



## Full wwPDB EM Validation Report ⓘ

Sep 23, 2025 – 04:21 PM EDT

PDB ID : 9E84 / pdb\_00009e84  
EMDB ID : EMD-47706  
Title : De Novo Mycobacterium tuberculosis transcription initiation promoter complex with 6-mer RNA and disordered Sigma-A region 4 domain (RNA Polymerase with Sigma-A, CarD, and RbpA)  
Authors : Brewer, J.J.; Campbell, E.A.; Darst, S.A.  
Deposited on : 2024-11-05  
Resolution : 3.60 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:

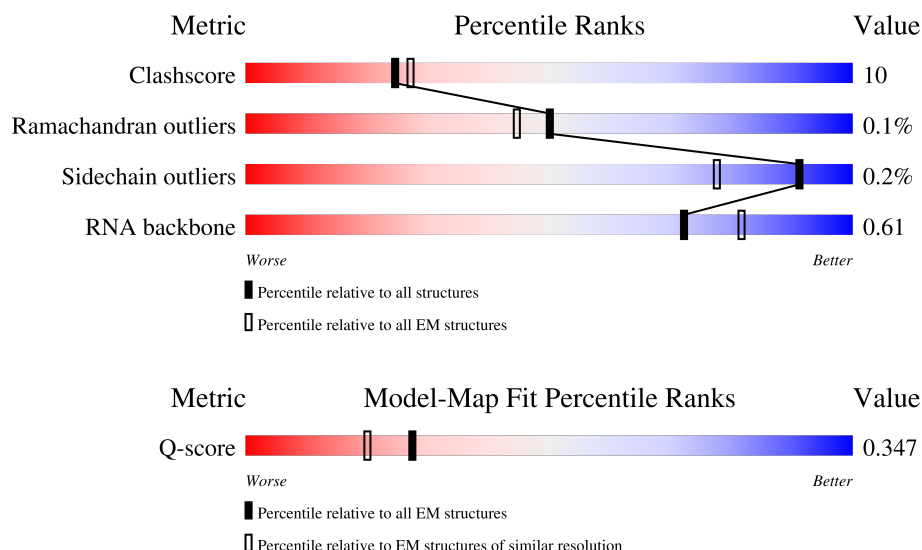
EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB 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 3.60 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.



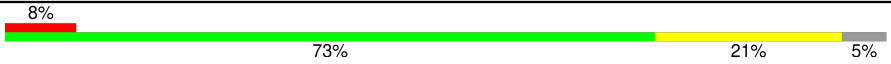



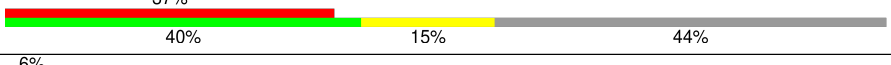

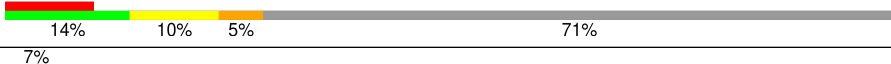

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	12797 ( 3.10 - 4.10 )

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	1178	

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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 [i](#)

There are 13 unique types of molecules in this entry. The entry contains 28008 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	223	Total	C	N	O	S	0	0
			1700	1070	293	335	2		
1	B	227	Total	C	N	O	S	0	0
			1695	1069	291	333	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1096	Total	C	N	O	S	0	0
			8484	5312	1491	1642	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1263	Total	C	N	O	S	0	0
			9861	6176	1792	1852	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	245	Total	C	N	O	S	0	0
			1928	1208	343	369	8		

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	88	Total	C	N	O	S	0	0
			720	448	133	136	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
			1231	772	221	237	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 (123-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	39	Total	C	N	O	P	0	0
			804	382	155	228	39		

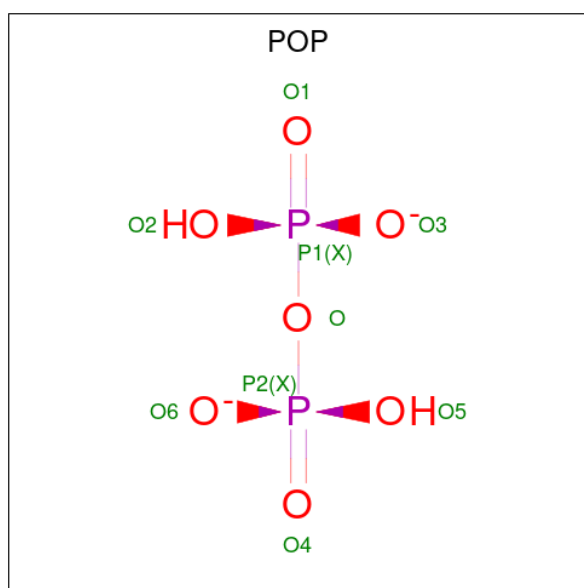
- Molecule 9 is a RNA chain called RNA (21-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	6	Total	C	N	O	P	0	0
			133	59	28	40	6		

- Molecule 10 is a DNA chain called DNA (127-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	39	Total	C	N	O	P	0	0
			791	378	132	242	39		

- Molecule 11 is PYROPHOSPHATE 2- (CCD ID: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

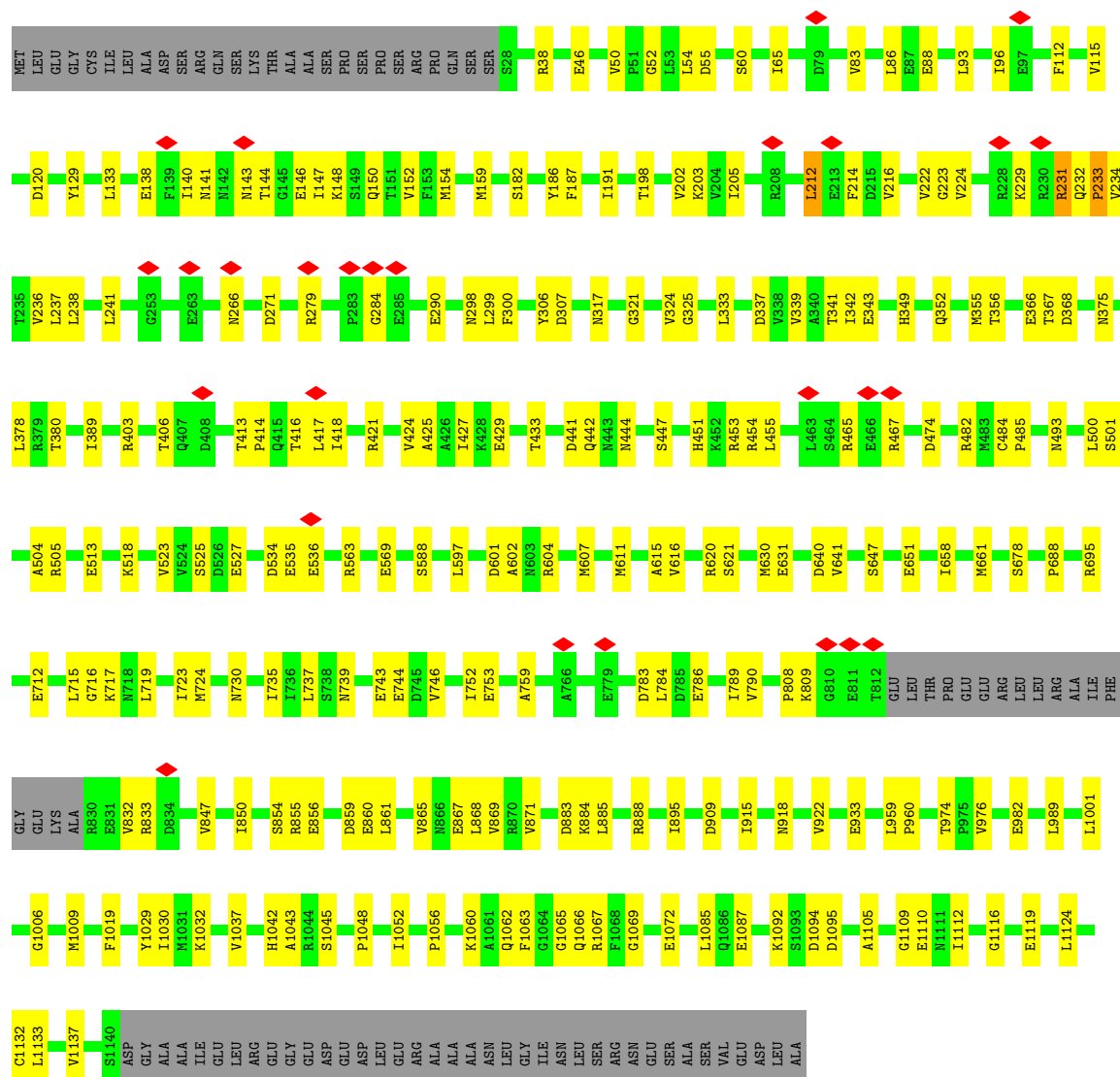
Mol	Chain	Residues	Atoms		AltConf
12	D	2	Total	Zn	0
			2	2	

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

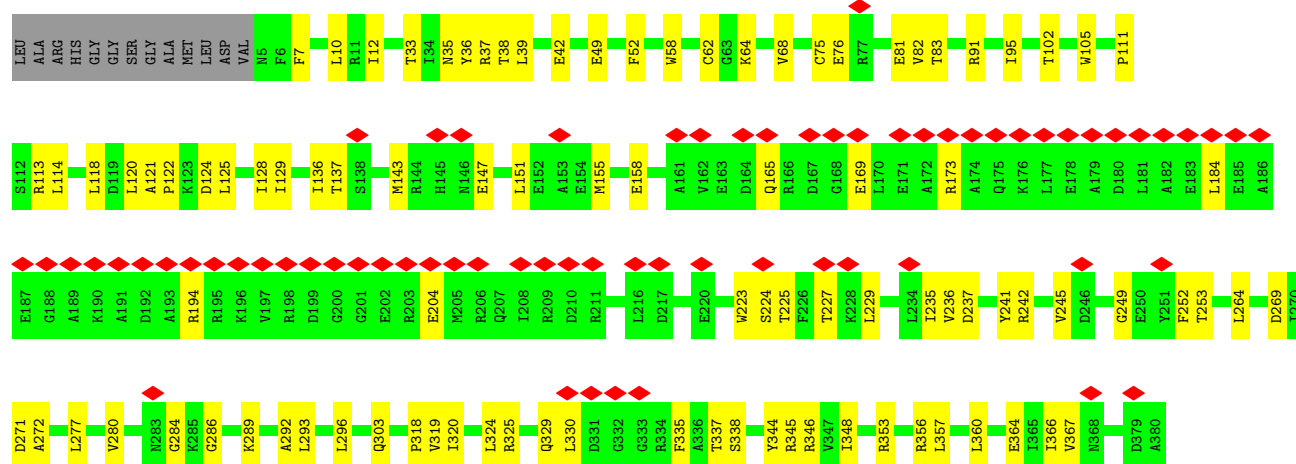
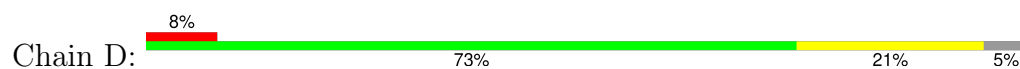
Mol	Chain	Residues	Atoms		AltConf
13	R	1	Total	Mg	0
			1	1	

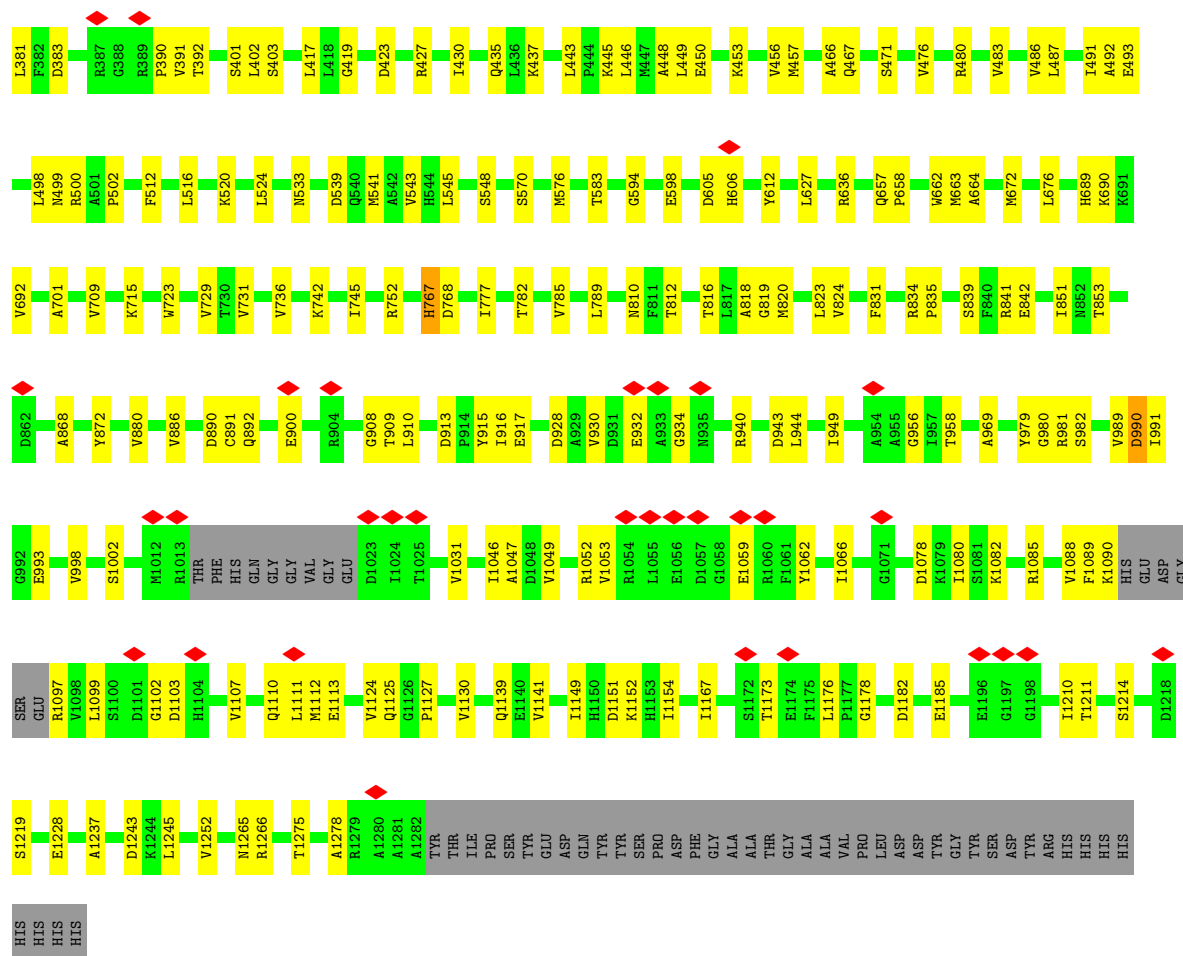




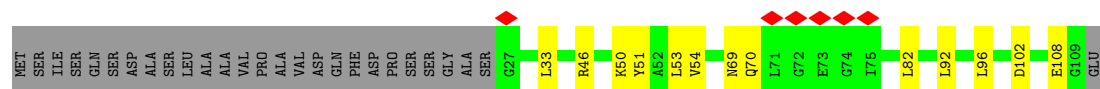


• Molecule 3: DNA-directed RNA polymerase subunit beta'

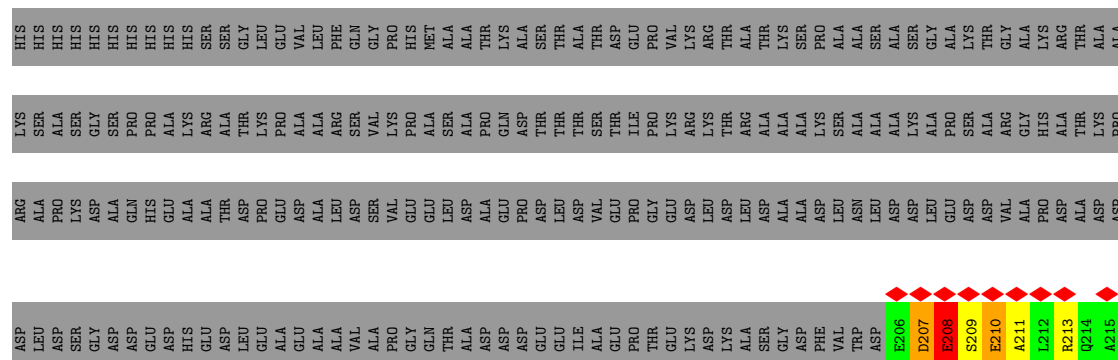
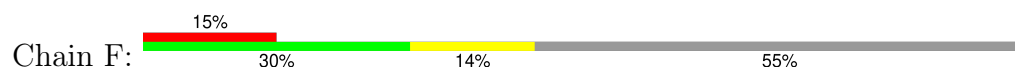




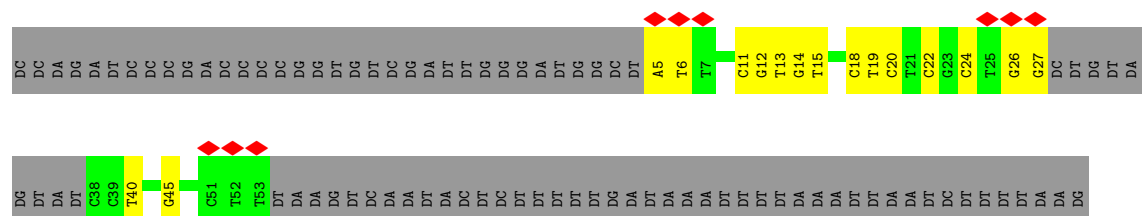
• Molecule 4: DNA-directed RNA polymerase subunit omega



• 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	43549	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	1.962	Depositor
Minimum map value	-1.273	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.169	Depositor
Map size ( $\text{\AA}$ )	275.456, 275.456, 275.456	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.076, 1.076, 1.076	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: POP, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.17	0/1726	0.36	0/2348
1	B	0.16	0/1721	0.38	0/2346
2	C	0.20	0/8640	0.38	1/11716 (0.0%)
3	D	0.21	1/10025 (0.0%)	0.37	2/13553 (0.0%)
4	E	0.18	0/662	0.41	0/901
5	F	0.23	0/1951	0.46	0/2632
6	J	0.32	0/734	0.70	2/991 (0.2%)
7	M	0.22	0/1247	0.41	0/1688
8	N	0.22	0/903	0.46	0/1389
9	R	0.20	0/149	0.37	0/231
10	T	0.23	0/881	0.49	0/1354
All	All	0.21	1/28639 (0.0%)	0.40	5/39149 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1088	VAL	C-N	12.46	1.51	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	51	PRO	CA-N-CD	-7.34	101.73	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1088	VAL	CA-C-N	-6.00	110.09	121.54
3	D	1088	VAL	C-N-CA	-6.00	110.09	121.54
2	C	233	PRO	CA-N-CD	-5.71	104.01	112.00
6	J	51	PRO	N-CD-CG	-5.36	95.16	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	229	LYS	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	1700	0	1739	26	0
1	B	1695	0	1714	32	0
2	C	8484	0	8412	195	0
3	D	9861	0	9924	218	0
4	E	649	0	645	12	0
5	F	1928	0	1920	76	0
6	J	720	0	705	20	0
7	M	1231	0	1244	37	0
8	N	804	0	439	5	0
9	R	133	0	67	3	0
10	T	791	0	444	15	0
11	C	9	0	0	0	0
12	D	2	0	0	0	0
13	R	1	0	0	0	0
All	All	28008	0	27253	575	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 10.

All (575) 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)
3:D:1089:PHE:CZ	3:D:1099:LEU:HA	2.10	0.87
3:D:539:ASP:OD1	9:R:5:A:O2'	1.95	0.85
5:F:448:VAL:O	5:F:452:SER:OG	1.96	0.83
3:D:449:LEU:HD11	3:D:476:VAL:HG13	1.61	0.82
2:C:525:SER:OG	2:C:527:GLU:OE1	1.98	0.80
2:C:442:GLN:O	2:C:678:SER:OG	1.99	0.80
2:C:719:LEU:HD12	2:C:1030:ILE:HD11	1.65	0.78
3:D:1265:ASN:OD1	3:D:1266:ARG:N	2.17	0.78
3:D:900:GLU:OE2	3:D:900:GLU:N	2.16	0.77
2:C:717:LYS:NZ	2:C:746:VAL:O	2.18	0.77
5:F:347:ALA:O	5:F:351:ILE:HD12	1.86	0.76
7:M:82:PRO:O	7:M:87:ARG:NH2	2.18	0.76
2:C:1087:GLU:OE2	3:D:548:SER:OG	2.03	0.76
2:C:982:GLU:OE1	3:D:841:ARG:NH1	2.20	0.75
3:D:383:ASP:OD2	3:D:403:SER:OG	2.05	0.75
2:C:883:ASP:OD1	2:C:884:LYS:N	2.20	0.75
3:D:33:THR:OG1	5:F:365:THR:O	2.05	0.74
3:D:1089:PHE:HE1	3:D:1103:ASP:OD2	1.70	0.73
2:C:1065:GLY:O	2:C:1066:GLN:NE2	2.22	0.73
2:C:467:ARG:NH1	8:N:73:DA:OP1	2.21	0.73
2:C:789:ILE:HD12	2:C:850:ILE:HG21	1.68	0.73
3:D:1151:ASP:O	3:D:1154:ILE:N	2.21	0.73
2:C:52:GLY:O	2:C:55:ASP:N	2.21	0.73
2:C:65:ILE:HD11	2:C:159:MET:HE1	1.71	0.73
7:M:2:ILE:HG22	7:M:3:PHE:CE1	2.24	0.72
2:C:182:SER:O	2:C:186:TYR:OH	2.07	0.72
3:D:35:ASN:OD1	3:D:38:THR:N	2.22	0.72
3:D:1089:PHE:HZ	3:D:1099:LEU:HA	1.52	0.72
1:B:108:GLY:N	1:B:121:PRO:O	2.23	0.72
2:C:366:GLU:OE1	2:C:366:GLU:N	2.22	0.72
1:B:75:GLU:N	1:B:75:GLU:OE1	2.23	0.71
5:F:238:VAL:HG11	5:F:297:GLU:HB3	1.73	0.71
5:F:344:SER:O	5:F:348:THR:HG23	1.91	0.71
7:M:2:ILE:HG22	7:M:3:PHE:CD1	2.25	0.71
7:M:86:SER:OG	7:M:90:LYS:NZ	2.18	0.71
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.72	0.70
5:F:261:GLN:OE1	5:F:264:THR:OG1	2.09	0.70
3:D:1066:ILE:HD11	3:D:1111:LEU:HD11	1.73	0.70
3:D:111:PRO:O	3:D:113:ARG:NH1	2.24	0.70
1:B:87:SER:OG	1:B:89:GLU:OE1	2.08	0.70
3:D:767:HIS:CE1	3:D:768:ASP:OD1	2.45	0.70
3:D:224:SER:O	3:D:227:THR:OG1	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:146:ASP:O	7:M:149:LYS:N	2.24	0.70
3:D:143:MET:HE2	3:D:143:MET:O	1.92	0.69
7:M:109:ARG:NH2	7:M:110:ASP:OD1	2.25	0.69
3:D:95:ILE:HG21	3:D:348:ILE:HD11	1.75	0.69
3:D:280:VAL:O	3:D:284:GLY:N	2.26	0.69
2:C:187:PHE:O	2:C:367:THR:OG1	2.09	0.68
2:C:441:ASP:OD2	2:C:451:HIS:ND1	2.26	0.68
3:D:35:ASN:OD1	3:D:38:THR:HG22	1.94	0.68
2:C:86:LEU:HD11	2:C:133:LEU:HD11	1.76	0.68
2:C:133:LEU:CD2	2:C:154:MET:HB2	2.24	0.68
1:A:57:ASP:OD2	1:A:58:GLY:N	2.28	0.67
2:C:465:ARG:NH1	2:C:493:ASN:OD1	2.27	0.67
2:C:716:GLY:N	2:C:1029:TYR:OH	2.26	0.67
2:C:640:ASP:OD1	2:C:641:VAL:HG13	1.94	0.67
3:D:443:LEU:HD23	3:D:448:ALA:HB2	1.75	0.67
3:D:320:ILE:O	3:D:325:ARG:NH1	2.28	0.67
3:D:81:GLU:OE2	3:D:82:VAL:N	2.28	0.67
3:D:155:MET:HE1	3:D:223:TRP:CD2	2.30	0.67
2:C:284:GLY:H	5:F:219:ALA:HB1	1.58	0.67
1:B:41:THR:HG21	1:B:215:LEU:HG	1.77	0.66
4:E:108:GLU:OE2	4:E:108:GLU:N	2.29	0.66
3:D:319:VAL:HG22	3:D:344:TYR:CE1	2.30	0.66
2:C:737:LEU:HG	2:C:895:ILE:HD12	1.78	0.65
2:C:93:LEU:HD21	2:C:96:ILE:HD11	1.77	0.65
3:D:125:LEU:HG	3:D:129:ILE:HD11	1.76	0.65
5:F:258:TYR:OH	6:J:91:ILE:HG23	1.96	0.65
2:C:234:VAL:HG22	2:C:238:LEU:HD11	1.77	0.65
2:C:453:ARG:NH2	2:C:501:SER:O	2.29	0.65
2:C:753:GLU:OE1	2:C:753:GLU:N	2.29	0.65
2:C:378:LEU:HD11	2:C:455:LEU:HD22	1.78	0.65
3:D:1031:VAL:HG23	3:D:1141:VAL:HG11	1.79	0.65
7:M:4:LYS:N	7:M:7:ASP:OD2	2.30	0.65
3:D:1167:ILE:O	3:D:1178:GLY:N	2.29	0.65
2:C:759:ALA:HB3	2:C:867:GLU:HG3	1.77	0.64
3:D:928:ASP:OD1	3:D:940:ARG:N	2.30	0.64
3:D:943:ASP:OD1	3:D:981:ARG:NH1	2.30	0.64
3:D:1219:SER:OG	3:D:1243:ASP:OD2	2.15	0.64
5:F:435:LEU:HG	5:F:439:ILE:HD11	1.78	0.63
3:D:1185:GLU:OE1	3:D:1185:GLU:N	2.30	0.63
2:C:640:ASP:OD1	2:C:641:VAL:N	2.31	0.63
5:F:351:ILE:O	5:F:355:ILE:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:50:LYS:O	4:E:54:VAL:HG23	1.98	0.63
7:M:124:GLU:OE1	7:M:124:GLU:N	2.30	0.63
1:A:95:MET:HE3	1:A:140:VAL:HG21	1.81	0.63
3:D:742:LYS:NZ	3:D:819:GLY:O	2.27	0.63
2:C:115:VAL:HG11	2:C:129:TYR:CE2	2.34	0.63
2:C:337:ASP:O	2:C:341:THR:HG23	1.98	0.62
2:C:212:LEU:HD21	2:C:214:PHE:HE1	1.64	0.62
3:D:173:ARG:NH1	3:D:204:GLU:OE1	2.32	0.62
5:F:257:LEU:HD13	6:J:81:HIS:NE2	2.15	0.62
2:C:855:ARG:NH2	2:C:865:VAL:O	2.33	0.62
5:F:334:LYS:O	5:F:346:TYR:OH	2.11	0.62
7:M:121:SER:OG	10:T:40:DT:OP1	2.17	0.62
3:D:49:GLU:OE1	3:D:49:GLU:N	2.32	0.61
2:C:786:GLU:N	2:C:786:GLU:OE1	2.33	0.61
3:D:137:THR:OG1	3:D:253:THR:OG1	2.17	0.61
3:D:445:LYS:HB3	3:D:516:LEU:HD12	1.82	0.61
2:C:1069:GLY:N	2:C:1072:GLU:OE1	2.33	0.61
5:F:427:ILE:HD11	10:T:26:DG:N1	2.16	0.61
5:F:207:ASP:C	5:F:209:SER:H	2.09	0.61
3:D:62:CYS:SG	3:D:64:LYS:NZ	2.73	0.61
3:D:1089:PHE:CZ	3:D:1099:LEU:CA	2.83	0.61
2:C:133:LEU:HD22	2:C:154:MET:HB2	1.81	0.61
3:D:345:ARG:NH2	5:F:365:THR:OG1	2.34	0.61
5:F:283:TRP:HE3	5:F:284:ILE:HD13	1.65	0.61
5:F:257:LEU:HD21	6:J:85:LEU:HD23	1.83	0.60
2:C:616:VAL:HG12	2:C:1032:LYS:O	2.01	0.60
3:D:435:GLN:N	3:D:435:GLN:OE1	2.33	0.60
2:C:234:VAL:HG22	2:C:238:LEU:CD1	2.31	0.60
2:C:186:TYR:OH	2:C:375:ASN:OD1	2.09	0.60
2:C:485:PRO:HB2	3:D:853:THR:HG21	1.83	0.60
2:C:352:GLN:N	2:C:352:GLN:OE1	2.35	0.59
5:F:299:ASN:HD22	5:F:328:LEU:HD11	1.67	0.59
3:D:114:LEU:HD23	3:D:125:LEU:HD21	1.83	0.59
2:C:868:LEU:HD23	2:C:869:VAL:N	2.18	0.59
6:J:24:LEU:HD12	6:J:25:ALA:N	2.18	0.59
3:D:498:LEU:HD12	3:D:512:PHE:CD1	2.37	0.59
2:C:441:ASP:OD1	2:C:447:SER:OG	2.17	0.58
2:C:1009:MET:HA	2:C:1009:MET:HE2	1.85	0.58
6:J:84:MET:SD	6:J:84:MET:N	2.76	0.58
3:D:502:PRO:HG3	9:R:6:G:H21	1.68	0.58
2:C:138:GLU:OE2	2:C:148:LYS:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:58:TRP:CD1	3:D:68:VAL:HG22	2.39	0.58
3:D:121:ALA:HB3	3:D:124:ASP:OD1	2.03	0.58
3:D:165:GLN:NE2	3:D:169:GLU:OE2	2.37	0.58
3:D:337:THR:OG1	3:D:338:SER:N	2.37	0.58
3:D:991:ILE:O	3:D:991:ILE:HG22	2.04	0.58
1:B:104:GLU:N	1:B:104:GLU:OE1	2.37	0.57
2:C:1137:VAL:HG12	3:D:10:LEU:CD1	2.34	0.57
7:M:8:THR:HG21	7:M:141:LEU:HD11	1.86	0.57
2:C:65:ILE:CD1	2:C:159:MET:HE1	2.33	0.57
3:D:225:THR:O	3:D:229:LEU:N	2.38	0.57
7:M:8:THR:HG22	7:M:141:LEU:HD21	1.86	0.57
2:C:647:SER:OG	2:C:695:ARG:NH1	2.38	0.57
1:A:151:GLN:N	1:A:151:GLN:OE1	2.37	0.57
2:C:569:GLU:OE1	2:C:569:GLU:N	2.38	0.57
2:C:1137:VAL:HG12	3:D:10:LEU:HD13	1.86	0.57
1:A:185:GLN:OE1	1:A:187:THR:HG23	2.05	0.57
2:C:505:ARG:NH2	2:C:513:GLU:OE1	2.37	0.57
3:D:353:ARG:NH2	5:F:319:ASP:OD1	2.37	0.57
3:D:745:ILE:HD11	3:D:785:VAL:HG22	1.86	0.57
2:C:850:ILE:HD12	2:C:871:VAL:HG22	1.86	0.56
3:D:245:VAL:O	3:D:249:GLY:N	2.38	0.56
2:C:224:VAL:HG12	2:C:224:VAL:O	2.05	0.56
3:D:39:LEU:HD22	3:D:335:PHE:CZ	2.39	0.56
3:D:271:ASP:OD1	3:D:303:GLN:NE2	2.38	0.56
3:D:736:VAL:O	3:D:841:ARG:NE	2.38	0.56
3:D:155:MET:HE1	3:D:223:TRP:CG	2.39	0.56
3:D:293:LEU:HD23	3:D:1176:LEU:HD21	1.87	0.56
7:M:8:THR:CG2	7:M:141:LEU:HD21	2.35	0.56
2:C:1124:LEU:HD22	3:D:417:LEU:HD11	1.87	0.56
2:C:237:LEU:HD23	2:C:241:LEU:HD23	1.88	0.56
1:B:55:ARG:NH1	1:B:137:GLU:OE2	2.39	0.56
3:D:124:ASP:O	3:D:128:ILE:HD12	2.06	0.56
2:C:307:ASP:OD1	2:C:307:ASP:N	2.39	0.56
3:D:993:GLU:OE1	4:E:51:TYR:OH	2.24	0.55
1:B:60:LEU:HD23	1:B:60:LEU:H	1.71	0.55
2:C:783:ASP:OD2	2:C:784:LEU:N	2.39	0.55
2:C:414:PRO:HA	2:C:417:LEU:HD13	1.87	0.55
3:D:891:CYS:SG	3:D:969:ALA:N	2.75	0.55
1:B:7:PRO:HB3	1:B:26:LEU:HD23	1.88	0.55
2:C:150:GLN:HG3	7:M:44:LEU:HD12	1.89	0.55
2:C:421:ARG:HH12	2:C:424:VAL:HG11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:437:LYS:HE2	4:E:33:LEU:HD11	1.88	0.55
2:C:237:LEU:HD23	2:C:241:LEU:CD2	2.37	0.55
3:D:1053:VAL:O	3:D:1102:GLY:N	2.40	0.55
3:D:1089:PHE:O	3:D:1097:ARG:NH1	2.40	0.55
5:F:210:GLU:O	5:F:213:ARG:HG3	2.06	0.55
7:M:85:TRP:CE3	7:M:86:SER:HA	2.42	0.55
2:C:809:LYS:O	2:C:833:ARG:NH2	2.40	0.55
3:D:329:GLN:HA	3:D:335:PHE:HA	1.89	0.55
3:D:982:SER:HB2	3:D:989:VAL:HG22	1.87	0.55
2:C:1066:GLN:OE1	3:D:427:ARG:NE	2.40	0.54
3:D:533:ASN:ND2	3:D:533:ASN:O	2.39	0.54
2:C:854:SER:OG	2:C:856:GLU:OE1	2.25	0.54
7:M:140:ALA:O	7:M:144:SER:N	2.38	0.54
2:C:290:GLU:OE1	2:C:290:GLU:N	2.41	0.54
2:C:989:LEU:HD21	2:C:1006:GLY:CA	2.38	0.54
2:C:909:ASP:OD1	2:C:1001:LEU:HD21	2.08	0.54
3:D:1139:GLN:NE2	3:D:1149:ILE:O	2.40	0.54
2:C:1062:GLN:OE1	2:C:1062:GLN:N	2.41	0.54
7:M:8:THR:CG2	7:M:141:LEU:HD11	2.37	0.54
3:D:913:ASP:HB3	3:D:916:ILE:HD11	1.90	0.54
2:C:343:GLU:OE1	2:C:355:MET:HE3	2.08	0.54
3:D:1049:VAL:HA	3:D:1107:VAL:HG12	1.89	0.54
3:D:1059:GLU:OE1	3:D:1059:GLU:N	2.41	0.54
2:C:159:MET:HE3	2:C:159:MET:HA	1.89	0.54
2:C:224:VAL:CG1	2:C:237:LEU:HD12	2.38	0.53
2:C:1094:ASP:OD1	2:C:1119:GLU:N	2.40	0.53
3:D:487:LEU:O	3:D:491:ILE:HG22	2.09	0.53
3:D:701:ALA:HA	3:D:709:VAL:HG21	1.90	0.53
2:C:715:LEU:N	2:C:1029:TYR:OH	2.41	0.53
3:D:663:MET:HE3	3:D:663:MET:HA	1.88	0.53
3:D:910:LEU:HD11	3:D:956:GLY:HA2	1.90	0.53
3:D:1046:ILE:HG22	3:D:1110:GLN:HA	1.90	0.53
3:D:42:GLU:N	3:D:42:GLU:OE1	2.41	0.53
3:D:52:PHE:O	3:D:91:ARG:NE	2.37	0.53
5:F:371:HIS:O	5:F:375:VAL:HG13	2.08	0.53
1:A:24:GLU:OE2	1:A:24:GLU:N	2.42	0.53
10:T:12:DG:H2'	10:T:13:DT:H72	1.89	0.53
2:C:317:ASN:O	2:C:321:GLY:N	2.41	0.53
3:D:979:TYR:CD2	3:D:989:VAL:HG21	2.44	0.53
2:C:465:ARG:NH2	9:R:2:G:OP2	2.41	0.52
2:C:133:LEU:HD23	2:C:154:MET:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:389:ILE:HD11	2:C:427:ILE:HD11	1.91	0.52
3:D:1053:VAL:HG22	3:D:1066:ILE:HG23	1.92	0.52
2:C:339:VAL:O	2:C:342:ILE:HG22	2.10	0.52
1:B:30:PHE:O	1:B:33:THR:OG1	2.23	0.52
3:D:1062:TYR:OH	3:D:1082:LYS:O	2.22	0.52
3:D:499:ASN:OD1	3:D:500:ARG:N	2.43	0.52
2:C:152:VAL:HG11	2:C:418:ILE:HG21	1.91	0.51
3:D:296:LEU:HD12	3:D:296:LEU:O	2.11	0.51
1:A:179:ASP:OD1	1:A:179:ASP:N	2.43	0.51
2:C:216:VAL:HG23	2:C:216:VAL:O	2.08	0.51
2:C:724:MET:HE1	2:C:1019:PHE:CE2	2.46	0.51
1:B:57:ASP:OD1	1:B:57:ASP:N	2.41	0.51
1:A:64:THR:OG1	1:A:65:THR:N	2.44	0.51
2:C:233:PRO:HD2	2:C:236:VAL:HG22	1.92	0.51
5:F:438:PHE:O	5:F:439:ILE:HD13	2.11	0.51
1:B:30:PHE:O	1:B:34:LEU:HD22	2.11	0.51
3:D:10:LEU:CD2	3:D:1245:LEU:HD11	2.40	0.51
5:F:300:LEU:O	5:F:304:VAL:HG23	2.11	0.51
3:D:136:ILE:HD11	3:D:235:ILE:HD11	1.93	0.50
1:A:61:HIS:NE2	1:A:63:PHE:O	2.45	0.50
5:F:325:ASN:O	5:F:329:ILE:HG13	2.11	0.50
2:C:140:ILE:HG23	2:C:146:GLU:O	2.12	0.50
2:C:860:GLU:O	2:C:861:LEU:HD23	2.11	0.50
3:D:932:GLU:OE1	3:D:932:GLU:N	2.45	0.50
2:C:620:ARG:O	2:C:621:SER:OG	2.26	0.50
2:C:1052:ILE:HD12	2:C:1052:ILE:H	1.76	0.50
3:D:980:GLY:O	3:D:989:VAL:HG23	2.12	0.50
5:F:308:LYS:O	5:F:311:THR:HG22	2.12	0.50
7:M:86:SER:HG	7:M:90:LYS:HZ1	1.50	0.50
7:M:127:MET:SD	7:M:127:MET:N	2.85	0.50
1:B:26:LEU:HD13	1:B:34:LEU:HD23	1.93	0.50
3:D:492:ALA:HB1	3:D:493:GLU:OE1	2.10	0.50
2:C:222:VAL:HG11	2:C:342:ILE:HD11	1.94	0.50
1:B:73:VAL:O	1:B:77:ILE:HG23	2.12	0.49
2:C:922:VAL:HG11	3:D:731:VAL:HG21	1.93	0.49
3:D:872:TYR:HB2	10:T:19:DT:H4'	1.94	0.49
2:C:723:ILE:HG22	2:C:723:ILE:O	2.12	0.49
2:C:739:ASN:ND2	2:C:743:GLU:OE1	2.45	0.49
2:C:1132:CYS:SG	3:D:318:PRO:HD3	2.52	0.49
2:C:112:PHE:CZ	2:C:133:LEU:HD12	2.47	0.49
2:C:413:THR:O	2:C:416:THR:OG1	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:790:VAL:HG11	2:C:847:VAL:HG21	1.92	0.49
3:D:491:ILE:HD13	3:D:516:LEU:CD2	2.43	0.49
2:C:202:VAL:HG12	2:C:214:PHE:HB2	1.94	0.49
2:C:601:ASP:OD2	2:C:602:ALA:N	2.45	0.49
3:D:105:TRP:NE1	3:D:383:ASP:OD1	2.44	0.49
5:F:258:TYR:HB2	6:J:94:LEU:HD12	1.94	0.49
1:A:76:ILE:HD11	1:A:126:ALA:HB2	1.94	0.49
2:C:885:LEU:HG	2:C:895:ILE:HD11	1.93	0.49
3:D:480:ARG:O	3:D:483:VAL:HG22	2.13	0.49
3:D:605:ASP:OD1	3:D:606:HIS:N	2.46	0.49
3:D:834:ARG:O	3:D:834:ARG:NE	2.42	0.49
3:D:908:GLY:O	3:D:909:THR:OG1	2.24	0.49
2:C:444:ASN:HB2	2:C:447:SER:H	1.77	0.49
2:C:46:GLU:OE1	2:C:46:GLU:N	2.37	0.48
5:F:235:ILE:HD12	5:F:238:VAL:HB	1.95	0.48
5:F:257:LEU:CD2	6:J:85:LEU:HD23	2.43	0.48
3:D:729:VAL:HG13	3:D:729:VAL:O	2.13	0.48
2:C:1067:ARG:NH1	3:D:419:GLY:O	2.45	0.48
3:D:319:VAL:HG22	3:D:344:TYR:HE1	1.77	0.48
2:C:233:PRO:HD2	2:C:236:VAL:CG2	2.43	0.48
2:C:279:ARG:CZ	5:F:219:ALA:HB2	2.43	0.48
2:C:413:THR:O	2:C:416:THR:N	2.47	0.48
3:D:789:LEU:HD22	3:D:818:ALA:O	2.13	0.48
5:F:210:GLU:O	5:F:211:ALA:C	2.56	0.48
5:F:257:LEU:HD12	5:F:257:LEU:O	2.14	0.48
3:D:35:ASN:CG	3:D:38:THR:HG22	2.38	0.48
4:E:92:LEU:CD2	4:E:96:LEU:HD11	2.44	0.48
2:C:888:ARG:NH2	2:C:933:GLU:OE2	2.47	0.48
3:D:524:LEU:HD13	3:D:541:MET:HE1	1.96	0.48
3:D:662:TRP:CZ3	3:D:664:ALA:HB2	2.49	0.48
5:F:231:TYR:O	5:F:235:ILE:HG22	2.14	0.48
5:F:316:ALA:HB3	5:F:319:ASP:HB2	1.96	0.48
7:M:24:THR:HB	7:M:31:GLN:HB3	1.95	0.48
3:D:1089:PHE:CE1	3:D:1099:LEU:HA	2.49	0.48
2:C:974:THR:HG23	2:C:974:THR:O	2.14	0.47
3:D:915:TYR:O	3:D:916:ILE:HD13	2.14	0.47
2:C:355:MET:SD	2:C:356:THR:N	2.87	0.47
3:D:236:VAL:HG12	3:D:237:ASP:H	1.79	0.47
3:D:277:LEU:HA	3:D:280:VAL:HG12	1.96	0.47
7:M:88:ARG:O	7:M:92:ASN:ND2	2.48	0.47
1:A:30:PHE:CZ	1:B:41:THR:HG22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:O	1:A:77:ILE:HD12	2.13	0.47
2:C:1133:LEU:HD13	3:D:12:ILE:HD11	1.97	0.47
5:F:427:ILE:HD12	10:T:27:DG:C2	2.49	0.47
7:M:3:PHE:HE2	7:M:60:ASP:OD2	1.97	0.47
7:M:70:VAL:HG11	7:M:101:VAL:HG22	1.95	0.47
2:C:505:ARG:O	2:C:513:GLU:N	2.43	0.47
1:B:24:GLU:OE1	1:B:24:GLU:N	2.47	0.47
2:C:1085:LEU:HD21	3:D:1252:VAL:HG22	1.96	0.47
3:D:241:TYR:CE1	3:D:245:VAL:HG21	2.49	0.47
5:F:235:ILE:HD13	5:F:300:LEU:HB2	1.96	0.47
2:C:500:LEU:HD22	2:C:504:ALA:HB3	1.96	0.47
4:E:53:LEU:HD23	4:E:53:LEU:O	2.14	0.47
7:M:28:LYS:HD2	7:M:32:LYS:HZ3	1.80	0.47
3:D:834:ARG:HE	3:D:834:ARG:C	2.23	0.47
3:D:1228:GLU:N	10:T:18:DC:OP1	2.35	0.47
5:F:245:GLU:O	5:F:249:LEU:HD23	2.14	0.47
5:F:364:ARG:NH2	5:F:368:ILE:HD13	2.30	0.47
10:T:14:DG:H2'	10:T:15:DT:H72	1.96	0.47
1:A:15:THR:HG22	1:A:18:ARG:HG2	1.96	0.47
2:C:484:CYS:HG	2:C:588:SER:HG	0.55	0.47
3:D:136:ILE:HD12	3:D:136:ILE:H	1.80	0.47
3:D:1211:THR:O	3:D:1214:SER:OG	2.25	0.47
5:F:303:VAL:HG23	5:F:351:ILE:HG21	1.96	0.47
2:C:1042:HIS:NE2	2:C:1063:PHE:O	2.48	0.47
1:A:95:MET:HE3	1:A:140:VAL:CG2	2.44	0.47
1:A:98:ARG:NH2	1:A:135:GLU:OE2	2.48	0.46
2:C:1056:PRO:HG3	3:D:423:ASP:OD1	2.15	0.46
2:C:141:ASN:OD1	2:C:144:THR:HG22	2.14	0.46
2:C:607:MET:O	2:C:611:MET:HG2	2.15	0.46
3:D:812:THR:O	3:D:816:THR:HG23	2.16	0.46
5:F:207:ASP:O	5:F:209:SER:N	2.46	0.46
3:D:184:LEU:O	3:D:194:ARG:NH1	2.47	0.46
3:D:676:LEU:O	3:D:715:LYS:NZ	2.41	0.46
2:C:224:VAL:HG11	2:C:237:LEU:HD12	1.97	0.46
7:M:3:PHE:CE1	7:M:58:VAL:HG12	2.50	0.46
2:C:389:ILE:CD1	2:C:427:ILE:HD11	2.45	0.46
3:D:445:LYS:HG3	3:D:446:LEU:HD12	1.98	0.46
3:D:823:LEU:HD12	3:D:831:PHE:HB3	1.97	0.46
6:J:28:GLN:NE2	6:J:45:ALA:O	2.48	0.46
7:M:7:ASP:O	7:M:18:LEU:HD12	2.16	0.46
7:M:54:GLU:OE1	7:M:54:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:100:ASP:OD1	7:M:102:ASN:N	2.49	0.46
1:A:111:VAL:HG23	1:A:111:VAL:O	2.16	0.46
2:C:298:ASN:C	2:C:298:ASN:OD1	2.58	0.46
3:D:576:MET:HE3	3:D:690:LYS:HE3	1.97	0.46
1:A:185:GLN:O	1:A:186:ARG:HB2	2.16	0.46
2:C:216:VAL:HG21	2:C:349:HIS:ND1	2.31	0.46
3:D:102:THR:HG21	3:D:129:ILE:HG21	1.97	0.46
3:D:118:LEU:HD12	3:D:264:LEU:CD2	2.45	0.46
3:D:498:LEU:HD23	3:D:543:VAL:HG22	1.98	0.46
3:D:944:LEU:HD21	3:D:949:ILE:HD11	1.96	0.46
5:F:395:THR:HG23	5:F:398:GLU:H	1.81	0.46
1:A:219:PHE:CE1	1:B:34:LEU:HD12	2.51	0.46
2:C:266:ASN:ND2	2:C:266:ASN:O	2.49	0.46
3:D:886:VAL:HG13	3:D:886:VAL:O	2.15	0.46
7:M:95:LYS:HD2	7:M:103:LYS:HE2	1.98	0.46
2:C:1137:VAL:HG11	3:D:7:PHE:CE2	2.50	0.46
7:M:126:ARG:NH1	7:M:127:MET:SD	2.89	0.46
10:T:14:DG:C2'	10:T:15:DT:H72	2.46	0.46
1:B:83:LEU:HD11	1:B:85:VAL:HG13	1.98	0.46
2:C:730:ASN:O	2:C:918:ASN:ND2	2.41	0.46
3:D:483:VAL:HA	3:D:486:VAL:HG12	1.98	0.46
5:F:304:VAL:HG22	5:F:321:ILE:HD12	1.98	0.46
8:N:48:DC:O2	10:T:45:DG:N2	2.49	0.46
1:A:181:THR:HG21	1:A:189:PHE:CE1	2.51	0.45
1:B:71:GLU:OE1	1:B:71:GLU:N	2.48	0.45
2:C:482:ARG:NH2	2:C:536:GLU:OE1	2.50	0.45
3:D:357:LEU:HD21	3:D:366:ILE:HG22	1.97	0.45
2:C:232:GLN:OE1	2:C:232:GLN:N	2.49	0.45
5:F:207:ASP:C	5:F:209:SER:N	2.74	0.45
3:D:120:LEU:HD12	3:D:125:LEU:CD1	2.47	0.45
3:D:1085:ARG:O	3:D:1113:GLU:HB3	2.15	0.45
5:F:249:LEU:HD13	5:F:291:ALA:HB1	1.99	0.45
2:C:474:ASP:OD1	2:C:474:ASP:C	2.58	0.45
3:D:81:GLU:HG3	3:D:83:THR:HG23	1.98	0.45
6:J:30:ALA:CB	6:J:50:ILE:HG23	2.46	0.45
8:N:81:DG:H1	10:T:11:DC:H42	1.65	0.45
3:D:277:LEU:HD12	3:D:292:ALA:O	2.16	0.45
3:D:917:GLU:OE1	3:D:917:GLU:N	2.49	0.45
2:C:191:ILE:HG12	2:C:198:THR:HG22	1.98	0.45
3:D:121:ALA:HB1	3:D:122:PRO:HD2	1.98	0.45
3:D:423:ASP:OD1	3:D:423:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:868:ALA:HA	10:T:20:DC:C6	2.52	0.45
2:C:418:ILE:O	5:F:388:GLN:NE2	2.50	0.45
2:C:658:ILE:HD11	2:C:688:PRO:CB	2.42	0.45
3:D:269:ASP:OD2	3:D:272:ALA:N	2.48	0.45
2:C:1048:PRO:HB3	5:F:440:GLU:HG2	1.99	0.45
3:D:242:ARG:NH2	3:D:364:GLU:OE2	2.49	0.45
3:D:453:LYS:HD3	3:D:476:VAL:HG11	1.99	0.45
5:F:207:ASP:CG	5:F:208:GLU:H	2.24	0.45
5:F:226:ASP:OD1	5:F:228:VAL:HG12	2.16	0.45
2:C:989:LEU:HD21	2:C:1006:GLY:HA2	1.99	0.45
3:D:1046:ILE:HG22	3:D:1110:GLN:HG3	1.99	0.45
5:F:208:GLU:C	5:F:210:GLU:H	2.25	0.45
5:F:323:GLU:OE2	5:F:358:ALA:HB1	2.17	0.45
3:D:319:VAL:HG22	3:D:344:TYR:CD1	2.51	0.44
6:J:27:ARG:HH21	6:J:43:PRO:HB3	1.81	0.44
2:C:1105:ALA:O	2:C:1109:GLY:N	2.49	0.44
3:D:58:TRP:CE2	3:D:68:VAL:HG13	2.53	0.44
3:D:915:TYR:C	3:D:916:ILE:HD13	2.42	0.44
5:F:347:ALA:C	5:F:351:ILE:HD12	2.43	0.44
5:F:424:ASP:OD1	5:F:424:ASP:C	2.59	0.44
1:A:213:LYS:O	1:A:216:VAL:HG22	2.16	0.44
7:M:26:THR:HA	7:M:31:GLN:HA	2.00	0.44
2:C:433:THR:O	2:C:433:THR:OG1	2.35	0.44
2:C:1124:LEU:HD22	3:D:417:LEU:CD1	2.48	0.44
3:D:155:MET:HA	3:D:158:GLU:HG3	2.00	0.44
3:D:330:LEU:HD22	5:F:439:ILE:HD12	1.99	0.44
3:D:1089:PHE:HB2	3:D:1090:LYS:HD2	1.99	0.44
5:F:286:ARG:O	5:F:290:ARG:HD3	2.17	0.44
3:D:839:SER:OG	3:D:842:GLU:OE1	2.30	0.44
5:F:258:TYR:OH	6:J:91:ILE:HD12	2.18	0.44
5:F:399:LEU:HB2	5:F:410:VAL:HG11	1.98	0.44
1:B:95:MET:SD	1:B:95:MET:N	2.91	0.44
3:D:381:LEU:HD12	3:D:402:LEU:HD13	2.00	0.44
1:A:158:GLU:OE1	1:A:158:GLU:N	2.44	0.44
2:C:367:THR:HG23	2:C:367:THR:O	2.17	0.44
5:F:210:GLU:O	5:F:213:ARG:N	2.49	0.44
2:C:518:LYS:O	2:C:525:SER:OG	2.36	0.43
1:A:30:PHE:CE2	1:B:41:THR:HG22	2.52	0.43
1:B:38:LEU:O	1:B:39:ARG:C	2.61	0.43
1:B:186:ARG:O	1:B:187:THR:OG1	2.32	0.43
3:D:147:GLU:O	3:D:151:LEU:HG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:338:THR:HG23	6:J:89:ARG:NH2	2.33	0.43
7:M:100:ASP:OD1	7:M:103:LYS:N	2.40	0.43
1:A:62:GLU:OE2	1:A:74:THR:HB	2.17	0.43
1:B:12:ASP:OD1	1:B:12:ASP:C	2.61	0.43
2:C:1092:LYS:NZ	3:D:545:LEU:O	2.44	0.43
3:D:594:GLY:N	3:D:598:GLU:OE2	2.51	0.43
3:D:1124:VAL:HG23	3:D:1125:GLN:HG3	2.00	0.43
5:F:263:MET:CE	5:F:266:LEU:HD11	2.48	0.43
5:F:283:TRP:CE3	5:F:284:ILE:HD13	2.48	0.43
2:C:83:VAL:HG11	2:C:88:GLU:OE1	2.18	0.43
2:C:375:ASN:OD1	2:C:375:ASN:O	2.37	0.43
3:D:324:LEU:HD12	3:D:324:LEU:N	2.33	0.43
3:D:466:ALA:HB1	3:D:471:SER:OG	2.19	0.43
3:D:1173:THR:O	3:D:1173:THR:OG1	2.37	0.43
1:A:76:ILE:CD1	1:A:126:ALA:HB2	2.49	0.43
2:C:306:TYR:CE2	2:C:333:LEU:HD12	2.53	0.43
2:C:421:ARG:NH1	2:C:424:VAL:HG11	2.33	0.43
5:F:208:GLU:C	5:F:210:GLU:N	2.75	0.43
2:C:284:GLY:N	5:F:219:ALA:HB1	2.30	0.43
2:C:299:LEU:HG	2:C:300:PHE:CD1	2.54	0.43
2:C:534:ASP:OD1	2:C:535:GLU:N	2.52	0.43
2:C:859:ASP:OD1	2:C:860:GLU:N	2.52	0.43
3:D:672:MET:HE1	3:D:723:TRP:CZ2	2.54	0.43
5:F:311:THR:OG1	5:F:312:GLY:N	2.51	0.43
2:C:271:ASP:OD1	2:C:271:ASP:N	2.52	0.43
2:C:324:VAL:HG12	2:C:325:GLY:H	1.84	0.43
2:C:597:LEU:HD23	2:C:976:VAL:CG1	2.49	0.43
2:C:604:ARG:NH2	2:C:607:MET:HE1	2.34	0.43
7:M:3:PHE:HB3	7:M:7:ASP:OD2	2.18	0.43
2:C:1045:SER:OG	3:D:450:GLU:OE2	2.30	0.43
3:D:834:ARG:HB3	3:D:835:PRO:HA	2.01	0.43
3:D:1089:PHE:O	3:D:1090:LYS:C	2.62	0.43
6:J:30:ALA:HB3	6:J:44:PHE:HE1	1.84	0.43
1:B:88:GLU:N	1:B:115:GLY:O	2.50	0.43
2:C:50:VAL:HG11	2:C:630:MET:HE1	2.01	0.43
2:C:186:TYR:CZ	2:C:375:ASN:OD1	2.72	0.43
2:C:1133:LEU:HD22	3:D:1237:ALA:HB2	2.01	0.43
3:D:453:LYS:O	3:D:457:MET:HG3	2.19	0.43
5:F:254:GLU:HB3	6:J:94:LEU:HD11	2.00	0.43
7:M:129:ALA:O	7:M:133:GLN:HG3	2.19	0.43
1:B:22:VAL:HG22	1:B:24:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:SER:OG	2:C:380:THR:HG21	2.19	0.42
2:C:1110:GLU:HG3	4:E:69:ASN:ND2	2.34	0.42
3:D:390:PRO:O	3:D:392:THR:HG23	2.19	0.42
3:D:612:TYR:CZ	3:D:627:LEU:HD22	2.55	0.42
3:D:930:VAL:HG13	3:D:934:GLY:O	2.19	0.42
5:F:240:LEU:HD12	5:F:240:LEU:H	1.83	0.42
3:D:36:TYR:CE2	3:D:37:ARG:HB2	2.54	0.42
5:F:335:PHE:O	6:J:88:ARG:NH1	2.47	0.42
6:J:34:THR:OG1	6:J:38:GLU:OE1	2.36	0.42
7:M:28:LYS:HD2	7:M:32:LYS:HE2	2.01	0.42
2:C:203:LYS:HD2	2:C:205:ILE:HD11	2.02	0.42
2:C:236:VAL:HG23	2:C:237:LEU:N	2.35	0.42
3:D:752:ARG:HD2	3:D:777:ILE:HD12	2.01	0.42
4:E:69:ASN:OD1	4:E:70:GLN:HG3	2.19	0.42
3:D:824:VAL:HG11	3:D:851:ILE:HG22	2.01	0.42
3:D:890:ASP:OD1	3:D:892:GLN:N	2.46	0.42
1:B:22:VAL:HG22	1:B:24:GLU:CD	2.45	0.42
1:B:41:THR:HG21	1:B:215:LEU:CG	2.47	0.42
2:C:223:GLY:HA2	2:C:231:ARG:HE	1.84	0.42
2:C:421:ARG:HA	2:C:421:ARG:CZ	2.49	0.42
2:C:455:LEU:N	2:C:455:LEU:HD23	2.35	0.42
3:D:1151:ASP:O	3:D:1152:LYS:C	2.63	0.42
1:A:176:TYR:HB3	1:A:194:LEU:HD12	2.02	0.42
1:B:32:TYR:O	1:B:33:THR:C	2.62	0.42
2:C:216:VAL:O	2:C:216:VAL:CG2	2.67	0.42
2:C:808:PRO:HA	2:C:832:VAL:HG12	2.00	0.42
2:C:1060:LYS:N	10:T:24:DC:OP1	2.53	0.42
3:D:75:CYS:SG	3:D:76:GLU:N	2.91	0.42
3:D:1182:ASP:OD1	3:D:1182:ASP:C	2.62	0.42
4:E:53:LEU:HD23	4:E:53:LEU:C	2.44	0.42
5:F:434:GLN:OE1	5:F:436:GLY:N	2.52	0.42
6:J:81:HIS:HA	6:J:84:MET:HG2	2.02	0.42
2:C:147:ILE:HG12	7:M:47:ARG:HB2	2.00	0.42
3:D:319:VAL:HA	3:D:344:TYR:CE1	2.55	0.42
3:D:346:ARG:NH2	3:D:391:VAL:HG21	2.35	0.42
5:F:243:ALA:O	5:F:247:VAL:HG23	2.20	0.42
1:A:221:LEU:HD11	1:B:6:ARG:HD2	2.01	0.42
2:C:403:ARG:O	2:C:406:THR:HG22	2.19	0.42
2:C:752:ILE:C	2:C:753:GLU:OE1	2.62	0.42
3:D:453:LYS:HA	3:D:456:VAL:HG22	2.02	0.42
3:D:1052:ARG:HB2	3:D:1102:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1090:LYS:HD2	3:D:1090:LYS:N	2.34	0.42
1:B:111:VAL:O	1:B:111:VAL:HG13	2.20	0.42
3:D:689:HIS:O	3:D:692:VAL:N	2.49	0.42
7:M:27:ILE:HG23	7:M:28:LYS:HG3	2.02	0.42
1:B:73:VAL:O	1:B:76:ILE:HG22	2.20	0.42
2:C:523:VAL:HG13	2:C:523:VAL:O	2.20	0.41
3:D:235:ILE:HD12	3:D:235:ILE:N	2.35	0.41
5:F:374:GLU:O	5:F:377:ASN:OD1	2.37	0.41
2:C:563:ARG:HG2	2:C:569:GLU:OE1	2.21	0.41
3:D:1078:ASP:C	3:D:1080:ILE:HD12	2.46	0.41
3:D:1089:PHE:C	3:D:1090:LYS:HD2	2.45	0.41
3:D:236:VAL:HG12	3:D:237:ASP:N	2.34	0.41
3:D:430:ILE:HG21	3:D:541:MET:HE2	2.01	0.41
3:D:636:ARG:HB2	3:D:663:MET:HE1	2.01	0.41
5:F:226:ASP:OD1	5:F:228:VAL:CG1	2.69	0.41
10:T:5:DA:C2'	10:T:6:DT:H72	2.51	0.41
2:C:112:PHE:CE1	2:C:133:LEU:HD12	2.56	0.41
2:C:442:GLN:O	2:C:442:GLN:HG3	2.20	0.41
3:D:998:VAL:O	3:D:1002:SER:OG	2.30	0.41
5:F:348:THR:HG21	8:N:58:DC:C5	2.56	0.41
2:C:424:VAL:HG13	2:C:425:ALA:N	2.36	0.41
2:C:735:ILE:HG21	2:C:915:ILE:HD11	2.02	0.41
2:C:1112:ILE:HD12	2:C:1112:ILE:N	2.36	0.41
3:D:467:GLN:HA	3:D:467:GLN:OE1	2.19	0.41
3:D:900:GLU:O	3:D:958:THR:OG1	2.35	0.41
3:D:1275:THR:HG23	3:D:1278:ALA:H	1.85	0.41
1:A:45:SER:C	1:A:46:ILE:HD13	2.45	0.41
3:D:944:LEU:HD23	3:D:944:LEU:O	2.20	0.41
3:D:1127:PRO:HA	3:D:1130:VAL:HG12	2.03	0.41
6:J:30:ALA:HB2	6:J:50:ILE:HG23	2.02	0.41
2:C:959:LEU:HD23	2:C:960:PRO:HD2	2.01	0.41
3:D:782:THR:HA	3:D:820:MET:HE2	2.03	0.41
3:D:989:VAL:HG12	3:D:990:ASP:N	2.35	0.41
2:C:38:ARG:NH2	2:C:712:GLU:OE1	2.54	0.41
2:C:631:GLU:HA	2:C:631:GLU:OE1	2.20	0.41
3:D:356:ARG:O	3:D:360:LEU:HG	2.20	0.41
3:D:364:GLU:HA	3:D:367:VAL:HG12	2.03	0.41
5:F:321:ILE:O	5:F:325:ASN:OD1	2.39	0.41
5:F:393:GLU:O	5:F:393:GLU:HG3	2.21	0.41
2:C:120:ASP:OD1	2:C:120:ASP:N	2.52	0.41
2:C:339:VAL:O	2:C:343:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:744:GLU:O	2:C:744:GLU:HG3	2.21	0.41
2:C:1009:MET:HE2	2:C:1009:MET:CA	2.48	0.41
2:C:1067:ARG:NE	10:T:22:DC:OP1	2.54	0.41
3:D:498:LEU:HD12	3:D:512:PHE:CE1	2.56	0.41
3:D:1085:ARG:O	3:D:1112:MET:SD	2.79	0.41
5:F:208:GLU:N	5:F:208:GLU:CD	2.78	0.41
1:B:54:ILE:HD11	1:B:164:VAL:HG11	2.02	0.41
2:C:1042:HIS:CD2	2:C:1043:ALA:N	2.89	0.41
3:D:10:LEU:CD2	3:D:1245:LEU:CD1	2.99	0.41
3:D:570:SER:O	3:D:570:SER:OG	2.35	0.41
3:D:1176:LEU:C	3:D:1176:LEU:HD23	2.46	0.41
4:E:46:ARG:NH2	4:E:102:ASP:OD2	2.54	0.41
7:M:11:TYR:CD1	7:M:11:TYR:O	2.74	0.41
8:N:81:DG:H22	10:T:11:DC:N4	2.20	0.41
2:C:1037:VAL:HG11	3:D:520:LYS:HB2	2.02	0.40
3:D:286:GLY:O	3:D:289:LYS:N	2.54	0.40
3:D:289:LYS:O	3:D:293:LEU:HD13	2.21	0.40
6:J:51:PRO:O	6:J:51:PRO:HD2	2.21	0.40
2:C:141:ASN:ND2	2:C:143:ASN:OD1	2.54	0.40
2:C:233:PRO:HD2	2:C:233:PRO:O	2.21	0.40
2:C:237:LEU:O	2:C:241:LEU:HD23	2.21	0.40
2:C:368:ASP:OD2	2:C:368:ASP:N	2.53	0.40
2:C:1095:ASP:OD1	2:C:1116:GLY:N	2.51	0.40
5:F:228:VAL:HA	5:F:318:LEU:HD11	2.03	0.40
3:D:151:LEU:O	3:D:155:MET:HG3	2.21	0.40
3:D:1265:ASN:OD1	3:D:1265:ASN:C	2.64	0.40
4:E:46:ARG:NE	4:E:102:ASP:OD1	2.54	0.40
6:J:83:ASP:HA	6:J:86:LEU:HB2	2.03	0.40
2:C:279:ARG:NE	5:F:219:ALA:HB2	2.36	0.40
2:C:651:GLU:OE2	2:C:661:MET:HE3	2.21	0.40
3:D:583:THR:HG21	3:D:729:VAL:HG11	2.03	0.40
2:C:52:GLY:O	2:C:54:LEU:N	2.54	0.40
2:C:425:ALA:O	2:C:429:GLU:N	2.46	0.40
2:C:444:ASN:OD1	2:C:615:ALA:O	2.40	0.40
2:C:454:ARG:C	2:C:455:LEU:HD23	2.47	0.40
3:D:95:ILE:CG2	3:D:348:ILE:HD11	2.49	0.40
3:D:657:GLN:N	3:D:658:PRO:CD	2.85	0.40
3:D:880:VAL:HG21	3:D:1210:ILE:HB	2.03	0.40
3:D:1047:ALA:HB2	3:D:1111:LEU:HD21	2.04	0.40
3:D:1278:ALA:HB1	4:E:82:LEU:HD13	2.02	0.40
5:F:300:LEU:HA	5:F:303:VAL:HG12	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	221/347 (64%)	206 (93%)	15 (7%)	0	100	100
1	B	225/347 (65%)	209 (93%)	16 (7%)	0	100	100
2	C	1092/1178 (93%)	1003 (92%)	88 (8%)	1 (0%)	48	79
3	D	1257/1333 (94%)	1183 (94%)	74 (6%)	0	100	100
4	E	81/110 (74%)	79 (98%)	2 (2%)	0	100	100
5	F	239/550 (44%)	224 (94%)	11 (5%)	4 (2%)	7	37
6	J	86/111 (78%)	75 (87%)	11 (13%)	0	100	100
7	M	157/285 (55%)	142 (90%)	15 (10%)	0	100	100
All	All	3358/4261 (79%)	3121 (93%)	232 (7%)	5 (0%)	50	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	224	SER
5	F	207	ASP
5	F	208	GLU
5	F	210	GLU
2	C	231	ARG

### 5.3.2 Protein sidechains [i](#)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/297 (65%)	192 (100%)	0	100	100
1	B	187/297 (63%)	187 (100%)	0	100	100
2	C	925/998 (93%)	924 (100%)	1 (0%)	92	97
3	D	1042/1107 (94%)	1037 (100%)	5 (0%)	86	93
4	E	69/90 (77%)	69 (100%)	0	100	100
5	F	197/447 (44%)	196 (100%)	1 (0%)	86	93
6	J	76/97 (78%)	76 (100%)	0	100	100
7	M	127/240 (53%)	127 (100%)	0	100	100
All	All	2815/3573 (79%)	2808 (100%)	7 (0%)	91	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	212	LEU
3	D	252	PHE
3	D	401	SER
3	D	767	HIS
3	D	810	ASN
3	D	990	ASP
5	F	208	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	36	ASN
1	B	124	HIS
2	C	375	ASN
2	C	610	ASN
2	C	941	HIS
3	D	767	HIS
3	D	771	ASN
4	E	65	ASN
5	F	299	ASN
5	F	461	GLN
6	J	58	ASN

### 5.3.3 RNA ⓘ



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	R	5/21 (23%)	1 (20%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	R	6	G

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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	0.77	0	12,13,13	0.87	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.

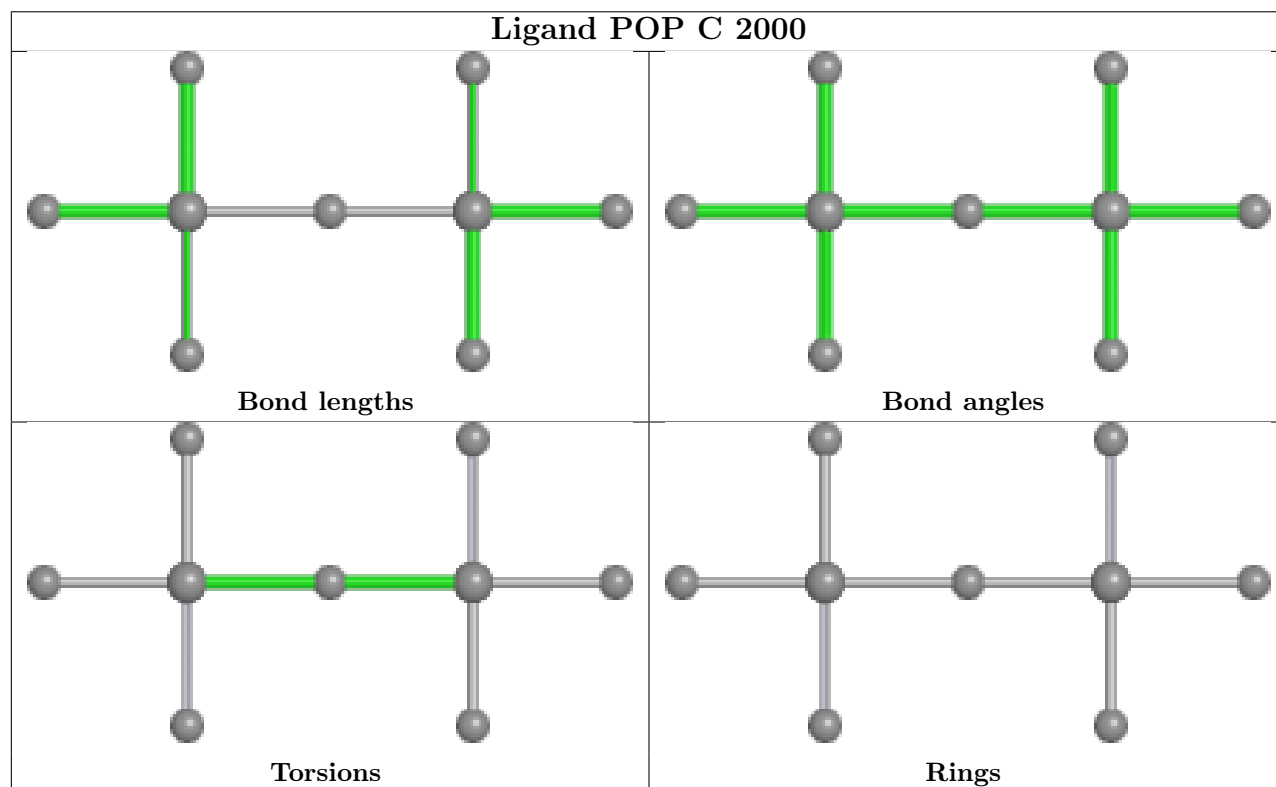
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

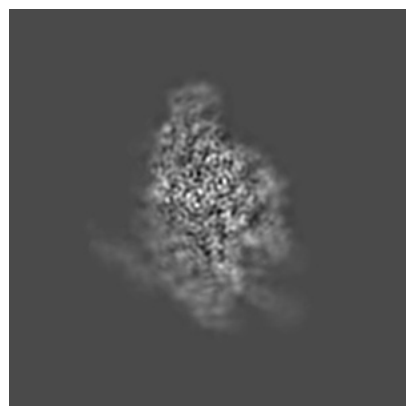
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47706. These allow visual inspection of the internal detail of the map and identification of artifacts.

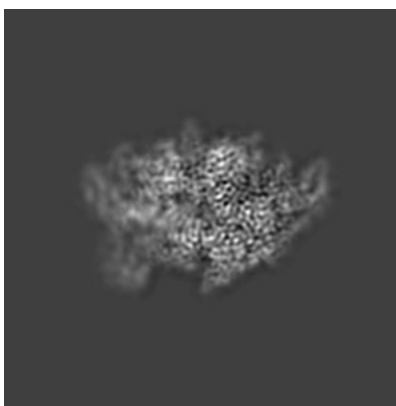
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

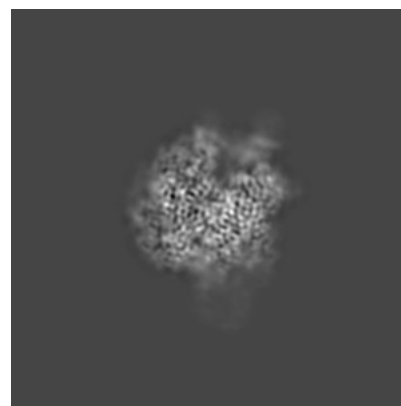
#### 6.1.1 Primary map



X

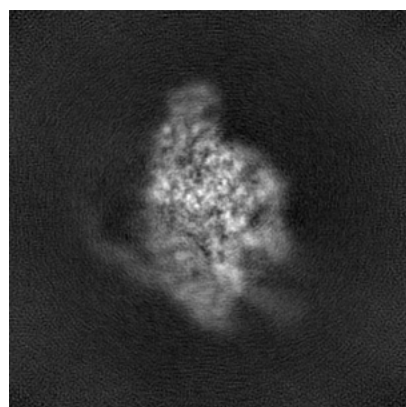


Y

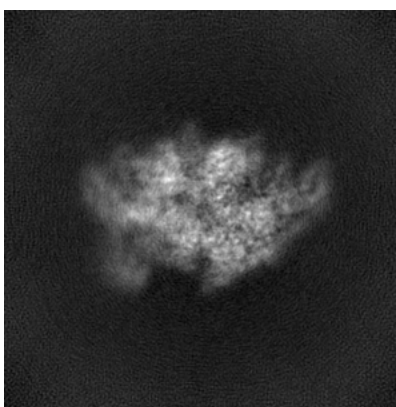


Z

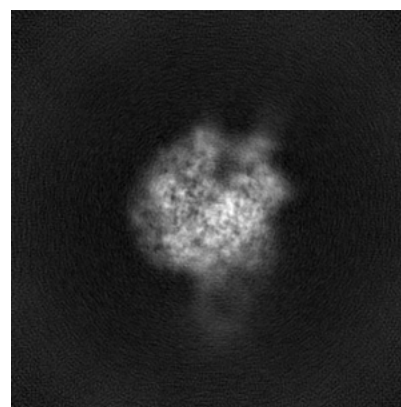
#### 6.1.2 Raw map



X



Y

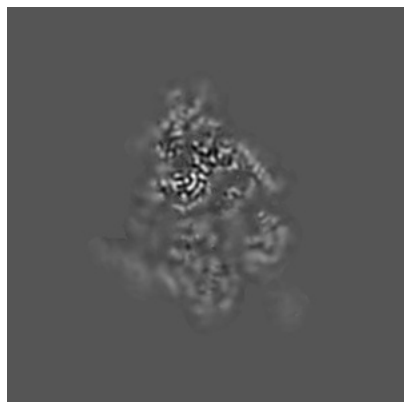


Z

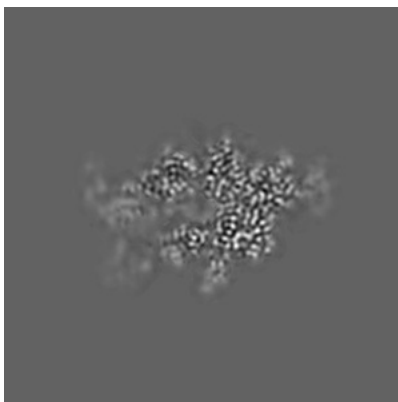
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 128

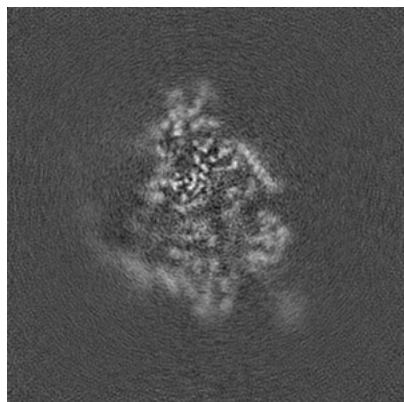


Y Index: 128

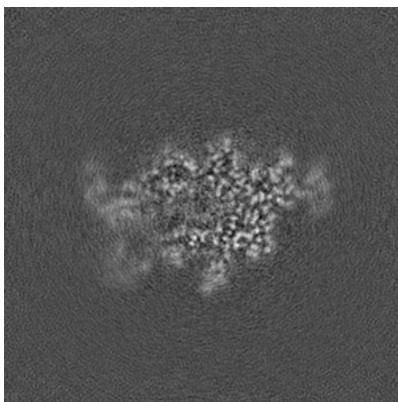


Z Index: 128

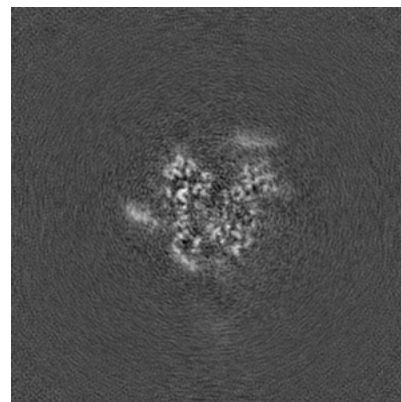
### 6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

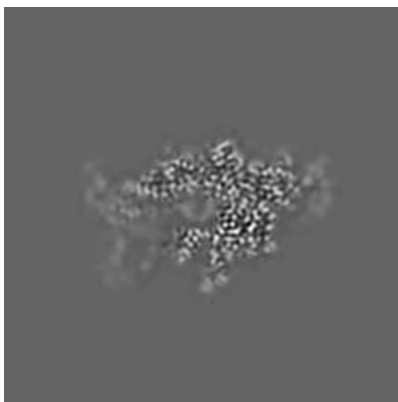
The images above show central slices of the map in three orthogonal directions.

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

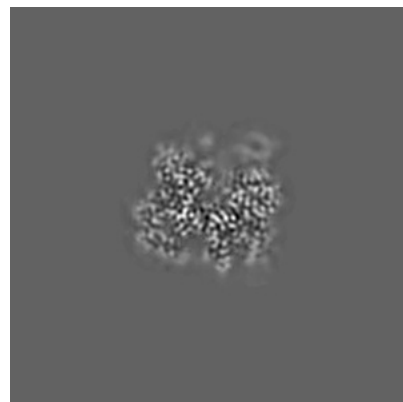
### 6.3.1 Primary map



X Index: 109

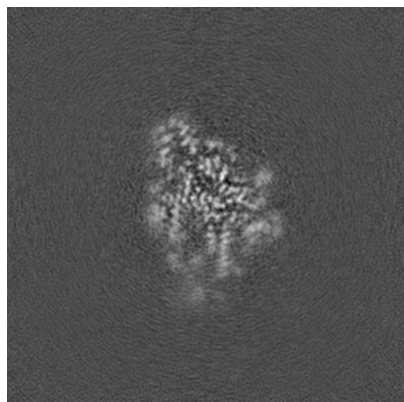


Y Index: 126

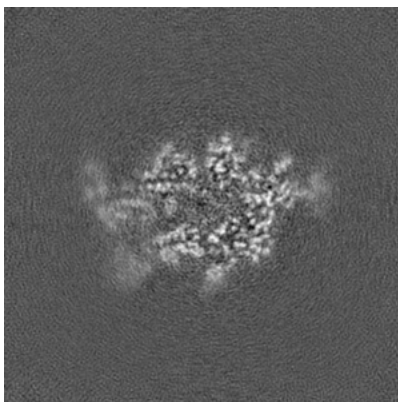


Z Index: 139

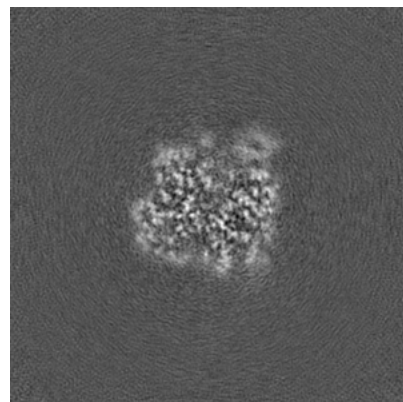
### 6.3.2 Raw map



X Index: 109



Y Index: 130

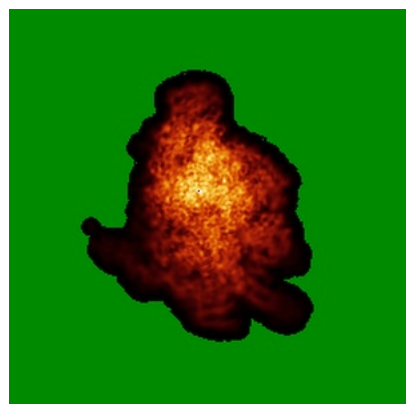


Z Index: 138

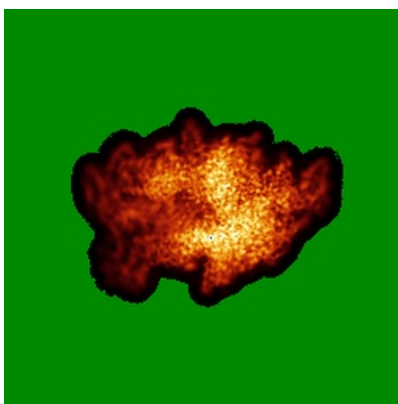
The images above show the largest variance slices of the map in three orthogonal directions.

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

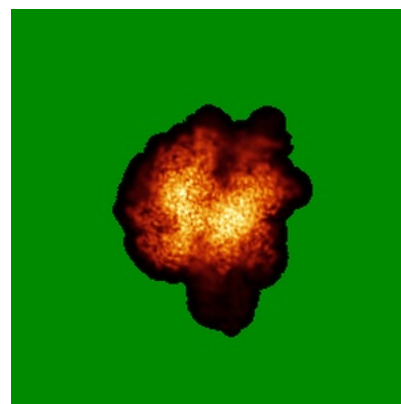
### 6.4.1 Primary map



X

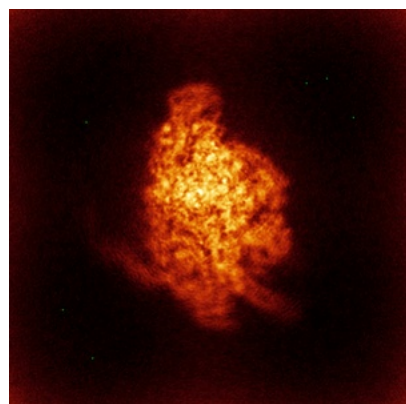


Y

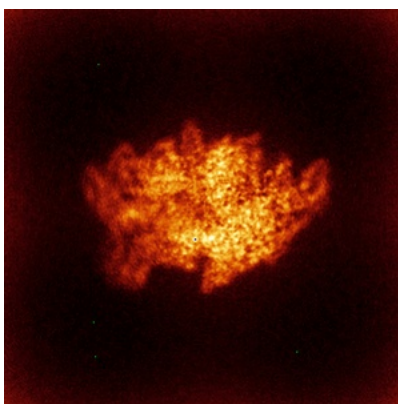


Z

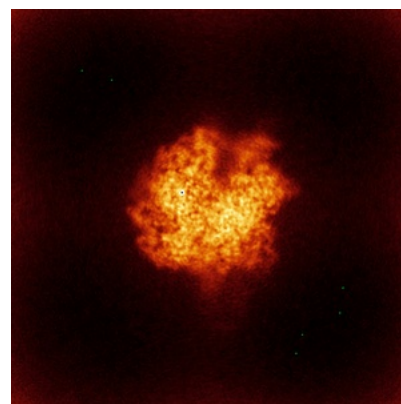
### 6.4.2 Raw map



X



Y



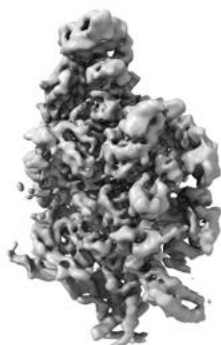
Z

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.

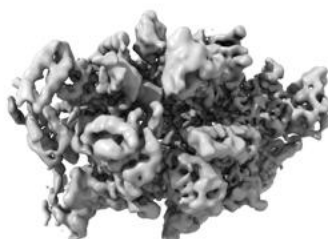


## 6.5 Orthogonal surface views [i](#)

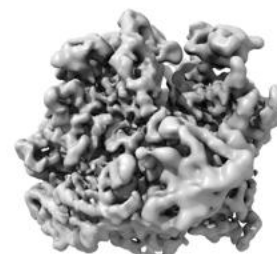
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.169. 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.



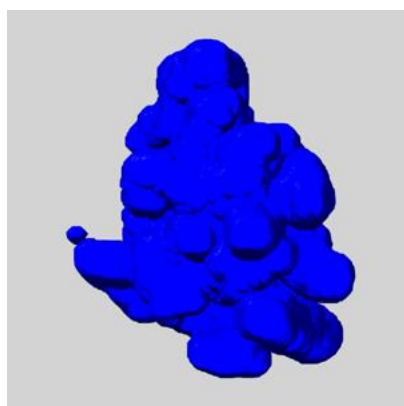
## 6.6 Mask visualisation [i](#)

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

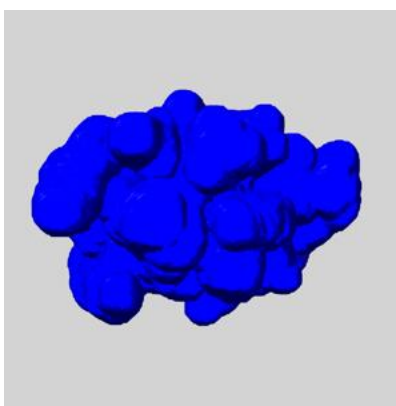
A mask typically either:

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

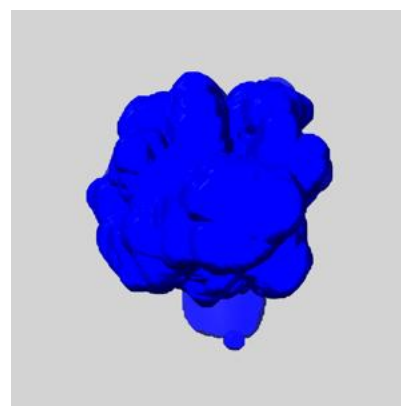
### 6.6.1 emd\_47706\_msk\_1.map [i](#)



X



Y

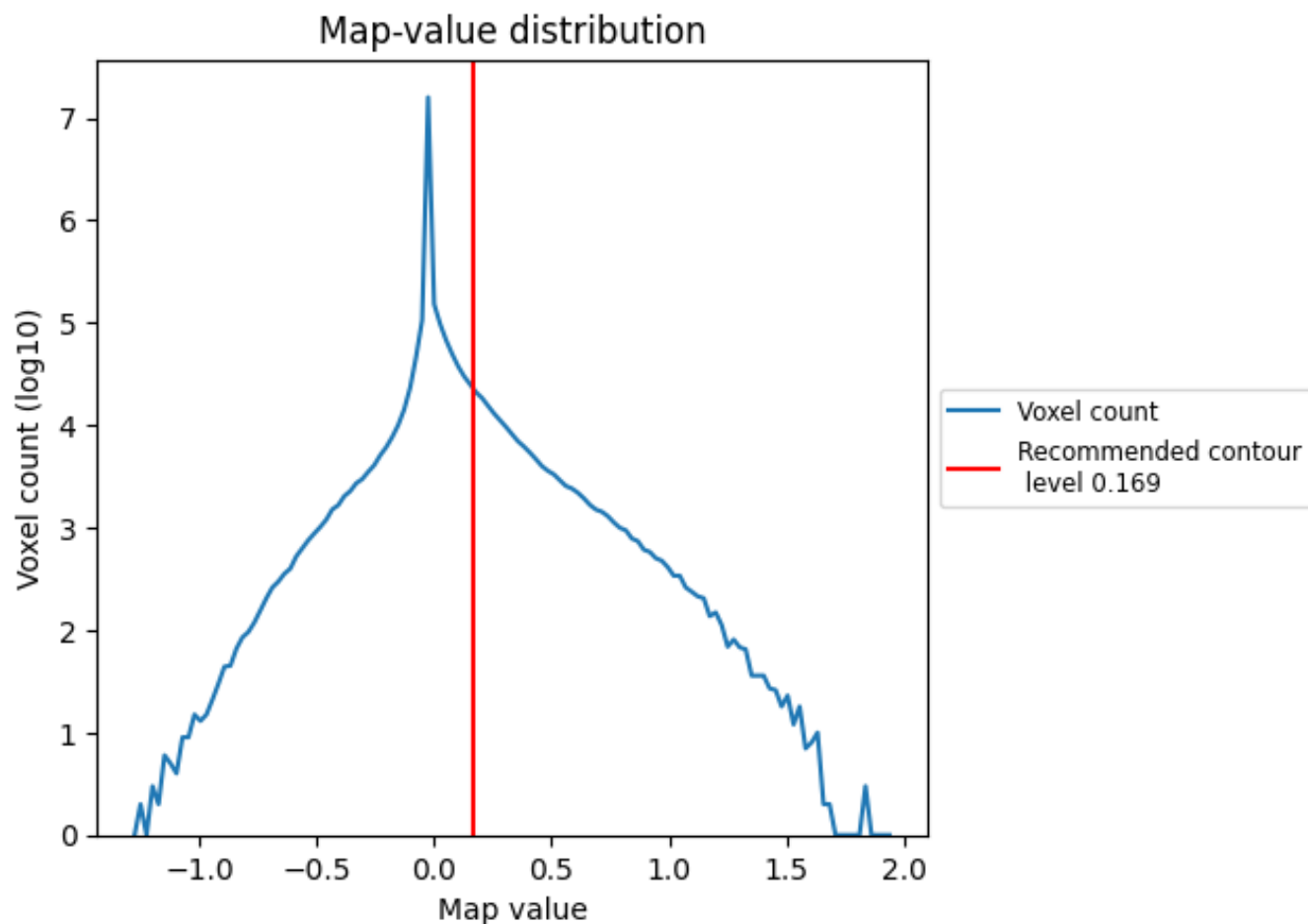


Z

## 7 Map analysis [i](#)

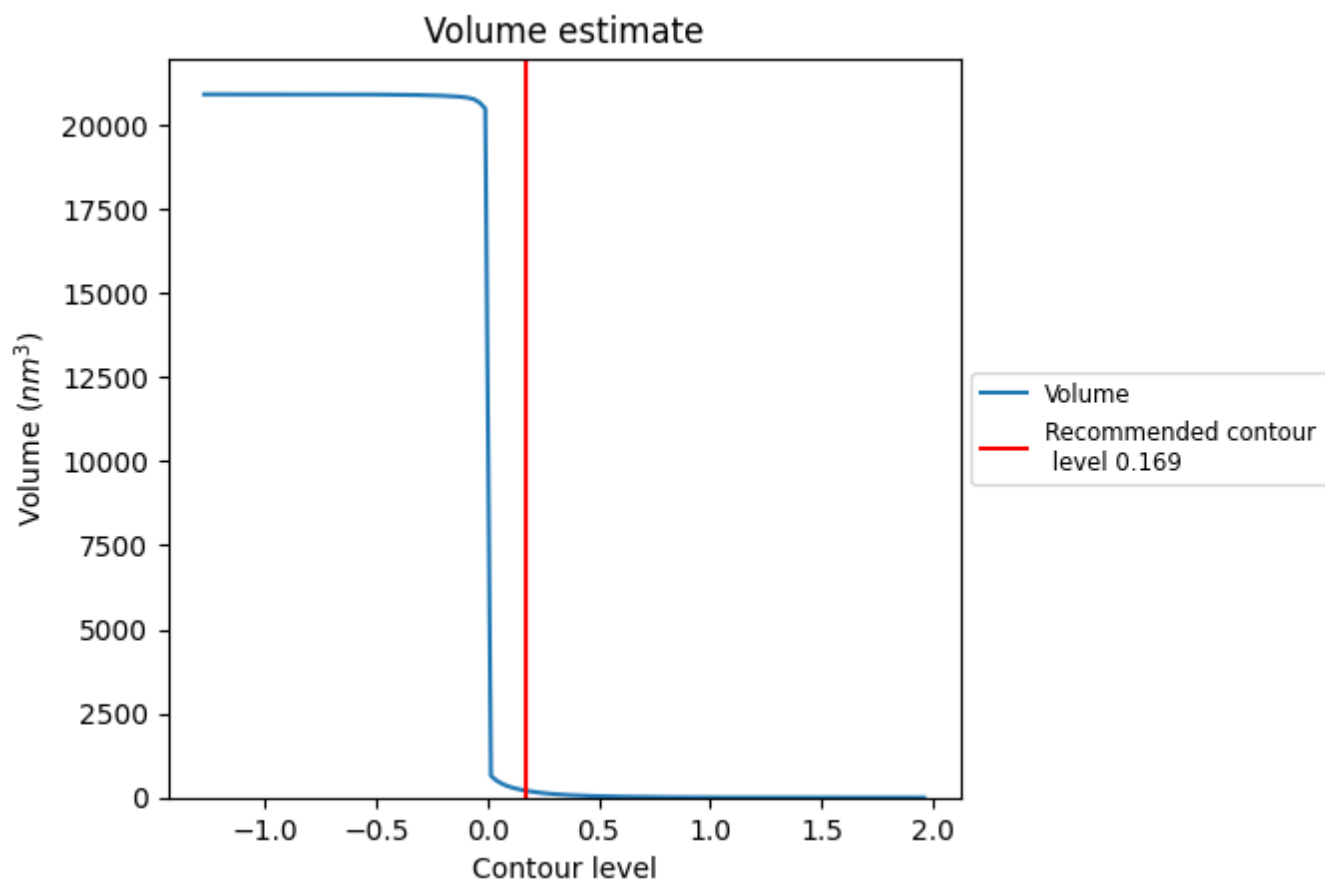
This section contains the results of statistical analysis of the map.

### 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.

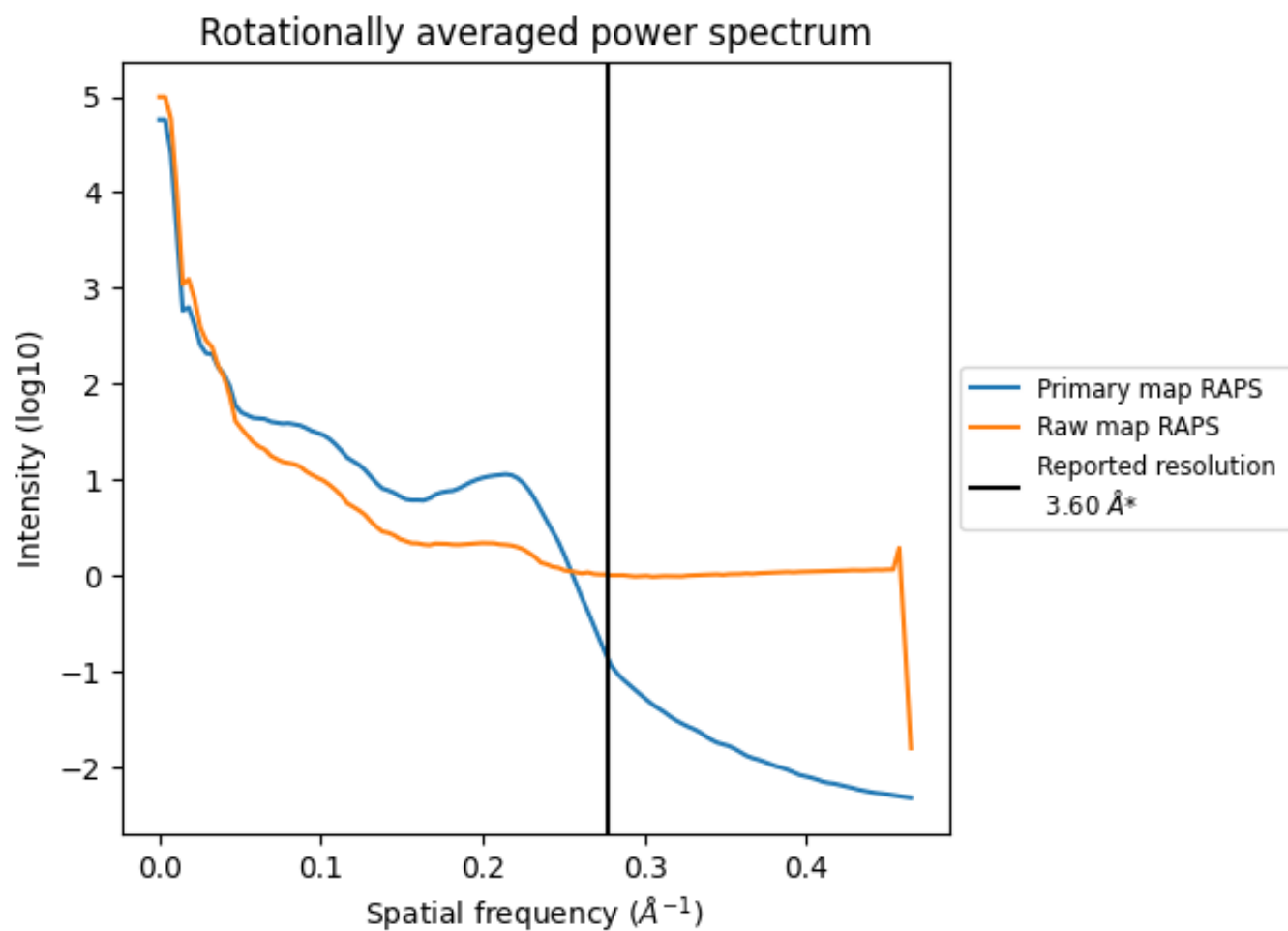
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 [i](#)

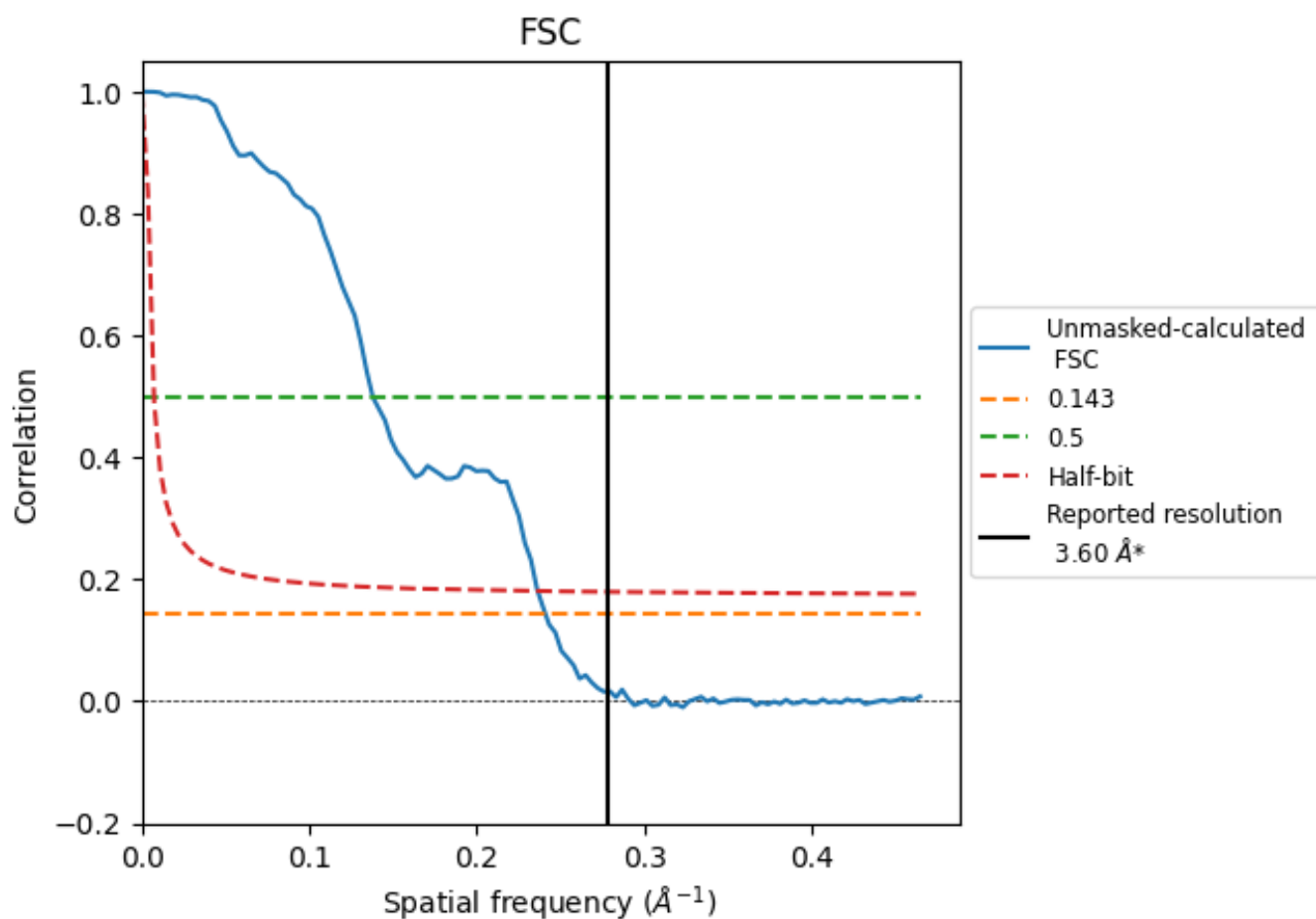


\*Reported resolution corresponds to spatial frequency of  $0.278 \text{ \AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

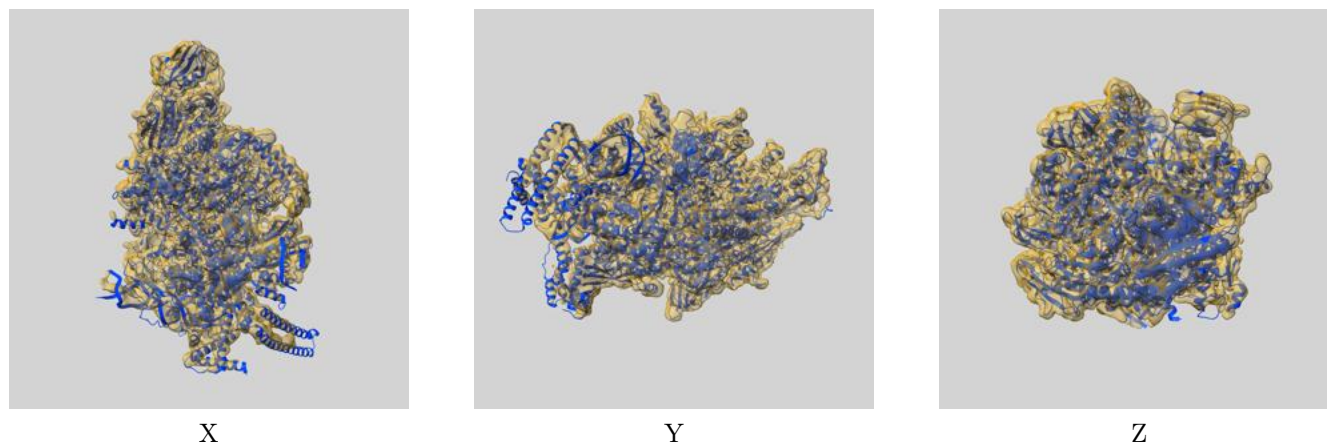
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.15	7.26	4.23

\*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 4.15 differs from the reported value 3.6 by more than 10 %

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

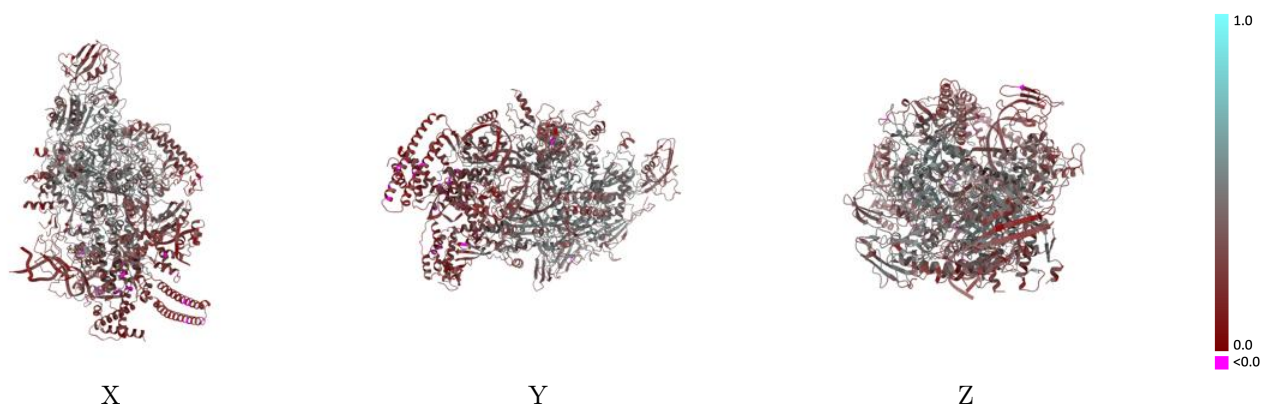
This section contains information regarding the fit between EMDB map EMD-47706 and PDB model 9E84. Per-residue inclusion information can be found in section 3 on page 9.

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



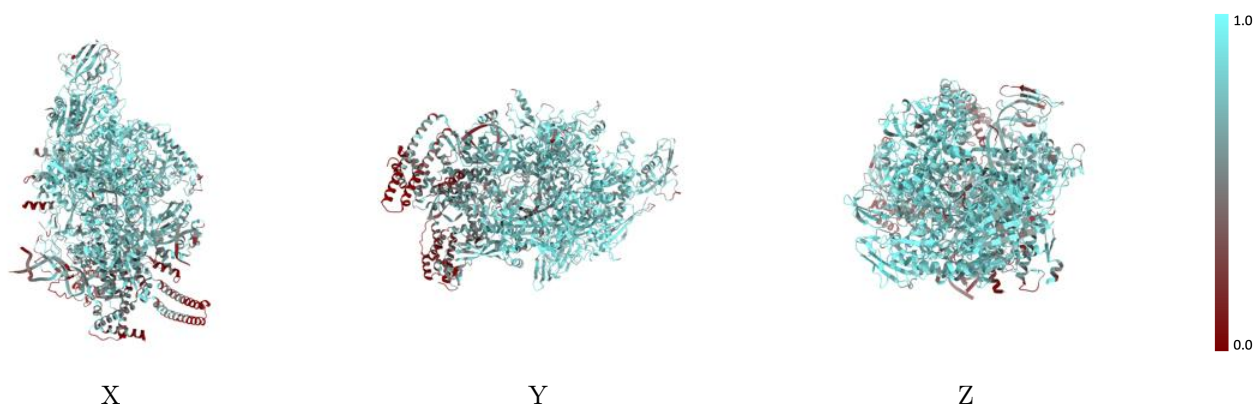
The images above show the 3D surface view of the map at the recommended contour level 0.169 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

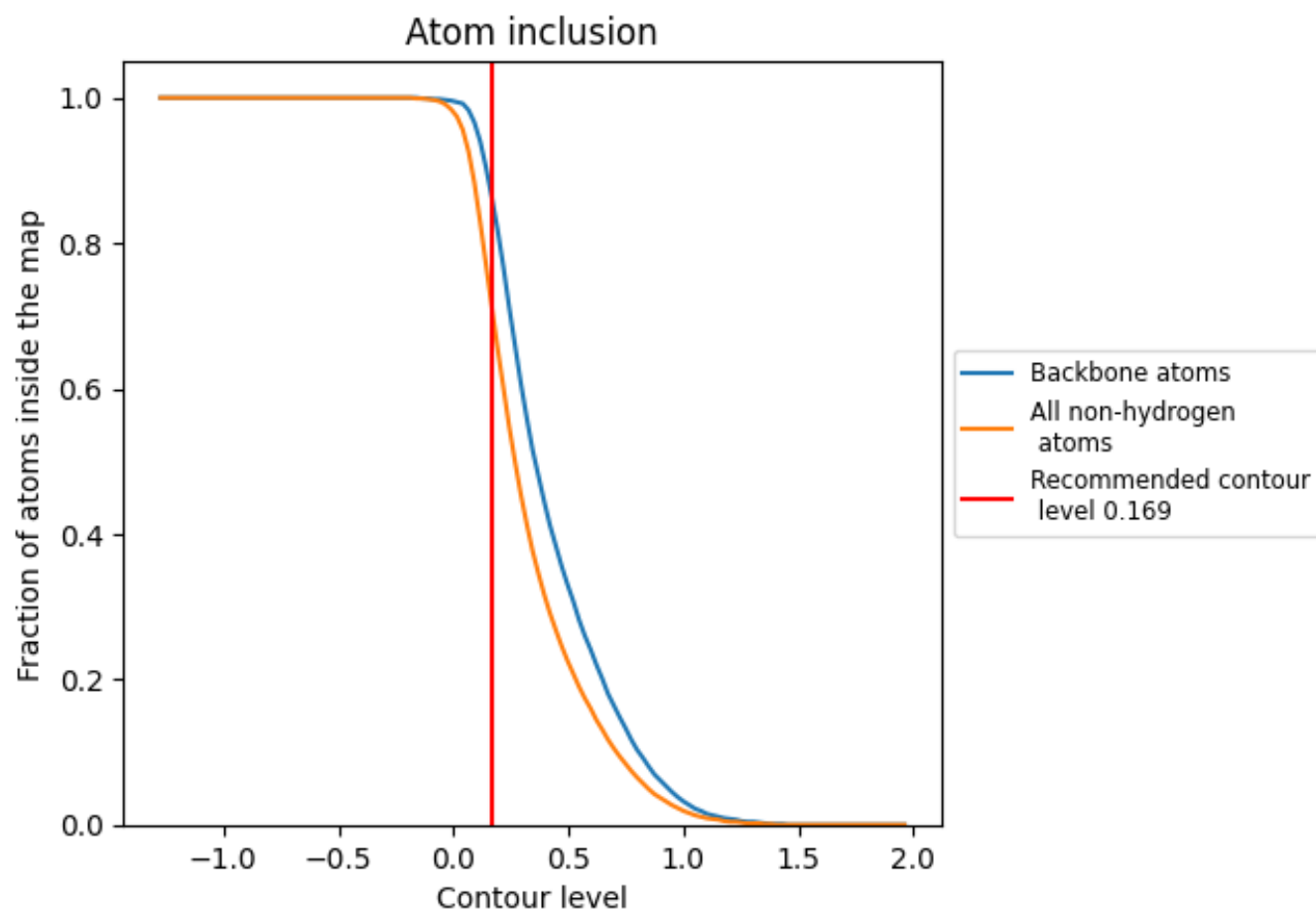
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.169).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 71% 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 (0.169) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7080	<div></div> 0.3470
A	<div></div> 0.8290	<div></div> 0.4140
B	<div></div> 0.7170	<div></div> 0.3300
C	<div></div> 0.8040	<div></div> 0.4000
D	<div></div> 0.7530	<div></div> 0.3630
E	<div></div> 0.6870	<div></div> 0.3510
F	<div></div> 0.4760	<div></div> 0.2260
J	<div></div> 0.3930	<div></div> 0.2220
M	<div></div> 0.2580	<div></div> 0.1790
N	<div></div> 0.6030	<div></div> 0.2230
R	<div></div> 0.4100	<div></div> 0.2610
T	<div></div> 0.5800	<div></div> 0.2660

1.0

0.0

<0.0