



## Full wwPDB EM Validation Report ⓘ

Sep 23, 2025 – 04:21 PM EDT

PDB ID : 9E86 / pdb\_00009e86  
EMDB ID : EMD-47708  
Title : De Novo Mycobacterium tuberculosis transcription initiation promoter complex with 5-mer RNA and open Beta' clamp (RNA Polymerase with Sigma-A, CarD, and RbpA)  
Authors : Brewer, J.J.; Campbell, E.A.; Darst, S.A.  
Deposited on : 2024-11-05  
Resolution : 3.80 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

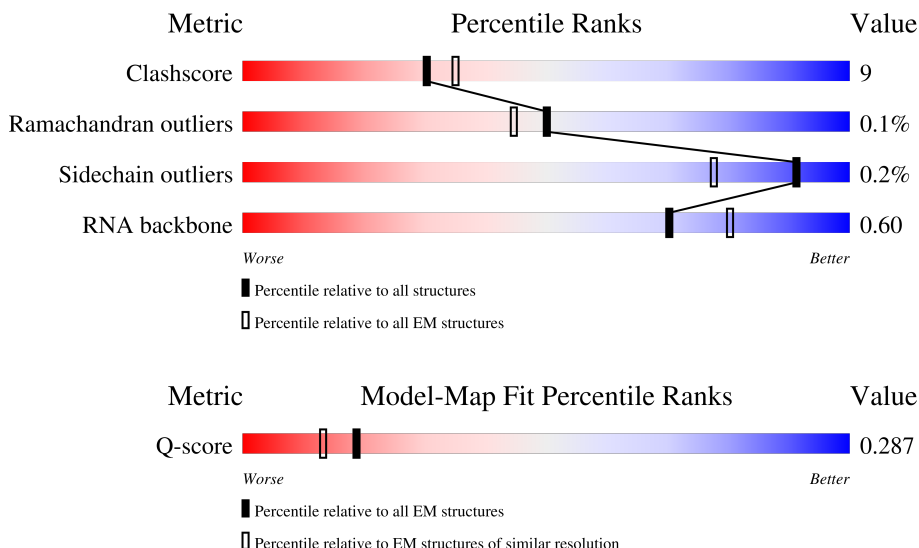
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

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



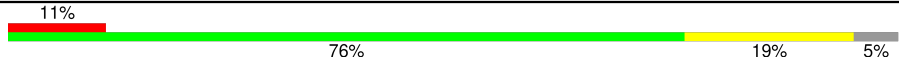

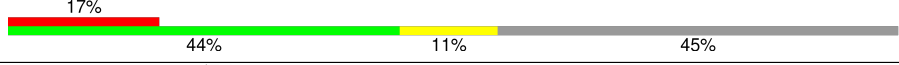
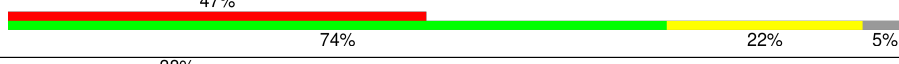
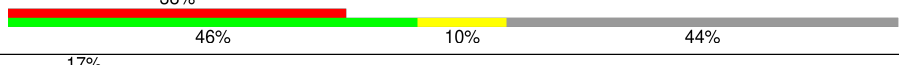

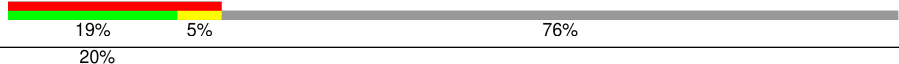

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	10198 ( 3.30 - 4.30 )

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  $\geq 3$ , 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	347	
1	B	347	
2	C	1177	

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Mol	Chain	Length	Quality of chain
3	D	1333	
4	E	110	
5	F	550	
6	J	111	
7	M	285	
8	N	127	
9	R	21	
10	T	127	

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 29207 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
1	A	225	Total	C	N	O	S	0	0
			1716	1080	296	338	2		
1	B	231	Total	C	N	O	S	0	0
			1724	1088	295	339	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1113	Total	C	N	O	S	0	0
			8571	5370	1498	1664	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1270	Total	C	N	O	S	0	0
			9904	6203	1804	1856	41		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	LEU	-	expression tag	UNP P0A675
D	-7	ALA	-	expression tag	UNP P0A675
D	-6	ARG	-	expression tag	UNP P0A675
D	-5	HIS	-	expression tag	UNP P0A675
D	-4	GLY	-	expression tag	UNP P0A675
D	-3	GLY	-	expression tag	UNP P0A675
D	-2	SER	-	expression tag	UNP P0A675
D	-1	GLY	-	expression tag	UNP P0A675
D	0	ALA	-	expression tag	UNP P0A675
D	1317	HIS	-	expression tag	UNP P0A675
D	1318	HIS	-	expression tag	UNP P0A675
D	1319	HIS	-	expression tag	UNP P0A675
D	1320	HIS	-	expression tag	UNP P0A675

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1321	HIS	-	expression tag	UNP P0A675
D	1322	HIS	-	expression tag	UNP P0A675
D	1323	HIS	-	expression tag	UNP P0A675
D	1324	HIS	-	expression tag	UNP P0A675

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	301	Total	C	N	O	S	0	0
			2373	1487	427	450	9		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-21	HIS	-	expression tag	UNP P0A603
F	-20	HIS	-	expression tag	UNP P0A603
F	-19	HIS	-	expression tag	UNP P0A603
F	-18	HIS	-	expression tag	UNP P0A603
F	-17	HIS	-	expression tag	UNP P0A603
F	-16	HIS	-	expression tag	UNP P0A603
F	-15	HIS	-	expression tag	UNP P0A603
F	-14	HIS	-	expression tag	UNP P0A603
F	-13	HIS	-	expression tag	UNP P0A603
F	-12	HIS	-	expression tag	UNP P0A603
F	-11	SER	-	expression tag	UNP P0A603
F	-10	SER	-	expression tag	UNP P0A603
F	-9	GLY	-	expression tag	UNP P0A603
F	-8	LEU	-	expression tag	UNP P0A603
F	-7	GLU	-	expression tag	UNP P0A603
F	-6	VAL	-	expression tag	UNP P0A603
F	-5	LEU	-	expression tag	UNP P0A603
F	-4	PHE	-	expression tag	UNP P0A603
F	-3	GLN	-	expression tag	UNP P0A603
F	-2	GLY	-	expression tag	UNP P0A603
F	-1	PRO	-	expression tag	UNP P0A603
F	0	HIS	-	expression tag	UNP P0A603

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	106	Total	C	N	O	S	0	0
			862	532	162	165	3		

- Molecule 7 is a protein called Ubiquitin-like protein SMT3,RNA polymerase-binding transcription factor CarD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	159	Total	C	N	O	S	0	0
			1241	777	224	239	1		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-122	MET	-	expression tag	UNP Q12306
M	-121	GLY	-	expression tag	UNP Q12306
M	-120	HIS	-	expression tag	UNP Q12306
M	-119	HIS	-	expression tag	UNP Q12306
M	-118	HIS	-	expression tag	UNP Q12306
M	-117	HIS	-	expression tag	UNP Q12306
M	-116	HIS	-	expression tag	UNP Q12306
M	-115	HIS	-	expression tag	UNP Q12306
M	-114	HIS	-	expression tag	UNP Q12306
M	-113	HIS	-	expression tag	UNP Q12306
M	-112	HIS	-	expression tag	UNP Q12306
M	-111	HIS	-	expression tag	UNP Q12306
M	-110	SER	-	expression tag	UNP Q12306
M	-109	SER	-	expression tag	UNP Q12306
M	-108	GLY	-	expression tag	UNP Q12306
M	-107	HIS	-	expression tag	UNP Q12306
M	-106	ILE	-	expression tag	UNP Q12306
M	-105	GLU	-	expression tag	UNP Q12306
M	-104	GLY	-	expression tag	UNP Q12306
M	-103	ARG	-	expression tag	UNP Q12306
M	-102	HIS	-	expression tag	UNP Q12306
M	-101	MET	-	expression tag	UNP Q12306
M	-100	ALA	-	expression tag	UNP Q12306
M	-99	SER	-	expression tag	UNP Q12306
M	0	SER	-	linker	UNP Q12306

- Molecule 8 is a DNA chain called DNA (52-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	52	Total	C	N	O	P	0	0
			1073	511	203	307	52		

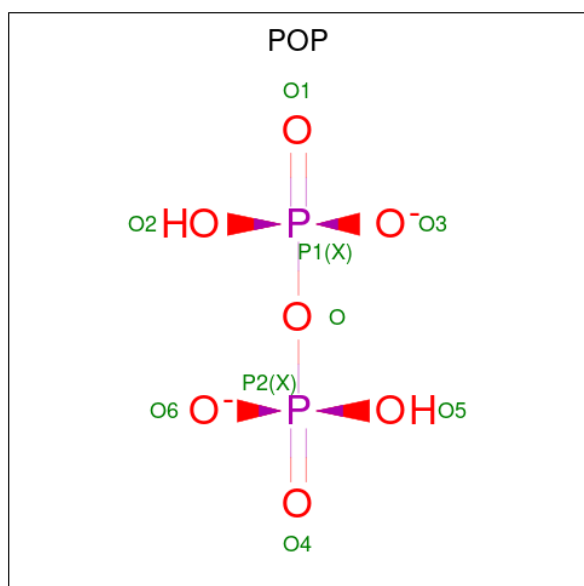
- Molecule 9 is a RNA chain called RNA (5'-R(P\*AP\*GP\*CP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	5	Total	C	N	O	P	0	0
			110	49	23	33	5		

- Molecule 10 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	48	Total	C	N	O	P	0	0
			972	466	164	294	48		

- Molecule 11 is PYROPHOSPHATE 2- (CCD ID: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms			AltConf
11	C	1	Total	O	P	0
			9	7	2	

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ).

Mol	Chain	Residues	Atoms		AltConf
12	D	2	Total	Zn	0
			2	2	

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

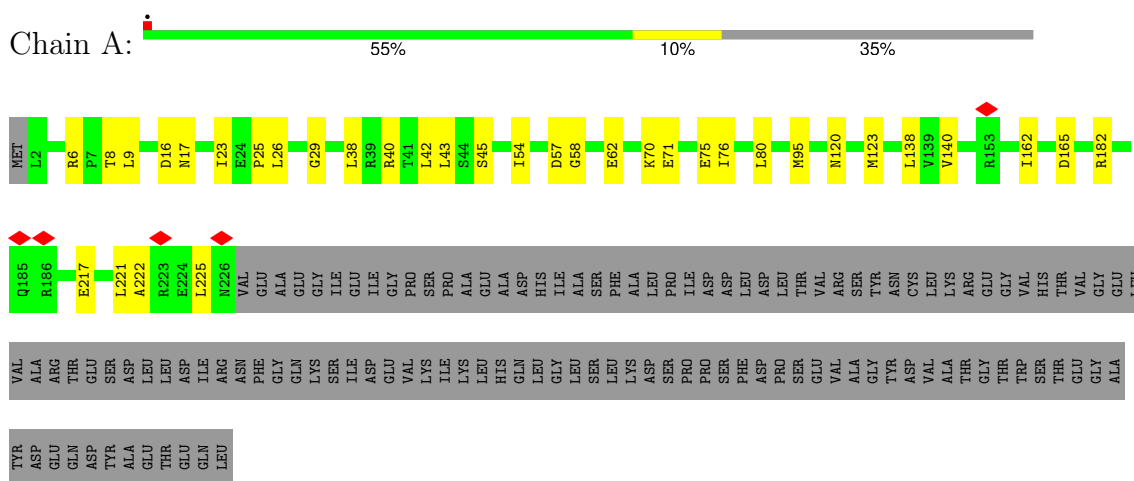
Mol	Chain	Residues	Atoms		AltConf
13	D	1	Total	Mg	0
			1	1	



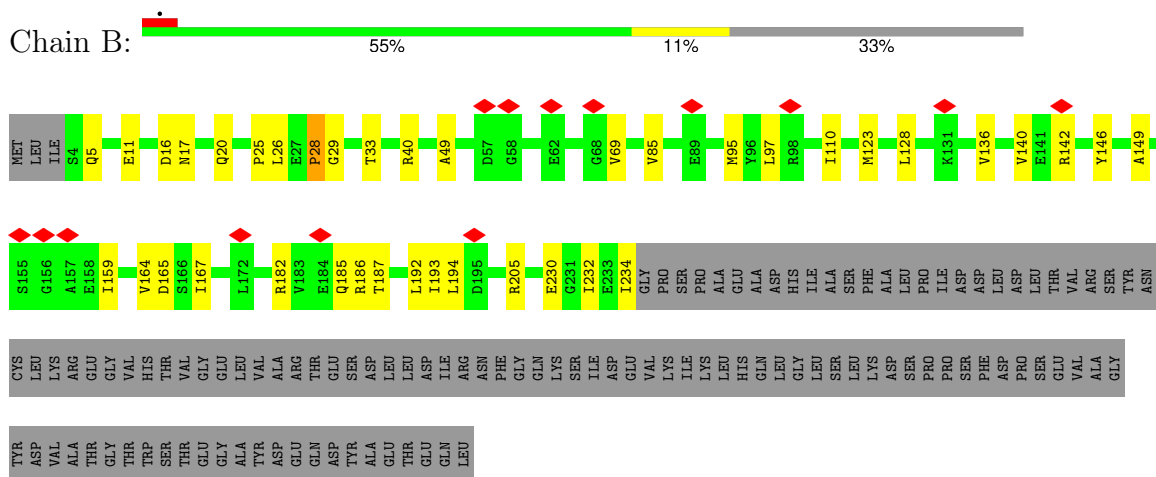
### 3 Residue-property plots

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

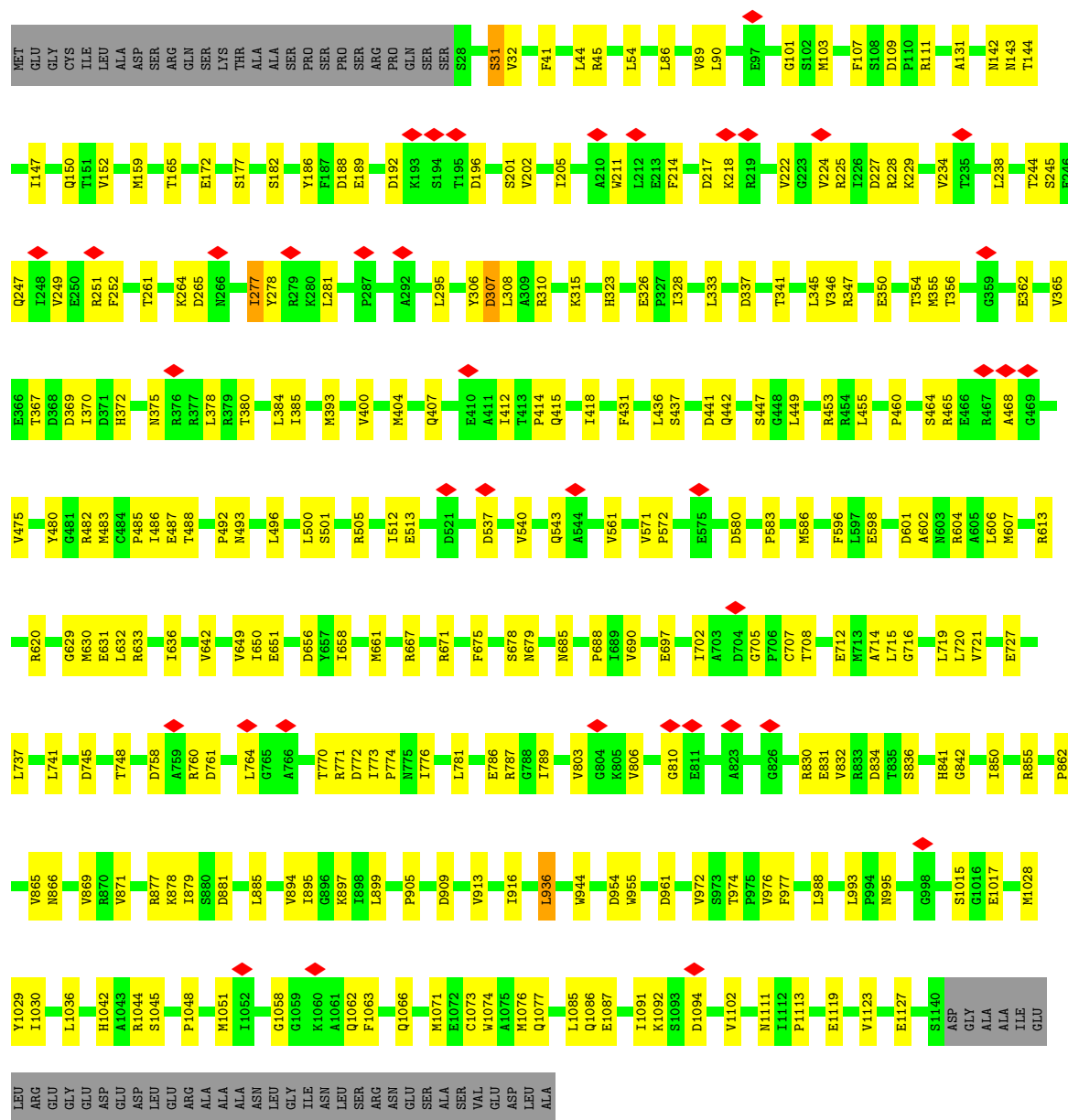


- Molecule 1: DNA-directed RNA polymerase subunit alpha

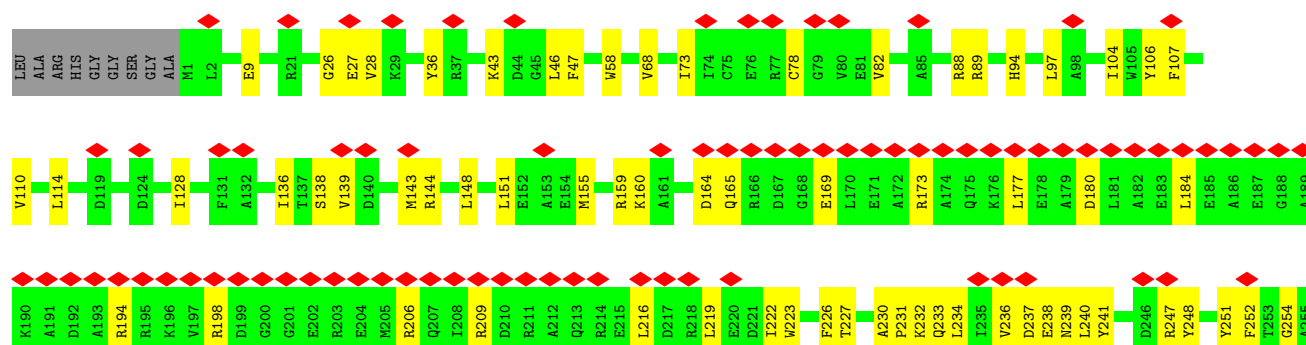
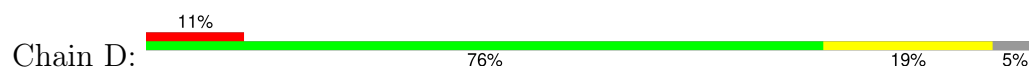


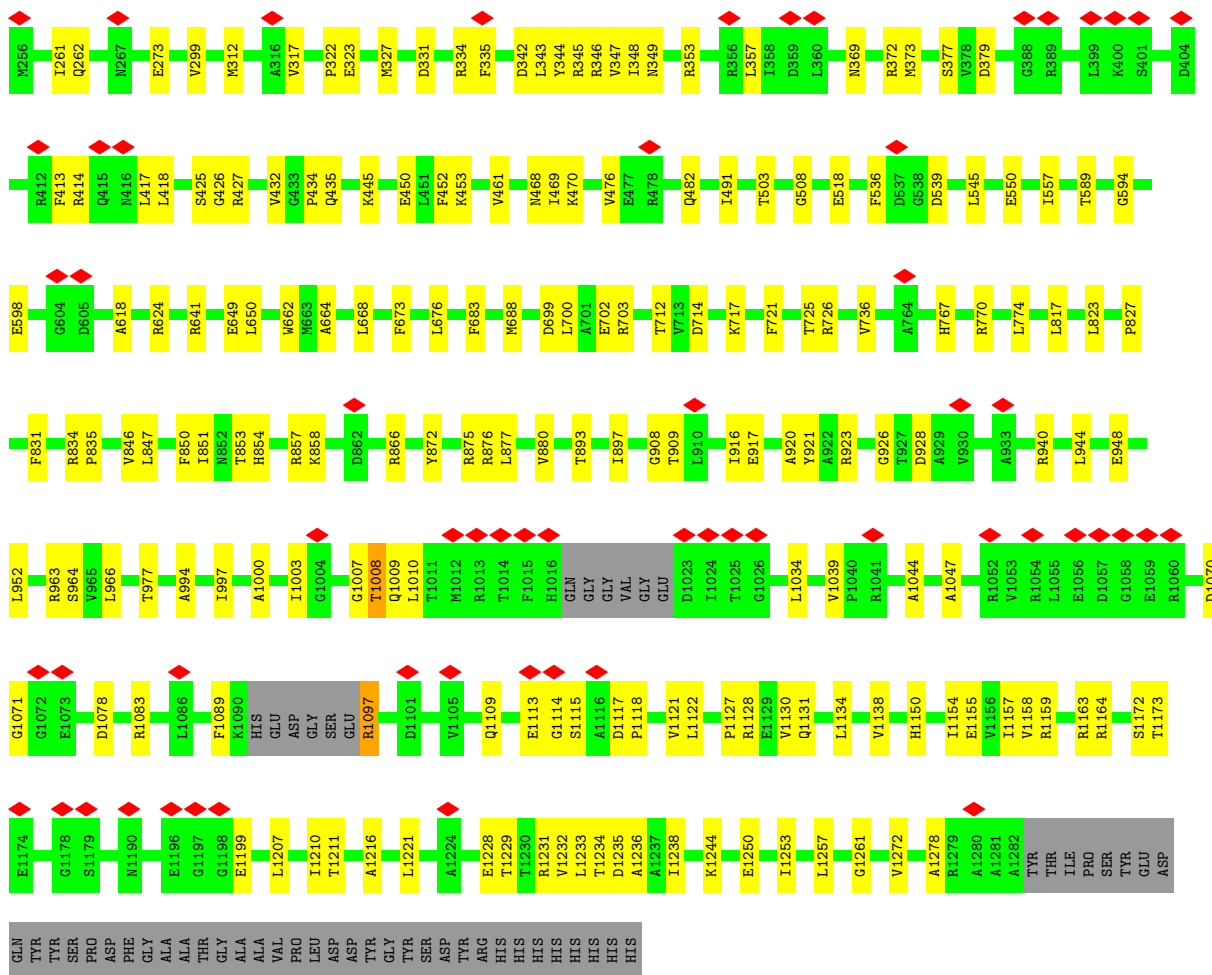
- Molecule 2: DNA-directed RNA polymerase subunit beta



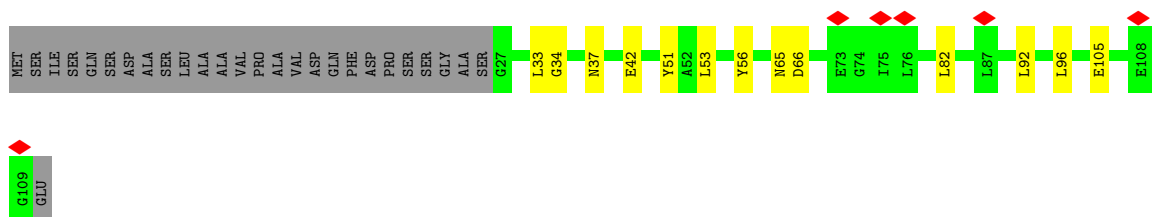


• Molecule 3: DNA-directed RNA polymerase subunit beta'

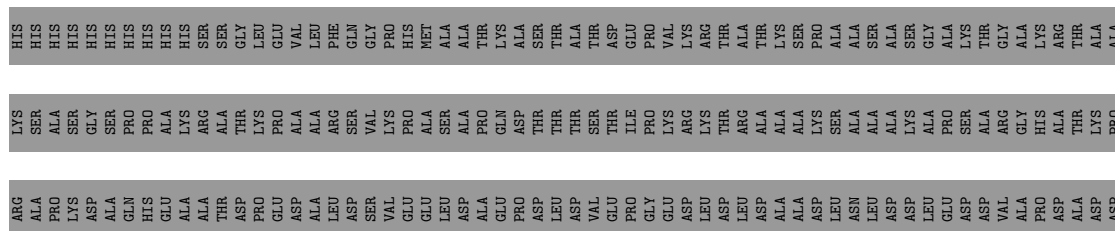




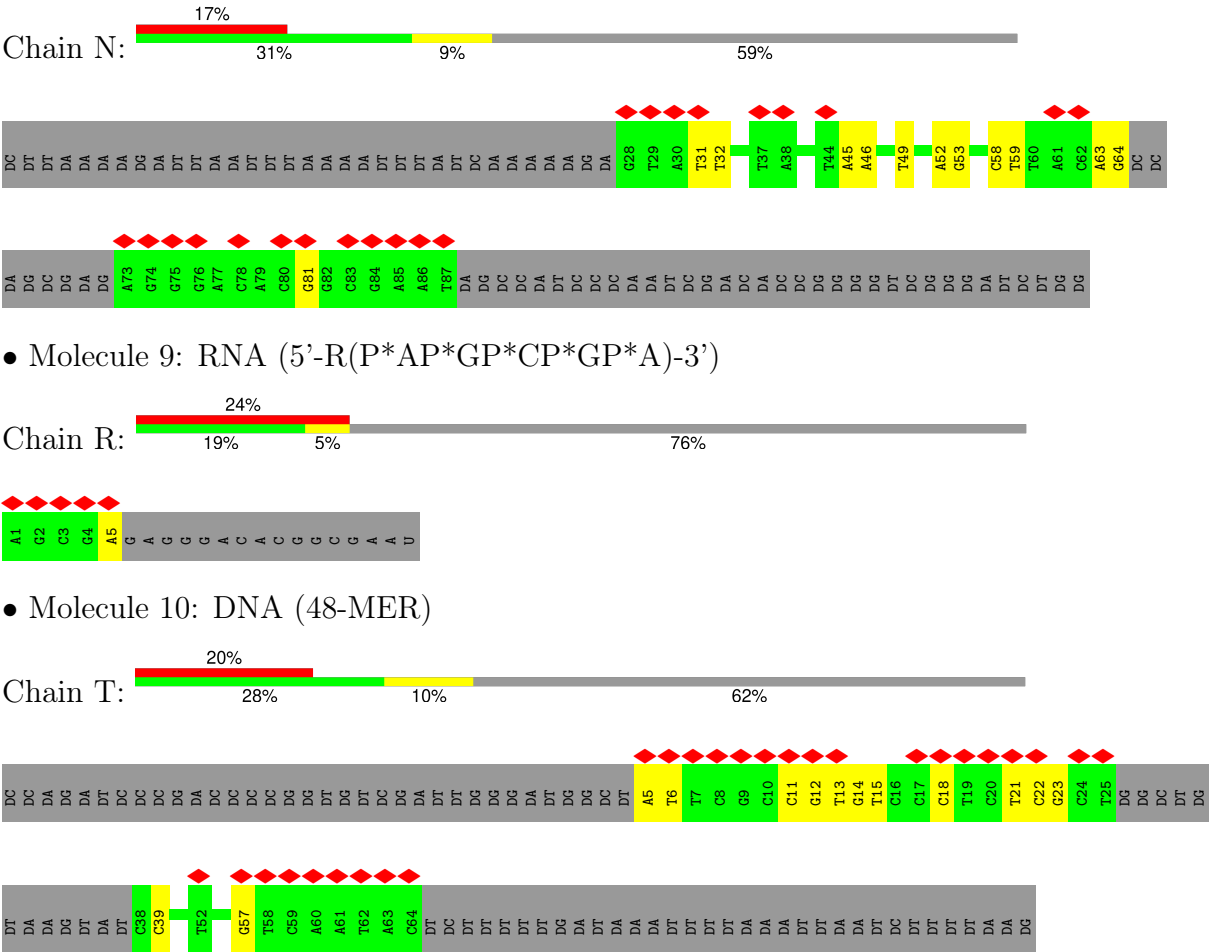
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor SigA







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10964	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	51.83	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.402	Depositor
Minimum map value	-0.974	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.194	Depositor
Map size (Å)	275.456, 275.456, 275.456	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.076, 1.076, 1.076	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POP, 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	0.17	0/1742	0.37	0/2370
1	B	0.15	0/1750	0.41	2/2385 (0.1%)
2	C	0.18	0/8730	0.40	0/11849
3	D	0.18	0/10068	0.40	0/13613
4	E	0.17	0/662	0.38	0/901
5	F	0.19	0/2403	0.41	0/3246
6	J	0.23	0/877	0.46	0/1182
7	M	0.18	0/1257	0.45	0/1700
8	N	0.22	0/1205	0.48	0/1856
9	R	0.12	0/123	0.29	0/190
10	T	0.23	0/1084	0.49	0/1666
All	All	0.18	0/29901	0.41	2/40958 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
3	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	PRO	CA-C-N	5.21	131.09	121.70
1	B	28	PRO	C-N-CA	5.21	131.09	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	307	ASP	Peptide
3	D	1173	THR	Peptide

## 5.2 Too-close contacts

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	1716	0	1756	24	0
1	B	1724	0	1745	28	0
2	C	8571	0	8457	194	0
3	D	9904	0	9967	184	0
4	E	649	0	645	12	0
5	F	2373	0	2384	50	0
6	J	862	0	845	19	0
7	M	1241	0	1259	22	0
8	N	1073	0	587	11	0
9	R	110	0	56	1	0
10	T	972	0	546	14	0
11	C	9	0	0	0	0
12	D	2	0	0	0	0
13	D	1	0	0	0	0
All	All	29207	0	28247	505	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 9.

All (505) 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)
5:F:492:ILE:HD12	5:F:503:ILE:HG21	1.44	0.97
3:D:369:ASN:OD1	3:D:372:ARG:NH2	2.04	0.90
7:M:70:VAL:HG11	7:M:101:VAL:HG12	1.55	0.87
2:C:441:ASP:OD1	2:C:447:SER:OG	1.95	0.84
3:D:964:SER:OG	3:D:1155:GLU:OE1	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1089:PHE:O	3:D:1097:ARG:N	2.13	0.82
2:C:745:ASP:OD1	2:C:748:THR:OG1	1.98	0.81
2:C:787:ARG:O	2:C:787:ARG:NH1	2.15	0.79
3:D:917:GLU:N	3:D:917:GLU:OE1	2.17	0.78
3:D:897:ILE:HD11	3:D:966:LEU:HD12	1.67	0.77
3:D:966:LEU:HD21	3:D:1158:VAL:HG23	1.67	0.77
4:E:42:GLU:OE1	4:E:42:GLU:N	2.17	0.77
3:D:239:ASN:OD1	3:D:240:LEU:N	2.18	0.77
6:J:79:ARG:NH2	8:N:53:DG:OP1	2.19	0.76
2:C:1058:GLY:O	2:C:1062:GLN:NE2	2.19	0.76
3:D:926:GLY:O	3:D:940:ARG:NH1	2.19	0.75
2:C:109:ASP:OD2	2:C:111:ARG:NH1	2.20	0.75
5:F:488:THR:OG1	5:F:491:GLU:OE1	2.02	0.75
1:B:5:GLN:NE2	1:B:25:PRO:O	2.20	0.74
2:C:632:LEU:HD12	2:C:633:ARG:N	2.02	0.74
2:C:369:ASP:O	2:C:375:ASN:ND2	2.21	0.74
2:C:182:SER:O	2:C:186:TYR:OH	2.03	0.73
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.22	0.73
2:C:879:ILE:HD11	2:C:895:ILE:CD1	2.18	0.73
7:M:23:GLU:N	7:M:34:TYR:O	2.23	0.72
3:D:1083:ARG:O	3:D:1083:ARG:NH1	2.23	0.71
4:E:34:GLY:O	4:E:37:ASN:ND2	2.22	0.71
1:B:123:MET:HA	1:B:123:MET:HE2	1.72	0.71
2:C:586:MET:HE2	3:D:846:VAL:HG13	1.73	0.71
2:C:1042:HIS:NE2	2:C:1063:PHE:O	2.24	0.70
3:D:594:GLY:N	3:D:598:GLU:OE2	2.24	0.70
5:F:351:ILE:HG22	5:F:355:ILE:HD11	1.73	0.69
3:D:9:GLU:OE2	3:D:1244:LYS:NZ	2.21	0.69
1:A:70:LYS:NZ	2:C:690:VAL:O	2.26	0.69
3:D:184:LEU:O	3:D:194:ARG:NH1	2.25	0.69
3:D:1128:ARG:NH1	3:D:1131:GLN:OE1	2.24	0.69
2:C:651:GLU:OE2	2:C:667:ARG:NH1	2.26	0.69
6:J:79:ARG:NH1	8:N:52:DA:O3'	2.25	0.69
1:A:62:GLU:HG3	1:A:162:ILE:HG23	1.75	0.68
2:C:326:GLU:OE1	2:C:326:GLU:N	2.26	0.68
5:F:256:GLY:HA2	5:F:284:ILE:HG22	1.74	0.68
3:D:966:LEU:HD13	3:D:1131:GLN:OE1	1.94	0.67
3:D:435:GLN:N	3:D:435:GLN:OE1	2.27	0.67
3:D:699:ASP:OD1	3:D:703:ARG:NH1	2.28	0.67
2:C:150:GLN:NE2	2:C:415:GLN:OE1	2.28	0.67
2:C:631:GLU:N	2:C:631:GLU:OE1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:27:GLU:N	3:D:27:GLU:OE1	2.27	0.67
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.76	0.67
2:C:855:ARG:NH2	2:C:865:VAL:O	2.28	0.66
2:C:571:VAL:HG22	2:C:572:PRO:HD2	1.77	0.66
3:D:963:ARG:NH1	3:D:977:THR:OG1	2.28	0.66
1:A:29:GLY:O	1:B:40:ARG:NH1	2.28	0.66
5:F:440:GLU:OE2	5:F:442:SER:N	2.28	0.66
2:C:192:ASP:O	2:C:196:ASP:N	2.24	0.66
3:D:880:VAL:HG21	3:D:1210:ILE:HB	1.76	0.65
2:C:604:ARG:NH1	2:C:607:MET:SD	2.70	0.65
3:D:241:TYR:OH	3:D:254:GLY:O	2.16	0.64
3:D:923:ARG:NH2	3:D:1155:GLU:OE2	2.30	0.64
2:C:505:ARG:NH2	2:C:513:GLU:OE1	2.30	0.64
2:C:1111:ASN:OD1	4:E:65:ASN:ND2	2.30	0.64
2:C:431:PHE:O	2:C:437:SER:OG	2.14	0.64
3:D:148:LEU:HD21	3:D:227:THR:HG22	1.80	0.64
7:M:30:GLU:OE1	7:M:32:LYS:NZ	2.30	0.64
3:D:1007:GLY:O	3:D:1009:GLN:N	2.31	0.64
2:C:656:ASP:OD1	2:C:671:ARG:NH1	2.31	0.63
2:C:772:ASP:O	2:C:830:ARG:NH2	2.29	0.63
7:M:104:VAL:CG2	7:M:135:LEU:HD21	2.28	0.63
2:C:909:ASP:OD2	2:C:995:ASN:ND2	2.32	0.63
2:C:705:GLY:N	2:C:708:THR:OG1	2.32	0.63
3:D:1118:PRO:HA	3:D:1121:VAL:HG12	1.81	0.62
6:J:90:SER:OG	6:J:92:GLU:OE1	2.16	0.62
2:C:214:PHE:CD1	2:C:224:VAL:HG13	2.35	0.62
2:C:897:LYS:HG3	2:C:899:LEU:HD23	1.81	0.62
5:F:463:VAL:O	5:F:466:THR:OG1	2.12	0.62
5:F:464:LEU:HD22	5:F:472:ALA:HA	1.81	0.62
3:D:97:LEU:HD21	3:D:317:VAL:HG23	1.81	0.62
3:D:68:VAL:HG21	6:J:17:GLU:HG2	1.82	0.62
5:F:299:ASN:OD1	8:N:59:DT:N3	2.32	0.62
2:C:1015:SER:OG	2:C:1017:GLU:OE1	2.17	0.61
5:F:492:ILE:CD1	5:F:503:ILE:HG21	2.25	0.61
5:F:255:ALA:HB2	6:J:97:LEU:HD22	1.83	0.60
1:A:25:PRO:C	1:A:26:LEU:HD12	2.27	0.60
2:C:879:ILE:HD11	2:C:895:ILE:HD12	1.83	0.60
5:F:277:GLN:NE2	5:F:281:MET:SD	2.73	0.60
2:C:31:SER:OG	2:C:32:VAL:N	2.34	0.60
2:C:44:LEU:HD12	2:C:45:ARG:N	2.15	0.60
1:B:167:ILE:HG23	1:B:167:ILE:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:716:GLY:N	2:C:1029:TYR:OH	2.35	0.60
2:C:715:LEU:N	2:C:1029:TYR:OH	2.35	0.60
5:F:351:ILE:HG22	5:F:355:ILE:CD1	2.32	0.60
1:B:16:ASP:OD1	1:B:17:ASN:N	2.34	0.59
1:A:40:ARG:HE	1:B:33:THR:HG22	1.67	0.59
2:C:147:ILE:HD11	7:M:47:ARG:HD3	1.84	0.59
2:C:1017:GLU:OE1	2:C:1017:GLU:N	2.35	0.59
5:F:306:LEU:HD11	5:F:348:THR:HG23	1.84	0.59
3:D:1121:VAL:HG13	3:D:1130:VAL:HG12	1.85	0.59
2:C:245:SER:O	2:C:249:VAL:HG23	2.01	0.59
2:C:347:ARG:NH1	2:C:355:MET:SD	2.75	0.59
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.85	0.59
3:D:503:THR:HG23	3:D:508:GLY:HA3	1.84	0.58
5:F:238:VAL:HG11	5:F:297:GLU:HB3	1.85	0.58
3:D:238:GLU:OE1	3:D:238:GLU:N	2.33	0.58
3:D:649:GLU:OE1	3:D:650:LEU:N	2.36	0.58
3:D:1250:GLU:OE1	3:D:1250:GLU:N	2.35	0.58
2:C:598:GLU:OE1	2:C:598:GLU:N	2.37	0.57
2:C:101:GLY:O	2:C:142:ASN:ND2	2.37	0.57
7:M:104:VAL:HG21	7:M:135:LEU:HD21	1.85	0.57
3:D:1229:THR:HG22	3:D:1233:LEU:HD11	1.86	0.57
1:B:11:GLU:OE1	1:B:11:GLU:N	2.37	0.57
5:F:498:VAL:HG21	5:F:502:ARG:NH2	2.19	0.57
2:C:372:HIS:NE2	2:C:537:ASP:OD2	2.38	0.57
2:C:675:PHE:N	2:C:685:ASN:OD1	2.38	0.57
2:C:468:ALA:HB1	2:C:496:LEU:HD11	1.87	0.56
2:C:601:ASP:OD1	2:C:602:ALA:N	2.38	0.56
3:D:1039:VAL:HG12	3:D:1117:ASP:HB3	1.87	0.56
2:C:993:LEU:HD12	2:C:993:LEU:O	2.05	0.56
3:D:236:VAL:HG12	3:D:237:ASP:H	1.70	0.56
3:D:1044:ALA:N	3:D:1115:SER:O	2.34	0.56
1:B:164:VAL:HG23	1:B:165:ASP:O	2.06	0.56
2:C:1111:ASN:ND2	4:E:66:ASP:OD1	2.39	0.55
3:D:151:LEU:HD13	3:D:248:TYR:CE1	2.41	0.55
1:B:95:MET:SD	1:B:95:MET:N	2.79	0.55
3:D:1138:VAL:HG11	3:D:1154:ILE:HD12	1.87	0.55
2:C:881:ASP:N	2:C:881:ASP:OD1	2.37	0.55
2:C:954:ASP:OD1	2:C:955:TRP:N	2.39	0.55
2:C:222:VAL:HG22	2:C:261:THR:HG21	1.88	0.55
2:C:936:LEU:HD11	2:C:972:VAL:HG11	1.89	0.55
2:C:1071:MET:HE2	10:T:21:DT:H4'	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:445:LYS:NZ	3:D:518:GLU:OE2	2.40	0.54
2:C:315:LYS:NZ	2:C:375:ASN:OD1	2.36	0.54
2:C:540:VAL:HG22	2:C:561:VAL:HG22	1.88	0.54
3:D:866:ARG:HD2	3:D:1008:THR:O	2.07	0.54
1:A:23:ILE:HG22	1:A:26:LEU:HD11	1.90	0.54
2:C:485:PRO:O	3:D:857:ARG:NH2	2.40	0.54
2:C:831:GLU:OE1	2:C:831:GLU:N	2.40	0.54
2:C:261:THR:O	2:C:265:ASP:N	2.41	0.54
3:D:539:ASP:OD2	9:R:5:A:O2'	2.22	0.54
3:D:1008:THR:O	3:D:1010:LEU:N	2.41	0.54
3:D:1034:LEU:HD11	3:D:1134:LEU:HD23	1.90	0.54
2:C:1076:MET:HB3	2:C:1085:LEU:HD13	1.89	0.54
2:C:278:TYR:HE1	2:C:295:LEU:HD22	1.73	0.54
2:C:540:VAL:HG22	2:C:561:VAL:CG2	2.38	0.54
3:D:331:ASP:O	3:D:334:ARG:NH2	2.41	0.54
2:C:488:THR:O	2:C:606:LEU:HD11	2.08	0.53
5:F:287:ASP:OD2	6:J:101:ARG:NH2	2.40	0.53
5:F:372:MET:HA	5:F:375:VAL:HG12	1.90	0.53
5:F:501:GLU:HG2	8:N:32:DT:H71	1.91	0.53
3:D:877:LEU:HD23	3:D:877:LEU:O	2.08	0.53
3:D:160:LYS:NZ	3:D:164:ASP:OD1	2.42	0.53
2:C:278:TYR:CE1	2:C:295:LEU:HD22	2.43	0.53
3:D:1172:SER:OG	3:D:1199:GLU:OE2	2.27	0.53
1:B:149:ALA:N	1:B:165:ASP:OD1	2.42	0.52
2:C:143:ASN:OD1	2:C:144:THR:N	2.42	0.52
3:D:28:VAL:HG21	3:D:46:LEU:HD13	1.91	0.52
3:D:641:ARG:O	3:D:683:PHE:N	2.42	0.52
3:D:966:LEU:HD22	3:D:1131:GLN:NE2	2.24	0.52
3:D:1134:LEU:O	3:D:1138:VAL:HG12	2.10	0.52
2:C:834:ASP:OD1	2:C:834:ASP:N	2.42	0.52
3:D:850:PHE:O	3:D:853:THR:OG1	2.28	0.52
3:D:1250:GLU:O	3:D:1253:ILE:HG22	2.09	0.52
2:C:354:THR:HA	2:C:365:VAL:HG23	1.91	0.52
3:D:413:PHE:HA	3:D:417:LEU:HD12	1.91	0.52
1:B:230:GLU:OE1	1:B:230:GLU:N	2.38	0.52
2:C:152:VAL:HG11	2:C:418:ILE:HG21	1.91	0.52
1:B:95:MET:CB	1:B:110:ILE:HD11	2.40	0.52
5:F:351:ILE:CG2	5:F:355:ILE:HD11	2.39	0.52
1:A:221:LEU:HD23	1:A:222:ALA:N	2.25	0.52
2:C:244:THR:O	2:C:247:GLN:N	2.43	0.52
2:C:586:MET:HE3	2:C:586:MET:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:MET:HB3	1:B:110:ILE:HD11	1.91	0.51
1:B:146:TYR:O	3:D:624:ARG:NH2	2.43	0.51
3:D:1235:ASP:OD1	3:D:1236:ALA:N	2.44	0.51
3:D:335:PHE:O	5:F:421:ILE:N	2.43	0.51
5:F:315:MET:HE1	5:F:362:GLN:HB2	1.92	0.51
2:C:189:GLU:OE1	2:C:367:THR:HG21	2.11	0.51
3:D:1127:PRO:HA	3:D:1130:VAL:HG22	1.93	0.51
1:B:186:ARG:O	1:B:187:THR:OG1	2.21	0.51
2:C:885:LEU:HD13	2:C:895:ILE:HD11	1.92	0.51
3:D:173:ARG:NH2	3:D:180:ASP:OD2	2.44	0.51
2:C:281:LEU:HD23	2:C:295:LEU:HD23	1.93	0.51
3:D:1234:THR:O	3:D:1238:ILE:HG13	2.11	0.51
2:C:789:ILE:HG21	2:C:869:VAL:HG21	1.93	0.51
3:D:700:LEU:HD23	3:D:712:THR:HG21	1.93	0.51
2:C:1074:TRP:O	3:D:997:ILE:HD11	2.11	0.50
3:D:482:GLN:OE1	3:D:482:GLN:N	2.38	0.50
3:D:1207:LEU:HD23	3:D:1207:LEU:O	2.11	0.50
7:M:4:LYS:N	7:M:7:ASP:OD2	2.45	0.50
2:C:774:PRO:O	2:C:776:ILE:HG22	2.11	0.50
3:D:877:LEU:HD22	3:D:1000:ALA:CB	2.40	0.50
2:C:234:VAL:HG22	2:C:238:LEU:HD23	1.92	0.50
3:D:1003:ILE:HD11	3:D:1154:ILE:HD13	1.93	0.50
3:D:1117:ASP:OD1	3:D:1117:ASP:N	2.40	0.50
2:C:455:LEU:HD12	2:C:483:MET:HG3	1.93	0.50
3:D:767:HIS:O	3:D:770:ARG:HG3	2.12	0.50
2:C:86:LEU:O	2:C:89:VAL:HG12	2.11	0.50
7:M:70:VAL:HG11	7:M:101:VAL:CG1	2.35	0.50
2:C:789:ILE:HD13	2:C:850:ILE:HD13	1.93	0.50
3:D:1159:ARG:O	3:D:1163:ARG:NE	2.45	0.50
2:C:487:GLU:OE2	2:C:613:ARG:NH2	2.45	0.49
3:D:345:ARG:O	3:D:349:ASN:OD1	2.30	0.49
2:C:1092:LYS:NZ	3:D:545:LEU:O	2.38	0.49
3:D:1113:GLU:OE1	3:D:1114:GLY:N	2.45	0.49
5:F:456:LEU:O	5:F:460:LEU:HG	2.12	0.49
2:C:480:TYR:OH	2:C:580:ASP:OD2	2.19	0.49
3:D:908:GLY:O	3:D:909:THR:HG23	2.11	0.49
2:C:177:SER:HB3	2:C:378:LEU:HD11	1.94	0.49
2:C:707:CYS:O	2:C:714:ALA:N	2.44	0.49
1:B:85:VAL:HG21	1:B:140:VAL:HG21	1.95	0.49
2:C:251:ARG:HG3	2:C:252:PHE:CD2	2.48	0.49
2:C:1051:MET:HE1	5:F:441:ASP:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:73:ILE:CG2	6:J:27:ARG:HD3	2.43	0.49
5:F:345:THR:HG23	8:N:58:DC:H5	1.78	0.49
10:T:12:DG:H2'	10:T:13:DT:H72	1.95	0.49
1:B:69:VAL:HG12	1:B:128:LEU:HG	1.94	0.49
3:D:165:GLN:NE2	3:D:169:GLU:OE2	2.42	0.49
3:D:1070:ASP:N	3:D:1071:GLY:HA2	2.28	0.49
3:D:468:ASN:OD1	3:D:470:LYS:N	2.46	0.49
3:D:618:ALA:HB1	3:D:668:LEU:HD12	1.94	0.49
2:C:214:PHE:CE1	2:C:224:VAL:HG13	2.48	0.48
3:D:47:PHE:CD2	3:D:322:PRO:HB3	2.48	0.48
3:D:230:ALA:HB1	3:D:231:PRO:HD2	1.95	0.48
2:C:356:THR:HA	2:C:362:GLU:HA	1.96	0.48
2:C:453:ARG:NH2	2:C:501:SER:O	2.46	0.48
2:C:789:ILE:HG22	2:C:803:VAL:HG22	1.95	0.48
3:D:353:ARG:NE	5:F:323:GLU:OE2	2.46	0.48
4:E:92:LEU:HD13	4:E:96:LEU:HD13	1.96	0.48
5:F:328:LEU:CD2	5:F:351:ILE:HD11	2.43	0.48
2:C:642:VAL:O	2:C:702:ILE:HG22	2.12	0.48
2:C:1017:GLU:OE2	3:D:726:ARG:NH2	2.45	0.48
3:D:893:THR:O	3:D:940:ARG:NH2	2.46	0.48
1:B:192:LEU:HD23	1:B:193:ILE:N	2.29	0.48
2:C:107:PHE:HZ	2:C:418:ILE:HD12	1.78	0.48
2:C:1036:LEU:N	2:C:1036:LEU:HD12	2.29	0.48
2:C:721:VAL:HG21	2:C:1028:MET:CE	2.44	0.48
2:C:737:LEU:HB3	2:C:741:LEU:HD12	1.95	0.48
3:D:434:PRO:O	3:D:717:LYS:NZ	2.40	0.48
1:A:76:ILE:O	1:A:80:LEU:HG	2.14	0.48
3:D:155:MET:HE1	3:D:223:TRP:CD1	2.49	0.48
5:F:324:GLY:O	5:F:328:LEU:HG	2.14	0.48
5:F:317:PHE:O	5:F:321:ILE:HG13	2.14	0.48
2:C:346:VAL:O	2:C:350:GLU:HG3	2.14	0.47
2:C:764:LEU:HD13	2:C:810:GLY:N	2.29	0.47
5:F:525:ASP:N	5:F:525:ASP:OD1	2.44	0.47
2:C:308:LEU:H	2:C:308:LEU:HD23	1.79	0.47
2:C:712:GLU:OE1	2:C:712:GLU:N	2.46	0.47
2:C:758:ASP:OD2	2:C:760:ARG:NH2	2.47	0.47
5:F:333:GLU:O	6:J:81:HIS:NE2	2.47	0.47
2:C:211:TRP:O	2:C:227:ASP:N	2.47	0.47
2:C:407:GLN:HB3	2:C:412:ILE:HG21	1.95	0.47
3:D:468:ASN:OD1	3:D:468:ASN:C	2.58	0.47
6:J:75:VAL:HG12	6:J:76:LYS:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:345:LEU:O	2:C:345:LEU:HD23	2.15	0.47
2:C:697:GLU:OE1	2:C:697:GLU:N	2.48	0.47
2:C:1045:SER:N	3:D:450:GLU:OE2	2.48	0.47
5:F:246:GLU:HA	5:F:249:LEU:HD12	1.97	0.47
1:A:217:GLU:OE1	1:B:234:ILE:HD12	2.14	0.47
2:C:277:ILE:O	2:C:281:LEU:HD13	2.15	0.47
2:C:442:GLN:NE2	2:C:679:ASN:OD1	2.48	0.47
3:D:427:ARG:NE	10:T:23:DG:H4'	2.30	0.47
5:F:277:GLN:O	5:F:281:MET:HG3	2.14	0.47
1:A:16:ASP:OD2	1:A:17:ASN:N	2.48	0.47
2:C:369:ASP:OD1	2:C:370:ILE:N	2.45	0.47
5:F:235:ILE:HG22	5:F:300:LEU:HD13	1.95	0.47
3:D:823:LEU:HD12	3:D:831:PHE:HB3	1.96	0.47
1:A:165:ASP:N	1:A:165:ASP:OD1	2.47	0.47
2:C:961:ASP:N	2:C:961:ASP:OD1	2.45	0.47
3:D:1221:LEU:HD11	3:D:1253:ILE:HG21	1.97	0.47
1:A:8:THR:OG1	1:A:9:LEU:N	2.44	0.46
3:D:461:VAL:HG21	3:D:469:ILE:HD13	1.97	0.46
3:D:1154:ILE:O	3:D:1158:VAL:HG22	2.15	0.46
2:C:165:THR:HG21	2:C:172:GLU:OE1	2.15	0.46
3:D:994:ALA:HB1	3:D:997:ILE:HG22	1.97	0.46
2:C:678:SER:OG	2:C:679:ASN:N	2.49	0.46
2:C:737:LEU:HD11	2:C:895:ILE:HD13	1.96	0.46
2:C:737:LEU:HD11	2:C:895:ILE:CD1	2.44	0.46
3:D:177:LEU:HD11	3:D:198:ARG:HD3	1.98	0.46
3:D:414:ARG:HA	3:D:418:LEU:HD13	1.97	0.46
3:D:928:ASP:OD1	3:D:940:ARG:N	2.49	0.46
3:D:1078:ASP:OD1	3:D:1078:ASP:N	2.44	0.46
7:M:6:GLY:H	7:M:19:VAL:HG23	1.80	0.46
2:C:586:MET:HE2	3:D:846:VAL:CG1	2.42	0.46
7:M:85:TRP:CD1	7:M:85:TRP:O	2.68	0.46
2:C:222:VAL:H	2:C:261:THR:HG21	1.79	0.46
2:C:475:VAL:HG23	3:D:854:HIS:ND1	2.30	0.46
2:C:482:ARG:HB3	2:C:512:ILE:HG21	1.98	0.46
2:C:486:ILE:O	2:C:606:LEU:HD13	2.15	0.46
2:C:771:ARG:O	2:C:773:ILE:HD12	2.16	0.46
3:D:88:ARG:O	3:D:322:PRO:HD2	2.15	0.46
2:C:632:LEU:O	2:C:636:ILE:HG23	2.16	0.46
2:C:758:ASP:N	2:C:758:ASP:OD1	2.46	0.46
2:C:1073:CYS:O	2:C:1077:GLN:NE2	2.49	0.46
3:D:47:PHE:CZ	3:D:327:MET:HE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:3:PHE:HE2	7:M:58:VAL:HG11	1.81	0.46
2:C:862:PRO:HG2	2:C:865:VAL:HG21	1.98	0.46
2:C:1044:ARG:NH2	2:C:1048:PRO:O	2.41	0.46
2:C:1123:VAL:O	2:C:1127:GLU:HG3	2.15	0.46
2:C:727:GLU:H	3:D:725:THR:HG22	1.81	0.46
3:D:345:ARG:O	3:D:346:ARG:C	2.58	0.46
6:J:64:LEU:HD23	6:J:65:ILE:N	2.31	0.46
2:C:307:ASP:OD1	2:C:307:ASP:N	2.49	0.46
3:D:110:VAL:O	3:D:1231:ARG:NH1	2.48	0.46
3:D:834:ARG:HB3	3:D:835:PRO:HA	1.98	0.45
5:F:284:ILE:HG23	6:J:101:ARG:NH1	2.31	0.45
2:C:393:MET:HE3	2:C:393:MET:HA	1.97	0.45
2:C:465:ARG:NH1	2:C:492:PRO:O	2.49	0.45
3:D:699:ASP:HA	3:D:702:GLU:HG2	1.99	0.45
2:C:414:PRO:O	2:C:418:ILE:HG22	2.16	0.45
3:D:58:TRP:CD2	3:D:68:VAL:HG22	2.51	0.45
5:F:498:VAL:HG21	5:F:502:ARG:CZ	2.47	0.45
7:M:85:TRP:HZ3	10:T:39:DC:O3'	1.99	0.45
3:D:43:LYS:NZ	3:D:78:CYS:O	2.50	0.45
7:M:107:VAL:O	7:M:111:LEU:HD23	2.15	0.45
10:T:14:DG:H2'	10:T:15:DT:H72	1.99	0.45
3:D:106:TYR:HB3	3:D:312:MET:HE1	1.97	0.45
3:D:136:ILE:HD12	3:D:252:PHE:CD2	2.51	0.45
3:D:1272:VAL:HG13	4:E:56:TYR:HE1	1.82	0.45
1:A:43:LEU:O	1:A:43:LEU:HD12	2.17	0.45
2:C:1086:GLN:OE1	3:D:1257:LEU:N	2.50	0.45
3:D:345:ARG:O	3:D:348:ILE:N	2.50	0.45
3:D:966:LEU:HD22	3:D:1131:GLN:CD	2.41	0.45
1:A:45:SER:HB3	1:B:232:ILE:HD11	1.98	0.45
2:C:894:VAL:HG22	3:D:536:PHE:O	2.17	0.45
3:D:331:ASP:OD1	3:D:331:ASP:N	2.50	0.45
2:C:202:VAL:HG12	2:C:214:PHE:HB2	1.97	0.45
5:F:241:LEU:HD13	5:F:249:LEU:HD11	1.99	0.45
7:M:6:GLY:N	7:M:19:VAL:HG23	2.32	0.45
7:M:146:ASP:O	7:M:149:LYS:N	2.50	0.45
7:M:148:ALA:O	7:M:152:THR:HG23	2.16	0.45
2:C:629:GLY:C	2:C:630:MET:HE2	2.42	0.44
3:D:872:TYR:OH	3:D:876:ARG:NH2	2.50	0.44
5:F:500:ARG:NH1	10:T:57:DG:N7	2.65	0.44
3:D:1207:LEU:HD23	3:D:1207:LEU:C	2.43	0.44
3:D:770:ARG:O	3:D:774:LEU:HG	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:500:LEU:HD11	2:C:512:ILE:HD12	2.00	0.44
3:D:230:ALA:HB3	3:D:233:GLN:NE2	2.33	0.44
3:D:342:ASP:OD1	3:D:343:LEU:N	2.51	0.44
2:C:44:LEU:HD12	2:C:45:ARG:C	2.42	0.44
2:C:188:ASP:OD1	2:C:188:ASP:N	2.51	0.44
2:C:841:HIS:ND1	2:C:842:GLY:N	2.66	0.44
3:D:714:ASP:OD1	3:D:714:ASP:C	2.61	0.44
3:D:948:GLU:O	3:D:952:LEU:HG	2.18	0.44
2:C:380:THR:O	2:C:384:LEU:HD22	2.18	0.44
2:C:649:VAL:HG22	2:C:650:ILE:H	1.83	0.44
2:C:761:ASP:OD1	2:C:866:ASN:ND2	2.51	0.44
3:D:1003:ILE:CD1	3:D:1154:ILE:HD13	2.48	0.44
3:D:1229:THR:O	3:D:1233:LEU:HG	2.18	0.44
5:F:266:LEU:HA	5:F:270:GLY:HA3	1.99	0.44
1:A:75:GLU:OE2	2:C:620:ARG:NH1	2.44	0.44
1:A:182:ARG:O	1:A:182:ARG:NH1	2.49	0.44
3:D:736:VAL:HG11	3:D:817:LEU:HD23	2.00	0.44
5:F:328:LEU:HD21	5:F:351:ILE:HD11	1.99	0.44
2:C:103:MET:HG3	2:C:404:MET:HE2	2.00	0.44
3:D:273:GLU:OE2	3:D:299:VAL:HG21	2.18	0.44
3:D:688:MET:HE2	3:D:688:MET:HA	1.99	0.44
6:J:18:THR:OG1	6:J:19:ASP:N	2.51	0.44
7:M:2:ILE:HD12	7:M:3:PHE:CE2	2.52	0.44
1:B:26:LEU:HD12	1:B:26:LEU:N	2.33	0.43
1:B:159:ILE:HD12	1:B:159:ILE:H	1.83	0.43
1:A:38:LEU:O	1:A:42:LEU:HG	2.18	0.43
2:C:356:THR:HG23	2:C:356:THR:O	2.17	0.43
2:C:806:VAL:HG12	2:C:832:VAL:HB	1.99	0.43
2:C:1066:GLN:HA	10:T:23:DG:OP1	2.17	0.43
3:D:73:ILE:O	3:D:82:VAL:HG12	2.19	0.43
1:A:57:ASP:OD1	1:A:58:GLY:N	2.52	0.43
2:C:32:VAL:CG2	2:C:636:ILE:HD13	2.49	0.43
2:C:586:MET:H	2:C:586:MET:CE	2.31	0.43
3:D:262:GLN:C	3:D:262:GLN:OE1	2.61	0.43
3:D:206:ARG:O	3:D:209:ARG:HG3	2.19	0.43
3:D:877:LEU:HD21	3:D:1157:ILE:HD12	2.01	0.43
5:F:319:ASP:O	5:F:323:GLU:HG2	2.18	0.43
1:B:28:PRO:HA	1:B:29:GLY:HA2	1.82	0.43
8:N:81:DG:H22	10:T:11:DC:N4	2.15	0.43
2:C:44:LEU:HD21	2:C:583:PRO:CD	2.49	0.43
2:C:306:TYR:CE2	2:C:333:LEU:HG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:465:ARG:NH2	2:C:493:ASN:OD1	2.48	0.43
3:D:550:GLU:OE1	3:D:550:GLU:N	2.47	0.43
3:D:673:PHE:HA	3:D:676:LEU:CD1	2.49	0.43
2:C:905:PRO:HD2	2:C:916:ILE:HD11	2.01	0.43
3:D:144:ARG:NH1	3:D:226:PHE:O	2.52	0.43
4:E:105:GLU:N	4:E:105:GLU:OE1	2.51	0.43
5:F:372:MET:HE1	8:N:49:DT:OP2	2.19	0.43
7:M:138:GLU:O	7:M:141:LEU:HD12	2.19	0.43
10:T:14:DG:C2'	10:T:15:DT:H72	2.48	0.43
2:C:596:PHE:HE1	2:C:974:THR:HG21	1.84	0.43
2:C:770:THR:OG1	2:C:771:ARG:N	2.50	0.43
3:D:128:ILE:HG21	3:D:261:ILE:HD11	2.01	0.43
3:D:453:LYS:HG3	3:D:476:VAL:HG11	2.01	0.43
6:J:53:THR:HG1	6:J:62:GLY:C	2.22	0.43
10:T:5:DA:C2'	10:T:6:DT:H72	2.49	0.43
3:D:425:SER:OG	3:D:426:GLY:N	2.52	0.43
2:C:103:MET:HG3	2:C:404:MET:CE	2.49	0.42
2:C:261:THR:HA	2:C:264:LYS:HB3	2.01	0.42
2:C:464:SER:O	2:C:468:ALA:N	2.48	0.42
3:D:432:VAL:HG13	3:D:434:PRO:HD3	2.01	0.42
3:D:1199:GLU:N	3:D:1199:GLU:OE1	2.51	0.42
3:D:897:ILE:CD1	3:D:966:LEU:HD12	2.42	0.42
2:C:205:ILE:O	2:C:205:ILE:HG23	2.19	0.42
2:C:944:TRP:CG	2:C:988:LEU:HD22	2.54	0.42
3:D:36:TYR:OH	8:N:49:DT:OP2	2.37	0.42
3:D:369:ASN:O	3:D:373:MET:HG3	2.19	0.42
3:D:1261:GLY:HA2	4:E:51:TYR:CE1	2.54	0.42
2:C:131:ALA:HB3	2:C:159:MET:HE3	2.00	0.42
2:C:310:ARG:HE	2:C:328:ILE:CG2	2.33	0.42
2:C:1094:ASP:HB3	2:C:1119:GLU:H	1.85	0.42
4:E:33:LEU:N	4:E:33:LEU:HD23	2.33	0.42
7:M:104:VAL:HG23	7:M:135:LEU:HD21	1.99	0.42
2:C:976:VAL:HG23	2:C:977:PHE:N	2.35	0.42
3:D:876:ARG:HE	3:D:1211:THR:HG22	1.83	0.42
2:C:201:SER:OG	2:C:202:VAL:N	2.53	0.42
3:D:138:SER:O	3:D:139:VAL:HG23	2.19	0.42
2:C:690:VAL:HG21	2:C:702:ILE:HD11	2.00	0.42
6:J:36:ASN:OD1	6:J:36:ASN:N	2.51	0.42
6:J:56:CYS:SG	6:J:58:ASN:N	2.92	0.42
7:M:108:VAL:HG11	7:M:135:LEU:HD12	2.01	0.42
2:C:803:VAL:O	2:C:836:SER:OG	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1051:MET:HE2	2:C:1051:MET:HA	2.01	0.42
3:D:347:VAL:HG12	3:D:377:SER:OG	2.20	0.42
3:D:721:PHE:O	3:D:725:THR:HG23	2.20	0.42
5:F:446:VAL:HG12	5:F:448:VAL:HG12	2.01	0.42
1:A:120:ASN:ND2	1:A:123:MET:SD	2.92	0.42
1:A:225:LEU:HD13	1:B:205:ARG:NH1	2.34	0.42
3:D:452:PHE:CE2	3:D:491:ILE:HD11	2.55	0.42
3:D:921:TYR:O	3:D:1150:HIS:NE2	2.48	0.42
7:M:120:LEU:HD23	7:M:124:GLU:HG3	2.02	0.42
1:A:54:ILE:HG22	1:A:138:LEU:HG	2.00	0.42
2:C:400:VAL:O	2:C:404:MET:HB2	2.20	0.42
3:D:26:GLY:O	3:D:94:HIS:ND1	2.53	0.42
3:D:159:ARG:HE	3:D:216:LEU:HD22	1.83	0.42
3:D:1228:GLU:N	10:T:18:DC:OP1	2.51	0.42
1:B:97:LEU:HD21	1:B:136:VAL:HB	2.02	0.41
2:C:86:LEU:O	2:C:90:LEU:HG	2.19	0.41
3:D:222:ILE:HD13	3:D:247:ARG:NH2	2.35	0.41
3:D:589:THR:HG21	3:D:688:MET:CG	2.50	0.41
3:D:877:LEU:HD21	3:D:1157:ILE:CD1	2.50	0.41
3:D:1047:ALA:N	3:D:1109:GLN:O	2.53	0.41
3:D:1122:LEU:HB2	3:D:1130:VAL:HG11	2.00	0.41
3:D:1272:VAL:HG13	4:E:56:TYR:CE1	2.55	0.41
10:T:21:DT:H2'	10:T:22:DC:H6	1.84	0.41
1:B:49:ALA:HA	1:B:142:ARG:HA	2.02	0.41
1:B:182:ARG:NE	1:B:185:GLN:OE1	2.52	0.41
2:C:773:ILE:HD13	2:C:781:LEU:HD11	2.02	0.41
3:D:966:LEU:HD23	3:D:1159:ARG:HB2	2.02	0.41
6:J:97:LEU:O	6:J:97:LEU:HD23	2.20	0.41
1:A:71:GLU:N	1:A:71:GLU:OE1	2.54	0.41
1:B:20:GLN:HA	1:B:194:LEU:O	2.21	0.41
2:C:217:ASP:OD1	2:C:218:LYS:N	2.52	0.41
2:C:385:ILE:HD11	2:C:431:PHE:CE2	2.55	0.41
2:C:720:LEU:HD23	2:C:913:VAL:HA	2.02	0.41
3:D:673:PHE:CE2	3:D:688:MET:SD	3.13	0.41
5:F:316:ALA:O	5:F:320:LEU:HD12	2.20	0.41
6:J:29:ILE:HA	6:J:43:PRO:HA	2.01	0.41
2:C:205:ILE:O	2:C:205:ILE:CG2	2.68	0.41
2:C:786:GLU:OE1	2:C:786:GLU:N	2.46	0.41
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	2.03	0.41
3:D:107:PHE:HA	3:D:114:LEU:HD12	2.02	0.41
5:F:237:LYS:HG2	5:F:238:VAL:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:499:THR:HG22	8:N:31:DT:OP2	2.20	0.41
2:C:877:ARG:HE	2:C:1036:LEU:CD2	2.34	0.41
3:D:151:LEU:HD13	3:D:248:TYR:HE1	1.84	0.41
3:D:344:TYR:O	3:D:347:VAL:HG22	2.19	0.41
3:D:345:ARG:C	3:D:349:ASN:OD1	2.64	0.41
3:D:557:ILE:HD13	4:E:53:LEU:CD1	2.51	0.41
3:D:916:ILE:HG23	3:D:920:ALA:HB3	2.03	0.41
6:J:80:THR:O	6:J:83:ASP:N	2.54	0.41
8:N:45:DA:H2''	8:N:46:DA:C8	2.56	0.41
2:C:436:LEU:HD13	2:C:460:PRO:HD2	2.03	0.41
2:C:632:LEU:HD12	2:C:633:ARG:H	1.84	0.41
2:C:748:THR:HG23	2:C:878:LYS:HA	2.01	0.41
2:C:850:ILE:HG12	2:C:871:VAL:HG23	2.03	0.41
2:C:1102:VAL:HG22	2:C:1113:PRO:HD2	2.02	0.41
3:D:944:LEU:HD23	3:D:944:LEU:O	2.21	0.41
2:C:107:PHE:CZ	2:C:418:ILE:HD12	2.55	0.41
3:D:136:ILE:O	3:D:232:LYS:N	2.54	0.41
3:D:1231:ARG:HA	3:D:1234:THR:HG22	2.02	0.41
8:N:63:DA:H2'	8:N:64:DG:C6	2.55	0.41
2:C:543:GLN:CD	3:D:847:LEU:HD21	2.46	0.41
2:C:719:LEU:HD22	2:C:1030:ILE:HD11	2.03	0.41
3:D:827:PRO:O	3:D:858:LYS:NZ	2.42	0.41
3:D:1232:VAL:O	3:D:1235:ASP:OD1	2.39	0.41
3:D:1278:ALA:HB1	4:E:82:LEU:HD21	2.02	0.41
2:C:468:ALA:CB	2:C:496:LEU:HD11	2.50	0.41
3:D:353:ARG:O	3:D:357:LEU:HD13	2.21	0.41
3:D:1221:LEU:HD23	3:D:1221:LEU:C	2.46	0.41
5:F:413:ILE:HD13	5:F:413:ILE:N	2.36	0.41
1:A:6:ARG:HA	1:A:6:ARG:NE	2.36	0.40
2:C:41:PHE:CD2	2:C:974:THR:HG22	2.57	0.40
3:D:89:ARG:HE	3:D:323:GLU:HG2	1.86	0.40
5:F:308:LYS:O	5:F:311:THR:HG22	2.21	0.40
5:F:328:LEU:HD23	5:F:351:ILE:CG1	2.51	0.40
2:C:54:LEU:HD21	2:C:449:LEU:HD12	2.01	0.40
2:C:337:ASP:O	2:C:341:THR:OG1	2.31	0.40
2:C:661:MET:SD	2:C:667:ARG:NH1	2.94	0.40
3:D:143:MET:HB2	3:D:251:TYR:CD1	2.56	0.40
3:D:662:TRP:CZ3	3:D:664:ALA:HB2	2.56	0.40
5:F:317:PHE:HA	5:F:320:LEU:HD13	2.02	0.40
5:F:409:LYS:O	5:F:413:ILE:HG12	2.21	0.40
1:A:95:MET:HE3	1:A:140:VAL:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:225:ARG:HG3	2:C:229:LYS:O	2.22	0.40
2:C:323:HIS:HB3	2:C:326:GLU:HB2	2.03	0.40
3:D:847:LEU:O	3:D:851:ILE:HG12	2.22	0.40
3:D:875:ARG:NH2	10:T:21:DT:OP1	2.53	0.40
6:J:40:PHE:CZ	6:J:58:ASN:HB2	2.57	0.40
7:M:114:ARG:HB3	7:M:120:LEU:HD21	2.03	0.40
10:T:5:DA:H2'	10:T:6:DT:H72	2.03	0.40
2:C:225:ARG:HD3	2:C:228:ARG:HA	2.03	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	223/347 (64%)	210 (94%)	13 (6%)	0	100	100
1	B	229/347 (66%)	209 (91%)	20 (9%)	0	100	100
2	C	1111/1177 (94%)	1015 (91%)	95 (9%)	1 (0%)	48	79
3	D	1264/1333 (95%)	1193 (94%)	70 (6%)	1 (0%)	48	79
4	E	81/110 (74%)	79 (98%)	2 (2%)	0	100	100
5	F	297/550 (54%)	283 (95%)	14 (5%)	0	100	100
6	J	104/111 (94%)	91 (88%)	13 (12%)	0	100	100
7	M	157/285 (55%)	149 (95%)	8 (5%)	0	100	100
All	All	3466/4260 (81%)	3229 (93%)	235 (7%)	2 (0%)	50	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	31	SER
3	D	1008	THR

### 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	194/297 (65%)	194 (100%)	0	100	100
1	B	190/297 (64%)	190 (100%)	0	100	100
2	C	929/997 (93%)	927 (100%)	2 (0%)	92	94
3	D	1044/1107 (94%)	1041 (100%)	3 (0%)	91	92
4	E	69/90 (77%)	69 (100%)	0	100	100
5	F	248/447 (56%)	248 (100%)	0	100	100
6	J	91/97 (94%)	91 (100%)	0	100	100
7	M	129/240 (54%)	129 (100%)	0	100	100
All	All	2894/3572 (81%)	2889 (100%)	5 (0%)	91	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	277	ILE
2	C	936	LEU
3	D	219	LEU
3	D	234	LEU
3	D	1097	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	61	HIS
2	C	981	GLN
2	C	1054	GLN
2	C	1077	GLN
3	D	510	GLN
3	D	564	ASN
3	D	1139	GLN
5	F	362	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	R	4/21 (19%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
11	POP	C	2000	-	6,8,8	0.75	0	12,13,13	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	POP	C	2000	-	-	0/6/6/6	-

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.



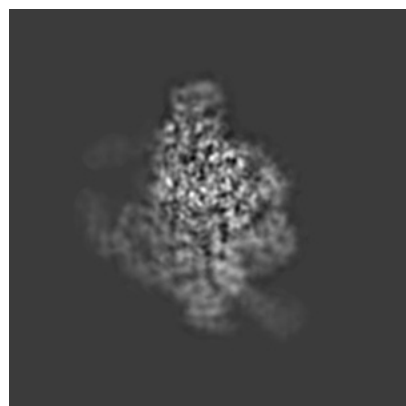
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47708. These allow visual inspection of the internal detail of the map and identification of artifacts.

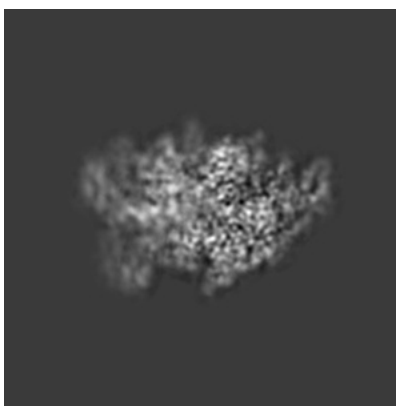
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

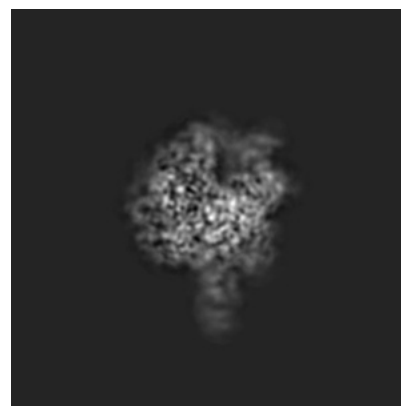
#### 6.1.1 Primary map



X

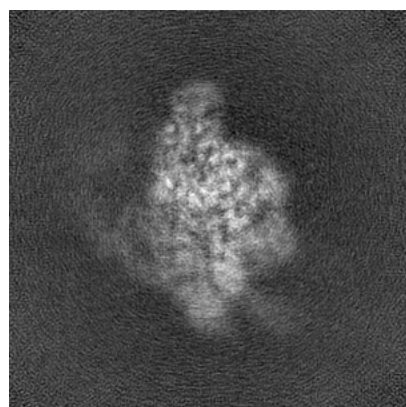


Y

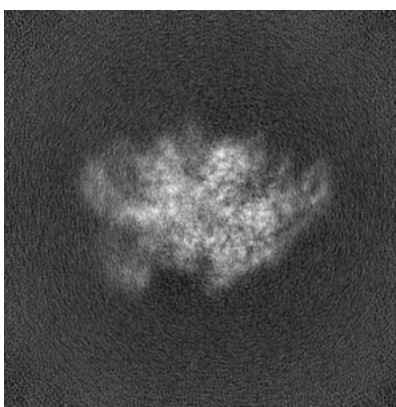


Z

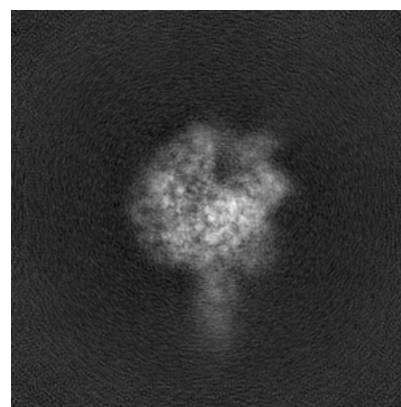
#### 6.1.2 Raw map



X



Y

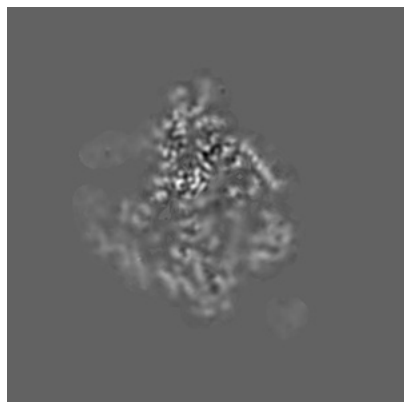


Z

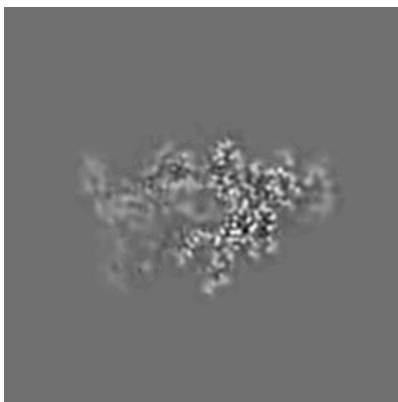
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

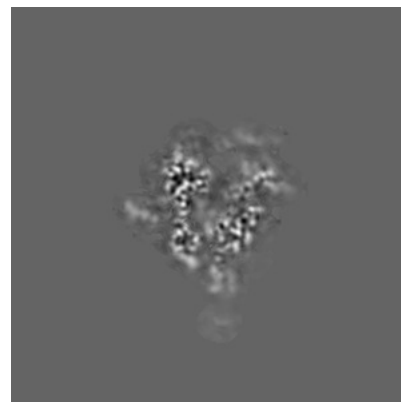
### 6.2.1 Primary map



X Index: 128

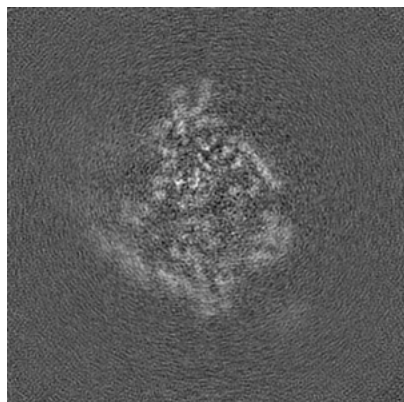


Y Index: 128

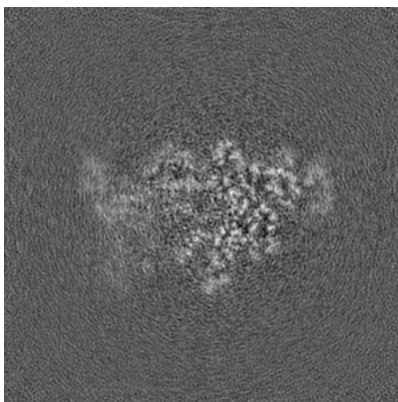


Z Index: 128

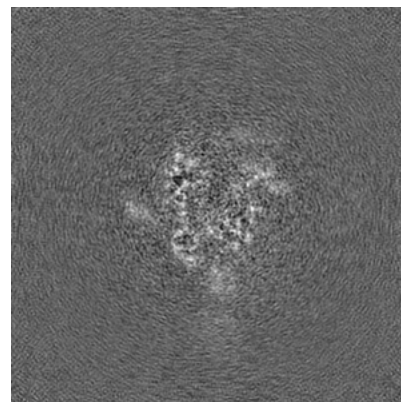
### 6.2.2 Raw map



X Index: 128



Y Index: 128

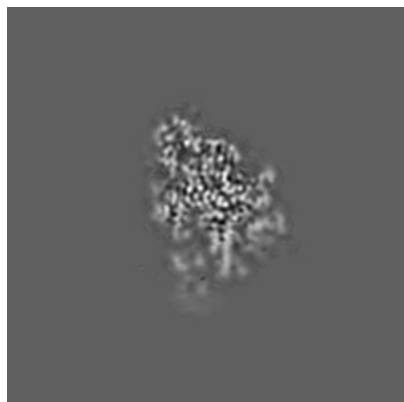


Z Index: 128

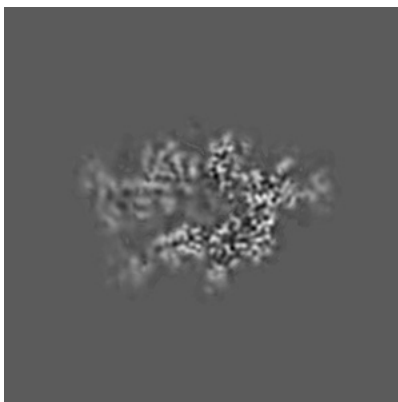
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

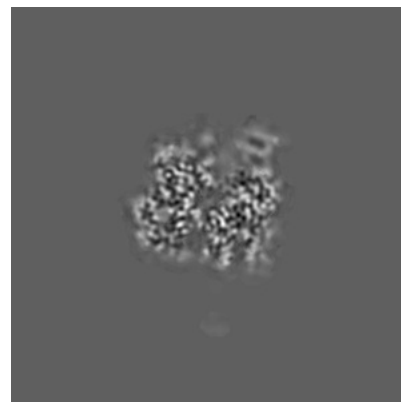
### 6.3.1 Primary map



X Index: 108

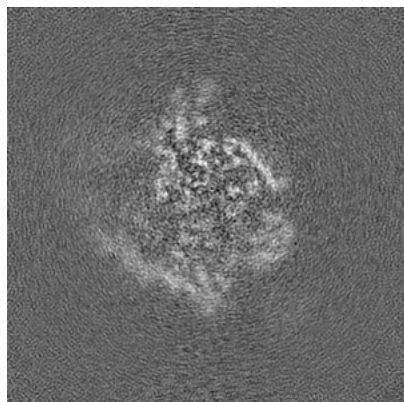


Y Index: 132

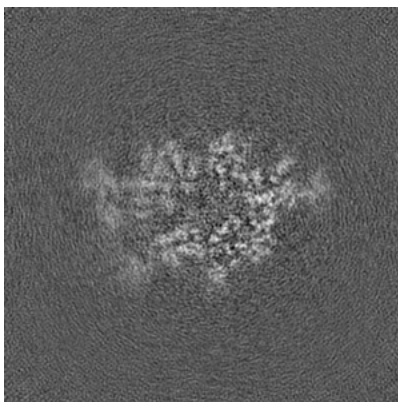


Z Index: 139

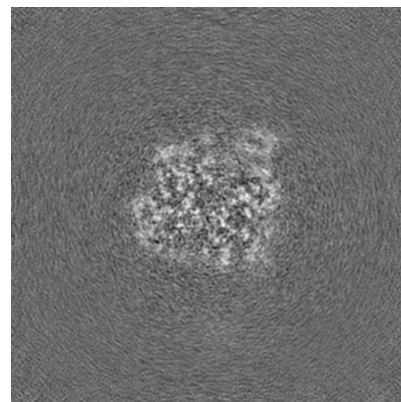
### 6.3.2 Raw map



X Index: 126



Y Index: 132

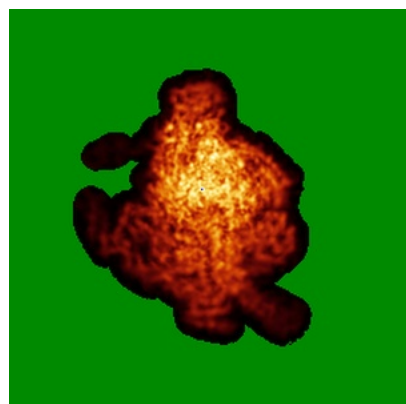


Z Index: 139

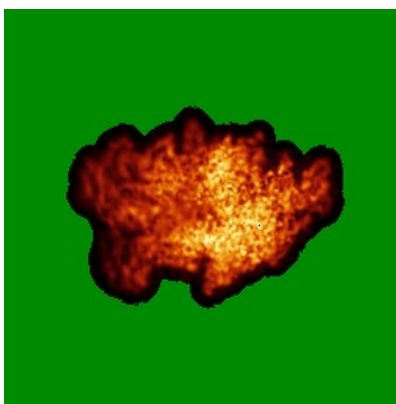
The images above show the largest variance slices of the map in three orthogonal directions.

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

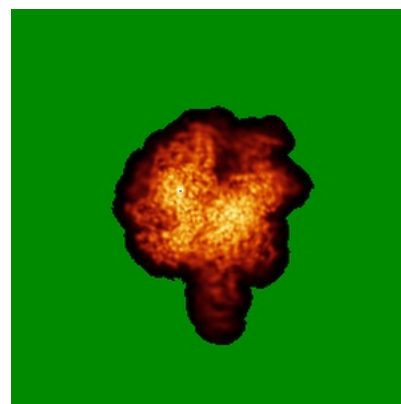
### 6.4.1 Primary map



X

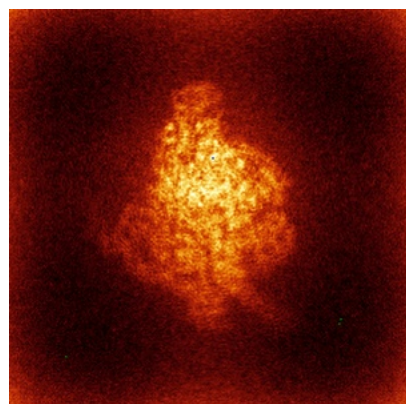


Y

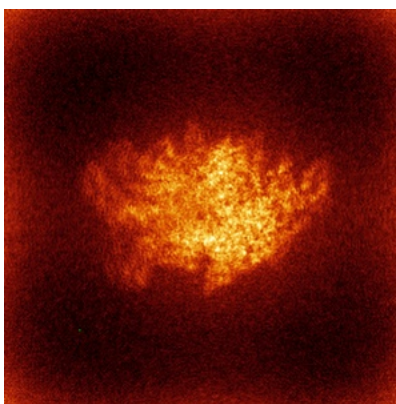


Z

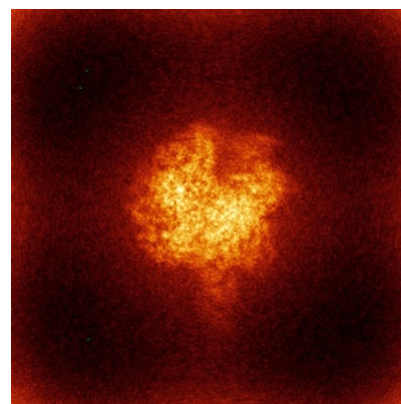
### 6.4.2 Raw map



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.

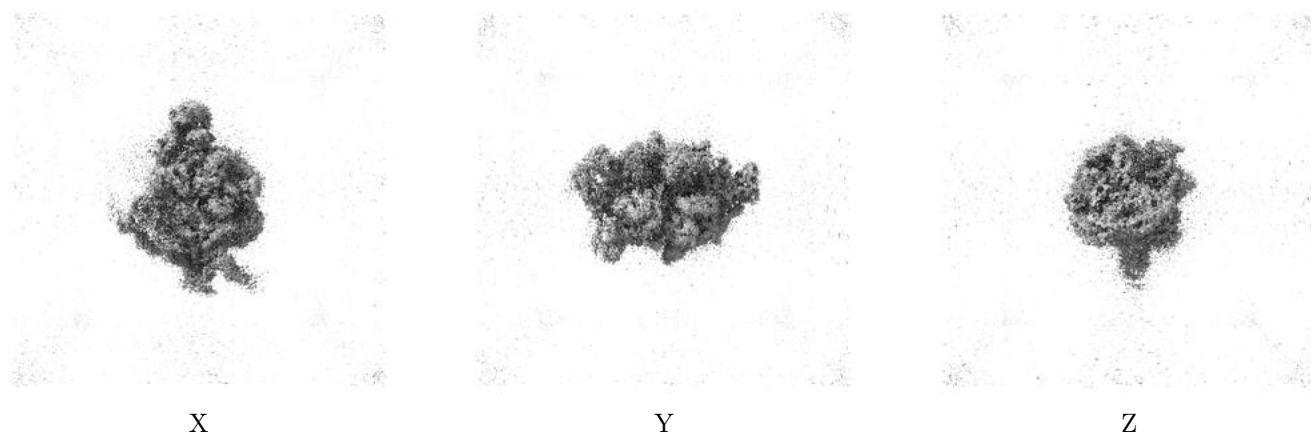
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.194. 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



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](#)

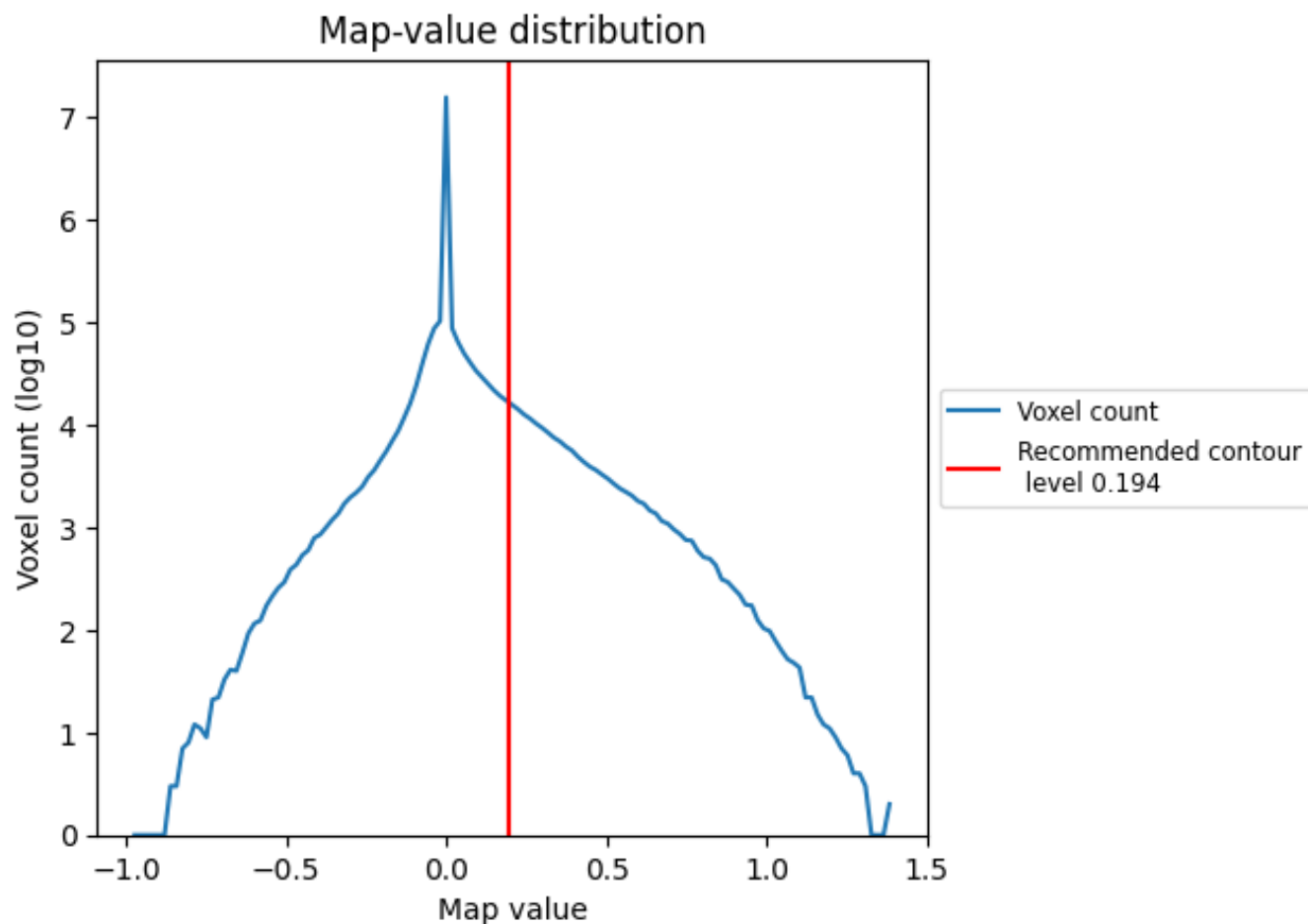
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

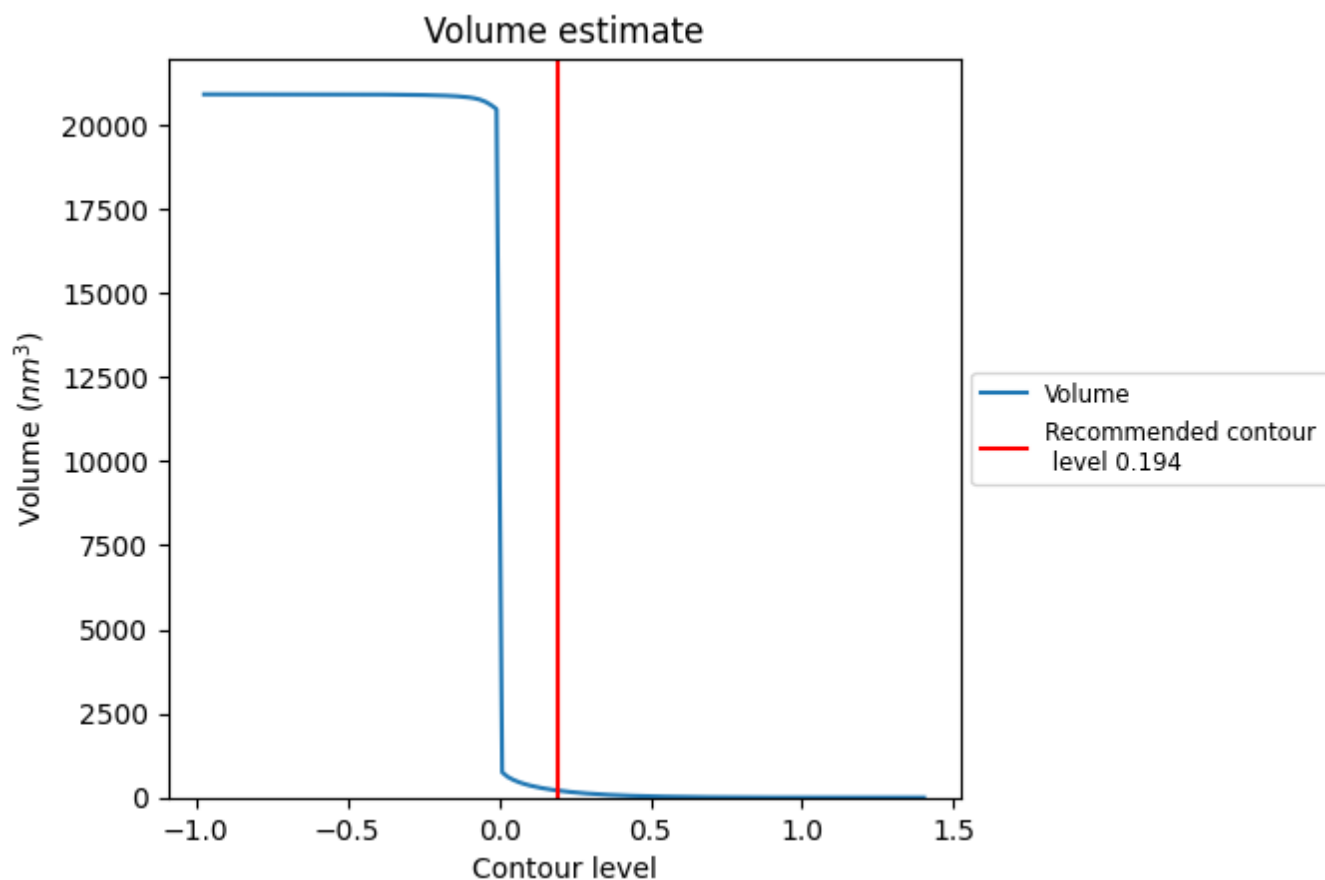
This section contains the results of statistical analysis of the map.

### 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.

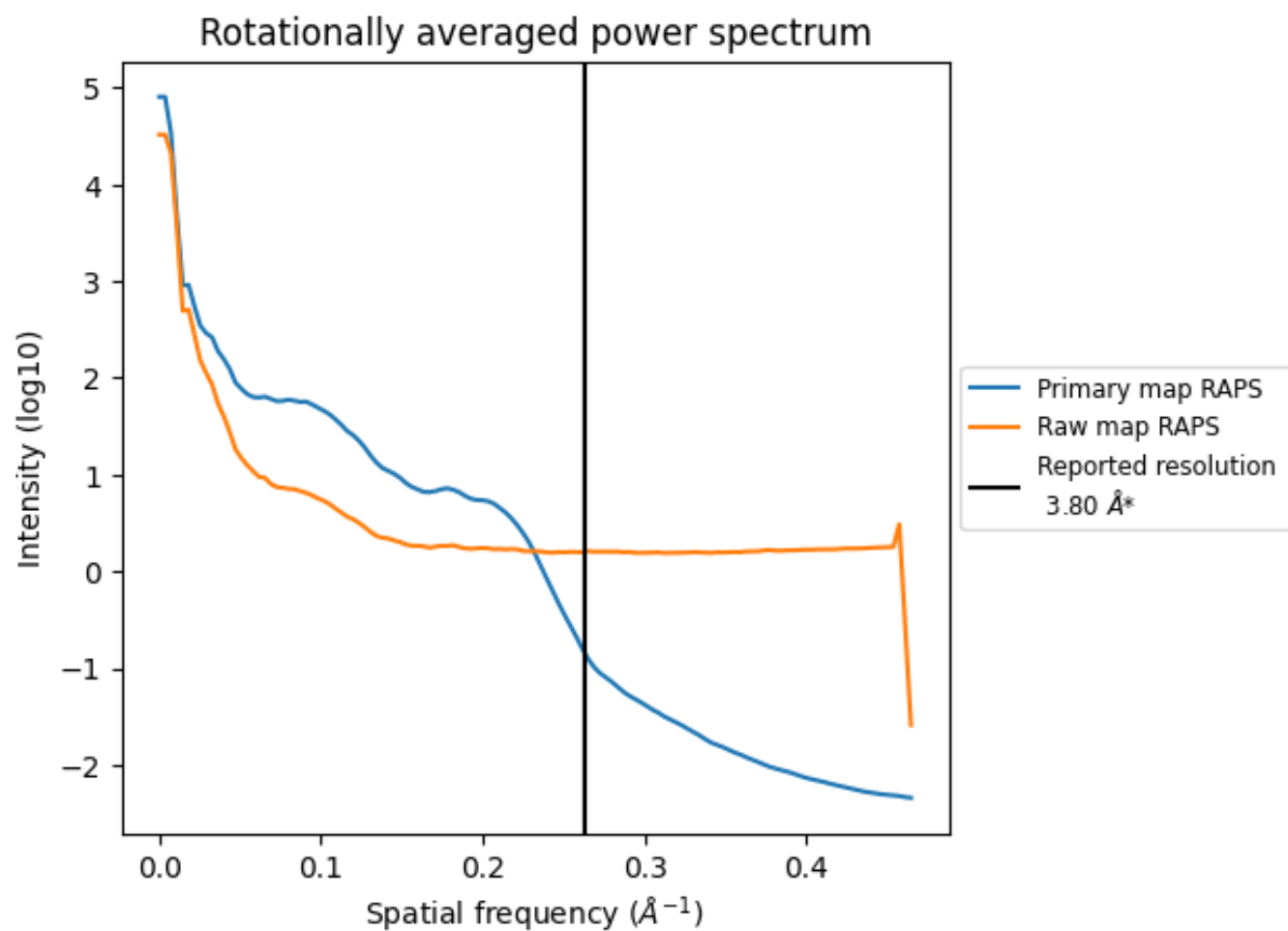
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 209 nm<sup>3</sup>; this corresponds to an approximate mass of 189 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 ⓘ



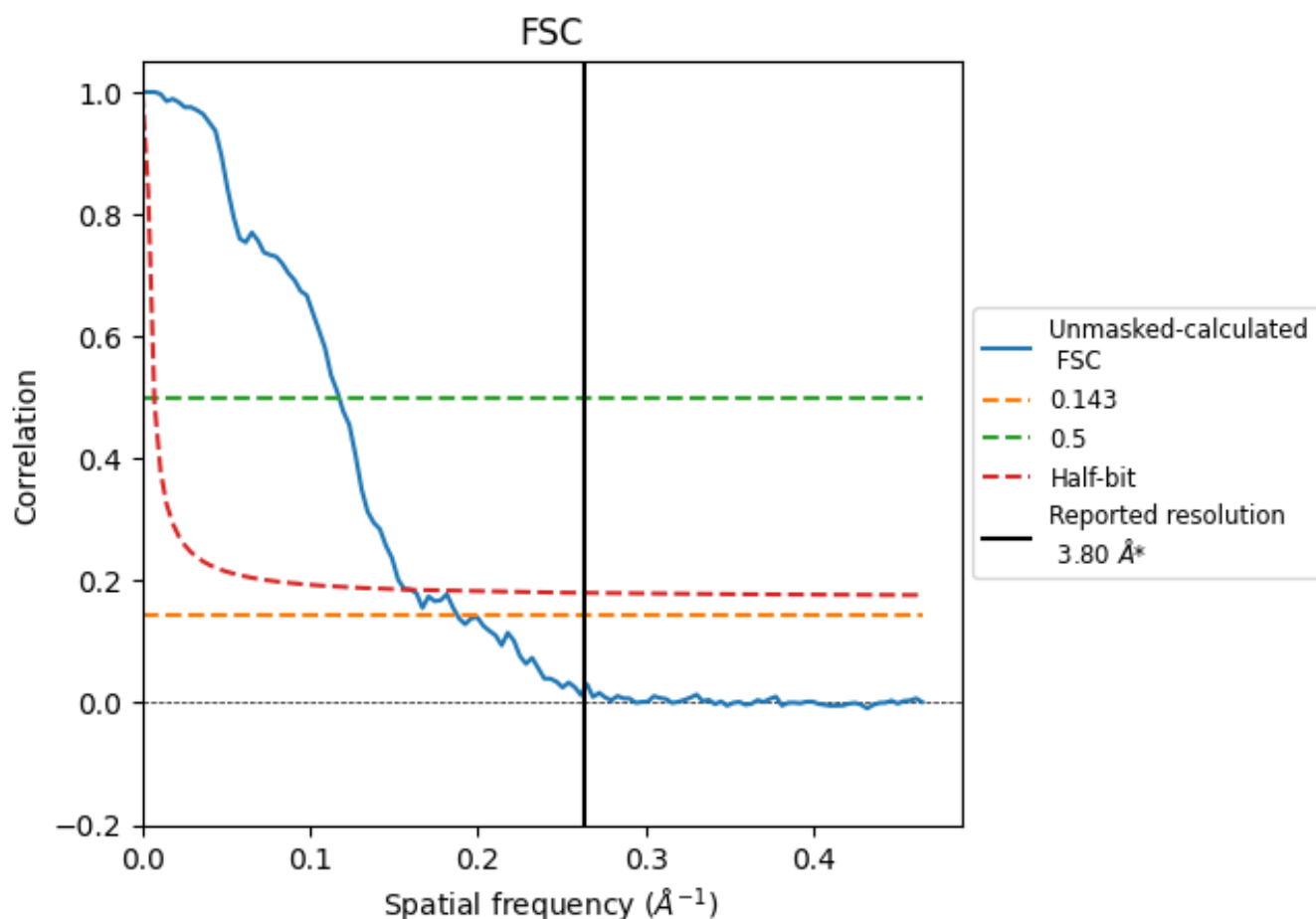
\*Reported resolution corresponds to spatial frequency of 0.263  $\text{\AA}^{-1}$



## 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 0.263  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

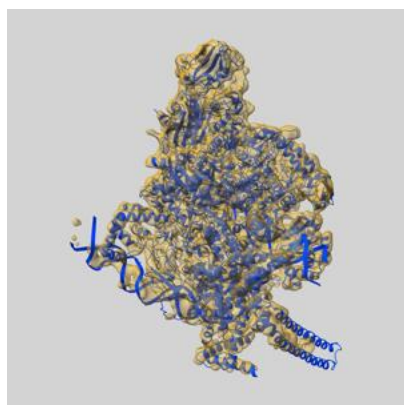
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.32	8.53	6.25

\*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 5.32 differs from the reported value 3.8 by more than 10 %

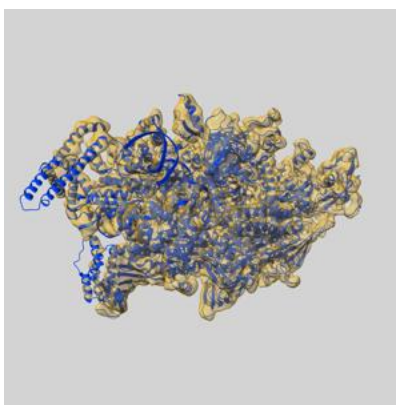
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47708 and PDB model 9E86. Per-residue inclusion information can be found in section [3](#) on page [9](#).

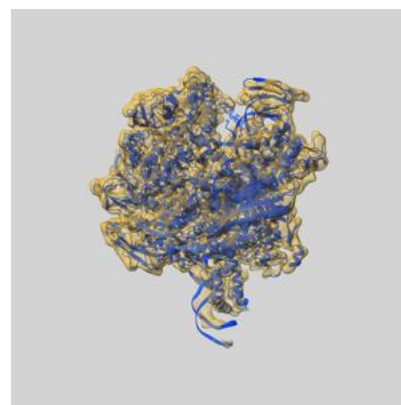
### 9.1 Map-model overlay [i](#)



X



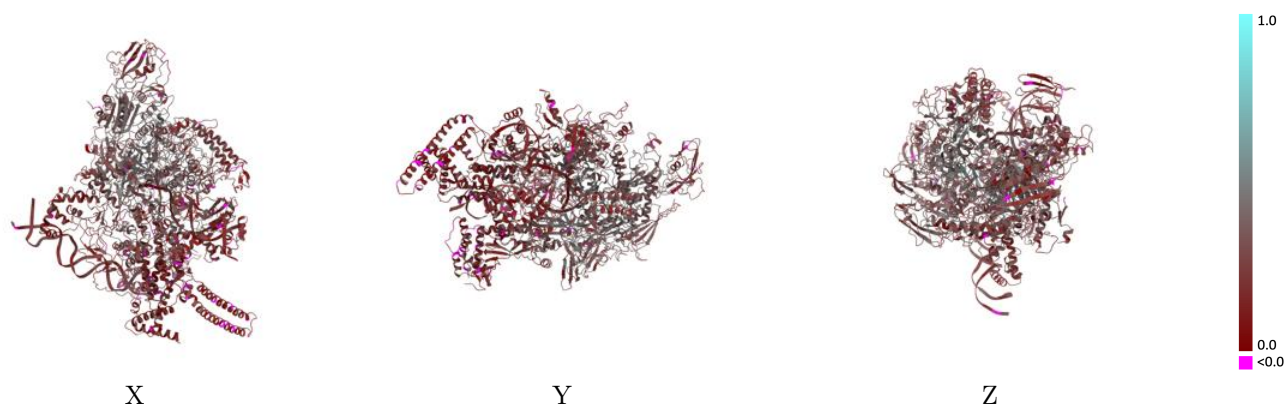
Y



Z

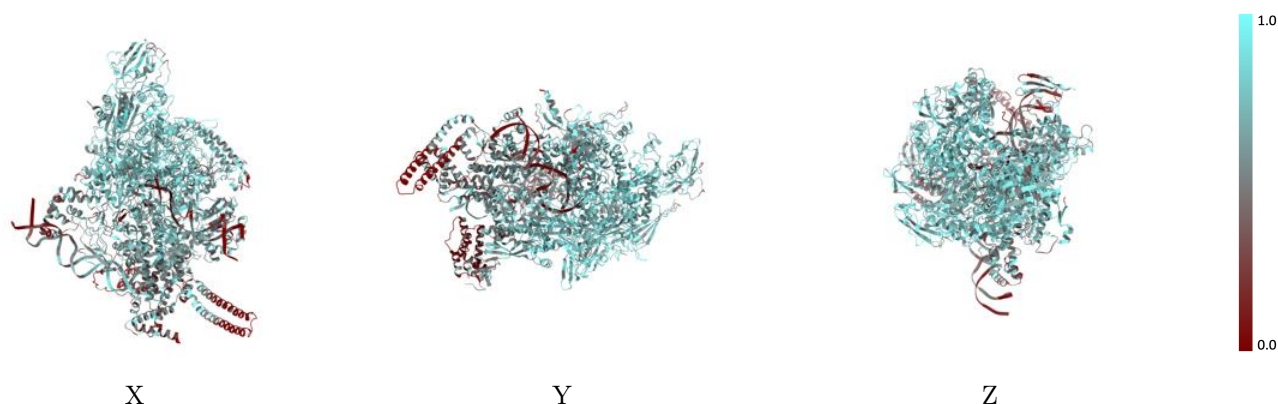
The images above show the 3D surface view of the map at the recommended contour level 0.194 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



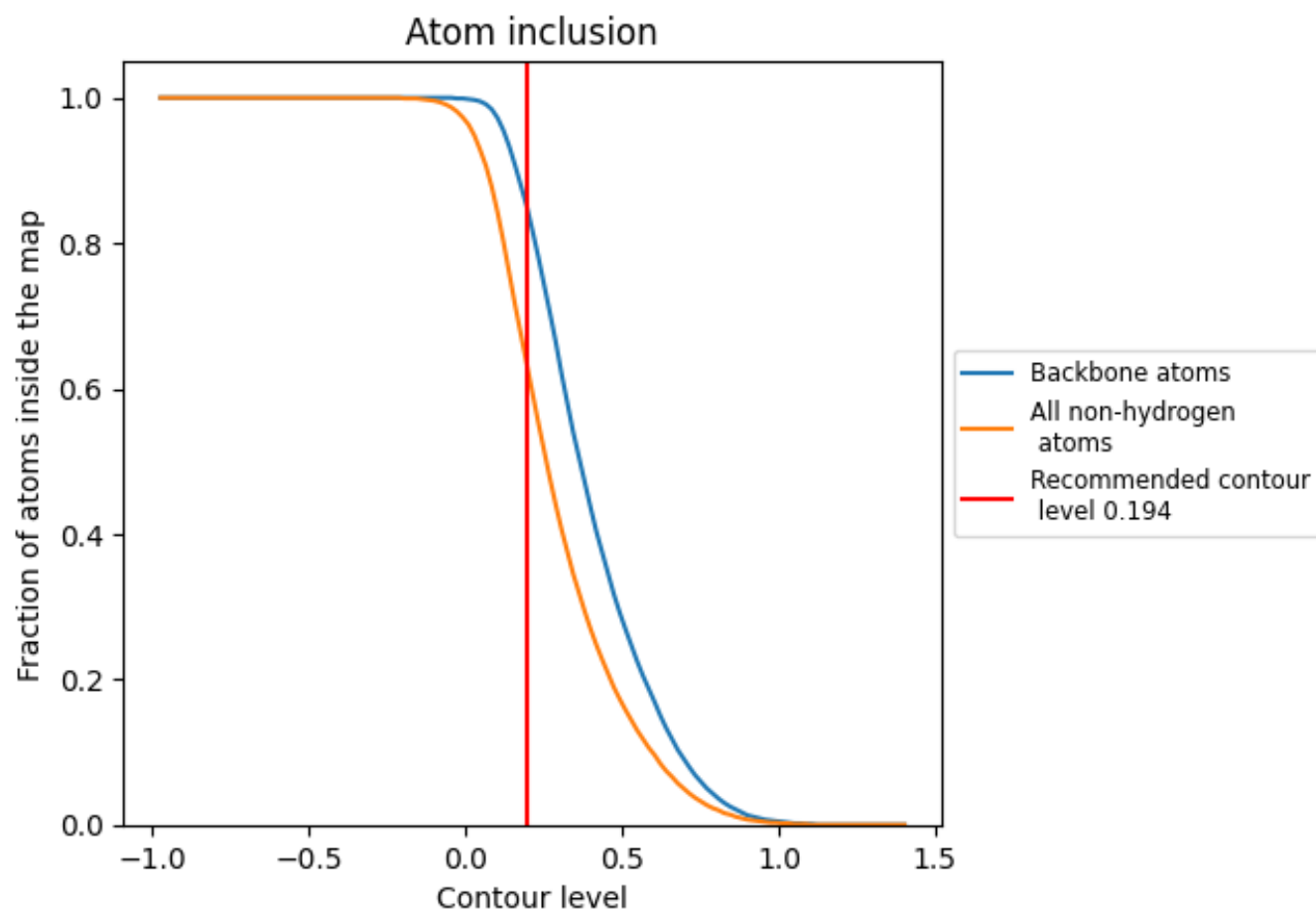
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.194).

























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 64% 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 (0.194) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6370	 0.2870
A	 0.7390	 0.3330
B	 0.7160	 0.2980
C	 0.7330	 0.3340
D	 0.6690	 0.2910
E	 0.6610	 0.3100
F	 0.5160	 0.1960
J	 0.4110	 0.2170
M	 0.2580	 0.1820
N	 0.4680	 0.2400
R	 0.0640	 0.2120
T	 0.3550	 0.1870

