



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 02:54 PM UTC

PDB ID : 7X76 / pdb_00007x76
EMDB ID : EMD-33033
Title : Cryo-EM structure of Streptomyces coelicolor RNAP-promoter open complex
with two Zur dimers
Authors : Yang, X.; Zheng, J.
Deposited on : 2022-03-09
Resolution : 3.67 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

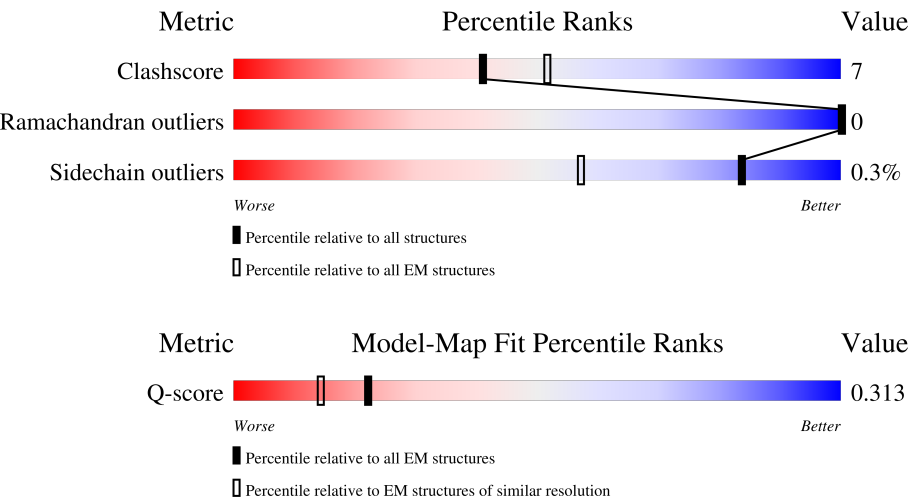
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.67 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.



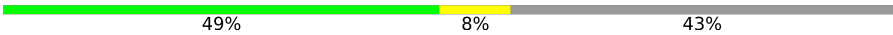
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11424 (3.17 - 4.17)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	340	
1	B	340	
1	S	340	
2	C	1161	

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Mol	Chain	Length	Quality of chain
3	D	1307	 81% 15% .
4	E	90	 63% 22% 14%
5	F	531	 49% 8% 43%
6	G	159	 77% 5% 18%
6	H	159	 68% 14% 18%
6	M	159	 68% 14% 18%
6	N	159	 69% 13% 18%
7	O	84	 80% 19% .
8	P	84	 79% 21%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 64334 atoms, of which 31436 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
1	A	226	Total	C	H	N	O	S	0	0
			3539	1102	1797	302	334	4		
1	B	233	Total	C	H	N	O	S	0	0
			3633	1131	1841	309	347	5		
1	S	57	Total	C	H	N	O	S	0	0
			891	274	453	77	85	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	1116	Total	C	H	N	O	S	0	0
			17325	5450	8633	1513	1698	31		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	1259	Total	C	H	N	O	S	0	0
			19864	6161	10018	1787	1857	41		

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
4	E	77	Total	C	H	N	O	0	0
			1202	382	605	98	117		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	301	Total	C	H	N	O	S	0	0
			4834	1509	2438	426	454	7		

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
6	G	131	Total	C	H	N	O	S	0	0
			1931	603	947	185	190	6		
6	H	131	Total	C	H	N	O	S	0	0
			1931	603	947	185	190	6		
6	M	131	Total	C	H	N	O	S	0	0
			1932	603	948	185	190	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
6	N	131	Total	C	H	N	O	S	0	0
			1931	603	947	185	190	6		

There are 80 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
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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
7	O	84	Total	C	H	N	O	P	0	0
			2648	810	934	315	505	84		

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

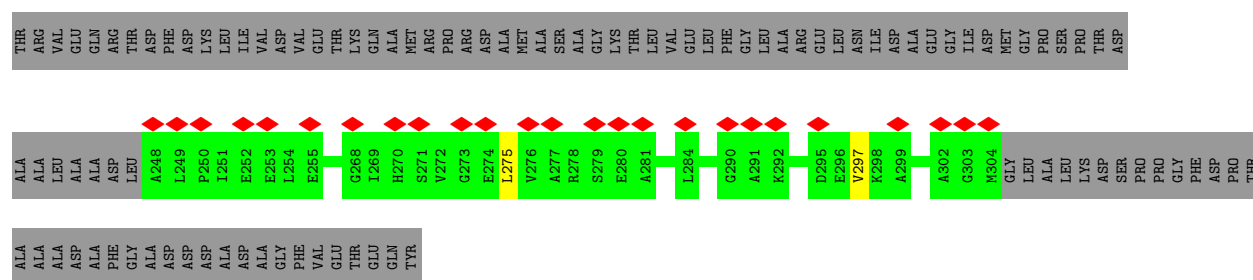
Mol	Chain	Residues	Atoms						AltConf	Trace
8	P	84	Total	C	H	N	O	P	0	0
			2658	815	928	328	503	84		

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

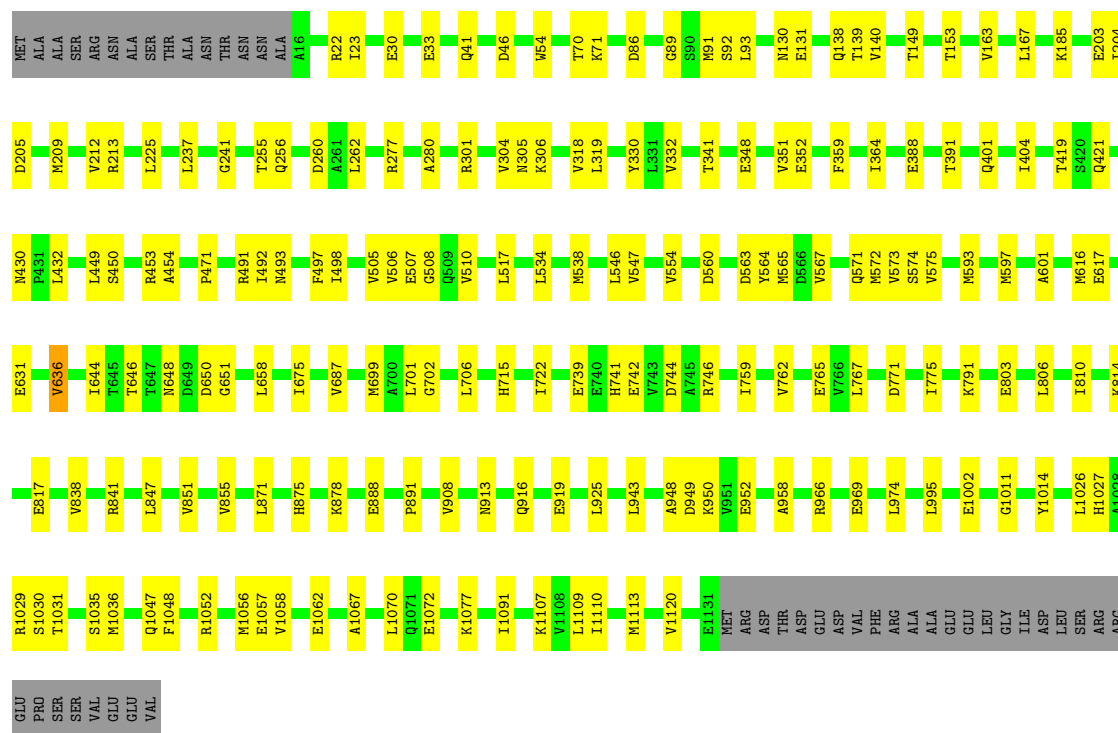
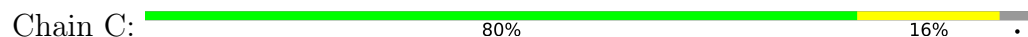
Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total	Mg	0
			1	1	

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

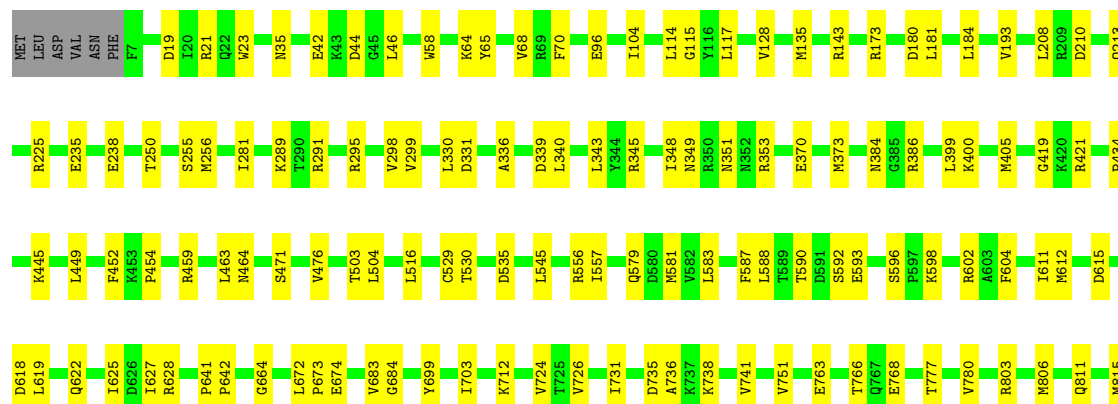
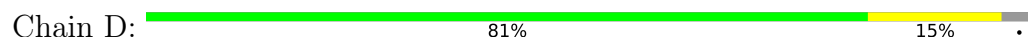
Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	
10	G	3	Total	Zn	0
			3	3	
10	H	3	Total	Zn	0
			3	3	
10	M	3	Total	Zn	0
			3	3	
10	N	3	Total	Zn	0
			3	3	

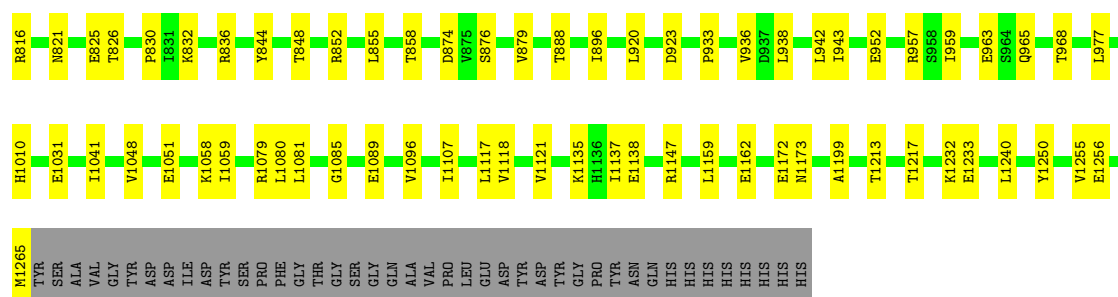


- Molecule 2: DNA-directed RNA polymerase subunit beta



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

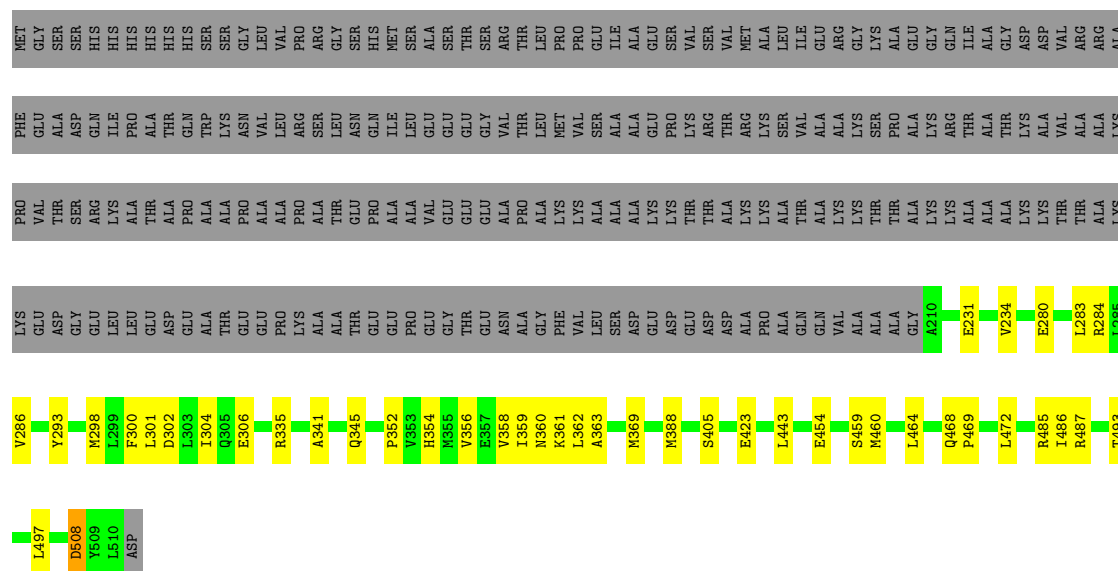




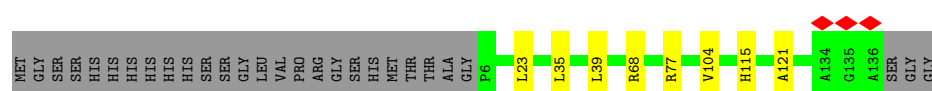
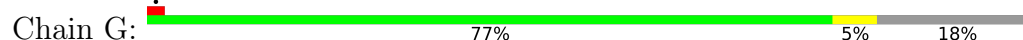
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase principal sigma factor HrdB

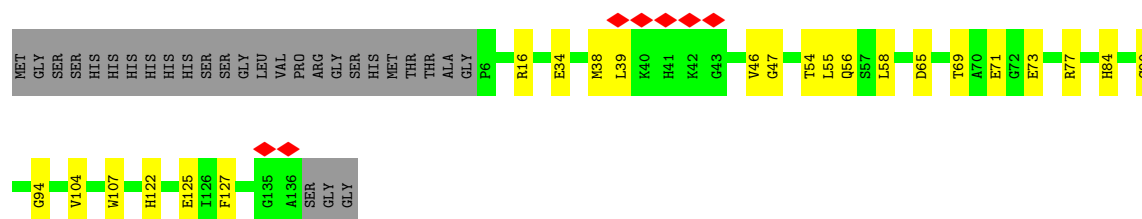


- Molecule 6: Putative metal uptake regulation protein



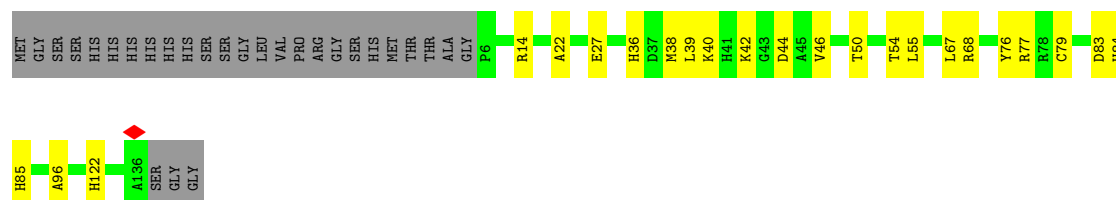
- Molecule 6: Putative metal uptake regulation protein





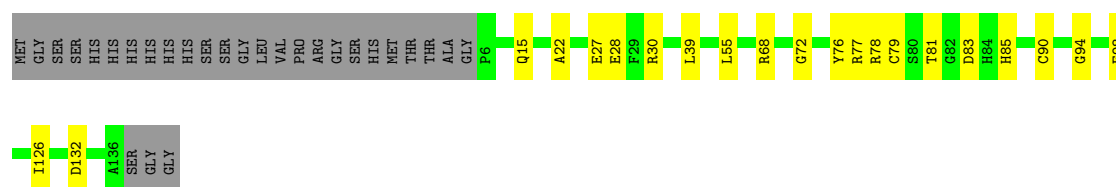
- Molecule 6: Putative metal uptake regulation protein

Chain M: 68% 14% 18%



- Molecule 6: Putative metal uptake regulation protein

Chain N: 69% 13% 18%



- Molecule 7: DNA (84-MER)

Chain O: 80% 19% 1%



- Molecule 8: DNA (84-MER)

Chain P: 79% 21% 0%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54779	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	2.275	Depositor
Minimum map value	-1.365	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.02	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: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/1768	0.43	0/2400
1	B	0.17	0/1818	0.43	0/2467
1	S	0.11	0/441	0.19	0/591
2	C	0.20	0/8848	0.39	0/11982
3	D	0.20	0/9998	0.42	0/13490
4	E	0.21	0/607	0.44	0/826
5	F	0.17	0/2431	0.41	0/3277
6	G	0.13	0/1001	0.31	0/1355
6	H	0.16	0/1001	0.38	0/1355
6	M	0.14	0/1001	0.30	0/1355
6	N	0.10	0/1001	0.25	0/1355
7	O	0.31	0/1920	0.60	1/2959 (0.0%)
8	P	0.27	0/1942	0.52	0/2997
All	All	0.20	0/33777	0.42	1/46409 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	23	DC	C4'-C3'-O3'	6.24	119.36	110.00

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	1797	1796	22	0
1	B	1792	1841	1841	31	0
1	S	438	453	452	1	0
2	C	8692	8633	8632	135	0
3	D	9846	10018	10017	140	0
4	E	597	605	604	16	0
5	F	2396	2438	2453	35	0
6	G	984	947	948	7	0
6	H	984	947	947	18	0
6	M	984	948	947	16	0
6	N	984	947	947	14	0
7	O	1714	934	940	31	0
8	P	1730	928	939	24	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	M	3	0	0	0	0
10	N	3	0	0	0	0
All	All	32898	31436	31463	440	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 7.

All (440) 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:505:VAL:HG22	2:C:510:VAL:HG12	1.39	1.03
8:P:23:DA:H2'	8:P:24:DG:C5	1.95	1.00
8:P:23:DA:H2'	8:P:24:DG:C6	2.10	0.87
2:C:1058:VAL:HG23	2:C:1070:LEU:HD11	1.57	0.85
3:D:583:LEU:HD21	3:D:724:VAL:HG11	1.58	0.84
6:H:84:HIS:NE2	6:H:122:HIS:NE2	2.27	0.81
2:C:817:GLU:N	2:C:817:GLU:OE1	2.18	0.76
2:C:806:LEU:HD12	5:F:464:LEU:HD21	1.70	0.74
3:D:896:ILE:HD11	3:D:943:ILE:HD11	1.70	0.74
6:G:104:VAL:HG12	6:H:104:VAL:HG12	1.69	0.72
3:D:421:ARG:NH1	8:P:18:DT:OP1	2.22	0.72
6:N:78:ARG:NH1	6:N:79:CYS:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:36:HIS:NE2	6:M:46:VAL:O	2.24	0.71
7:O:21:DT:H2''	7:O:22:DT:OP2	1.89	0.71
3:D:590:THR:CG2	3:D:622:GLN:HG2	2.21	0.71
3:D:920:LEU:CD1	3:D:938:LEU:HD21	2.21	0.70
5:F:485:ARG:NH2	7:O:33:DT:OP2	2.24	0.70
2:C:1113:MET:HE2	2:C:1120:VAL:HG21	1.74	0.70
3:D:888:THR:O	3:D:957:ARG:NH2	2.25	0.70
2:C:352:GLU:N	2:C:352:GLU:OE1	2.25	0.69
3:D:449:LEU:HD11	3:D:476:VAL:HG23	1.74	0.69
4:E:65:GLU:OE1	4:E:65:GLU:N	2.25	0.69
3:D:291:ARG:NH2	7:O:79:DG:OP2	2.25	0.69
3:D:579:GLN:OE1	3:D:803:ARG:NE	2.24	0.69
3:D:1048:VAL:O	3:D:1085:GLY:N	2.26	0.69
6:H:47:GLY:N	8:P:55:DC:OP2	2.26	0.69
2:C:966:ARG:N	2:C:969:GLU:OE1	2.25	0.69
3:D:874:ASP:OD1	3:D:1232:LYS:NZ	2.20	0.68
2:C:715:HIS:HB2	2:C:722:ILE:HD11	1.75	0.67
2:C:256:GLN:N	2:C:256:GLN:OE1	2.28	0.67
2:C:908:VAL:HG11	3:D:726:VAL:HG21	1.77	0.66
2:C:203:GLU:N	2:C:203:GLU:OE1	2.28	0.66
2:C:803:GLU:OE2	2:C:803:GLU:N	2.27	0.66
2:C:838:VAL:HG12	2:C:855:VAL:HG12	1.75	0.66
1:A:41:THR:HG21	1:A:215:LEU:HD21	1.77	0.66
3:D:434:PRO:O	3:D:712:LYS:NZ	2.20	0.66
4:E:61:THR:HG23	4:E:70:ILE:HD11	1.77	0.66
1:B:136:MET:HE1	1:B:138:LEU:HD23	1.79	0.65
2:C:648:ASN:ND2	2:C:650:ASP:OD2	2.29	0.65
6:N:28:GLU:OE1	6:N:30:ARG:NH2	2.30	0.65
3:D:952:GLU:N	3:D:952:GLU:OE1	2.30	0.65
2:C:505:VAL:CG2	2:C:510:VAL:HG12	2.22	0.65
2:C:1052:ARG:NH1	3:D:419:GLY:O	2.29	0.65
3:D:780:VAL:HG11	3:D:815:MET:HE3	1.78	0.64
5:F:359:ILE:HD12	5:F:362:LEU:HD11	1.80	0.64
2:C:33:GLU:OE1	2:C:33:GLU:N	2.30	0.64
2:C:746:ARG:NH1	3:D:331:ASP:OD1	2.30	0.64
6:H:84:HIS:CE1	6:H:122:HIS:HE2	2.16	0.64
3:D:844:TYR:O	3:D:848:THR:HG23	1.97	0.64
6:N:27:GLU:OE1	6:N:77:ARG:NH2	2.31	0.64
6:N:77:ARG:NH1	6:N:79:CYS:SG	2.71	0.64
2:C:364:ILE:HD11	2:C:492:ILE:HD12	1.78	0.63
7:O:23:DC:H2''	7:O:24:DA:O4'	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:50:THR:O	6:M:54:THR:HG23	1.97	0.63
1:B:154:GLN:N	1:B:154:GLN:OE1	2.30	0.63
3:D:295:ARG:O	3:D:299:VAL:HG23	1.99	0.63
2:C:744:ASP:O	2:C:791:LYS:NZ	2.32	0.63
1:B:42:LEU:CD2	1:B:171:VAL:HG11	2.29	0.62
2:C:70:THR:HG23	2:C:71:LYS:HD2	1.81	0.62
2:C:510:VAL:HG23	2:C:538:MET:SD	2.39	0.62
3:D:238:GLU:OE1	3:D:238:GLU:N	2.32	0.62
3:D:1255:VAL:HG13	4:E:80:LEU:HD21	1.82	0.62
2:C:597:MET:HE3	2:C:878:LYS:HE2	1.80	0.62
7:O:23:DC:H2''	7:O:24:DA:C4'	2.30	0.62
2:C:617:GLU:OE1	2:C:617:GLU:N	2.30	0.61
1:A:200:GLN:OE1	1:A:200:GLN:N	2.34	0.61
2:C:806:LEU:HD12	5:F:464:LEU:CD2	2.29	0.61
4:E:36:ARG:NE	4:E:74:GLU:OE1	2.32	0.61
6:H:125:GLU:OE1	6:H:125:GLU:N	2.33	0.61
1:A:38:LEU:HD21	1:A:208:MET:SD	2.41	0.60
2:C:506:VAL:HG22	2:C:507:GLU:OE1	2.01	0.60
2:C:759:ILE:HG22	2:C:767:LEU:HD11	1.83	0.60
3:D:923:ASP:OD1	3:D:933:PRO:HA	2.01	0.60
3:D:938:LEU:HD22	3:D:942:LEU:HD22	1.84	0.60
6:H:65:ASP:OD2	6:H:77:ARG:NH1	2.35	0.60
3:D:452:PHE:CE1	3:D:545:LEU:HD11	2.36	0.60
3:D:225:ARG:NH1	3:D:235:GLU:OE1	2.35	0.60
2:C:949:ASP:OD1	2:C:950:LYS:N	2.35	0.59
2:C:471:PRO:O	3:D:852:ARG:NH2	2.35	0.59
5:F:423:GLU:OE2	5:F:423:GLU:N	2.36	0.59
3:D:963:GLU:OE2	3:D:965:GLN:NE2	2.36	0.59
6:N:55:LEU:HD21	6:N:76:TYR:CD1	2.37	0.59
7:O:23:DC:H2''	7:O:24:DA:H5'	1.85	0.59
3:D:590:THR:HG23	3:D:622:GLN:HG2	1.84	0.59
1:A:157:GLN:N	1:A:157:GLN:OE1	2.33	0.59
2:C:1077:LYS:NZ	3:D:545:LEU:O	2.22	0.59
3:D:587:PHE:CE1	3:D:622:GLN:NE2	2.71	0.59
1:B:38:LEU:HD11	1:B:208:MET:SD	2.43	0.58
3:D:590:THR:CG2	3:D:622:GLN:CG	2.80	0.58
8:P:36:DT:H2''	8:P:37:DA:C8	2.38	0.58
3:D:1041:ILE:HD12	3:D:1107:ILE:HD11	1.85	0.58
2:C:510:VAL:HG11	2:C:565:MET:SD	2.43	0.58
2:C:742:GLU:N	2:C:742:GLU:OE1	2.35	0.58
7:O:25:DG:O6	8:P:59:DA:N6	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:814:LYS:HE2	2:C:814:LYS:HA	1.86	0.58
1:A:44:SER:OG	2:C:888:GLU:OE2	2.20	0.58
2:C:943:LEU:HD12	2:C:948:ALA:O	2.04	0.57
5:F:300:PHE:CZ	5:F:304:ILE:HD11	2.38	0.57
1:B:51:VAL:HG11	1:B:80:ILE:HD11	1.86	0.57
2:C:650:ASP:OD1	2:C:651:GLY:N	2.38	0.57
3:D:445:LYS:NZ	3:D:516:LEU:HD13	2.19	0.57
6:M:22:ALA:HB1	6:M:38:MET:HE3	1.86	0.57
6:M:122:HIS:HA	6:N:126:ILE:HG22	1.86	0.57
8:P:23:DA:H2'	8:P:24:DG:C4	2.39	0.57
2:C:22:ARG:NE	2:C:617:GLU:OE2	2.37	0.57
2:C:810:ILE:HD11	5:F:497:LEU:HD12	1.87	0.57
3:D:1121:VAL:HG11	3:D:1137:ILE:HD12	1.86	0.57
5:F:362:LEU:HD12	5:F:363:ALA:N	2.20	0.57
6:N:15:GLN:NE2	7:O:11:DG:OP2	2.38	0.57
2:C:305:ASN:OD1	2:C:306:LYS:N	2.38	0.56
8:P:23:DA:C8	8:P:24:DG:O6	2.58	0.56
1:B:42:LEU:HD21	1:B:171:VAL:HG11	1.86	0.56
2:C:421:GLN:N	2:C:421:GLN:OE1	2.38	0.56
3:D:58:TRP:CE3	3:D:68:VAL:HG12	2.40	0.56
3:D:1172:GLU:OE2	3:D:1173:ASN:ND2	2.38	0.56
3:D:143:ARG:NH1	3:D:250:THR:O	2.38	0.56
3:D:604:PHE:HE2	3:D:619:LEU:HD22	1.70	0.56
1:B:136:MET:CE	1:B:138:LEU:HD23	2.34	0.56
3:D:1147:ARG:NH2	3:D:1199:ALA:O	2.37	0.56
3:D:876:SER:O	3:D:879:VAL:HG12	2.06	0.56
2:C:91:MET:SD	2:C:92:SER:N	2.79	0.56
3:D:751:VAL:HG11	3:D:768:GLU:OE2	2.06	0.55
1:B:136:MET:SD	1:B:137:GLU:N	2.79	0.55
3:D:115:GLY:CA	3:D:298:VAL:HG21	2.36	0.55
3:D:581:MET:HE1	3:D:712:LYS:HG3	1.89	0.55
2:C:739:GLU:OE1	2:C:739:GLU:N	2.40	0.55
5:F:306:GLU:OE1	5:F:341:ALA:HB1	2.07	0.55
7:O:23:DC:H2''	7:O:24:DA:C5'	2.37	0.55
2:C:1026:LEU:HD23	2:C:1027:HIS:N	2.22	0.55
1:B:41:THR:OG1	1:B:215:LEU:HD21	2.07	0.55
3:D:96:GLU:O	3:D:351:ASN:ND2	2.39	0.55
3:D:855:LEU:O	3:D:858:THR:OG1	2.20	0.55
2:C:255:THR:OG1	2:C:260:ASP:OD2	2.22	0.55
2:C:952:GLU:OE1	2:C:952:GLU:N	2.39	0.55
2:C:574:SER:OG	2:C:575:VAL:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:167:LEU:HD23	2:C:364:ILE:HG22	1.88	0.54
7:O:23:DC:H4'	7:O:24:DA:OP1	2.07	0.54
6:G:23:LEU:O	6:G:77:ARG:NH1	2.40	0.54
2:C:364:ILE:CD1	2:C:492:ILE:HD12	2.38	0.54
3:D:588:LEU:HD21	3:D:664:GLY:O	2.07	0.54
6:M:14:ARG:NH1	7:O:29:DC:OP1	2.40	0.54
6:N:81:THR:OG1	6:N:98:GLU:OE1	2.26	0.54
2:C:508:GLY:N	2:C:560:ASP:OD1	2.41	0.54
2:C:341:THR:N	2:C:348:GLU:OE2	2.41	0.54
4:E:32:TYR:CE2	4:E:75:ILE:HD12	2.43	0.54
3:D:1118:VAL:HG21	3:D:1138:GLU:OE2	2.07	0.54
2:C:765:GLU:N	2:C:765:GLU:OE1	2.37	0.53
5:F:284:ARG:NH1	7:O:63:DG:O6	2.42	0.53
1:B:83:LEU:HD11	1:B:118:VAL:CG2	2.37	0.53
6:G:121:ALA:N	6:H:127:PHE:O	2.41	0.53
1:A:177:LYS:HG3	1:A:193:ILE:HG23	1.90	0.53
4:E:16:ILE:CG2	4:E:20:LEU:HD21	2.39	0.53
1:B:38:LEU:HD21	1:B:194:VAL:HG11	1.91	0.53
3:D:115:GLY:HA3	3:D:298:VAL:HG21	1.90	0.53
5:F:369:MET:SD	5:F:369:MET:N	2.82	0.53
3:D:977:LEU:HD11	3:D:1135:LYS:HZ1	1.73	0.53
2:C:91:MET:HE1	2:C:93:LEU:HG	1.90	0.52
1:B:228:ASP:OD1	1:B:229:ALA:N	2.41	0.52
4:E:32:TYR:CZ	4:E:75:ILE:HD12	2.45	0.52
7:O:21:DT:C2'	7:O:22:DT:OP2	2.56	0.52
2:C:430:ASN:ND2	2:C:701:LEU:HD22	2.24	0.52
3:D:35:ASN:N	3:D:42:GLU:OE2	2.43	0.52
1:B:120:ASN:N	1:B:120:ASN:OD1	2.42	0.52
2:C:185:LYS:NZ	2:C:205:ASP:OD1	2.39	0.52
2:C:715:HIS:CB	2:C:722:ILE:HD11	2.40	0.52
1:A:64:THR:OG1	1:A:65:THR:N	2.42	0.52
1:B:202:MET:SD	1:B:203:ARG:N	2.83	0.52
2:C:563:ASP:OD1	2:C:563:ASP:N	2.42	0.52
3:D:65:TYR:HB3	3:D:70:PHE:CE1	2.45	0.51
3:D:281:ILE:O	3:D:289:LYS:NZ	2.40	0.51
3:D:821:ASN:N	3:D:825:GLU:O	2.42	0.51
2:C:913:ASN:OD1	2:C:916:GLN:NE2	2.43	0.51
3:D:128:VAL:HG21	3:D:135:MET:SD	2.50	0.51
6:M:83:ASP:O	6:M:85:HIS:ND1	2.43	0.51
3:D:879:VAL:O	3:D:879:VAL:HG13	2.10	0.51
3:D:104:ILE:HD11	3:D:386:ARG:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:80:LEU:HD23	4:E:81:THR:N	2.26	0.51
3:D:19:ASP:OD1	3:D:23:TRP:NE1	2.44	0.51
3:D:384:ASN:ND2	3:D:399:LEU:O	2.43	0.51
1:A:7:PRO:HG3	1:B:218:LEU:HD13	1.92	0.51
2:C:759:ILE:CG2	2:C:767:LEU:HD11	2.41	0.51
3:D:339:ASP:OD1	5:F:405:SER:OG	2.28	0.51
3:D:1089:GLU:N	3:D:1089:GLU:OE1	2.44	0.51
1:A:41:THR:HG22	1:B:30:PHE:CE2	2.46	0.50
2:C:1107:LYS:HA	2:C:1110:ILE:HG22	1.91	0.50
2:C:330:TYR:CE1	2:C:351:VAL:HG23	2.46	0.50
2:C:1058:VAL:HG22	2:C:1062:GLU:OE2	2.10	0.50
3:D:1041:ILE:CD1	3:D:1107:ILE:HD11	2.41	0.50
6:N:68:ARG:NH2	6:N:72:GLY:O	2.45	0.50
1:B:38:LEU:CD2	1:B:194:VAL:HG11	2.42	0.50
2:C:149:THR:HG22	2:C:153:THR:O	2.12	0.50
2:C:806:LEU:HD13	5:F:443:LEU:HD21	1.94	0.50
5:F:472:LEU:HD13	5:F:487:ARG:HB2	1.93	0.50
2:C:86:ASP:OD1	2:C:89:GLY:N	2.45	0.50
3:D:210:ASP:O	3:D:213:GLN:NE2	2.45	0.50
6:H:16:ARG:NH1	8:P:54:DG:OP1	2.44	0.50
7:O:72:DG:H1	8:P:13:DC:H42	1.59	0.50
3:D:21:ARG:NH2	3:D:96:GLU:OE2	2.45	0.50
4:E:44:TYR:OH	4:E:61:THR:HG21	2.11	0.50
6:N:132:ASP:OD1	6:N:132:ASP:N	2.43	0.50
1:A:15:ASP:OD1	1:A:16:GLU:N	2.44	0.49
3:D:173:ARG:NE	3:D:208:LEU:HD23	2.27	0.49
4:E:25:SER:OG	4:E:26:LYS:N	2.44	0.49
1:B:120:ASN:ND2	1:B:123:LEU:HD11	2.27	0.49
1:B:202:MET:HA	1:B:202:MET:HE2	1.95	0.49
3:D:504:LEU:HD12	3:D:504:LEU:H	1.77	0.49
5:F:460:MET:N	5:F:460:MET:SD	2.85	0.49
5:F:301:LEU:HA	5:F:304:ILE:HD12	1.93	0.49
7:O:23:DC:C2'	7:O:24:DA:H5'	2.41	0.49
1:A:41:THR:HG21	1:A:215:LEU:CD2	2.41	0.49
2:C:1035:SER:OG	2:C:1036:MET:N	2.46	0.49
3:D:373:MET:SD	5:F:301:LEU:HD22	2.52	0.49
3:D:1256:GLU:OE1	3:D:1256:GLU:N	2.46	0.49
6:M:55:LEU:HD13	6:M:76:TYR:CE2	2.47	0.49
1:B:207:ALA:O	1:B:210:SER:OG	2.29	0.49
5:F:388:MET:SD	5:F:388:MET:N	2.86	0.49
5:F:454:GLU:HB3	5:F:493:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:920:LEU:HD13	3:D:938:LEU:HD21	1.93	0.49
1:A:69:VAL:HG12	1:A:128:LEU:HD12	1.95	0.49
2:C:517:LEU:HD21	2:C:564:TYR:CD2	2.48	0.49
3:D:777:THR:HA	3:D:780:VAL:HG12	1.94	0.49
6:N:83:ASP:O	6:N:85:HIS:ND1	2.44	0.49
2:C:318:VAL:CG1	2:C:319:LEU:HD23	2.43	0.48
3:D:977:LEU:HD11	3:D:1135:LYS:NZ	2.27	0.48
5:F:472:LEU:O	5:F:486:ILE:HG21	2.13	0.48
3:D:830:PRO:O	3:D:832:LYS:NZ	2.29	0.48
7:O:71:DG:H2'	7:O:71:DG:N3	2.27	0.48
2:C:875:HIS:NE2	2:C:919:GLU:OE1	2.42	0.48
2:C:1056:MET:HB3	3:D:503:THR:HG23	1.95	0.48
2:C:567:VAL:N	2:C:571:GLN:OE1	2.42	0.48
2:C:572:MET:HG3	2:C:573:VAL:HG13	1.95	0.48
7:O:30:DG:N2	8:P:56:DG:C2	2.82	0.48
1:A:122:ASP:OD1	1:A:122:ASP:N	2.47	0.48
2:C:851:VAL:O	2:C:851:VAL:HG23	2.13	0.48
2:C:1067:ALA:HB1	3:D:1240:LEU:HD22	1.95	0.48
6:M:39:LEU:HD12	6:M:40:LYS:N	2.29	0.48
6:M:77:ARG:NE	6:M:96:ALA:HB3	2.28	0.48
2:C:517:LEU:HD21	2:C:564:TYR:CE2	2.49	0.47
3:D:933:PRO:O	3:D:936:VAL:HG12	2.14	0.47
6:H:39:LEU:HD21	6:H:46:VAL:HG21	1.96	0.47
3:D:1162:GLU:N	3:D:1162:GLU:OE1	2.47	0.47
2:C:364:ILE:HD11	2:C:492:ILE:HG23	1.96	0.47
2:C:1030:SER:OG	2:C:1031:THR:N	2.46	0.47
5:F:360:ASN:OD1	5:F:361:LYS:N	2.47	0.47
1:B:129:ASN:OD1	1:B:129:ASN:N	2.45	0.47
1:B:77:ILE:HG23	1:B:164:VAL:HG23	1.97	0.47
2:C:505:VAL:HG22	2:C:510:VAL:CG1	2.28	0.47
8:P:62:DG:H2''	8:P:63:DA:C8	2.49	0.47
2:C:567:VAL:HG12	2:C:571:GLN:OE1	2.15	0.47
3:D:920:LEU:HD11	3:D:938:LEU:HD21	1.93	0.47
3:D:1117:LEU:O	3:D:1121:VAL:HG12	2.14	0.47
6:M:27:GLU:O	6:M:77:ARG:NE	2.48	0.47
2:C:41:GLN:NE2	2:C:163:VAL:O	2.41	0.47
2:C:493:ASN:N	2:C:497:PHE:O	2.40	0.47
3:D:641:PRO:HD2	3:D:642:PRO:CD	2.44	0.47
5:F:293:TYR:OH	5:F:335:ARG:NE	2.48	0.47
7:O:22:DT:C2	7:O:23:DC:C4	3.03	0.47
2:C:771:ASP:N	2:C:775:ILE:O	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:811:GLN:OE1	3:D:816:ARG:NH1	2.48	0.47
7:O:21:DT:H2'	7:O:22:DT:H72	1.97	0.47
7:O:71:DG:C2	7:O:72:DG:C2	3.03	0.47
5:F:468:GLN:NE2	5:F:469:PRO:O	2.46	0.47
2:C:702:GLY:O	2:C:1014:TYR:OH	2.33	0.46
3:D:641:PRO:HD2	3:D:642:PRO:HD2	1.97	0.46
1:A:110:ILE:HD11	1:A:138:LEU:HD13	1.96	0.46
2:C:419:THR:HA	8:P:23:DA:H2	1.80	0.46
3:D:627:ILE:HG22	3:D:628:ARG:O	2.15	0.46
2:C:759:ILE:HG23	2:C:762:VAL:HG21	1.98	0.46
5:F:369:MET:HE3	5:F:369:MET:HA	1.97	0.46
6:M:27:GLU:OE1	6:M:27:GLU:N	2.48	0.46
3:D:583:LEU:HD21	3:D:724:VAL:CG1	2.39	0.46
3:D:731:ILE:O	3:D:836:ARG:NE	2.48	0.46
2:C:225:LEU:C	2:C:225:LEU:HD23	2.41	0.46
3:D:1058:LYS:NZ	3:D:1059:ILE:O	2.48	0.46
6:H:55:LEU:HD12	6:H:56:GLN:N	2.30	0.46
7:O:22:DT:C2	7:O:23:DC:N3	2.84	0.46
2:C:30:GLU:N	2:C:30:GLU:OE1	2.48	0.46
2:C:1047:GLN:N	2:C:1047:GLN:OE1	2.49	0.46
2:C:644:ILE:HG22	2:C:658:LEU:HD11	1.98	0.46
3:D:1031:GLU:O	3:D:1031:GLU:HG2	2.15	0.46
8:P:69:DG:H2''	8:P:70:DT:C7	2.46	0.46
1:A:9:LEU:HD23	1:A:10:THR:N	2.30	0.45
1:B:30:PHE:O	1:B:33:THR:OG1	2.33	0.45
2:C:46:ASP:OD1	2:C:54:TRP:N	2.50	0.45
3:D:959:ILE:HD11	3:D:968:THR:HG21	1.97	0.45
2:C:91:MET:HE3	2:C:91:MET:C	2.42	0.45
2:C:209:MET:SD	2:C:209:MET:N	2.89	0.45
6:H:16:ARG:NH1	8:P:53:DC:O5'	2.49	0.45
6:M:77:ARG:NH1	6:M:79:CYS:SG	2.82	0.45
2:C:1002:GLU:N	2:C:1002:GLU:OE1	2.49	0.45
3:D:64:LYS:HG2	3:D:65:TYR:H	1.81	0.45
5:F:302:ASP:O	5:F:306:GLU:HG3	2.16	0.45
7:O:9:DA:H2'	7:O:10:DT:H71	1.99	0.45
1:B:172:LEU:O	3:D:612:MET:HE2	2.17	0.45
3:D:1250:TYR:O	4:E:31:ILE:HG21	2.16	0.45
6:H:90:CYS:O	6:H:94:GLY:N	2.49	0.45
2:C:841:ARG:NH2	2:C:847:LEU:O	2.50	0.45
6:G:35:LEU:O	6:G:39:LEU:HD23	2.16	0.45
3:D:180:ASP:OD1	3:D:181:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:34:GLU:O	6:H:38:MET:HE3	2.17	0.45
2:C:359:PHE:HE2	2:C:498:ILE:HD12	1.82	0.45
2:C:1058:VAL:HG23	2:C:1070:LEU:HD21	1.99	0.45
3:D:343:LEU:HD11	3:D:400:LYS:O	2.16	0.45
8:P:23:DA:C8	8:P:24:DG:C6	3.05	0.45
1:B:31:GLY:N	1:B:190:ASP:OD2	2.47	0.44
2:C:432:LEU:HB2	2:C:699:MET:HE3	1.99	0.44
2:C:1027:HIS:CE1	2:C:1048:PHE:HA	2.52	0.44
2:C:1029:ARG:NH1	2:C:1048:PHE:O	2.49	0.44
3:D:596:SER:O	3:D:598:LYS:N	2.49	0.44
3:D:738:LYS:O	3:D:741:VAL:HG12	2.17	0.44
2:C:23:ILE:O	2:C:958:ALA:N	2.49	0.44
3:D:674:GLU:OE1	3:D:674:GLU:N	2.48	0.44
3:D:340:LEU:HD11	3:D:405:MET:CE	2.47	0.44
3:D:529:CYS:SG	3:D:530:THR:N	2.91	0.44
1:B:137:GLU:N	1:B:137:GLU:OE1	2.50	0.44
3:D:1213:THR:O	3:D:1217:THR:OG1	2.28	0.44
5:F:298:MET:HE1	5:F:345:GLN:HB2	1.99	0.44
6:G:104:VAL:HG11	6:H:107:TRP:CE3	2.53	0.44
7:O:71:DG:N3	7:O:71:DG:C2'	2.80	0.44
1:A:57:ASP:OD2	1:A:133:LYS:NZ	2.50	0.44
2:C:130:ASN:OD1	2:C:131:GLU:N	2.50	0.44
2:C:204:ILE:CD1	2:C:332:VAL:HG12	2.47	0.44
2:C:212:VAL:O	2:C:213:ARG:NH2	2.50	0.44
7:O:30:DG:OP1	7:O:30:DG:C8	2.70	0.44
5:F:354:HIS:O	5:F:358:VAL:HG23	2.18	0.44
3:D:1233:GLU:OE2	3:D:1233:GLU:N	2.34	0.44
6:G:115:HIS:O	6:G:115:HIS:ND1	2.50	0.44
2:C:453:ARG:HA	7:O:71:DG:H1'	1.99	0.44
3:D:255:SER:OG	3:D:256:MET:N	2.50	0.44
7:O:79:DG:N2	8:P:7:DC:O2	2.51	0.44
8:P:69:DG:C2'	8:P:70:DT:H72	2.48	0.44
1:A:223:ARG:O	1:A:223:ARG:NH1	2.48	0.43
2:C:262:LEU:HD21	2:C:280:ALA:HB3	2.00	0.43
2:C:140:VAL:HG21	2:C:404:ILE:HD11	2.00	0.43
2:C:636:VAL:HG22	2:C:646:THR:HG22	2.00	0.43
2:C:1057:GLU:CD	3:D:503:THR:HG21	2.43	0.43
3:D:590:THR:HG23	3:D:622:GLN:CG	2.47	0.43
2:C:534:LEU:HD21	2:C:538:MET:SD	2.59	0.43
3:D:471:SER:HB3	5:F:508:ASP:OD2	2.18	0.43
7:O:29:DC:H1'	7:O:30:DG:OP1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:345:ARG:O	3:D:349:ASN:ND2	2.52	0.43
3:D:699:TYR:HD2	3:D:703:ILE:HG21	1.82	0.43
7:O:25:DG:N2	8:P:61:DT:O2	2.52	0.43
6:H:84:HIS:CE1	6:H:122:HIS:NE2	2.82	0.43
6:M:42:LYS:NZ	6:M:44:ASP:OD1	2.41	0.43
2:C:1072:GLU:OE2	2:C:1072:GLU:N	2.52	0.43
3:D:184:LEU:HD23	3:D:193:VAL:HB	2.01	0.43
3:D:459:ARG:HD3	3:D:463:LEU:HD23	2.00	0.43
3:D:1080:LEU:HD12	3:D:1081:LEU:N	2.33	0.43
2:C:706:LEU:HD12	2:C:1011:GLY:O	2.19	0.43
3:D:353:ARG:NH2	5:F:302:ASP:OD1	2.51	0.43
4:E:16:ILE:HG22	4:E:20:LEU:HD21	2.00	0.43
8:P:23:DA:C2'	8:P:24:DG:C5	2.85	0.43
1:A:120:ASN:OD1	1:A:120:ASN:N	2.52	0.43
6:M:39:LEU:HD13	6:M:46:VAL:HB	2.00	0.43
3:D:115:GLY:HA2	3:D:298:VAL:HG21	2.00	0.42
3:D:557:ILE:HD13	4:E:30:VAL:HG22	2.01	0.42
3:D:625:ILE:HD12	3:D:627:ILE:HD11	2.01	0.42
3:D:1159:LEU:HD12	3:D:1159:LEU:H	1.84	0.42
5:F:283:LEU:HA	5:F:286:VAL:HG12	2.00	0.42
5:F:300:PHE:CE2	5:F:304:ILE:HD11	2.54	0.42
7:O:23:DC:C6	7:O:23:DC:OP1	2.72	0.42
1:B:107:ALA:HA	1:B:110:ILE:HD12	2.01	0.42
2:C:631:GLU:N	2:C:631:GLU:OE1	2.52	0.42
3:D:445:LYS:HZ2	3:D:516:LEU:HD13	1.85	0.42
3:D:763:GLU:O	3:D:766:THR:OG1	2.33	0.42
6:M:84:HIS:NE2	6:M:122:HIS:CE1	2.88	0.42
7:O:57:DT:H5'	7:O:58:DT:H72	2.00	0.42
8:P:60:DC:H2'	8:P:61:DT:H72	2.02	0.42
2:C:262:LEU:HD23	2:C:277:ARG:HE	1.83	0.42
2:C:1027:HIS:HE1	2:C:1048:PHE:HA	1.83	0.42
3:D:641:PRO:CD	3:D:642:PRO:CD	2.98	0.42
1:A:171:VAL:HA	1:A:198:THR:HB	2.00	0.42
2:C:806:LEU:O	2:C:810:ILE:HG12	2.20	0.42
3:D:421:ARG:NH2	8:P:18:DT:OP2	2.52	0.42
2:C:138:GLN:NE2	2:C:139:THR:O	2.53	0.42
2:C:419:THR:HG1	8:P:23:DA:H2	1.56	0.42
1:A:223:ARG:NH1	1:A:226:ASN:O	2.53	0.42
2:C:546:LEU:HD23	2:C:547:VAL:N	2.35	0.42
3:D:449:LEU:HD11	3:D:476:VAL:CG2	2.47	0.42
3:D:602:ARG:NH1	3:D:618:ASP:OD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ARG:NH1	1:B:56:ILE:O	2.51	0.42
2:C:237:LEU:O	2:C:241:GLY:N	2.52	0.42
2:C:301:ARG:HA	2:C:304:VAL:HG12	2.00	0.42
3:D:1051:GLU:N	3:D:1051:GLU:OE1	2.53	0.42
6:G:68:ARG:NH1	6:H:69:THR:O	2.52	0.42
8:P:61:DT:O4	8:P:62:DG:C6	2.72	0.42
2:C:388:GLU:O	2:C:391:THR:OG1	2.37	0.42
3:D:806:MET:SD	3:D:806:MET:N	2.86	0.41
3:D:1265:MET:HA	3:D:1265:MET:HE2	2.02	0.41
3:D:64:LYS:HG2	3:D:65:TYR:CD1	2.55	0.41
3:D:556:ARG:HD2	4:E:11:ILE:HG23	2.01	0.41
3:D:1079:ARG:NH2	3:D:1096:VAL:HG11	2.35	0.41
2:C:554:VAL:HG22	2:C:554:VAL:O	2.21	0.41
2:C:1056:MET:CB	3:D:503:THR:HG23	2.49	0.41
2:C:430:ASN:ND2	2:C:601:ALA:O	2.54	0.41
3:D:735:ASP:OD1	3:D:736:ALA:N	2.53	0.41
5:F:352:PRO:O	5:F:356:VAL:HG23	2.21	0.41
6:H:71:GLU:OE1	6:H:73:GLU:N	2.53	0.41
3:D:370:GLU:HA	3:D:370:GLU:OE1	2.20	0.41
3:D:611:ILE:O	3:D:615:ASP:OD1	2.38	0.41
7:O:71:DG:C5	7:O:72:DG:C6	3.08	0.41
2:C:138:GLN:NE2	2:C:401:GLN:OE1	2.53	0.41
3:D:535:ASP:OD1	3:D:535:ASP:N	2.52	0.41
4:E:61:THR:HG22	4:E:62:HIS:O	2.21	0.41
1:B:27:GLU:HB3	1:B:28:PRO:HD3	2.03	0.41
5:F:280:GLU:HA	5:F:283:LEU:HG	2.02	0.41
6:M:67:LEU:HD12	6:M:68:ARG:N	2.35	0.41
1:A:52:THR:HG23	1:A:152:ASN:OD1	2.20	0.41
1:B:66:VAL:HG13	1:B:66:VAL:O	2.21	0.41
2:C:205:ASP:CG	2:C:205:ASP:O	2.63	0.41
2:C:449:LEU:HD11	2:C:454:ALA:HA	2.03	0.41
2:C:1091:ILE:HG21	3:D:454:PRO:HB2	2.02	0.41
2:C:1109:LEU:HD23	2:C:1109:LEU:C	2.45	0.41
3:D:592:SER:OG	3:D:593:GLU:N	2.54	0.41
3:D:672:LEU:HB3	3:D:673:PRO:HD2	2.03	0.41
3:D:826:THR:HG1	3:D:1010:HIS:CE1	2.34	0.41
1:S:275:LEU:HD21	1:S:297:VAL:HG13	2.02	0.41
1:B:171:VAL:O	3:D:612:MET:HE1	2.21	0.41
3:D:464:ASN:OD1	3:D:464:ASN:N	2.55	0.41
2:C:449:LEU:HD12	2:C:450:SER:O	2.21	0.40
3:D:46:LEU:HD21	3:D:348:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:330:LEU:HD11	3:D:336:ALA:HB2	2.03	0.40
5:F:459:SER:OG	5:F:460:MET:SD	2.79	0.40
6:N:55:LEU:HD21	6:N:76:TYR:CE1	2.55	0.40
3:D:64:LYS:CG	3:D:65:TYR:H	2.34	0.40
4:E:40:ILE:HG23	4:E:67:PRO:HB3	2.03	0.40
5:F:231:GLU:HA	5:F:234:VAL:HG22	2.03	0.40
2:C:575:VAL:HG22	2:C:616:MET:CE	2.51	0.40
2:C:1058:VAL:HG23	2:C:1070:LEU:CD1	2.40	0.40
6:H:54:THR:O	6:H:58:LEU:HG	2.21	0.40
2:C:675:ILE:HD11	2:C:687:VAL:O	2.22	0.40
2:C:891:PRO:HB2	2:C:995:LEU:HD12	2.03	0.40
3:D:114:LEU:HD12	3:D:117:LEU:CD2	2.51	0.40
6:N:22:ALA:HB2	6:N:39:LEU:HD21	2.04	0.40
1:A:42:LEU:O	1:A:171:VAL:HG21	2.21	0.40
2:C:491:ARG:C	2:C:492:ILE:HD13	2.47	0.40
2:C:925:LEU:HD21	2:C:974:LEU:HG	2.03	0.40
3:D:683:VAL:HG23	3:D:684:GLY:N	2.37	0.40
6:N:90:CYS:O	6:N:94:GLY:N	2.47	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%)	213 (95%)	11 (5%)	0	100	100
1	B	231/340 (68%)	222 (96%)	9 (4%)	0	100	100
1	S	55/340 (16%)	55 (100%)	0	0	100	100
2	C	1114/1161 (96%)	1059 (95%)	55 (5%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	299/531 (56%)	290 (97%)	9 (3%)	0	100	100
6	G	129/159 (81%)	128 (99%)	1 (1%)	0	100	100
6	H	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	3771/4745 (80%)	3634 (96%)	137 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/279 (70%)	191 (98%)	3 (2%)	57	68
1	B	199/279 (71%)	199 (100%)	0	100	100
1	S	47/279 (17%)	47 (100%)	0	100	100
2	C	942/979 (96%)	938 (100%)	4 (0%)	84	81
3	D	1054/1095 (96%)	1053 (100%)	1 (0%)	88	88
4	E	64/74 (86%)	64 (100%)	0	100	100
5	F	258/430 (60%)	257 (100%)	1 (0%)	84	81
6	G	99/120 (82%)	99 (100%)	0	100	100
6	H	99/120 (82%)	99 (100%)	0	100	100
6	M	99/120 (82%)	99 (100%)	0	100	100
6	N	99/120 (82%)	99 (100%)	0	100	100
All	All	3154/3895 (81%)	3145 (100%)	9 (0%)	84	83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU

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Mol	Chain	Res	Type
1	A	131	LYS
1	A	198	THR
2	C	593	MET
2	C	636	VAL
2	C	741	HIS
2	C	871	LEU
3	D	44	ASP
5	F	508	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	152	ASN
2	C	98	HIS
2	C	138	GLN
2	C	916	GLN
2	C	941	GLN
2	C	1071	GLN
3	D	767	GLN
3	D	1021	GLN
6	N	41	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 15 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

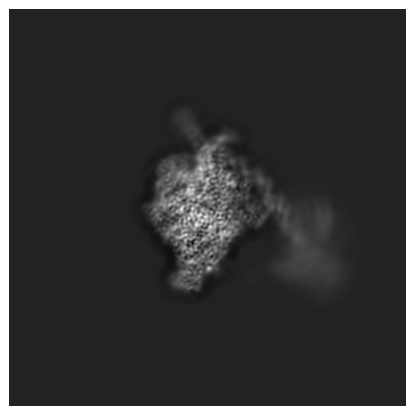
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33033. These allow visual inspection of the internal detail of the map and identification of artifacts.

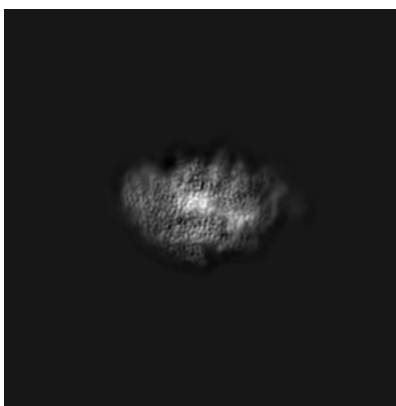
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

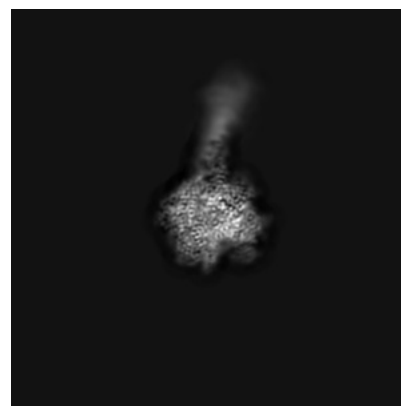
6.1.1 Primary map



X

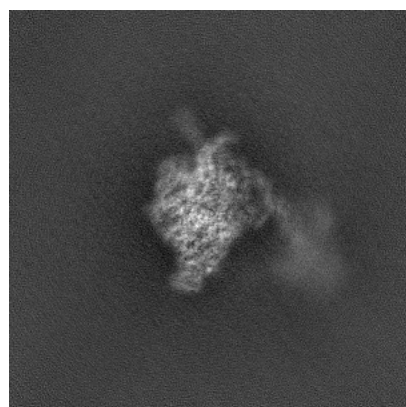


Y

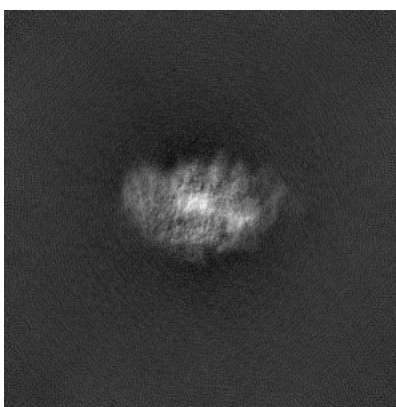


Z

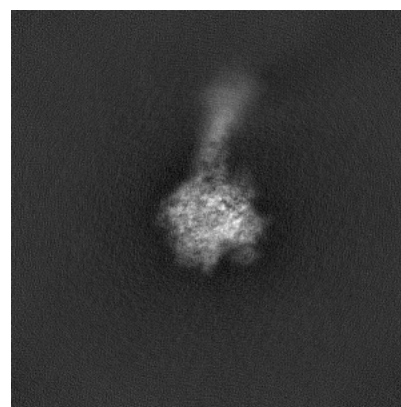
6.1.2 Raw map



X



Y

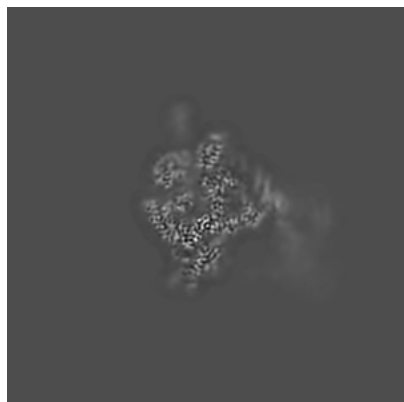


Z

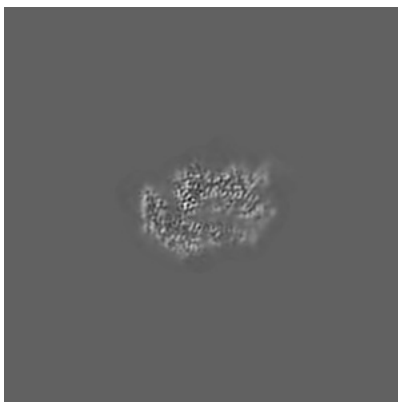
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

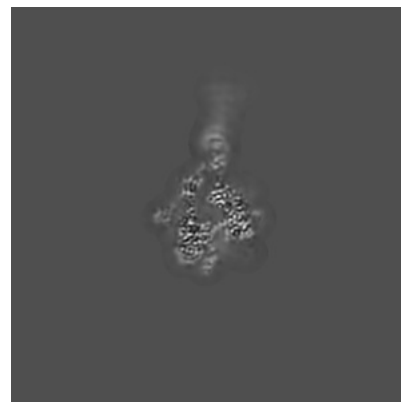
6.2.1 Primary map



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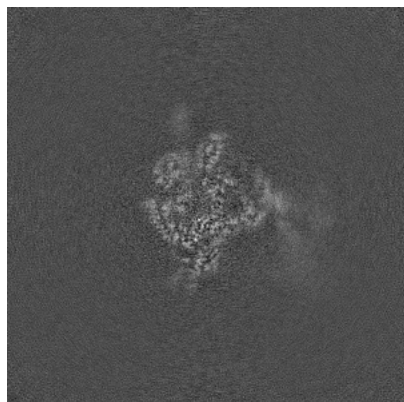


Y Index: 192

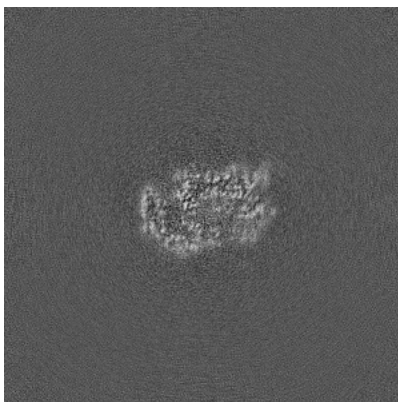


Z Index: 192

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: 201



Y Index: 193

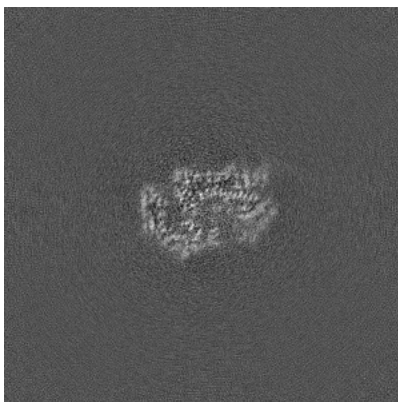


Z Index: 179

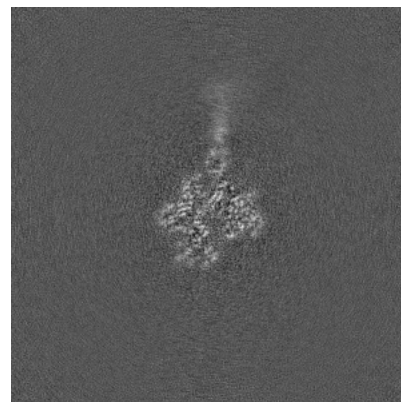
6.3.2 Raw map



X Index: 201



Y Index: 193

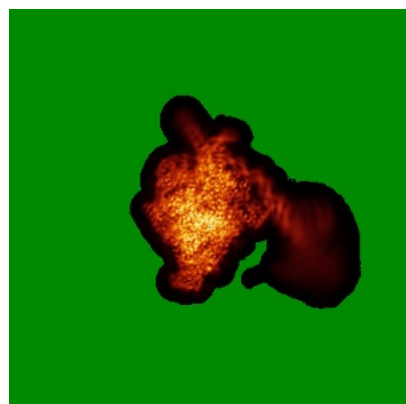


Z Index: 183

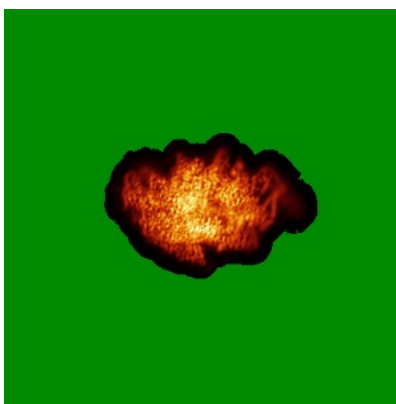
The images above show the largest variance slices of the map in three orthogonal directions.

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

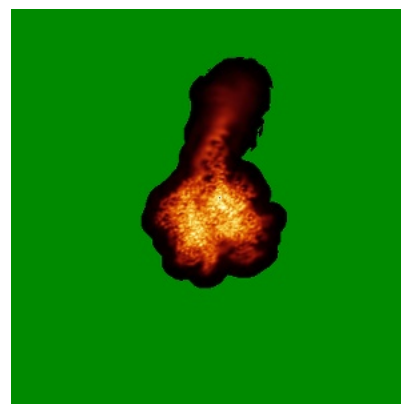
6.4.1 Primary map



X

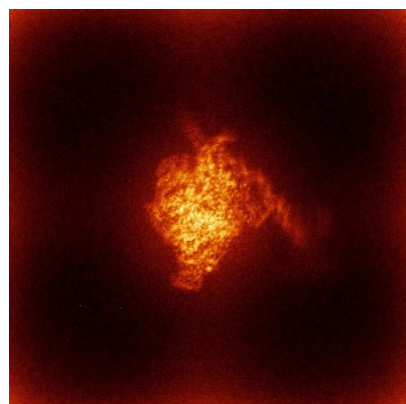


Y

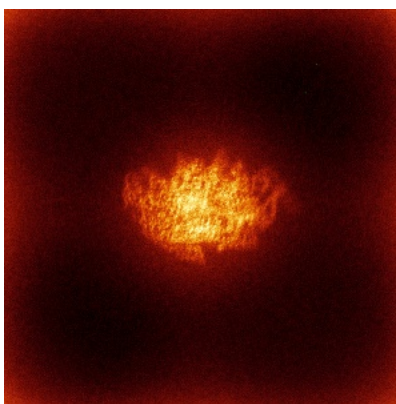


Z

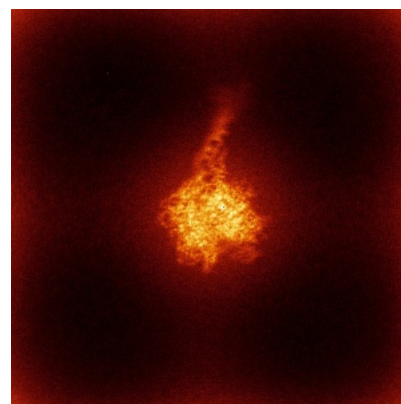
6.4.2 Raw map



X



Y

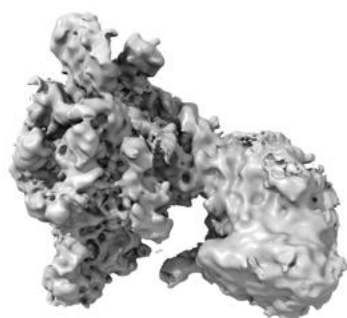


Z

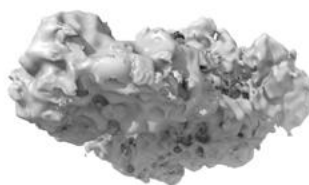
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



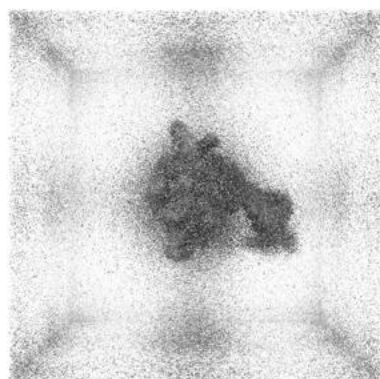
Y



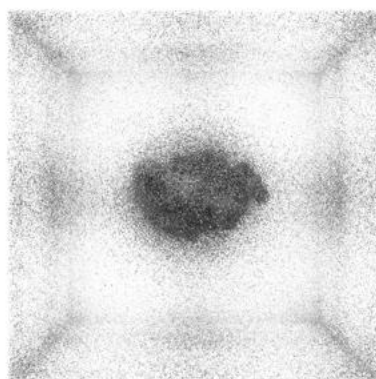
Z

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

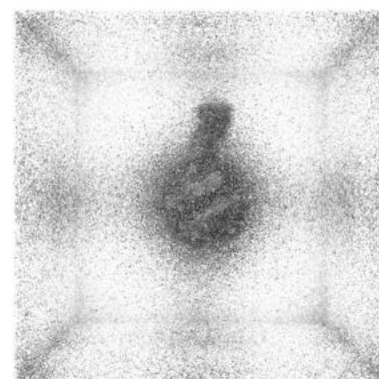
6.5.2 Raw map



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.

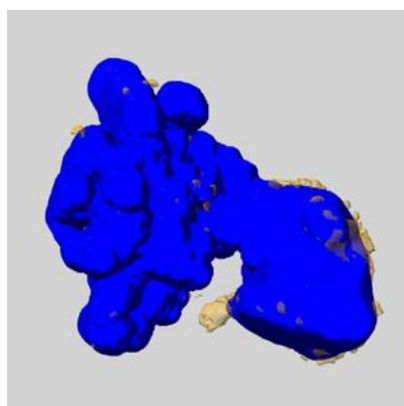
6.6 Mask visualisation [i](#)

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

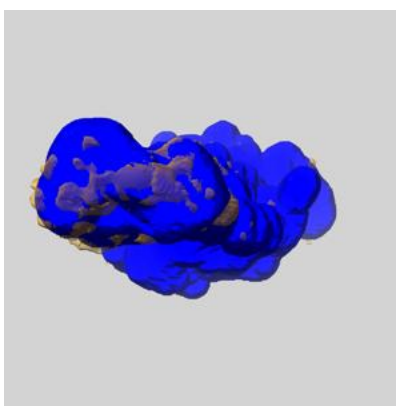
A mask typically either:

- 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_33033_msk_1.map [i](#)



X



Y

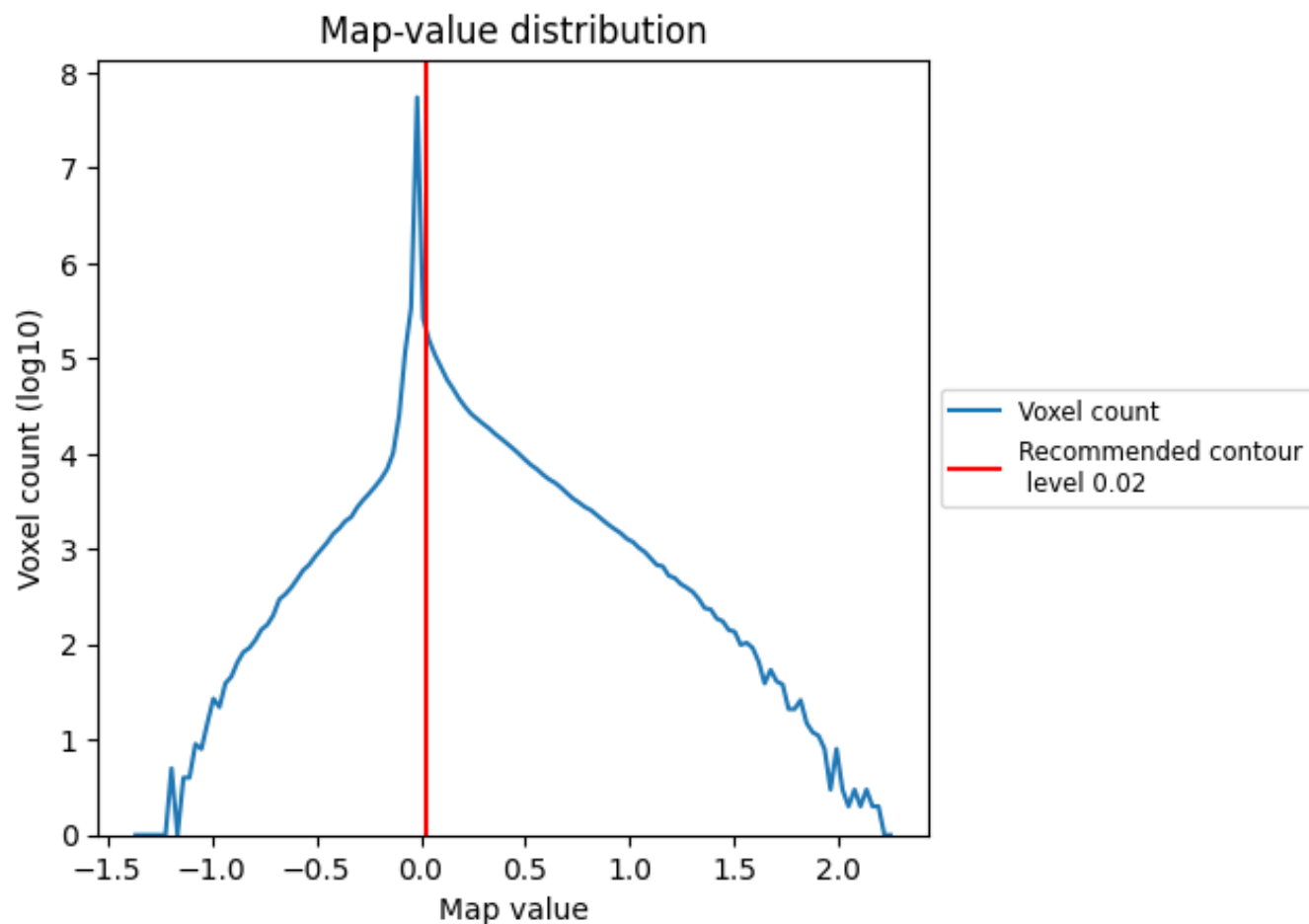


Z

7 Map analysis [i](#)

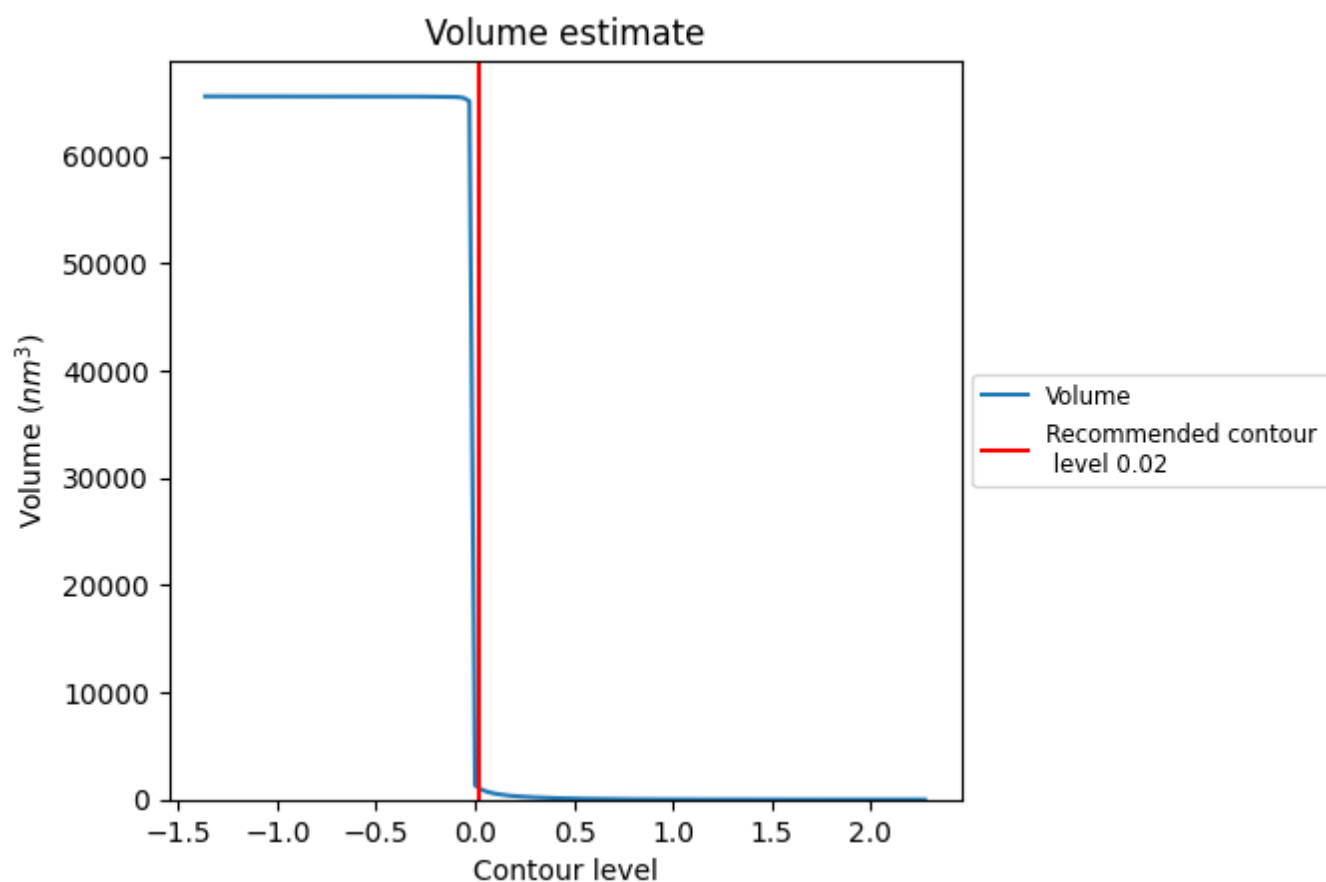
This section contains the results of statistical analysis of the map.

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.

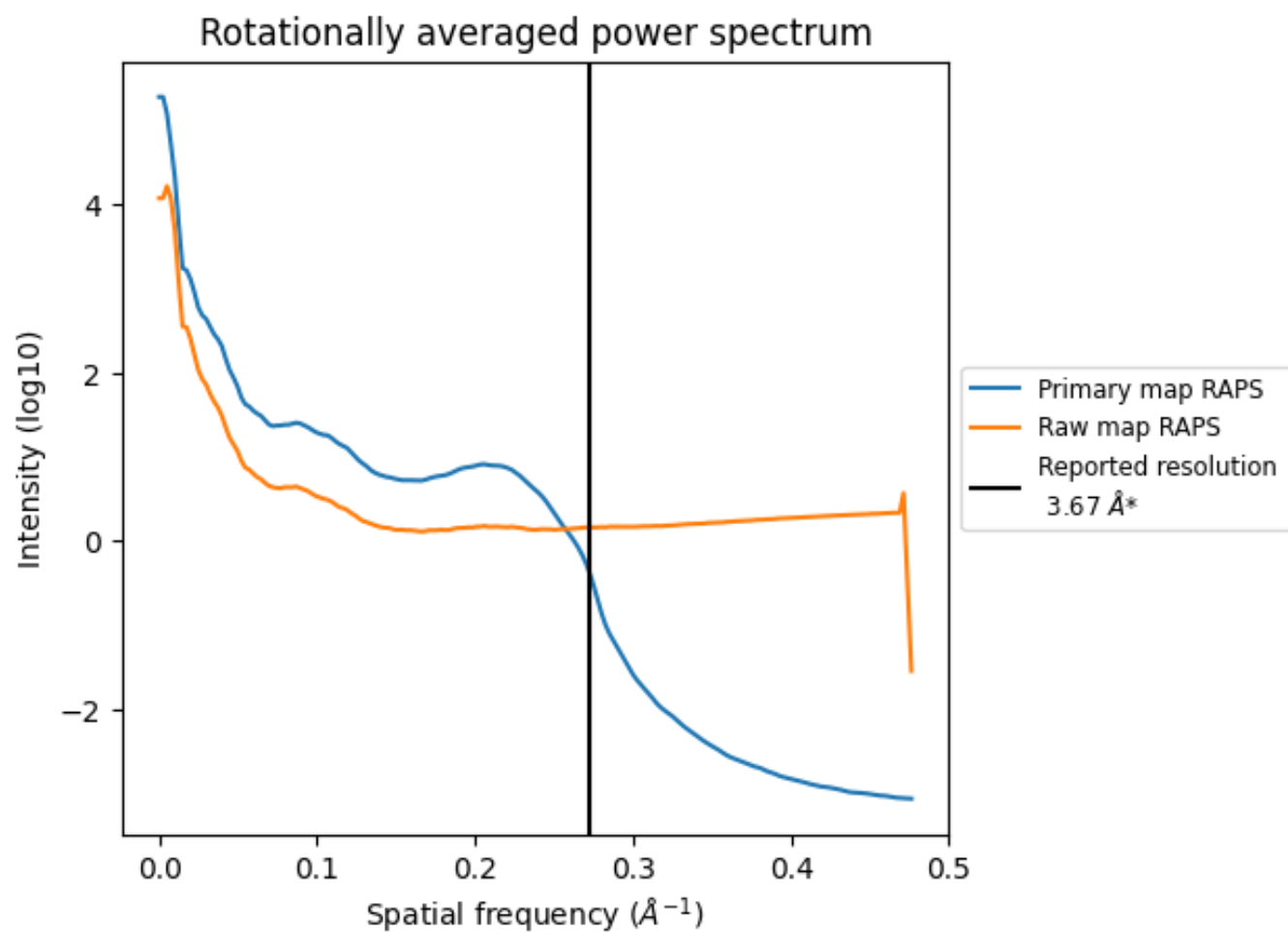
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1078 nm^3 ; this corresponds to an approximate mass of 973 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

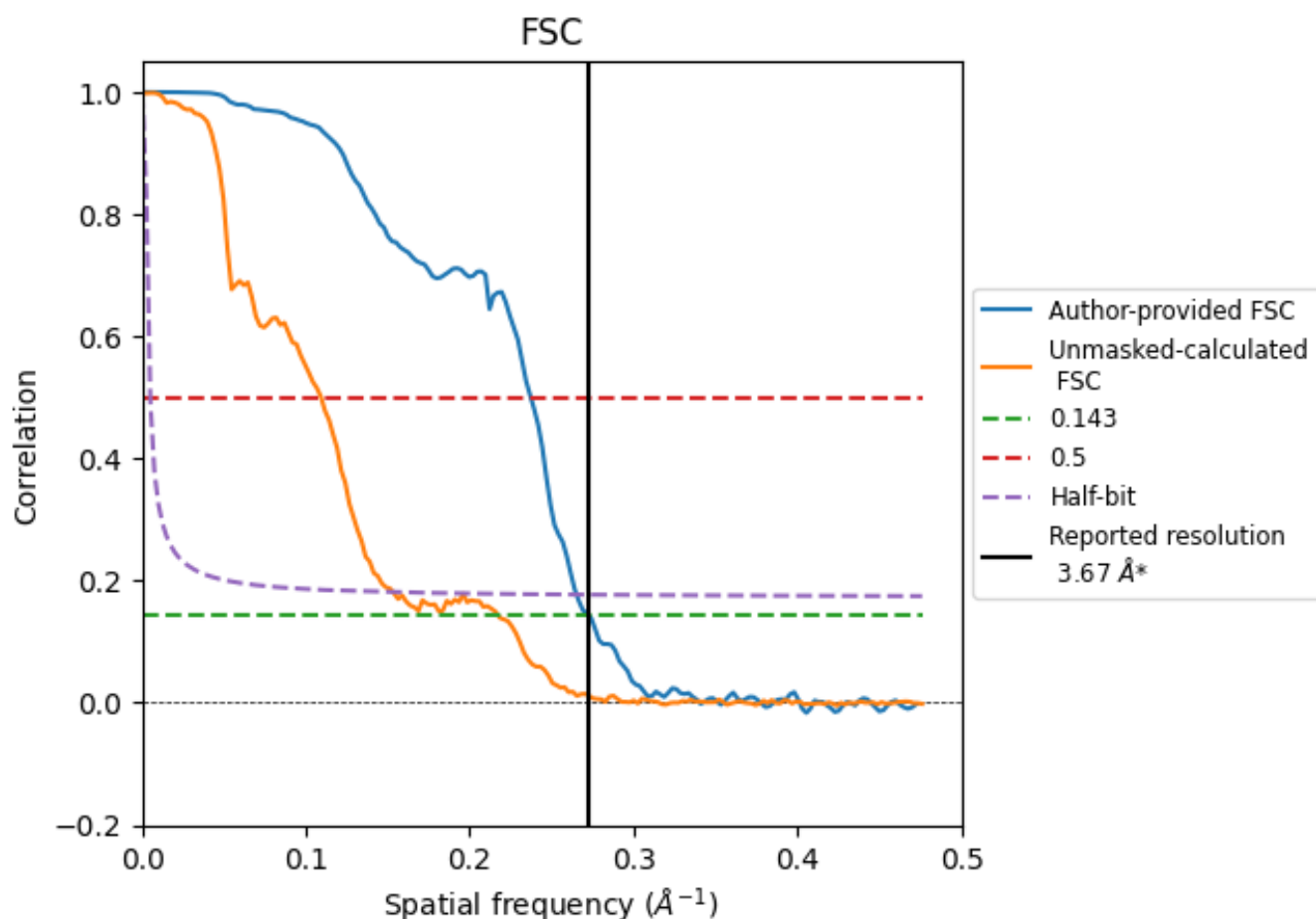


*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

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 0.272 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

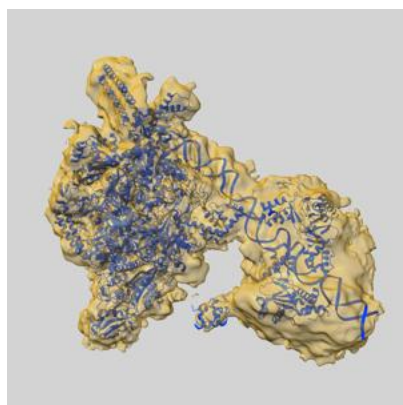
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.67	-	-
Author-provided FSC curve	3.67	4.22	3.77
Unmasked-calculated*	4.60	9.16	6.53

*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 4.60 differs from the reported value 3.67 by more than 10 %

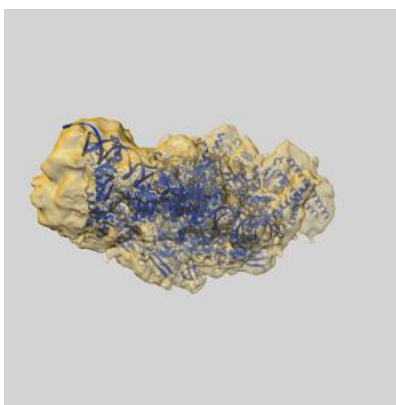
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33033 and PDB model 7X76. Per-residue inclusion information can be found in section [3](#) on page [9](#).

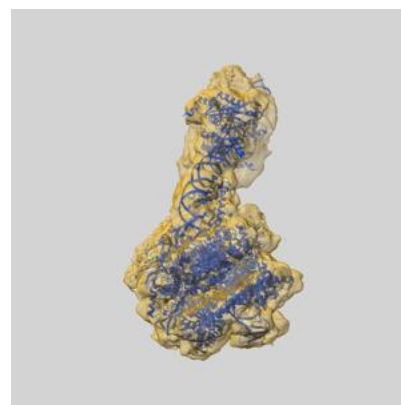
9.1 Map-model overlay [i](#)



X



Y



Z

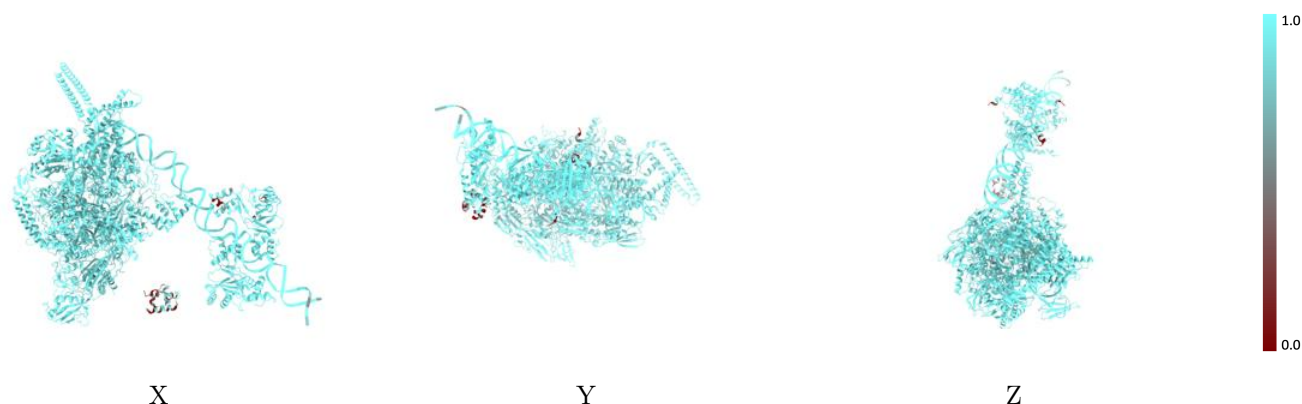
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



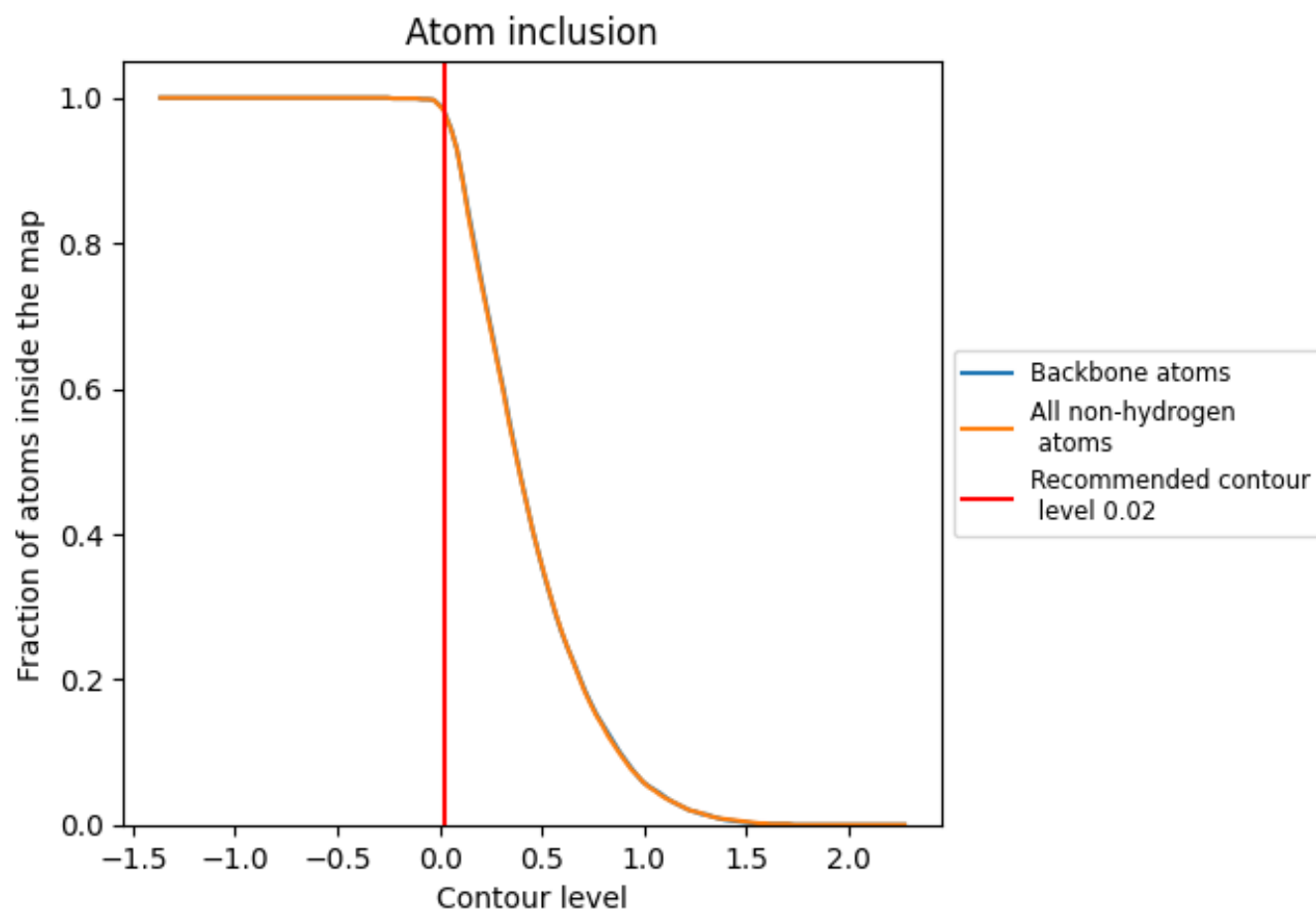
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

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

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	 0.9830	 0.3130
A	 0.9920	 0.3870
B	 0.9900	 0.3310
C	 0.9940	 0.4010
D	 0.9920	 0.3760
E	 0.9810	 0.3790
F	 0.9930	 0.2940
G	 0.9850	 0.0570
H	 0.9190	 0.0420
M	 0.9950	 0.0690
N	 1.0000	 0.0560
O	 0.9830	 0.2020
P	 0.9910	 0.1900
S	 0.5240	 0.0280

