	274	77	85	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1116	8692	5450	1513	1698	31	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1259	9846	6161	1787	1857	41	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1300	HIS	-	expression tag	UNP Q8CJT1
D	1301	HIS	-	expression tag	UNP Q8CJT1
D	1302	HIS	-	expression tag	UNP Q8CJT1
D	1303	HIS	-	expression tag	UNP Q8CJT1
D	1304	HIS	-	expression tag	UNP Q8CJT1
D	1305	HIS	-	expression tag	UNP Q8CJT1
D	1306	HIS	-	expression tag	UNP Q8CJT1
D	1307	HIS	-	expression tag	UNP Q8CJT1

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	77	597	382	98	117	0	0

- Molecule 5 is a protein called RNA polymerase principal sigma factor HrdB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	301	2396	1509	426	454	7	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP P18183
F	-18	GLY	-	expression tag	UNP P18183
F	-17	SER	-	expression tag	UNP P18183
F	-16	SER	-	expression tag	UNP P18183
F	-15	HIS	-	expression tag	UNP P18183
F	-14	HIS	-	expression tag	UNP P18183
F	-13	HIS	-	expression tag	UNP P18183
F	-12	HIS	-	expression tag	UNP P18183
F	-11	HIS	-	expression tag	UNP P18183
F	-10	HIS	-	expression tag	UNP P18183
F	-9	SER	-	expression tag	UNP P18183
F	-8	SER	-	expression tag	UNP P18183
F	-7	GLY	-	expression tag	UNP P18183
F	-6	LEU	-	expression tag	UNP P18183
F	-5	VAL	-	expression tag	UNP P18183
F	-4	PRO	-	expression tag	UNP P18183
F	-3	ARG	-	expression tag	UNP P18183
F	-2	GLY	-	expression tag	UNP P18183
F	-1	SER	-	expression tag	UNP P18183
F	0	HIS	-	expression tag	UNP P18183

- Molecule 6 is a protein called Putative metal uptake regulation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	131	984	603	185	190	6	0	0
6	H	131	984	603	185	190	6	0	0
6	K	131	984	603	185	190	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	131	984	603	185	190	6	0	0
			Total	C	N	O	S		
6	M	131	984	603	185	190	6	0	0
			Total	C	N	O	S		
6	N	131	984	603	185	190	6	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	MET	-	initiating methionine	UNP Q9L2H5
G	-18	GLY	-	expression tag	UNP Q9L2H5
G	-17	SER	-	expression tag	UNP Q9L2H5
G	-16	SER	-	expression tag	UNP Q9L2H5
G	-15	HIS	-	expression tag	UNP Q9L2H5
G	-14	HIS	-	expression tag	UNP Q9L2H5
G	-13	HIS	-	expression tag	UNP Q9L2H5
G	-12	HIS	-	expression tag	UNP Q9L2H5
G	-11	HIS	-	expression tag	UNP Q9L2H5
G	-10	HIS	-	expression tag	UNP Q9L2H5
G	-9	SER	-	expression tag	UNP Q9L2H5
G	-8	SER	-	expression tag	UNP Q9L2H5
G	-7	GLY	-	expression tag	UNP Q9L2H5
G	-6	LEU	-	expression tag	UNP Q9L2H5
G	-5	VAL	-	expression tag	UNP Q9L2H5
G	-4	PRO	-	expression tag	UNP Q9L2H5
G	-3	ARG	-	expression tag	UNP Q9L2H5
G	-2	GLY	-	expression tag	UNP Q9L2H5
G	-1	SER	-	expression tag	UNP Q9L2H5
G	0	HIS	-	expression tag	UNP Q9L2H5
H	-19	MET	-	initiating methionine	UNP Q9L2H5
H	-18	GLY	-	expression tag	UNP Q9L2H5
H	-17	SER	-	expression tag	UNP Q9L2H5
H	-16	SER	-	expression tag	UNP Q9L2H5
H	-15	HIS	-	expression tag	UNP Q9L2H5
H	-14	HIS	-	expression tag	UNP Q9L2H5
H	-13	HIS	-	expression tag	UNP Q9L2H5
H	-12	HIS	-	expression tag	UNP Q9L2H5
H	-11	HIS	-	expression tag	UNP Q9L2H5
H	-10	HIS	-	expression tag	UNP Q9L2H5
H	-9	SER	-	expression tag	UNP Q9L2H5
H	-8	SER	-	expression tag	UNP Q9L2H5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	GLY	-	expression tag	UNP Q9L2H5
H	-6	LEU	-	expression tag	UNP Q9L2H5
H	-5	VAL	-	expression tag	UNP Q9L2H5
H	-4	PRO	-	expression tag	UNP Q9L2H5
H	-3	ARG	-	expression tag	UNP Q9L2H5
H	-2	GLY	-	expression tag	UNP Q9L2H5
H	-1	SER	-	expression tag	UNP Q9L2H5
H	0	HIS	-	expression tag	UNP Q9L2H5
K	-19	MET	-	initiating methionine	UNP Q9L2H5
K	-18	GLY	-	expression tag	UNP Q9L2H5
K	-17	SER	-	expression tag	UNP Q9L2H5
K	-16	SER	-	expression tag	UNP Q9L2H5
K	-15	HIS	-	expression tag	UNP Q9L2H5
K	-14	HIS	-	expression tag	UNP Q9L2H5
K	-13	HIS	-	expression tag	UNP Q9L2H5
K	-12	HIS	-	expression tag	UNP Q9L2H5
K	-11	HIS	-	expression tag	UNP Q9L2H5
K	-10	HIS	-	expression tag	UNP Q9L2H5
K	-9	SER	-	expression tag	UNP Q9L2H5
K	-8	SER	-	expression tag	UNP Q9L2H5
K	-7	GLY	-	expression tag	UNP Q9L2H5
K	-6	LEU	-	expression tag	UNP Q9L2H5
K	-5	VAL	-	expression tag	UNP Q9L2H5
K	-4	PRO	-	expression tag	UNP Q9L2H5
K	-3	ARG	-	expression tag	UNP Q9L2H5
K	-2	GLY	-	expression tag	UNP Q9L2H5
K	-1	SER	-	expression tag	UNP Q9L2H5
K	0	HIS	-	expression tag	UNP Q9L2H5
L	-19	MET	-	initiating methionine	UNP Q9L2H5
L	-18	GLY	-	expression tag	UNP Q9L2H5
L	-17	SER	-	expression tag	UNP Q9L2H5
L	-16	SER	-	expression tag	UNP Q9L2H5
L	-15	HIS	-	expression tag	UNP Q9L2H5
L	-14	HIS	-	expression tag	UNP Q9L2H5
L	-13	HIS	-	expression tag	UNP Q9L2H5
L	-12	HIS	-	expression tag	UNP Q9L2H5
L	-11	HIS	-	expression tag	UNP Q9L2H5
L	-10	HIS	-	expression tag	UNP Q9L2H5
L	-9	SER	-	expression tag	UNP Q9L2H5
L	-8	SER	-	expression tag	UNP Q9L2H5
L	-7	GLY	-	expression tag	UNP Q9L2H5
L	-6	LEU	-	expression tag	UNP Q9L2H5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	-5	VAL	-	expression tag	UNP Q9L2H5
L	-4	PRO	-	expression tag	UNP Q9L2H5
L	-3	ARG	-	expression tag	UNP Q9L2H5
L	-2	GLY	-	expression tag	UNP Q9L2H5
L	-1	SER	-	expression tag	UNP Q9L2H5
L	0	HIS	-	expression tag	UNP Q9L2H5
M	-19	MET	-	initiating methionine	UNP Q9L2H5
M	-18	GLY	-	expression tag	UNP Q9L2H5
M	-17	SER	-	expression tag	UNP Q9L2H5
M	-16	SER	-	expression tag	UNP Q9L2H5
M	-15	HIS	-	expression tag	UNP Q9L2H5
M	-14	HIS	-	expression tag	UNP Q9L2H5
M	-13	HIS	-	expression tag	UNP Q9L2H5
M	-12	HIS	-	expression tag	UNP Q9L2H5
M	-11	HIS	-	expression tag	UNP Q9L2H5
M	-10	HIS	-	expression tag	UNP Q9L2H5
M	-9	SER	-	expression tag	UNP Q9L2H5
M	-8	SER	-	expression tag	UNP Q9L2H5
M	-7	GLY	-	expression tag	UNP Q9L2H5
M	-6	LEU	-	expression tag	UNP Q9L2H5
M	-5	VAL	-	expression tag	UNP Q9L2H5
M	-4	PRO	-	expression tag	UNP Q9L2H5
M	-3	ARG	-	expression tag	UNP Q9L2H5
M	-2	GLY	-	expression tag	UNP Q9L2H5
M	-1	SER	-	expression tag	UNP Q9L2H5
M	0	HIS	-	expression tag	UNP Q9L2H5
N	-19	MET	-	initiating methionine	UNP Q9L2H5
N	-18	GLY	-	expression tag	UNP Q9L2H5
N	-17	SER	-	expression tag	UNP Q9L2H5
N	-16	SER	-	expression tag	UNP Q9L2H5
N	-15	HIS	-	expression tag	UNP Q9L2H5
N	-14	HIS	-	expression tag	UNP Q9L2H5
N	-13	HIS	-	expression tag	UNP Q9L2H5
N	-12	HIS	-	expression tag	UNP Q9L2H5
N	-11	HIS	-	expression tag	UNP Q9L2H5
N	-10	HIS	-	expression tag	UNP Q9L2H5
N	-9	SER	-	expression tag	UNP Q9L2H5
N	-8	SER	-	expression tag	UNP Q9L2H5
N	-7	GLY	-	expression tag	UNP Q9L2H5
N	-6	LEU	-	expression tag	UNP Q9L2H5
N	-5	VAL	-	expression tag	UNP Q9L2H5
N	-4	PRO	-	expression tag	UNP Q9L2H5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	-3	ARG	-	expression tag	UNP Q9L2H5
N	-2	GLY	-	expression tag	UNP Q9L2H5
N	-1	SER	-	expression tag	UNP Q9L2H5
N	0	HIS	-	expression tag	UNP Q9L2H5

- Molecule 7 is a DNA chain called DNA (84-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	O	84	1714	810	315	505	84	0	0

- Molecule 8 is a DNA chain called DNA (84-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	P	84	1730	815	328	503	84	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
9	D	1	1	1	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

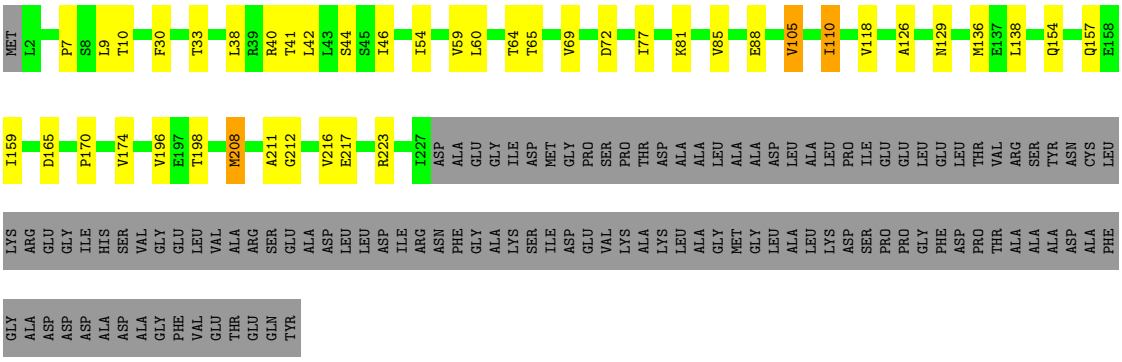
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
10	D	2	2	2	0
10	G	3	3	3	0
10	H	3	3	3	0
10	K	3	3	3	0
10	L	3	3	3	0
10	M	3	3	3	0
10	N	3	3	3	0

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.

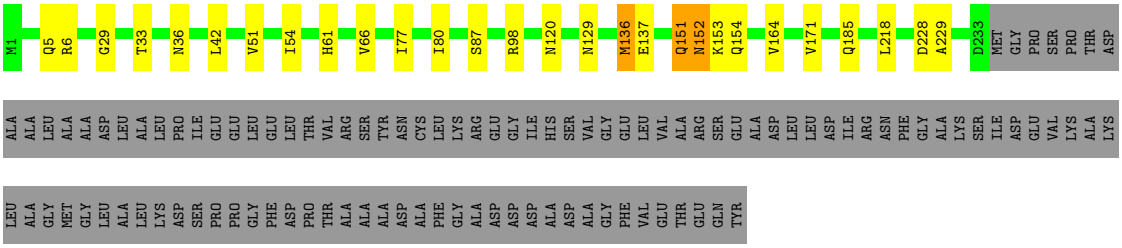
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



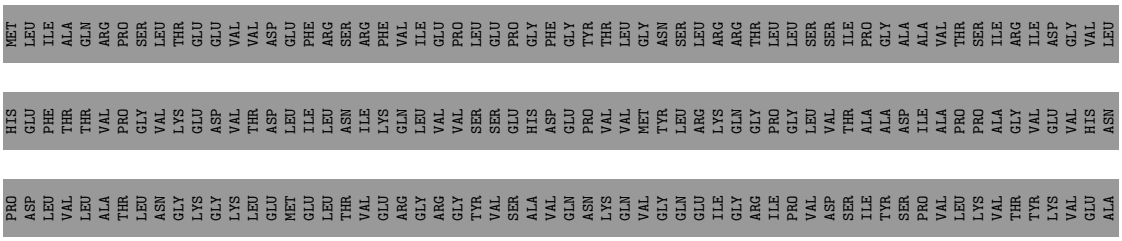
• Molecule 1: DNA-directed RNA polymerase subunit alpha

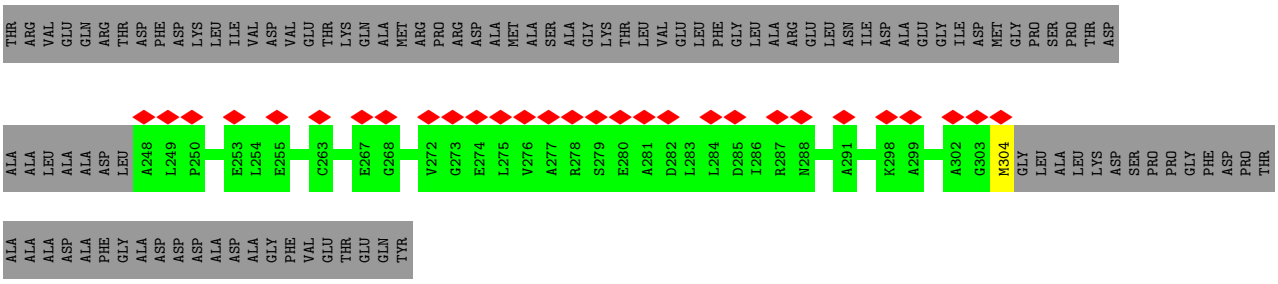
Chain B:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

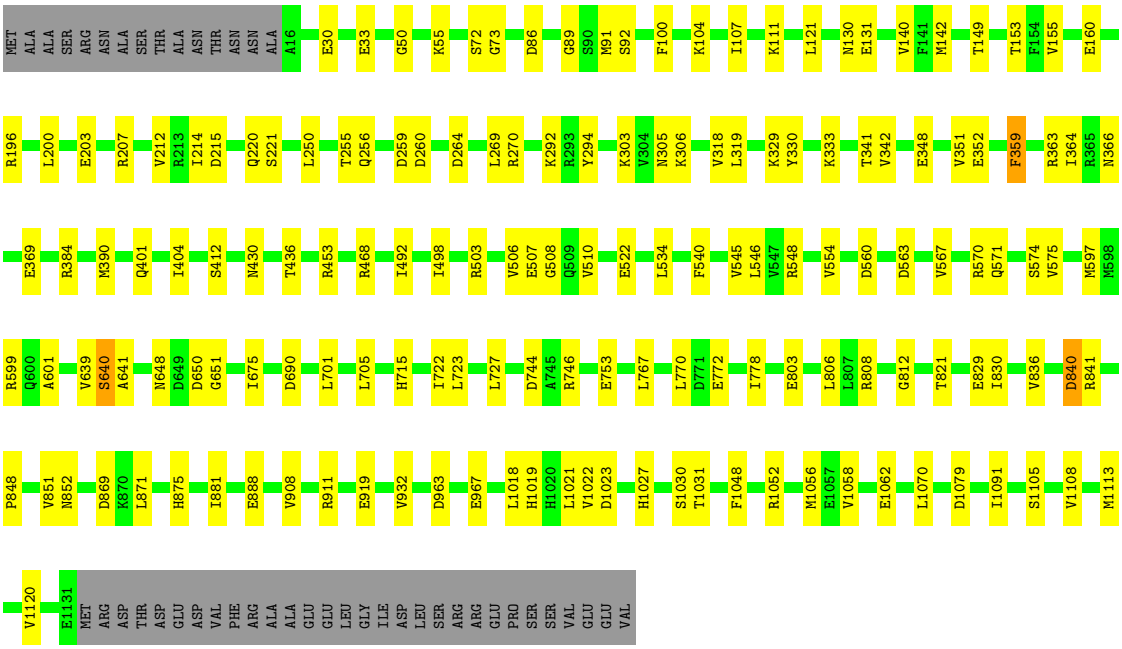
Chain S:





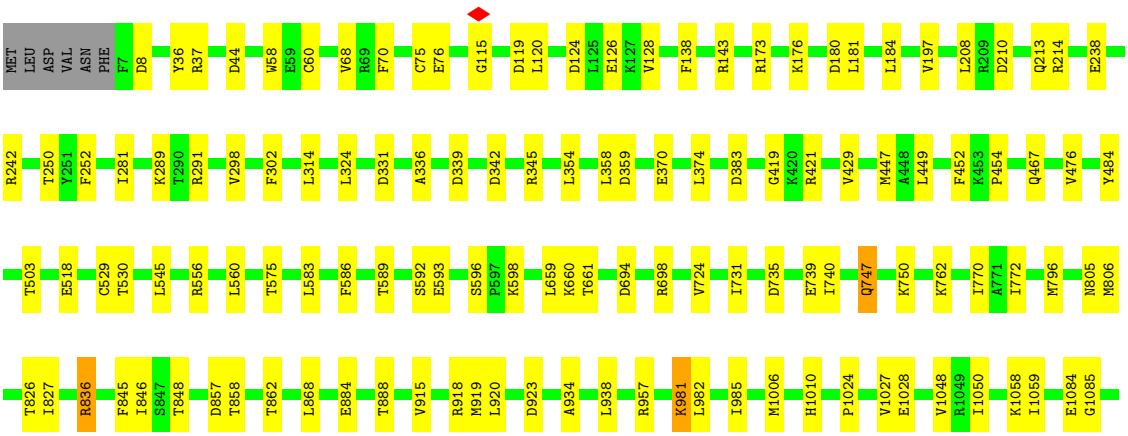
• Molecule 2: DNA-directed RNA polymerase subunit beta

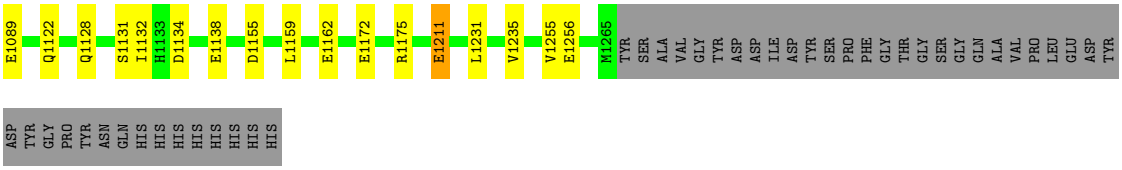
Chain C:



• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:



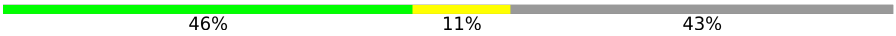


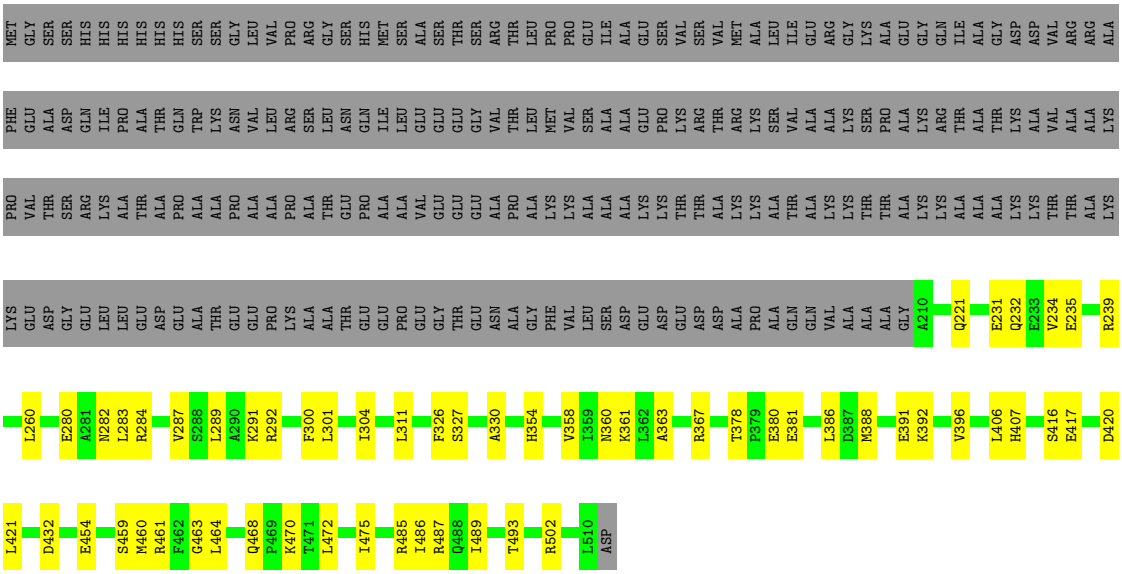
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:

• Molecule 5: RNA polymerase principal sigma factor HrdB

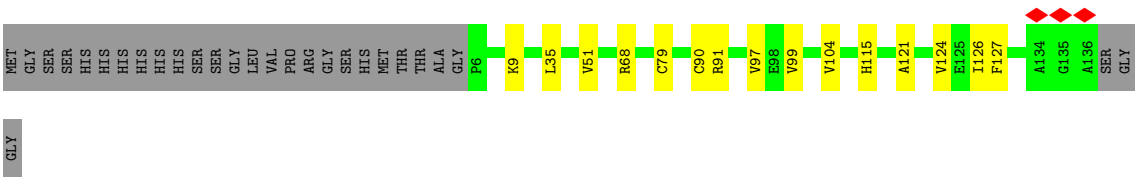
Chain F:





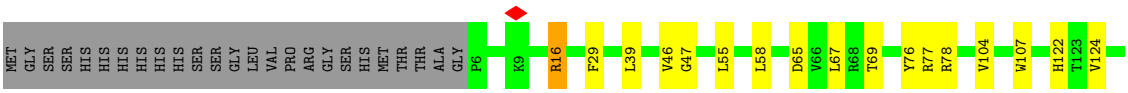
• Molecule 6: Putative metal uptake regulation protein

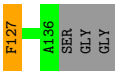
Chain G:



• Molecule 6: Putative metal uptake regulation protein

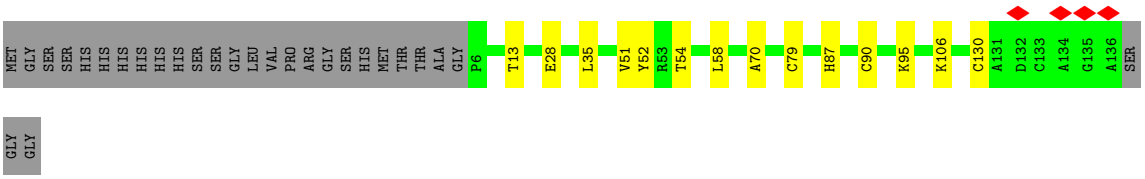
Chain H:





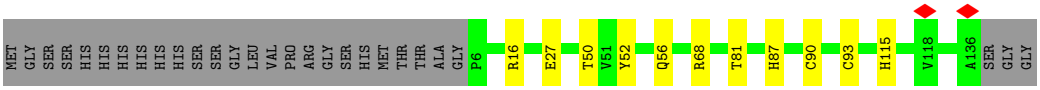
• Molecule 6: Putative metal uptake regulation protein

Chain K:



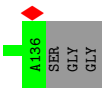
• Molecule 6: Putative metal uptake regulation protein

Chain L:



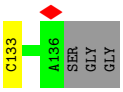
• Molecule 6: Putative metal uptake regulation protein

Chain M:



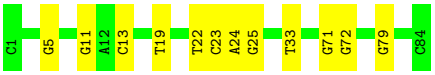
• Molecule 6: Putative metal uptake regulation protein

Chain N:



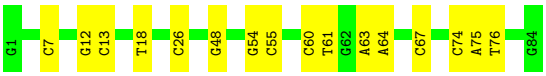
• Molecule 7: DNA (84-MER)

Chain O:



• Molecule 8: DNA (84-MER)

Chain P: 81% 19%


G1
C7
G12
C13
T18
C26
G48
G54
C55
C60
T61
G62
A63
A64
C67
C74
A75
T76
G84

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30218	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	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.899	Depositor
Minimum map value	-1.758	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	403.19998, 403.19998, 403.19998	wwPDB
Map dimensions	384, 384, 384	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	0.27	0/1768	0.60	0/2400
1	B	0.27	0/1818	0.59	0/2467
1	S	0.24	0/441	0.49	0/591
2	C	0.27	0/8848	0.57	0/11982
3	D	0.27	0/9998	0.60	0/13490
4	E	0.30	0/607	0.56	0/826
5	F	0.27	0/2431	0.60	0/3277
6	G	0.25	0/1001	0.55	0/1355
6	H	0.26	0/1001	0.55	0/1355
6	K	0.24	0/1001	0.56	0/1355
6	L	0.25	0/1001	0.50	0/1355
6	M	0.25	0/1001	0.55	0/1355
6	N	0.24	0/1001	0.52	0/1355
7	O	0.67	0/1920	0.94	0/2959
8	P	0.63	0/1942	0.89	0/2997
All	All	0.33	0/35779	0.63	0/49119

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	1742	0	1796	30	0
1	B	1792	0	1841	21	0
1	S	438	0	452	0	0
2	C	8692	0	8632	105	0
3	D	9846	0	10017	85	0
4	E	597	0	604	10	0
5	F	2396	0	2453	37	0
6	G	984	0	947	9	0
6	H	984	0	947	11	0
6	K	984	0	947	8	0
6	L	984	0	947	4	0
6	M	984	0	947	10	0
6	N	984	0	947	10	0
7	O	1714	0	940	17	0
8	P	1730	0	939	16	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
10	G	3	0	0	0	0
10	H	3	0	0	0	0
10	K	3	0	0	0	0
10	L	3	0	0	0	0
10	M	3	0	0	0	0
10	N	3	0	0	0	0
All	All	34872	0	33356	327	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (327) 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)
2:C:1058:VAL:HG23	2:C:1070:LEU:HD11	1.59	0.84
3:D:1255:VAL:HG13	4:E:80:LEU:HD21	1.65	0.78
6:G:104:VAL:HG12	6:H:104:VAL:HG12	1.67	0.76
2:C:522:GLU:OE2	2:C:548:ARG:NH2	2.22	0.73
3:D:923:ASP:OD1	3:D:934:ALA:N	2.22	0.72
6:M:36:HIS:NE2	6:M:46:VAL:O	2.22	0.72
6:N:78:ARG:NH1	6:N:79:CYS:O	2.23	0.71
2:C:107:ILE:HD11	2:C:155:VAL:HG21	1.73	0.71
2:C:364:ILE:HD11	2:C:492:ILE:HD12	1.73	0.71
3:D:770:ILE:HD11	3:D:826:THR:HG21	1.72	0.70
3:D:1128:GLN:N	3:D:1128:GLN:OE1	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:715:HIS:HB2	2:C:722:ILE:HD11	1.75	0.69
5:F:485:ARG:NH2	7:O:33:DT:OP2	2.25	0.69
2:C:352:GLU:N	2:C:352:GLU:OE1	2.26	0.69
3:D:529:CYS:SG	3:D:530:THR:N	2.65	0.68
3:D:339:ASP:OD1	5:F:407:HIS:ND1	2.26	0.68
6:H:47:GLY:N	8:P:55:DC:OP2	2.27	0.68
4:E:65:GLU:OE1	4:E:65:GLU:N	2.27	0.67
5:F:417:GLU:OE2	5:F:417:GLU:N	2.28	0.67
3:D:1058:LYS:NZ	3:D:1059:ILE:O	2.27	0.67
1:B:42:LEU:CD2	1:B:171:VAL:HG11	2.25	0.66
3:D:421:ARG:NH1	8:P:18:DT:OP1	2.28	0.66
3:D:1006:MET:SD	3:D:1128:GLN:NE2	2.69	0.66
2:C:256:GLN:N	2:C:256:GLN:OE1	2.29	0.66
6:N:28:GLU:OE1	6:N:30:ARG:NH2	2.30	0.65
2:C:33:GLU:OE1	2:C:33:GLU:N	2.30	0.65
6:N:77:ARG:NH1	6:N:79:CYS:SG	2.70	0.64
1:A:154:GLN:OE1	1:A:154:GLN:N	2.31	0.64
3:D:556:ARG:O	3:D:560:LEU:HD22	1.98	0.64
2:C:203:GLU:N	2:C:203:GLU:OE2	2.30	0.64
2:C:875:HIS:NE2	2:C:919:GLU:OE1	2.25	0.63
6:N:27:GLU:OE1	6:N:77:ARG:NH2	2.32	0.63
2:C:1019:HIS:O	2:C:1019:HIS:ND1	2.32	0.63
3:D:583:LEU:HD21	3:D:724:VAL:HG11	1.79	0.63
5:F:454:GLU:N	5:F:454:GLU:OE2	2.32	0.62
3:D:342:ASP:OD1	3:D:345:ARG:NH2	2.32	0.62
2:C:967:GLU:N	2:C:967:GLU:OE2	2.31	0.62
3:D:1048:VAL:O	3:D:1085:GLY:N	2.32	0.62
2:C:333:LYS:NZ	2:C:342:VAL:O	2.32	0.62
2:C:453:ARG:HA	7:O:71:DG:H1'	1.81	0.62
2:C:675:ILE:HD11	2:C:690:ASP:OD1	2.00	0.62
2:C:111:LYS:NZ	2:C:160:GLU:OE2	2.22	0.62
3:D:518:GLU:OE1	3:D:518:GLU:N	2.33	0.61
4:E:36:ARG:NE	4:E:74:GLU:OE1	2.32	0.61
2:C:806:LEU:HD13	5:F:464:LEU:HD21	1.82	0.61
3:D:238:GLU:OE1	3:D:238:GLU:N	2.33	0.61
4:E:46:GLN:N	4:E:46:GLN:OE1	2.34	0.61
2:C:746:ARG:NH1	3:D:331:ASP:OD1	2.33	0.61
2:C:508:GLY:N	2:C:560:ASP:OD1	2.34	0.60
3:D:143:ARG:NH1	3:D:250:THR:O	2.34	0.60
1:B:154:GLN:N	1:B:154:GLN:OE1	2.34	0.60
2:C:214:ILE:HG21	2:C:269:LEU:HD21	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:15:GLN:NE2	7:O:11:DG:OP2	2.35	0.59
3:D:291:ARG:NH2	7:O:79:DG:OP2	2.34	0.59
1:A:40:ARG:HE	1:B:33:THR:HG23	1.67	0.59
3:D:124:ASP:O	3:D:128:VAL:HG23	2.03	0.59
6:K:35:LEU:HD23	6:K:51:VAL:HG13	1.84	0.59
2:C:363:ARG:NH1	2:C:369:GLU:OE1	2.36	0.59
2:C:1052:ARG:NH1	3:D:419:GLY:O	2.36	0.59
2:C:753:GLU:OE1	2:C:753:GLU:N	2.31	0.59
2:C:1113:MET:CE	2:C:1120:VAL:HG21	2.33	0.59
1:A:40:ARG:NH2	1:B:29:GLY:O	2.36	0.58
2:C:574:SER:OG	2:C:575:VAL:N	2.37	0.58
2:C:1058:VAL:HG22	2:C:1062:GLU:OE2	2.02	0.58
3:D:115:GLY:CA	3:D:298:VAL:HG21	2.33	0.58
1:A:157:GLN:N	1:A:157:GLN:OE1	2.34	0.58
3:D:281:ILE:O	3:D:289:LYS:NZ	2.36	0.58
2:C:648:ASN:ND2	2:C:650:ASP:OD2	2.36	0.58
6:N:55:LEU:HD21	6:N:76:TYR:CD1	2.38	0.58
3:D:1122:GLN:NE2	3:D:1134:ASP:OD1	2.35	0.57
7:O:72:DG:H1	8:P:13:DC:H42	1.52	0.57
3:D:452:PHE:CE1	3:D:545:LEU:HD11	2.39	0.57
7:O:22:DT:H1'	7:O:23:DC:OP2	2.05	0.57
2:C:723:LEU:HD13	2:C:727:LEU:HD12	1.87	0.57
2:C:869:ASP:OD1	2:C:1022:VAL:HG12	2.05	0.56
6:H:16:ARG:NH1	8:P:54:DG:OP1	2.38	0.56
2:C:808:ARG:O	2:C:812:GLY:N	2.38	0.56
3:D:354:LEU:HD23	3:D:358:LEU:HD13	1.87	0.56
3:D:659:LEU:HD23	3:D:660:LYS:N	2.20	0.56
6:K:79:CYS:SG	6:K:87:HIS:CE1	2.98	0.56
6:H:65:ASP:OD2	6:H:77:ARG:NH1	2.38	0.56
5:F:367:ARG:NH1	8:P:26:DC:O3'	2.38	0.56
3:D:467:GLN:N	3:D:467:GLN:OE1	2.39	0.56
1:A:88:GLU:N	1:A:88:GLU:OE2	2.39	0.56
3:D:115:GLY:HA2	3:D:298:VAL:HG21	1.87	0.56
5:F:280:GLU:HA	5:F:283:LEU:HG	1.87	0.56
1:A:129:ASN:ND2	2:C:639:VAL:O	2.39	0.55
2:C:506:VAL:HG22	2:C:507:GLU:OE1	2.07	0.55
3:D:845:PHE:O	3:D:848:THR:OG1	2.21	0.55
4:E:80:LEU:HD23	4:E:81:THR:N	2.20	0.55
6:M:50:THR:O	6:M:54:THR:HG23	2.05	0.55
2:C:1027:HIS:HE1	2:C:1048:PHE:HA	1.71	0.55
2:C:650:ASP:OD1	2:C:651:GLY:N	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LEU:HD21	1:B:171:VAL:HG11	1.89	0.55
5:F:486:ILE:HD12	5:F:489:ILE:HD11	1.89	0.55
1:A:170:PRO:O	1:A:198:THR:OG1	2.20	0.54
2:C:829:GLU:OE1	2:C:830:ILE:N	2.40	0.54
3:D:1211:GLU:HG2	8:P:12:DG:H5"	1.88	0.54
5:F:388:MET:SD	5:F:388:MET:N	2.81	0.54
5:F:300:PHE:CZ	5:F:304:ILE:HD11	2.43	0.54
3:D:184:LEU:HD22	3:D:197:VAL:HG11	1.90	0.53
6:L:27:GLU:N	6:L:27:GLU:OE1	2.41	0.53
2:C:772:GLU:N	2:C:772:GLU:OE2	2.41	0.53
7:O:72:DG:OP2	7:O:72:DG:H3'	2.08	0.53
1:A:54:ILE:HD11	1:A:77:ILE:CD1	2.39	0.53
6:N:81:THR:OG1	6:N:98:GLU:OE1	2.26	0.53
1:A:174:VAL:HG22	1:A:196:VAL:HG23	1.91	0.53
6:K:52:TYR:OH	7:O:13:DC:OP2	2.26	0.53
3:D:731:ILE:O	3:D:836:ARG:NE	2.42	0.53
3:D:826:THR:OG1	3:D:1010:HIS:NE2	2.41	0.53
1:B:54:ILE:HD11	1:B:136:MET:SD	2.49	0.52
6:G:68:ARG:NH1	6:H:69:THR:O	2.41	0.52
6:M:83:ASP:O	6:M:85:HIS:ND1	2.42	0.52
2:C:72:SER:OG	2:C:73:GLY:N	2.42	0.52
2:C:468:ARG:NH2	2:C:522:GLU:OE1	2.42	0.52
2:C:744:ASP:OD2	2:C:746:ARG:NH2	2.43	0.52
1:A:64:THR:OG1	1:A:65:THR:N	2.42	0.52
1:B:137:GLU:OE1	1:B:137:GLU:N	2.43	0.52
2:C:1027:HIS:CE1	2:C:1048:PHE:HA	2.45	0.52
3:D:76:GLU:OE1	3:D:76:GLU:N	2.43	0.51
5:F:459:SER:O	5:F:463:GLY:N	2.43	0.51
1:A:85:VAL:HG12	1:A:118:VAL:HG22	1.92	0.51
8:P:74:DC:H2"	8:P:75:DA:C8	2.45	0.51
3:D:694:ASP:OD1	3:D:698:ARG:NE	2.42	0.51
1:B:5:GLN:OE1	1:B:6:ARG:N	2.44	0.51
2:C:1079:ASP:OD1	2:C:1105:SER:N	2.42	0.51
2:C:100:PHE:CE1	2:C:121:LEU:HD12	2.46	0.51
1:A:42:LEU:HD12	1:A:46:ILE:HD11	1.91	0.51
3:D:747:GLN:NE2	3:D:772:ILE:HD13	2.25	0.51
2:C:821:THR:HG22	2:C:821:THR:O	2.11	0.50
6:H:55:LEU:HD13	6:H:76:TYR:CE2	2.46	0.50
2:C:563:ASP:N	2:C:563:ASP:OD1	2.43	0.50
2:C:767:LEU:HD12	2:C:767:LEU:O	2.11	0.50
6:G:35:LEU:HD22	6:G:51:VAL:CG1	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HD22	1:A:159:ILE:HD12	1.93	0.50
1:B:228:ASP:OD1	1:B:229:ALA:N	2.42	0.50
3:D:1256:GLU:OE1	3:D:1256:GLU:N	2.44	0.50
6:N:68:ARG:NH2	6:N:72:GLY:O	2.45	0.50
2:C:570:ARG:NH2	2:C:963:ASP:OD2	2.44	0.50
3:D:173:ARG:NE	3:D:208:LEU:HD23	2.27	0.50
3:D:1231:LEU:O	3:D:1235:VAL:HG23	2.12	0.50
2:C:196:ARG:NH1	2:C:292:LYS:O	2.45	0.50
3:D:1162:GLU:N	3:D:1162:GLU:OE1	2.45	0.49
7:O:24:DA:H4'	7:O:25:DG:OP1	2.11	0.49
3:D:449:LEU:HD11	3:D:476:VAL:CG2	2.42	0.49
1:A:7:PRO:HG3	1:B:218:LEU:HD13	1.93	0.49
2:C:364:ILE:CD1	2:C:492:ILE:HD12	2.41	0.49
6:M:39:LEU:HD12	6:M:40:LYS:N	2.27	0.49
2:C:341:THR:N	2:C:348:GLU:OE2	2.46	0.49
6:N:83:ASP:O	6:N:85:HIS:ND1	2.43	0.49
6:K:28:GLU:OE1	6:K:28:GLU:N	2.46	0.49
2:C:1113:MET:HE2	2:C:1120:VAL:HG21	1.95	0.49
2:C:149:THR:HG22	2:C:153:THR:O	2.12	0.49
2:C:430:ASN:ND2	2:C:701:LEU:HD22	2.28	0.49
2:C:597:MET:SD	2:C:1018:LEU:HD21	2.52	0.49
1:A:110:ILE:HD11	1:A:138:LEU:HD22	1.95	0.48
7:O:23:DC:H1'	7:O:24:DA:H5'	1.95	0.48
2:C:86:ASP:OD1	2:C:89:GLY:N	2.47	0.48
2:C:803:GLU:OE1	2:C:803:GLU:N	2.44	0.48
3:D:210:ASP:O	3:D:213:GLN:NE2	2.47	0.48
3:D:314:LEU:HD23	3:D:314:LEU:H	1.79	0.48
4:E:32:TYR:CZ	4:E:75:ILE:HD12	2.49	0.48
5:F:360:ASN:OD1	5:F:361:LYS:N	2.46	0.48
3:D:36:TYR:OH	3:D:37:ARG:NH2	2.46	0.48
4:E:32:TYR:CE2	4:E:75:ILE:HD12	2.48	0.48
5:F:284:ARG:O	5:F:287:VAL:HG12	2.13	0.48
2:C:330:TYR:CE1	2:C:351:VAL:HG23	2.49	0.48
3:D:915:VAL:HG22	3:D:938:LEU:HD12	1.96	0.48
6:M:27:GLU:OE1	6:M:27:GLU:N	2.47	0.48
2:C:767:LEU:HA	2:C:770:LEU:HD23	1.94	0.47
5:F:282:ASN:HB2	5:F:311:LEU:HD11	1.96	0.47
2:C:214:ILE:HG23	2:C:214:ILE:O	2.13	0.47
2:C:359:PHE:HE2	2:C:498:ILE:HD12	1.78	0.47
2:C:318:VAL:HG13	2:C:319:LEU:HD23	1.96	0.47
3:D:184:LEU:HD22	3:D:197:VAL:CG1	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:71:DG:H2'	7:O:72:DG:C8	2.49	0.47
1:A:9:LEU:HD23	1:A:10:THR:N	2.29	0.47
2:C:330:TYR:CZ	2:C:351:VAL:HG23	2.50	0.47
2:C:510:VAL:HG21	2:C:534:LEU:CD2	2.45	0.47
3:D:596:SER:O	3:D:598:LYS:N	2.47	0.47
5:F:221:GLN:O	5:F:221:GLN:NE2	2.43	0.47
2:C:715:HIS:HB2	2:C:722:ILE:CD1	2.42	0.47
2:C:871:LEU:HB2	2:C:881:ILE:HD11	1.97	0.47
1:A:44:SER:HB3	2:C:888:GLU:OE2	2.15	0.47
1:A:72:ASP:OD1	1:A:72:ASP:N	2.48	0.47
1:A:38:LEU:HD21	1:A:208:MET:SD	2.55	0.46
1:B:51:VAL:HG11	1:B:80:ILE:HD11	1.97	0.46
5:F:354:HIS:O	5:F:358:VAL:HG23	2.15	0.46
3:D:115:GLY:HA3	3:D:298:VAL:HG21	1.98	0.46
3:D:1089:GLU:N	3:D:1089:GLU:OE1	2.48	0.46
2:C:1108:VAL:HG22	3:D:324:LEU:HD21	1.98	0.46
4:E:17:ASP:OD1	4:E:18:GLU:N	2.48	0.46
5:F:472:LEU:HD13	5:F:487:ARG:HB2	1.98	0.46
2:C:567:VAL:HG12	2:C:571:GLN:OE1	2.16	0.46
3:D:421:ARG:NH2	8:P:18:DT:OP2	2.48	0.46
6:G:121:ALA:N	6:H:127:PHE:O	2.47	0.46
1:A:33:THR:HG23	1:B:36:ASN:OD1	2.16	0.46
1:B:129:ASN:OD1	1:B:129:ASN:N	2.47	0.46
2:C:91:MET:SD	2:C:92:SER:N	2.88	0.46
1:A:42:LEU:HD21	1:A:196:VAL:HG21	1.97	0.46
2:C:140:VAL:HG21	2:C:404:ILE:HD11	1.96	0.46
6:G:35:LEU:HD22	6:G:51:VAL:HG11	1.98	0.46
2:C:318:VAL:CG1	2:C:319:LEU:HD23	2.47	0.45
3:D:180:ASP:OD1	3:D:181:LEU:N	2.49	0.45
3:D:575:THR:O	3:D:575:THR:HG22	2.17	0.45
8:P:63:DA:H1'	8:P:64:DA:H5'	1.97	0.45
5:F:391:GLU:N	5:F:391:GLU:OE1	2.47	0.45
5:F:416:SER:OG	5:F:417:GLU:OE2	2.35	0.45
6:N:129:THR:OG1	6:N:133:CYS:SG	2.74	0.45
2:C:390:MET:N	2:C:390:MET:HE2	2.32	0.45
3:D:1024:PRO:O	3:D:1028:GLU:HG3	2.17	0.45
6:L:50:THR:HG21	7:O:5:DG:O5'	2.17	0.45
2:C:851:VAL:O	2:C:851:VAL:HG23	2.17	0.45
3:D:586:PHE:HE2	3:D:796:MET:HG2	1.82	0.45
5:F:378:THR:OG1	5:F:380:GLU:OE2	2.34	0.45
5:F:454:GLU:HB3	5:F:493:THR:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:472:LEU:HD12	8:P:48:DG:OP2	2.16	0.45
6:L:90:CYS:SG	6:L:93:CYS:N	2.85	0.45
8:P:75:DA:H4'	8:P:76:DT:OP1	2.16	0.45
2:C:430:ASN:ND2	2:C:601:ALA:O	2.50	0.44
3:D:336:ALA:HB1	5:F:406:LEU:CD2	2.46	0.44
6:K:54:THR:O	6:K:58:LEU:HD23	2.16	0.44
7:O:72:DG:H3'	7:O:72:DG:P	2.57	0.44
2:C:130:ASN:OD1	2:C:131:GLU:N	2.50	0.44
2:C:540:PHE:CD2	2:C:545:VAL:HG11	2.51	0.44
2:C:1108:VAL:HG13	3:D:324:LEU:HD22	1.99	0.44
1:B:120:ASN:OD1	1:B:120:ASN:N	2.51	0.44
2:C:436:THR:HG21	2:C:599:ARG:HD3	2.00	0.44
3:D:739:GLU:OE1	3:D:740:ILE:HG23	2.17	0.44
6:K:13:THR:OG1	8:P:67:DC:OP1	2.31	0.44
2:C:1056:MET:HB3	3:D:503:THR:HG23	1.98	0.44
2:C:294:TYR:CE1	2:C:319:LEU:HD22	2.52	0.44
2:C:840:ASP:OD1	2:C:840:ASP:N	2.50	0.44
6:H:39:LEU:HD21	6:H:46:VAL:HG21	2.00	0.44
6:K:70:ALA:O	6:L:68:ARG:NH2	2.50	0.44
1:A:217:GLU:OE2	1:B:6:ARG:NH1	2.50	0.44
2:C:869:ASP:OD2	2:C:1021:LEU:HD22	2.17	0.44
8:P:60:DC:H2'	8:P:61:DT:H72	2.00	0.44
1:B:151:GLN:OE1	1:B:153:LYS:N	2.45	0.44
4:E:32:TYR:CE1	4:E:80:LEU:HD22	2.53	0.44
5:F:260:LEU:H	5:F:260:LEU:HD12	1.82	0.44
2:C:554:VAL:HG12	2:C:554:VAL:O	2.17	0.43
2:C:806:LEU:HD13	5:F:464:LEU:CD2	2.48	0.43
2:C:1030:SER:OG	2:C:1031:THR:N	2.50	0.43
5:F:301:LEU:HA	5:F:304:ILE:HD12	1.99	0.43
5:F:326:PHE:CE1	5:F:330:ALA:HB2	2.52	0.43
2:C:546:LEU:HD11	2:C:554:VAL:HG12	2.01	0.43
3:D:981:LYS:HD2	3:D:982:LEU:O	2.18	0.43
6:G:104:VAL:HG11	6:H:107:TRP:CE3	2.54	0.43
2:C:30:GLU:N	2:C:30:GLU:OE1	2.51	0.43
2:C:1091:ILE:HG21	3:D:454:PRO:HB2	1.99	0.43
3:D:918:ARG:NH2	3:D:1138:GLU:OE2	2.51	0.43
6:M:84:HIS:HE2	6:M:122:HIS:CE1	2.36	0.43
5:F:231:GLU:HA	5:F:234:VAL:HG22	2.00	0.43
6:G:115:HIS:O	6:G:115:HIS:ND1	2.51	0.43
6:M:39:LEU:HD13	6:M:46:VAL:HB	1.99	0.43
2:C:255:THR:OG1	2:C:260:ASP:OD2	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:119:ASP:C	3:D:120:LEU:HD12	2.38	0.43
3:D:1159:LEU:HD12	3:D:1159:LEU:H	1.84	0.43
1:A:69:VAL:O	2:C:641:ALA:HB2	2.19	0.43
1:A:105:VAL:HG12	1:A:126:ALA:H	1.84	0.43
2:C:215:ASP:OD1	2:C:215:ASP:O	2.36	0.43
2:C:329:LYS:O	2:C:333:LYS:HG3	2.19	0.43
3:D:592:SER:OG	3:D:593:GLU:N	2.52	0.43
3:D:858:THR:O	3:D:862:THR:OG1	2.36	0.43
7:O:79:DG:N2	8:P:7:DC:O2	2.52	0.43
5:F:289:LEU:O	5:F:292:ARG:HB2	2.18	0.42
2:C:366:ASN:OD1	2:C:366:ASN:N	2.52	0.42
2:C:723:LEU:HD23	2:C:881:ILE:HD12	2.01	0.42
3:D:354:LEU:HD12	3:D:374:LEU:HD22	2.02	0.42
5:F:416:SER:OG	5:F:420:ASP:OD2	2.37	0.42
3:D:58:TRP:CE3	3:D:68:VAL:HG12	2.55	0.42
2:C:705:LEU:HD13	2:C:727:LEU:HD11	2.01	0.42
2:C:778:ILE:HD11	2:C:836:VAL:HG12	2.01	0.42
3:D:919:MET:O	3:D:957:ARG:N	2.43	0.42
1:A:54:ILE:HD11	1:A:77:ILE:HD11	2.01	0.42
1:A:212:GLY:O	1:A:216:VAL:HG13	2.19	0.42
2:C:640:SER:OG	2:C:641:ALA:N	2.52	0.42
3:D:659:LEU:HD22	3:D:661:THR:HB	2.01	0.42
1:B:185:GLN:O	1:B:185:GLN:HG3	2.20	0.42
3:D:354:LEU:N	3:D:370:GLU:OE2	2.53	0.42
3:D:770:ILE:HD11	3:D:826:THR:CG2	2.44	0.42
5:F:363:ALA:O	5:F:367:ARG:HG3	2.20	0.42
1:B:152:ASN:N	1:B:152:ASN:OD1	2.52	0.42
2:C:50:GLY:O	2:C:55:LYS:NZ	2.53	0.42
2:C:430:ASN:HD22	2:C:701:LEU:HD22	1.85	0.42
5:F:386:LEU:H	5:F:386:LEU:HD12	1.84	0.42
5:F:392:LYS:O	5:F:396:VAL:HG23	2.20	0.42
2:C:1113:MET:HE3	2:C:1120:VAL:HG21	2.01	0.41
3:D:920:LEU:CD2	3:D:938:LEU:HD21	2.49	0.41
6:G:126:ILE:HD12	6:H:122:HIS:HA	2.02	0.41
1:A:59:VAL:HG13	1:A:64:THR:HG23	2.01	0.41
2:C:214:ILE:HG22	2:C:220:GLN:HE22	1.86	0.41
3:D:884:GLU:HA	3:D:985:ILE:HD11	2.02	0.41
7:O:23:DC:H2'	7:O:23:DC:OP1	2.20	0.41
3:D:888:THR:O	3:D:957:ARG:NH2	2.54	0.41
3:D:1172:GLU:OE1	3:D:1175:ARG:NH1	2.53	0.41
6:M:58:LEU:O	6:M:62:GLY:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:841:ARG:NH2	2:C:848:PRO:O	2.53	0.41
4:E:42:ALA:HB3	4:E:54:TYR:CE2	2.55	0.41
3:D:1050:ILE:HG22	3:D:1084:GLU:HG2	2.02	0.41
8:P:12:DG:H2'	8:P:13:DC:C6	2.56	0.41
1:A:7:PRO:CG	1:B:218:LEU:HD13	2.51	0.41
6:G:124:VAL:HG22	6:H:124:VAL:HG13	2.03	0.41
7:O:23:DC:C1'	7:O:24:DA:H5'	2.51	0.41
2:C:305:ASN:OD1	2:C:306:LYS:N	2.53	0.41
3:D:449:LEU:HD22	3:D:484:TYR:HE1	1.86	0.41
6:M:52:TYR:OH	7:O:19:DT:OP1	2.39	0.41
2:C:200:LEU:HD11	2:C:212:VAL:CG1	2.51	0.41
2:C:1022:VAL:HG23	3:D:429:VAL:HG12	2.02	0.41
3:D:1131:SER:C	3:D:1132:ILE:HD13	2.41	0.41
2:C:932:VAL:O	2:C:932:VAL:HG23	2.21	0.40
5:F:461:ARG:CA	5:F:475:ILE:HD11	2.51	0.40
1:A:41:THR:HG23	1:A:211:ALA:HB1	2.02	0.40
1:A:81:LYS:NZ	1:A:165:ASP:OD1	2.41	0.40
1:B:66:VAL:HG13	1:B:66:VAL:O	2.21	0.40
3:D:827:ILE:HD13	3:D:846:ILE:HD12	2.04	0.40
3:D:868:LEU:HD13	3:D:1027:VAL:HG12	2.02	0.40
5:F:235:GLU:OE1	5:F:239:ARG:NH1	2.55	0.40
1:B:77:ILE:HG23	1:B:164:VAL:HG23	2.02	0.40
3:D:805:ASN:OD1	3:D:806:MET:N	2.51	0.40
3:D:1211:GLU:CG	8:P:12:DG:H5"	2.51	0.40
5:F:460:MET:SD	5:F:470:LYS:NZ	2.94	0.40
6:K:95:LYS:NZ	6:K:130:CYS:SG	2.86	0.40
3:D:354:LEU:CD2	3:D:358:LEU:HD13	2.52	0.40
5:F:378:THR:HG23	5:F:381:GLU:H	1.87	0.40
6:M:42:LYS:NZ	6:M:44:ASP:OD1	2.40	0.40

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	224/340 (66%)	215 (96%)	9 (4%)	0	100	100
1	B	231/340 (68%)	221 (96%)	10 (4%)	0	100	100
1	S	55/340 (16%)	55 (100%)	0	0	100	100
2	C	1114/1161 (96%)	1071 (96%)	43 (4%)	0	100	100
3	D	1257/1307 (96%)	1212 (96%)	45 (4%)	0	100	100
4	E	75/90 (83%)	73 (97%)	2 (3%)	0	100	100
5	F	299/531 (56%)	292 (98%)	7 (2%)	0	100	100
6	G	129/159 (81%)	126 (98%)	3 (2%)	0	100	100
6	H	129/159 (81%)	128 (99%)	1 (1%)	0	100	100
6	K	129/159 (81%)	127 (98%)	2 (2%)	0	100	100
6	L	129/159 (81%)	127 (98%)	2 (2%)	0	100	100
6	M	129/159 (81%)	127 (98%)	2 (2%)	0	100	100
6	N	129/159 (81%)	128 (99%)	1 (1%)	0	100	100
All	All	4029/5063 (80%)	3902 (97%)	127 (3%)	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	194/279 (70%)	188 (97%)	6 (3%)	40	70
1	B	199/279 (71%)	193 (97%)	6 (3%)	41	70
1	S	47/279 (17%)	46 (98%)	1 (2%)	53	78
2	C	942/979 (96%)	922 (98%)	20 (2%)	53	78
3	D	1054/1095 (96%)	1029 (98%)	25 (2%)	49	76
4	E	64/74 (86%)	61 (95%)	3 (5%)	26	59
5	F	258/430 (60%)	251 (97%)	7 (3%)	44	73
6	G	99/120 (82%)	92 (93%)	7 (7%)	14	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	H	99/120 (82%)	93 (94%)	6 (6%)	18	51
6	K	99/120 (82%)	97 (98%)	2 (2%)	55	79
6	L	99/120 (82%)	93 (94%)	6 (6%)	18	51
6	M	99/120 (82%)	95 (96%)	4 (4%)	31	63
6	N	99/120 (82%)	96 (97%)	3 (3%)	41	70
All	All	3352/4135 (81%)	3256 (97%)	96 (3%)	45	71

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	PHE
1	A	105	VAL
1	A	110	ILE
1	A	136	MET
1	A	208	MET
1	A	223	ARG
1	B	61	HIS
1	B	87	SER
1	B	98	ARG
1	B	136	MET
1	B	151	GLN
1	B	152	ASN
2	C	104	LYS
2	C	142	MET
2	C	207	ARG
2	C	221	SER
2	C	250	LEU
2	C	259	ASP
2	C	264	ASP
2	C	270	ARG
2	C	303	LYS
2	C	359	PHE
2	C	384	ARG
2	C	401	GLN
2	C	412	SER
2	C	503	ARG
2	C	640	SER
2	C	840	ASP
2	C	852	ASN
2	C	908	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	911	ARG
2	C	1023	ASP
3	D	8	ASP
3	D	44	ASP
3	D	60	CYS
3	D	70	PHE
3	D	75	CYS
3	D	126	GLU
3	D	138	PHE
3	D	176	LYS
3	D	214	ARG
3	D	242	ARG
3	D	252	PHE
3	D	302	PHE
3	D	359	ASP
3	D	383	ASP
3	D	447	MET
3	D	589	THR
3	D	735	ASP
3	D	747	GLN
3	D	750	LYS
3	D	762	LYS
3	D	836	ARG
3	D	857	ASP
3	D	981	LYS
3	D	1155	ASP
3	D	1211	GLU
4	E	21	GLU
4	E	32	TYR
4	E	83	GLU
5	F	232	GLN
5	F	291	LYS
5	F	327	SER
5	F	421	LEU
5	F	432	ASP
5	F	468	GLN
5	F	502	ARG
6	G	9	LYS
6	G	79	CYS
6	G	90	CYS
6	G	91	ARG
6	G	97	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	G	99	VAL
6	G	127	PHE
6	H	16	ARG
6	H	29	PHE
6	H	58	LEU
6	H	67	LEU
6	H	78	ARG
6	H	127	PHE
6	K	90	CYS
6	K	106	LYS
6	L	16	ARG
6	L	52	TYR
6	L	56	GLN
6	L	81	THR
6	L	87	HIS
6	L	115	HIS
6	M	28	GLU
6	M	52	TYR
6	M	60	ASP
6	M	90	CYS
6	N	16	ARG
6	N	36	HIS
6	N	53	ARG
1	S	304	MET

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

Mol	Chain	Res	Type
2	C	916	GLN
6	H	122	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 21 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.

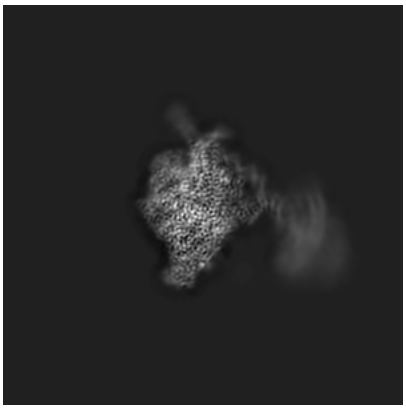
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-33032. These allow visual inspection of the internal detail of the map and identification of artifacts.

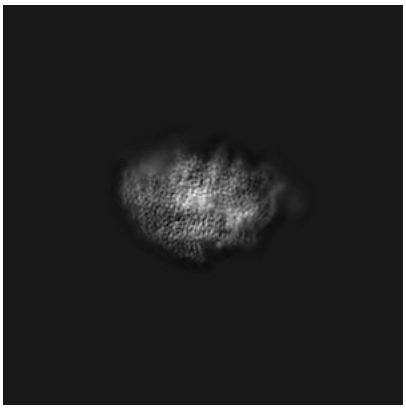
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

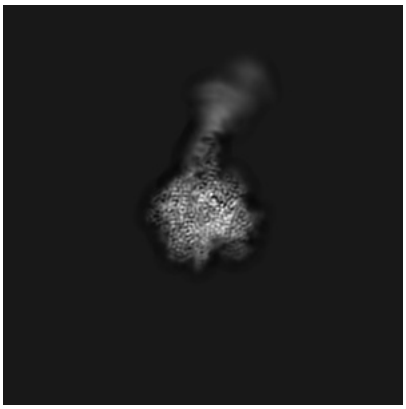
6.1.1 Primary map



X

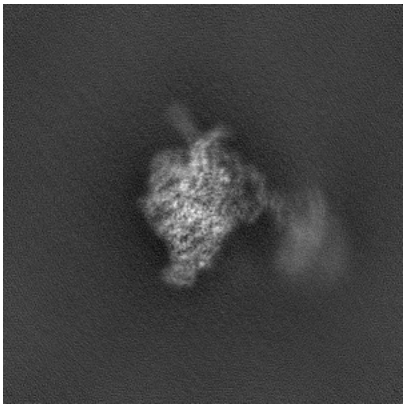


Y

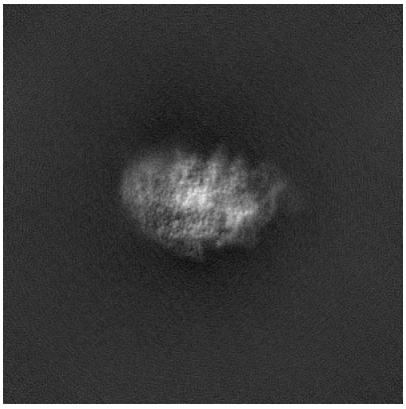


Z

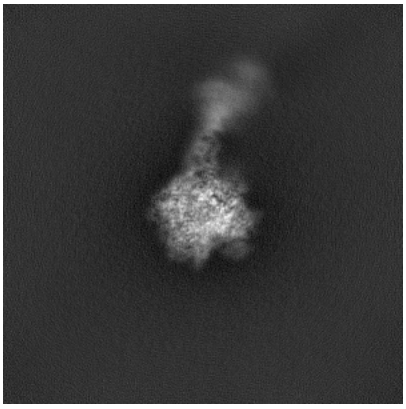
6.1.2 Raw map



X



Y

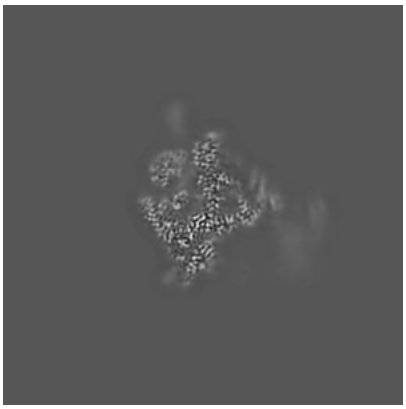


Z

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

6.2 Central slices (i)

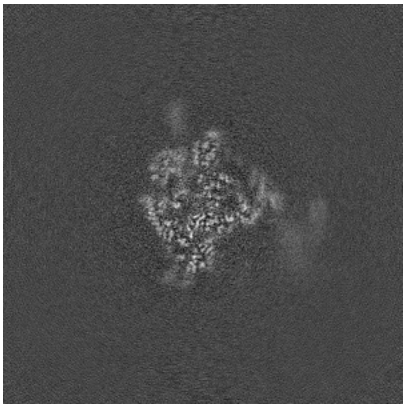
6.2.1 Primary map

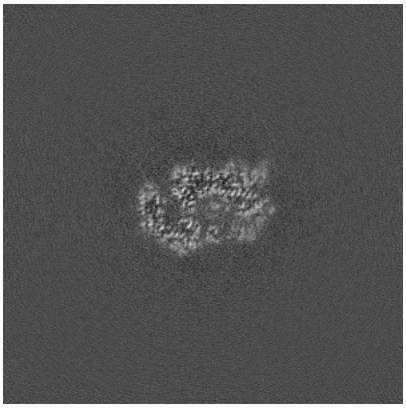

X Index: 192

Y Index: 192

Z Index: 192

6.2.2 Raw map


X Index: 192


Y Index: 192

Z Index: 192

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

6.3 Largest variance slices (i)

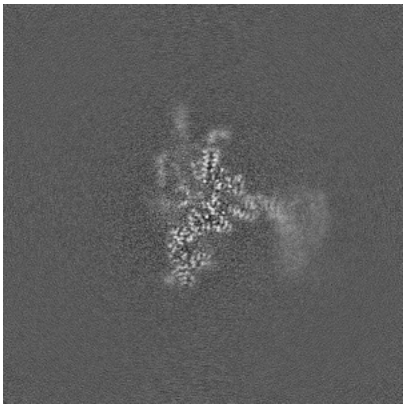
6.3.1 Primary map

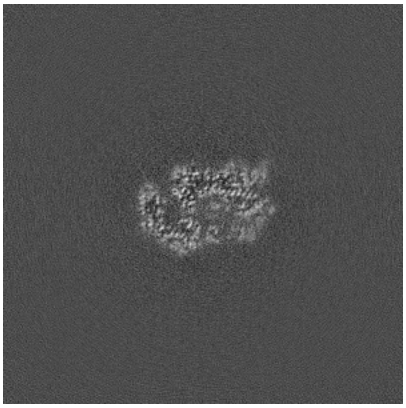
X Index: 200

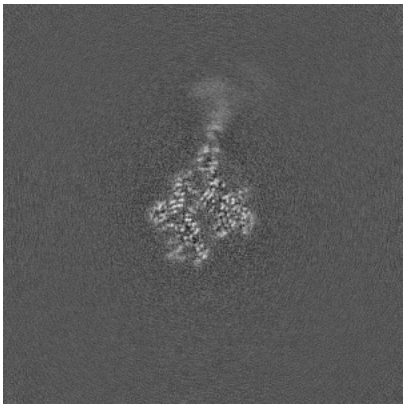
Y Index: 192

Z Index: 178

6.3.2 Raw map


X Index: 200

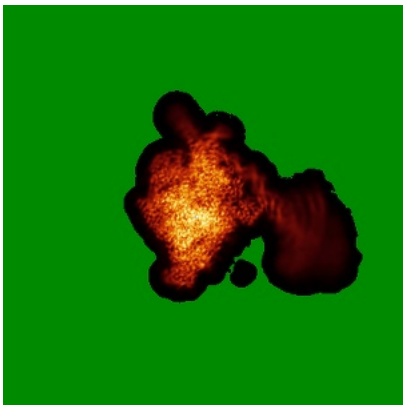

Y Index: 192

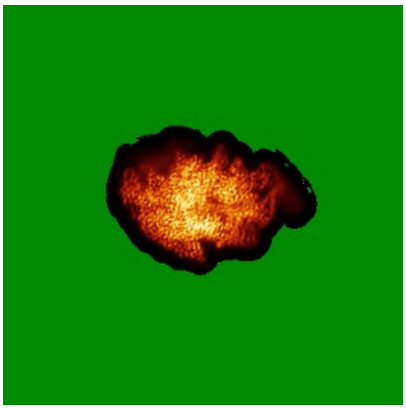

Z Index: 183

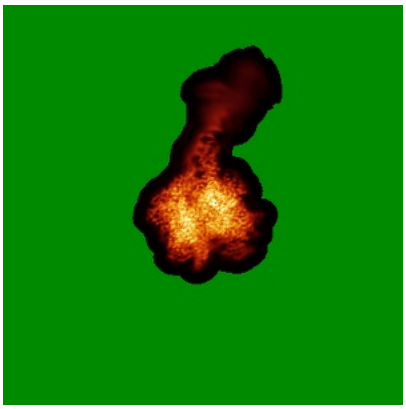
The images above show the largest variance slices of the map in three orthogonal directions.

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

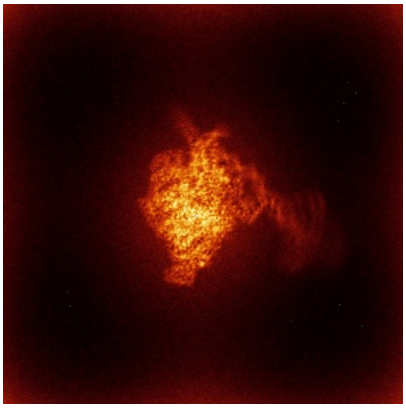
6.4.1 Primary map

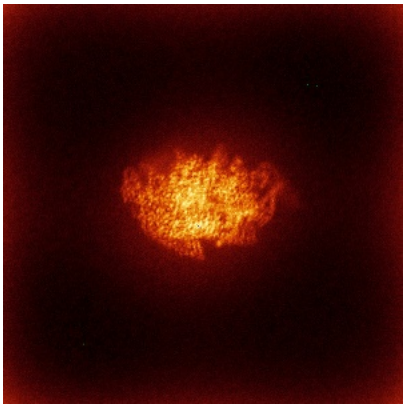

X

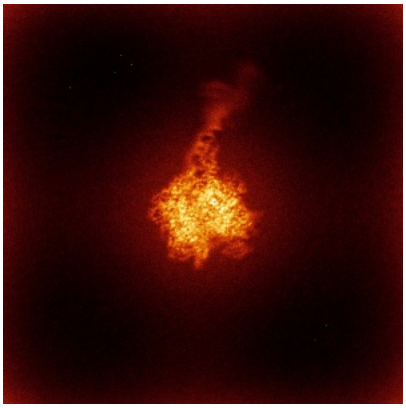

Y


Z

6.4.2 Raw map


X

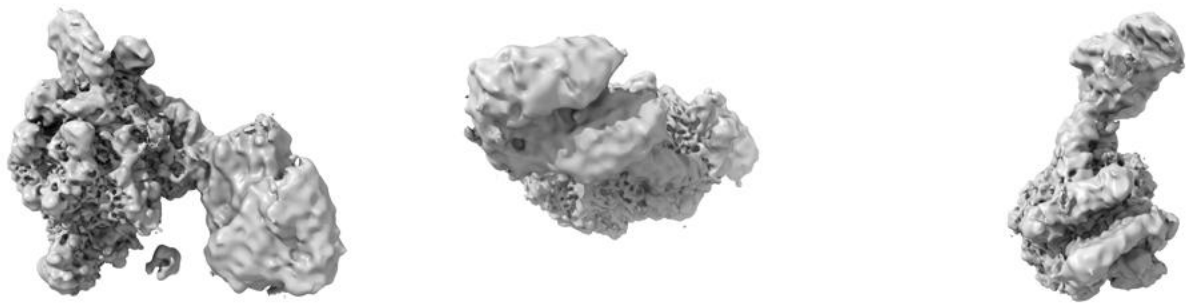

Y


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)

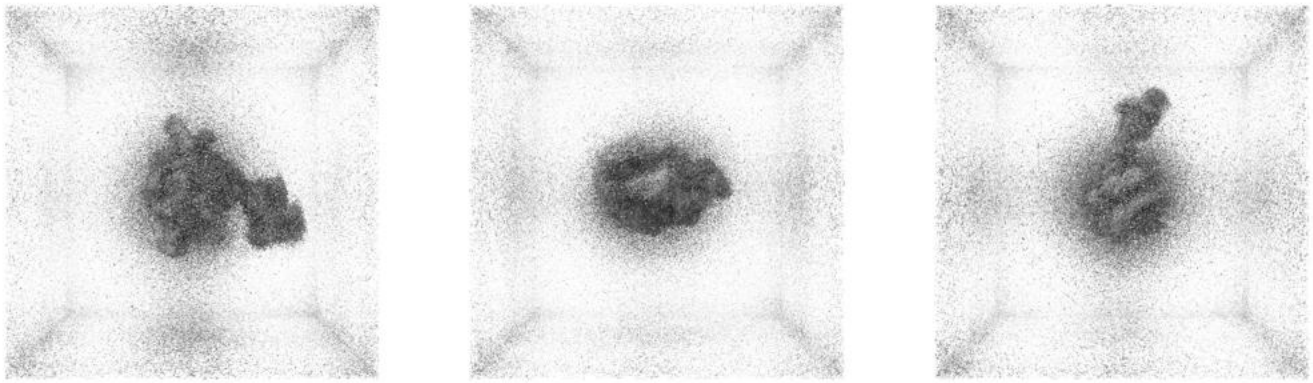
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

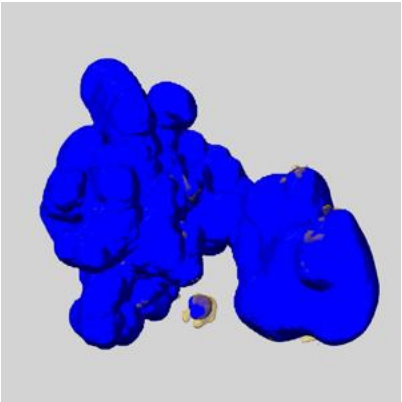
6.6 Mask visualisation (i)

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

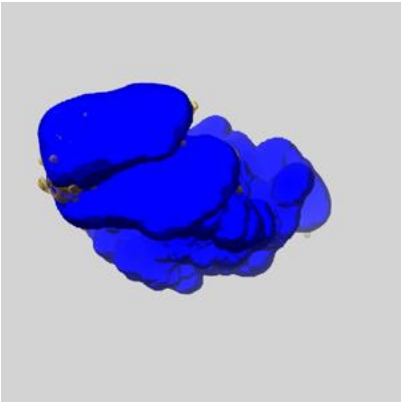
A mask typically either:

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

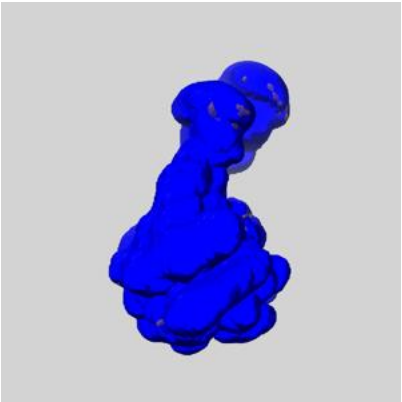
6.6.1 emd_33032_msk_1.map (i)



X



Y

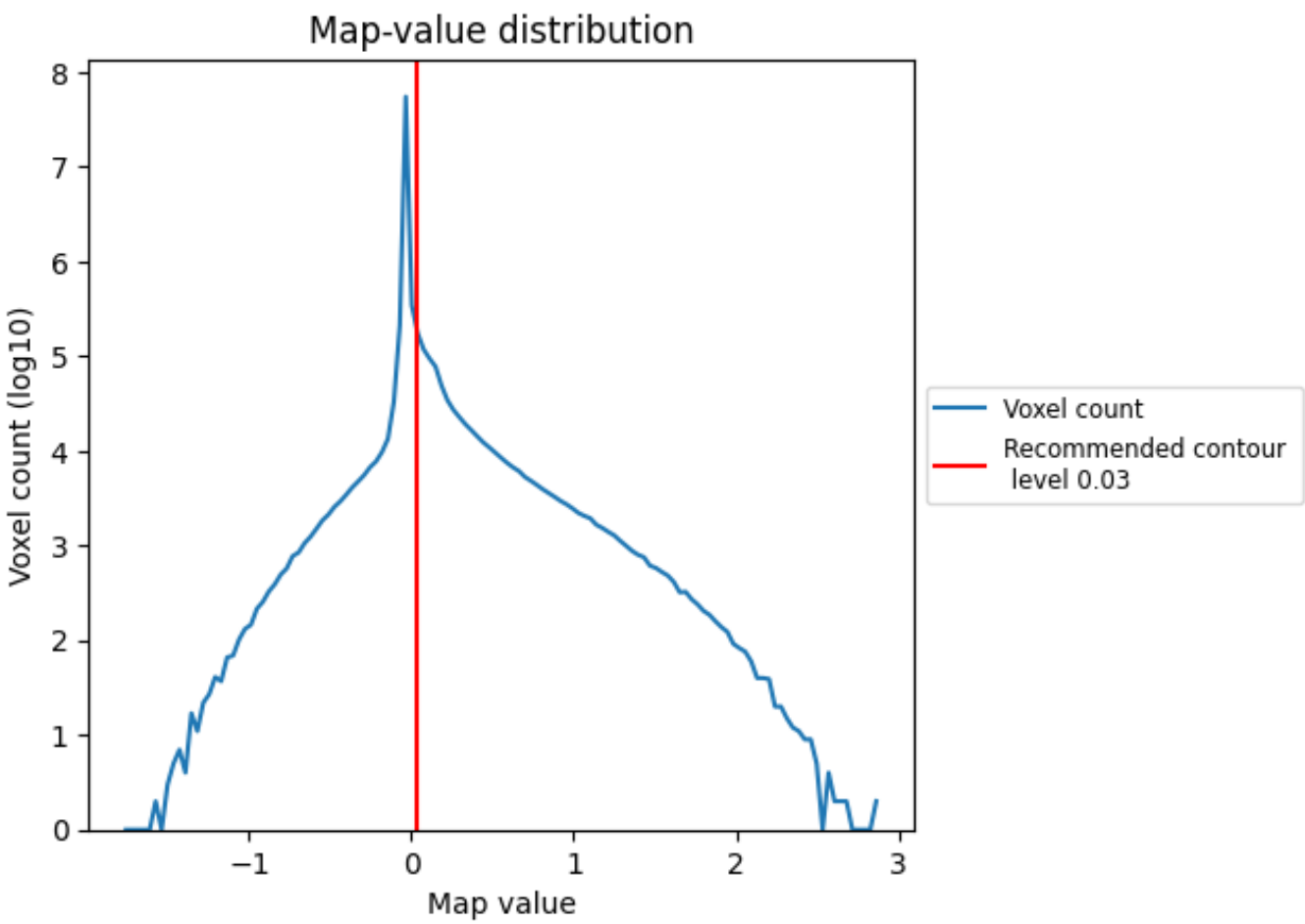


Z

7 Map analysis (i)

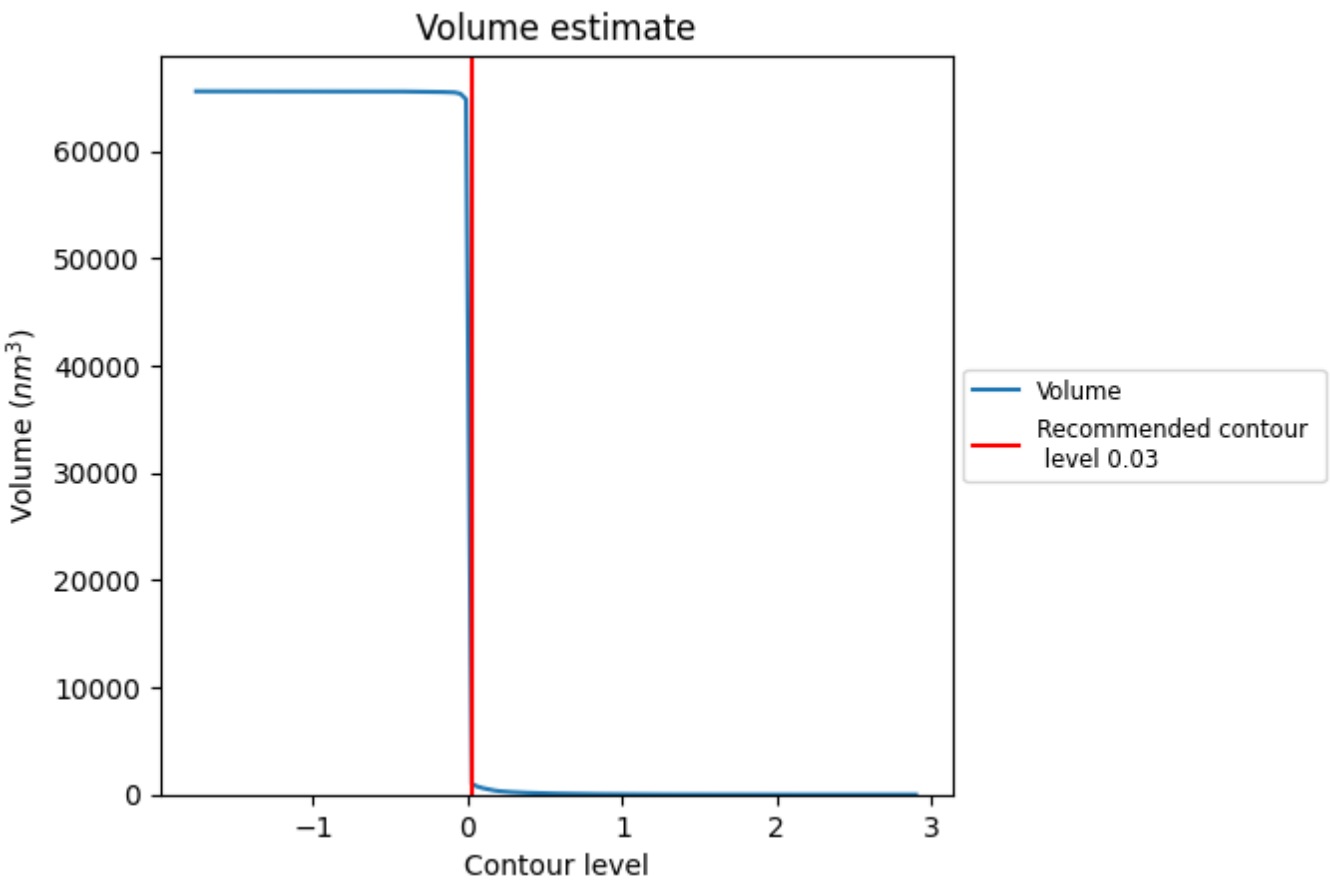
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

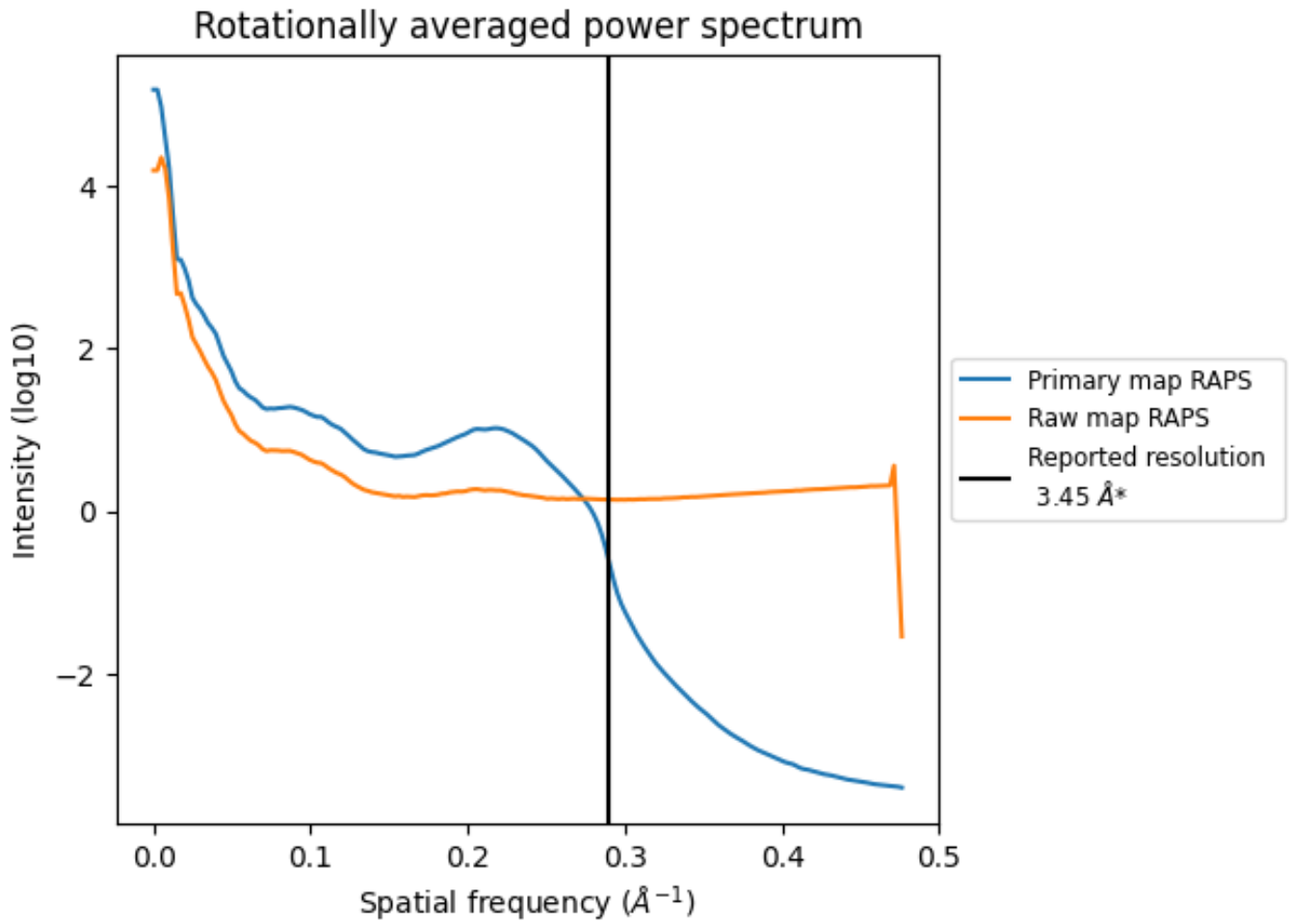
7.2 Volume estimate (i)



The volume at the recommended contour level is 972 nm^3; this corresponds to an approximate mass of 878 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)

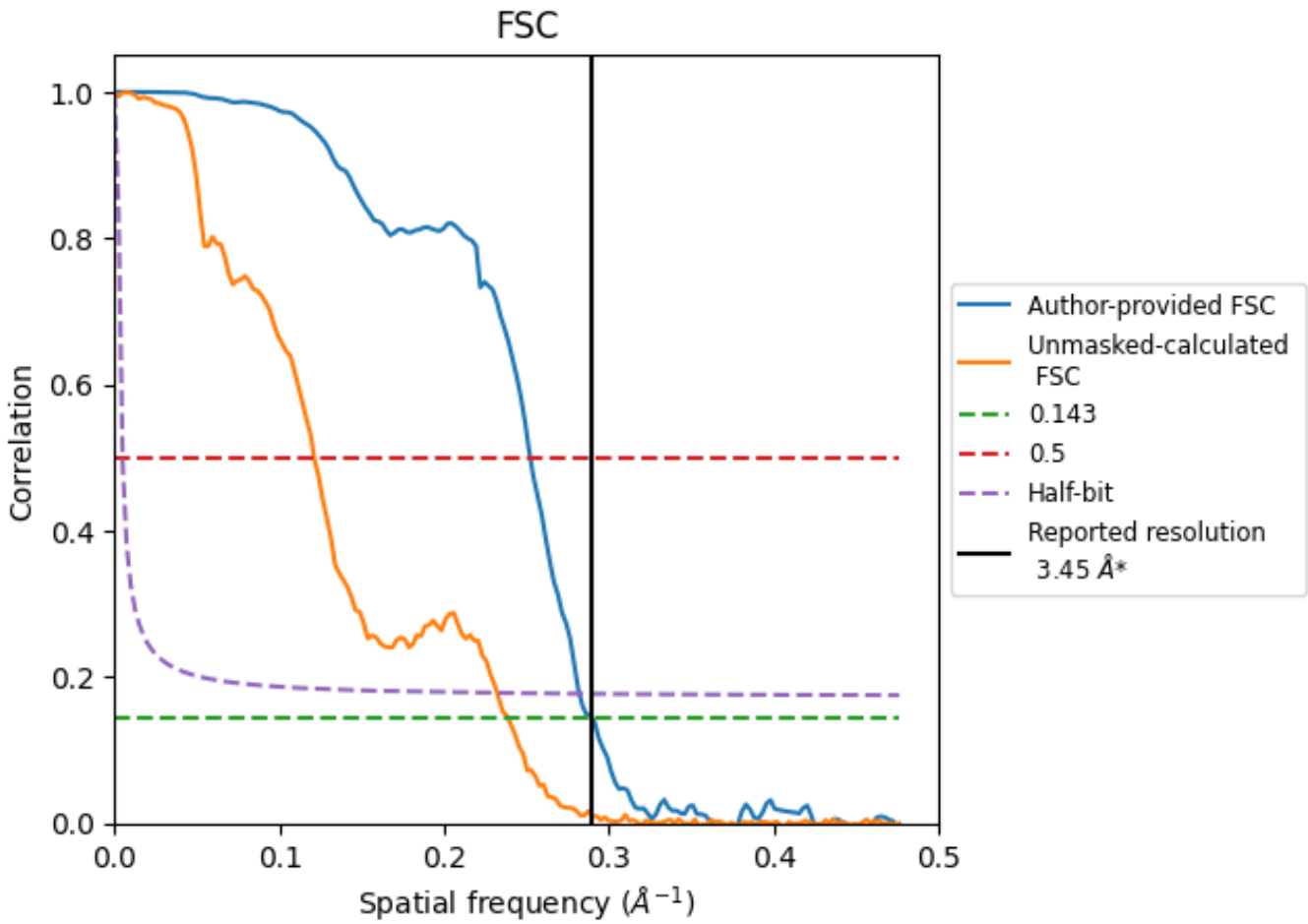


*Reported resolution corresponds to spatial frequency of 0.290 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.290 Å^{-1}

8.2 Resolution estimates (i)

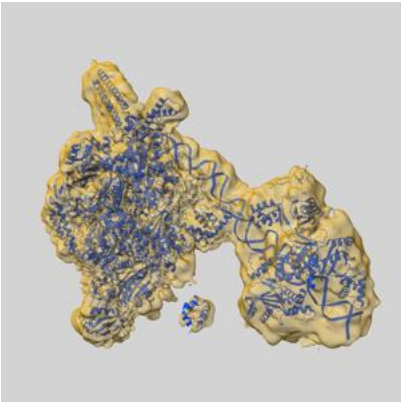
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	3.45	3.96	3.54
Unmasked-calculated*	4.19	8.25	4.31

*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 4.19 differs from the reported value 3.45 by more than 10 %

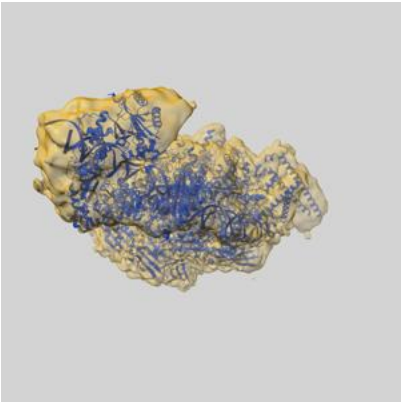
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-33032 and PDB model 7X75. Per-residue inclusion information can be found in section 3 on page 10.

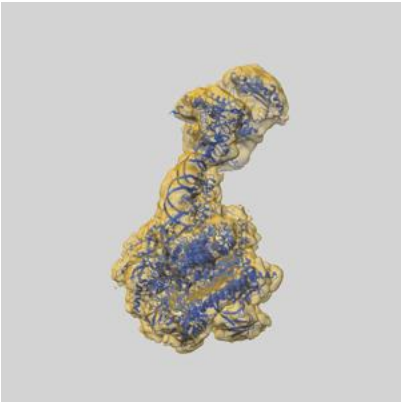
9.1 Map-model overlay (i)



X



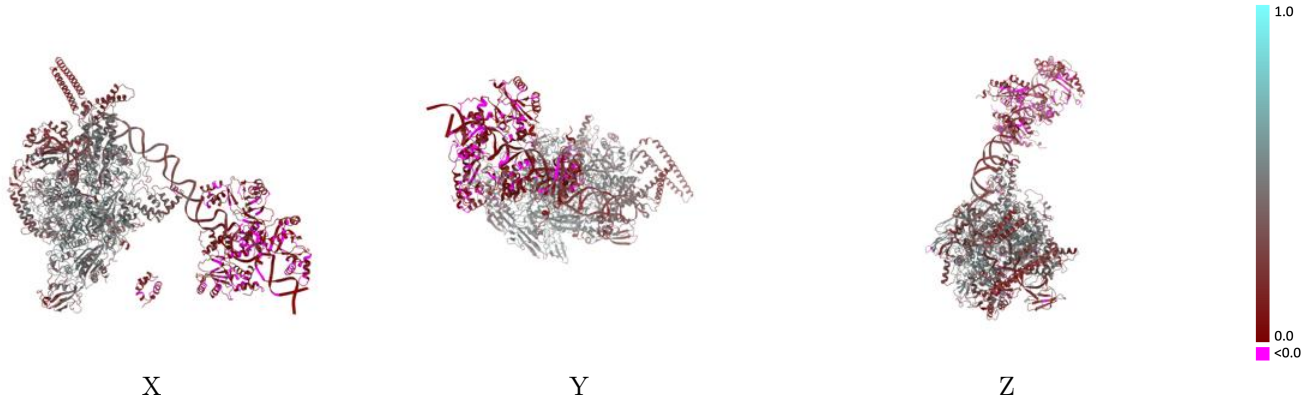
Y



Z

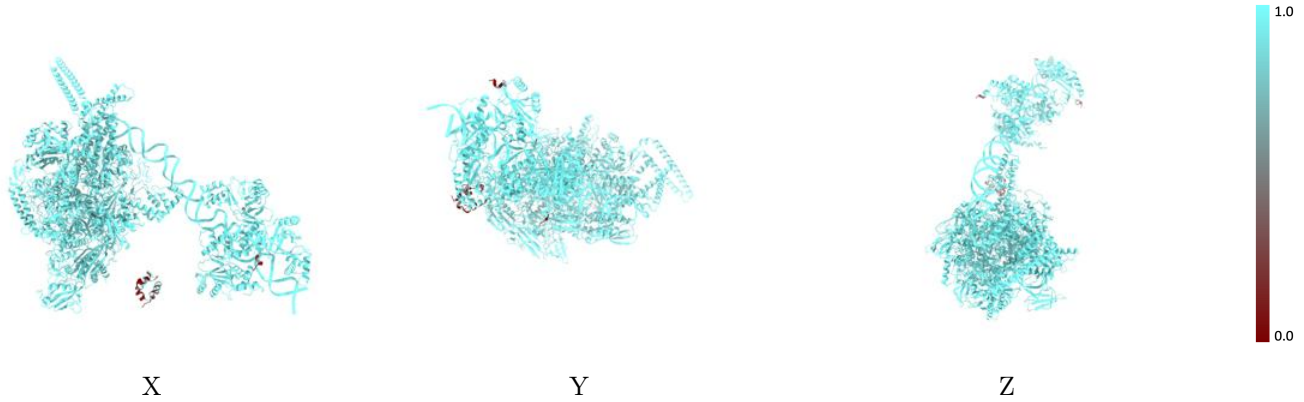
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



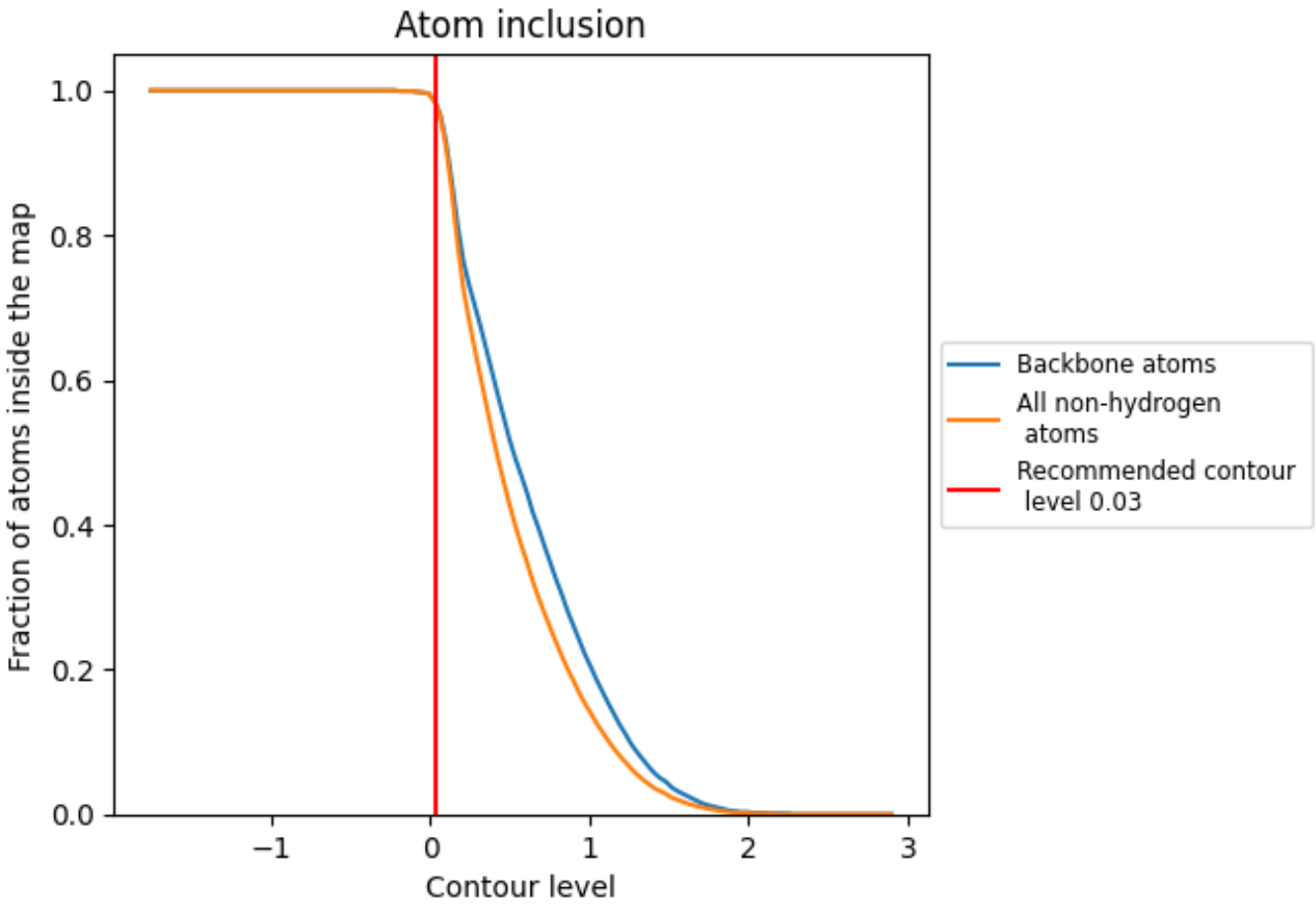
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9830	0.3300
A	0.9910	0.4370
B	0.9910	0.3820
C	0.9930	0.4330
D	0.9870	0.4130
E	0.9860	0.4070
F	0.9910	0.3360
G	0.9820	0.0770
H	0.9820	0.1010
K	0.9730	0.0490
L	0.9870	0.0640
M	0.9950	0.0900
N	0.9960	0.0720
O	0.9990	0.2180
P	0.9890	0.1910
S	0.4410	0.0860