



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 04:50 PM UTC

PDB ID : 9GDO / pdb_00009gdo
EMDB ID : EMD-51273
Title : Cryo-EM structure of Vibrio cholerae RNA polymerase holoenzyme bound to an ompU promoter DNA fragment
Authors : Alcaide-Jimenez, A.; Baudin, F.; Canals, A.; Machon, C.; Murciano, B.; Fabrega-Ferrer, M.; Bantysh, O.; Perez-Luque, R.; Krukoniš, E.S.; Muller, C.W.; Coll, M.
Deposited on : 2024-08-06
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

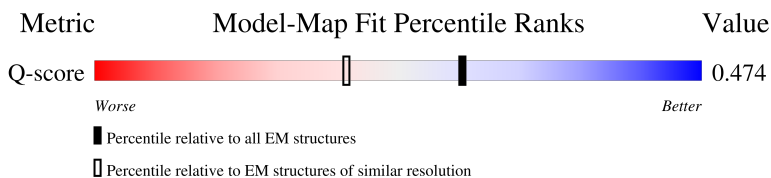
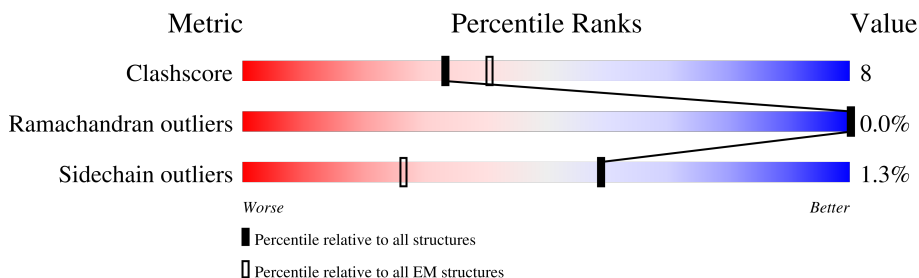
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	69	
2	N	69	
3	A	330	
3	B	330	

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Mol	Chain	Length	Quality of chain
3	G	330	<div><div></div><div>13%6%•</div><div>79%</div></div>
4	C	1341	<div><div></div><div>79%20%•</div></div>
5	D	1401	<div><div></div><div>69%17%14%</div></div>
6	E	90	<div><div></div><div>71%19%10%</div></div>
7	F	621	<div><div></div><div>•55%20%25%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 30695 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 DNA chain called ompU promoter template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	58	Total	C	N	O	P	0	0
			1180	566	211	346	57		

- Molecule 2 is a DNA chain called ompU promoter non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	58	Total	C	N	O	P	0	0
			1197	570	225	344	58		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	69	Total	C	N	O	S	0	0
			536	337	95	102	2		
3	A	231	Total	C	N	O	S	1	0
			1786	1117	315	349	5		
3	B	222	Total	C	N	O	S	0	0
			1697	1064	295	333	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	1328	Total	C	N	O	S	1	0
			10421	6547	1811	2025	38		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	1205	Total	C	N	O	S	0	0
			9435	5927	1680	1781	47		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	81	Total	C	N	O	S	0	0
			630	383	118	128	1		

- Molecule 7 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	468	Total	C	N	O	S	0	0
			3810	2384	690	719	17		

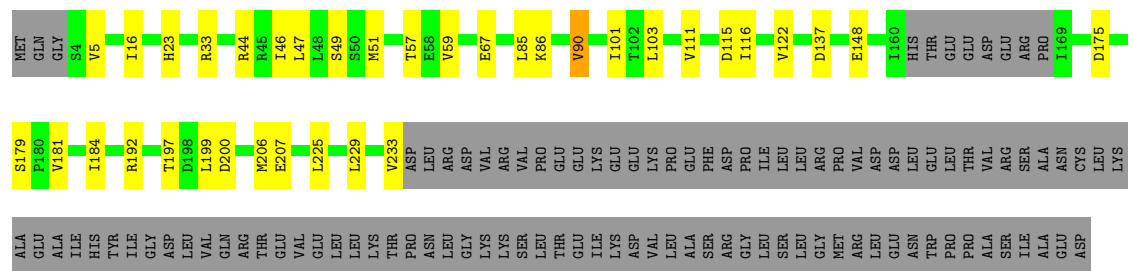
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

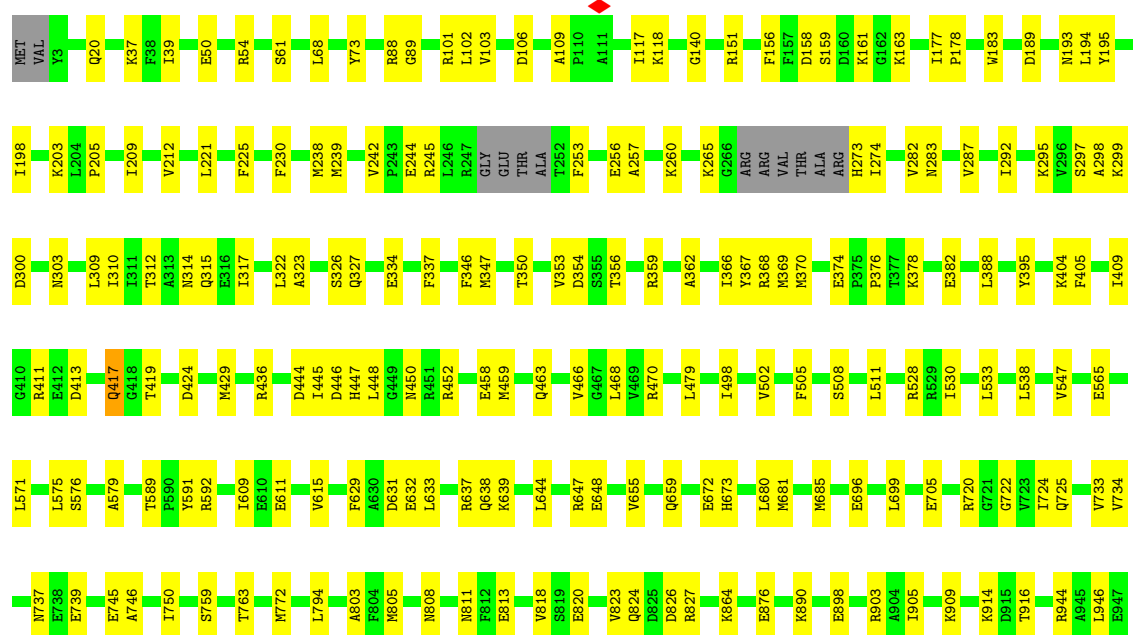
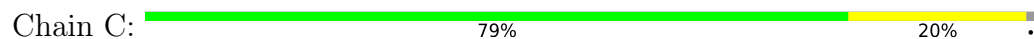
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

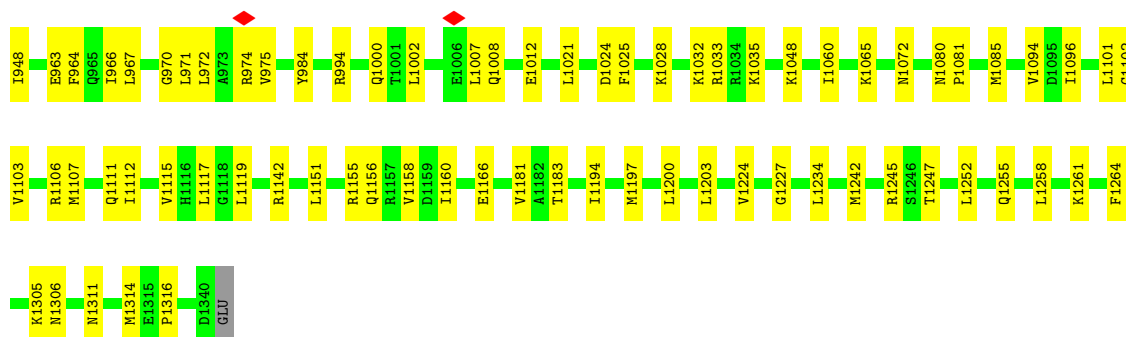
Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	

- Molecule 3: DNA-directed RNA polymerase subunit alpha



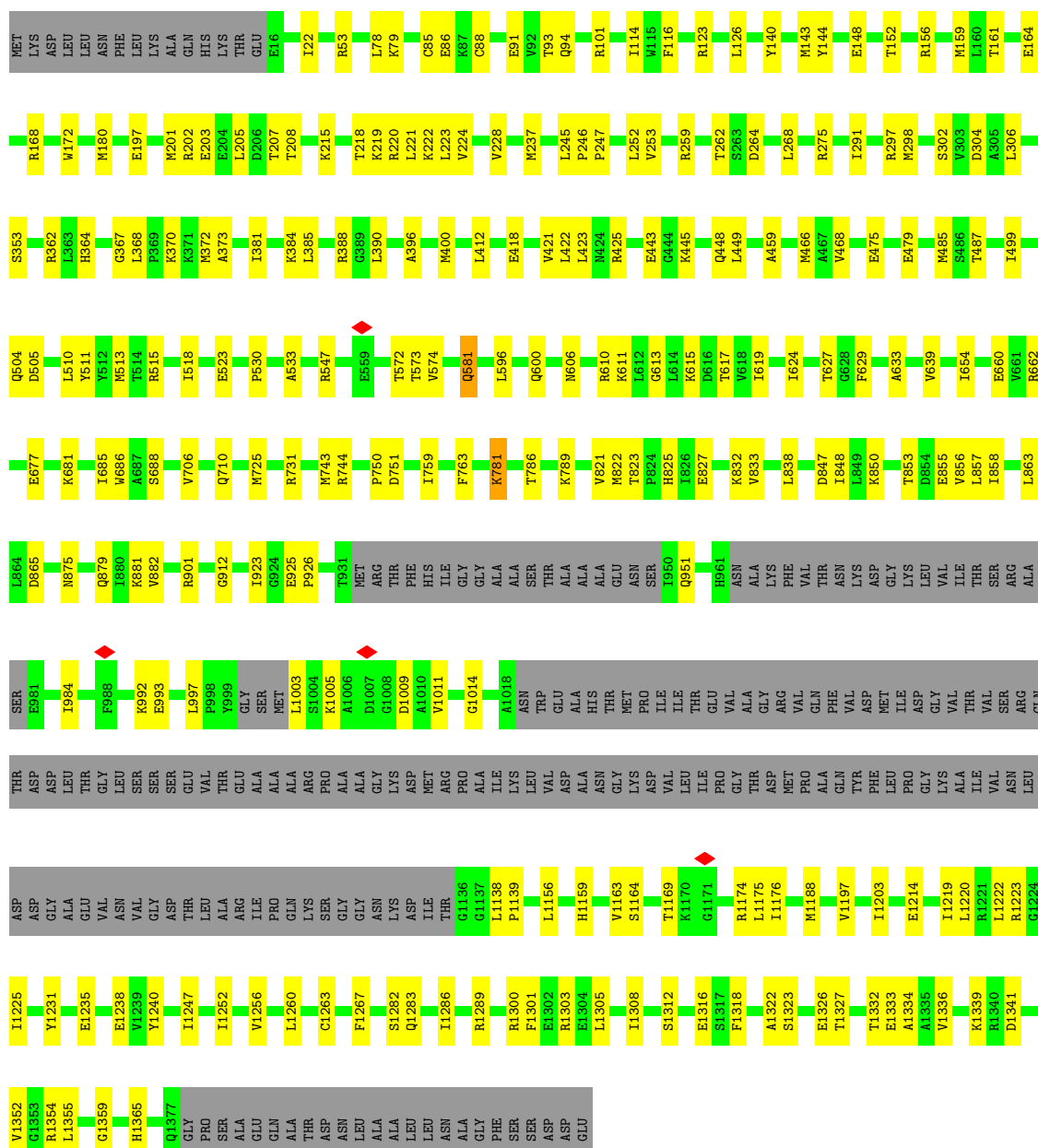
- Molecule 4: DNA-directed RNA polymerase subunit beta





• Molecule 5: DNA-directed RNA polymerase subunit beta'

Chain D:



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- The diagram illustrates a 16-bit bus architecture. It features a central horizontal bus line. On the left, a vertical stack of components is connected to the bus: A600 (green), K601 (yellow), R604 (green), K605 (green), L606 (yellow), and S610 (yellow). On the right, a vertical stack of components is connected to the bus: L619 (green), ASP (grey), and GLU (grey). The bus is labeled '16-bit' at both ends.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	199680	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 ($e^-/\text{\AA}^2$)	55.11	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.690	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.00455	Depositor
Map size (Å)	295.92, 295.92, 295.92	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	T	0.20	0/1322	0.40	0/2037
2	N	0.22	0/1345	0.40	0/2075
3	A	0.10	0/1809	0.29	0/2452
3	B	0.11	0/1717	0.28	0/2327
3	G	0.14	0/539	0.46	0/726
4	C	0.16	0/10585	0.33	0/14288
5	D	0.11	0/9579	0.29	0/12917
6	E	0.16	0/632	0.39	0/850
7	F	0.12	0/3861	0.31	0/5184
All	All	0.14	0/31389	0.32	0/42856

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	1180	0	657	26	0
2	N	1197	0	654	23	0
3	A	1786	0	1808	30	0
3	B	1697	0	1728	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	536	0	574	14	0
4	C	10421	0	10444	172	0
5	D	9435	0	9609	145	0
6	E	630	0	636	17	0
7	F	3810	0	3891	95	0
8	D	1	0	0	0	0
9	D	2	0	0	0	0
All	All	30695	0	30001	503	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 8.

All (503) 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:D:984:ILE:HB	5:D:993:GLU:HB2	1.57	0.87
5:D:857:LEU:HD22	5:D:875:ASN:HD22	1.44	0.83
2:N:-1:DT:H1'	2:N:0:DC:H5'	1.59	0.82
4:C:1103:VAL:HG11	4:C:1112:ILE:HD11	1.64	0.79
7:F:349:ILE:O	7:F:353:GLN:NE2	2.16	0.79
4:C:158:ASP:OD1	4:C:159:SER:N	2.19	0.76
6:E:3:ARG:HG2	6:E:48:VAL:HG13	1.69	0.75
5:D:202:ARG:HD3	5:D:221:LEU:HD21	1.67	0.75
5:D:275:ARG:HH11	5:D:302:SER:HB3	1.49	0.75
7:F:343:GLU:HA	7:F:346:ARG:HD2	1.67	0.75
5:D:79:LYS:HB3	7:F:577:THR:HG22	1.69	0.73
5:D:449:LEU:HD13	5:D:466:MET:HE1	1.70	0.72
4:C:805:MET:HE2	4:C:1224:VAL:HG11	1.71	0.72
4:C:368:ARG:HH12	4:C:376:PRO:HG3	1.56	0.71
5:D:140:TYR:HB3	7:F:102:MET:HE1	1.73	0.70
4:C:310:ILE:HD12	4:C:310:ILE:H	1.56	0.70
4:C:312:THR:OG1	4:C:315:GLN:OE1	2.09	0.69
4:C:1305:LYS:HZ1	7:F:542:SER:HB3	1.57	0.68
7:F:471:LEU:HD13	7:F:495:MET:HE2	1.75	0.68
3:B:86:LYS:HD3	3:B:175:ASP:HB2	1.76	0.68
5:D:1283:GLN:NE2	5:D:1316:GLU:OE2	2.27	0.68
7:F:369:ILE:HA	7:F:372:ARG:NH1	2.10	0.67
7:F:369:ILE:HA	7:F:372:ARG:HH12	1.59	0.67
6:E:3:ARG:NH2	6:E:55:GLU:OE2	2.28	0.67
7:F:350:GLN:HA	7:F:353:GLN:HE22	1.59	0.67
5:D:1164:SER:HB2	5:D:1176:ILE:HG13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:216:GLU:O	3:A:220:ARG:HG3	1.95	0.66
4:C:696:GLU:OE1	4:C:827:ARG:NH2	2.29	0.66
4:C:681:MET:O	4:C:685:MET:HG3	1.96	0.65
7:F:100:VAL:O	7:F:104:MET:HG2	1.96	0.65
5:D:660:GLU:OE2	5:D:685:ILE:HD13	1.96	0.65
4:C:1080:ASN:HB3	4:C:1085:MET:HE3	1.79	0.64
5:D:259:ARG:NH1	7:F:511:GLU:O	2.31	0.64
3:B:57:THR:HG21	3:B:148:GLU:HG3	1.79	0.64
4:C:463:GLN:HG3	4:C:505:PHE:HB2	1.79	0.64
4:C:198:ILE:HD12	4:C:369:MET:HE1	1.79	0.64
4:C:592:ARG:HG3	4:C:655:VAL:HG12	1.81	0.63
4:C:1002:LEU:HD13	4:C:1007:LEU:HB3	1.81	0.63
5:D:161:THR:HB	5:D:164:GLU:HG3	1.81	0.63
5:D:297:ARG:NH2	7:F:106:GLU:OE2	2.32	0.62
5:D:1352:VAL:HG23	5:D:1354:ARG:HG3	1.82	0.62
1:T:-7:DT:H2'	1:T:-6:DT:H71	1.81	0.62
4:C:772:MET:SD	3:A:75:GLN:NE2	2.72	0.62
5:D:164:GLU:O	5:D:168:ARG:HG2	1.99	0.62
4:C:1117:LEU:HD13	4:C:1194:ILE:HG12	1.82	0.61
3:G:293:THR:HG22	3:G:295:ASN:H	1.65	0.61
7:F:353:GLN:HA	7:F:356:GLU:HG3	1.83	0.61
5:D:1169:THR:OG1	5:D:1174:ARG:NH1	2.34	0.61
5:D:148:GLU:OE2	5:D:156:ARG:NH2	2.33	0.61
3:A:31:LEU:HD13	3:A:36:GLY:HA2	1.81	0.61
5:D:126:LEU:HD21	5:D:219:LYS:HG3	1.81	0.61
4:C:368:ARG:HG3	4:C:368:ARG:HH11	1.65	0.60
5:D:418:GLU:HB2	6:E:45:LYS:HG3	1.84	0.60
7:F:121:ILE:HG21	7:F:387:MET:HG3	1.82	0.60
6:E:3:ARG:NH1	6:E:6:VAL:HG22	2.17	0.60
6:E:3:ARG:HH12	6:E:6:VAL:HG22	1.66	0.60
5:D:850:LYS:HG3	5:D:875:ASN:HD21	1.67	0.60
3:A:21:THR:HG23	3:A:22:THR:HG23	1.83	0.60
7:F:371:HIS:O	7:F:375:ILE:HG13	2.02	0.59
5:D:1225:ILE:HD11	5:D:1303:ARG:HD3	1.84	0.59
6:E:3:ARG:HH22	6:E:6:VAL:HA	1.66	0.59
4:C:944:ARG:O	4:C:948:ILE:HG13	2.02	0.59
7:F:335:VAL:HA	7:F:338:VAL:HB	1.84	0.59
3:B:47:LEU:HD13	3:B:206:MET:HE3	1.84	0.59
4:C:528:ARG:NH2	4:C:576:SER:O	2.33	0.59
6:E:4:VAL:HG12	6:E:5:THR:HG23	1.85	0.59
5:D:847:ASP:HB3	5:D:856:VAL:HG13	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:133:GLN:NE2	7:F:264:PHE:O	2.36	0.58
2:N:-36:DC:OP2	7:F:594:ARG:NE	2.35	0.58
3:B:59:VAL:HG21	3:B:85:LEU:HD13	1.85	0.58
4:C:1025:PHE:HA	4:C:1028:LYS:HD2	1.85	0.58
1:T:7:DA:N6	4:C:508:SER:OG	2.36	0.58
2:N:-3:DT:C4	2:N:-2:DC:N4	2.71	0.58
5:D:677:GLU:O	5:D:681:LYS:HG2	2.04	0.58
4:C:1101:LEU:HD22	5:D:731:ARG:HB2	1.85	0.58
5:D:367:GLY:HA3	5:D:448:GLN:HB2	1.85	0.58
7:F:356:GLU:O	7:F:360:SER:N	2.28	0.58
4:C:725:GLN:HB3	4:C:733:VAL:HG12	1.85	0.57
3:A:235:LEU:HG	3:B:16:ILE:HD11	1.85	0.57
7:F:327:VAL:O	7:F:330:SER:OG	2.19	0.57
1:T:6:DG:H2'	1:T:7:DA:C8	2.39	0.57
5:D:201:MET:SD	5:D:220:ARG:NH1	2.76	0.57
5:D:1355:LEU:O	5:D:1365:HIS:NE2	2.36	0.57
1:T:1:DT:H2'	1:T:2:DC:C6	2.39	0.57
4:C:1115:VAL:HG13	4:C:1227:GLY:HA3	1.86	0.57
7:F:142:THR:HG23	7:F:277:LEU:HD13	1.85	0.57
7:F:349:ILE:HA	7:F:352:LEU:HD12	1.87	0.57
4:C:633:LEU:HD22	5:D:662:ARG:HH22	1.69	0.57
3:A:4:SER:OG	3:A:5:VAL:N	2.38	0.57
4:C:411:ARG:NE	4:C:413:ASP:OD1	2.36	0.57
5:D:1267:PHE:HB2	5:D:1300:ARG:HB3	1.86	0.57
5:D:518:ILE:HG12	5:D:547:ARG:HH21	1.69	0.57
1:T:16:DC:H2''	1:T:17:DA:C8	2.40	0.57
4:C:244:GLU:OE1	4:C:244:GLU:N	2.37	0.56
5:D:381:ILE:HD11	5:D:412:LEU:HD13	1.87	0.56
5:D:685:ILE:HG13	5:D:686:TRP:N	2.20	0.56
5:D:821:VAL:HG13	5:D:881:LYS:HE3	1.87	0.56
4:C:444:ASP:HB3	4:C:447:HIS:HB2	1.88	0.56
3:G:297:GLY:N	3:G:300:SER:OG	2.38	0.56
4:C:826:ASP:OD2	3:A:86:LYS:NZ	2.39	0.56
1:T:16:DC:H5''	7:F:159:ARG:HH22	1.71	0.56
5:D:1282:SER:O	5:D:1286:ILE:HG13	2.05	0.56
4:C:890:LYS:HE2	4:C:914:LYS:HB2	1.88	0.56
5:D:475:GLU:O	5:D:479:GLU:HG3	2.06	0.56
4:C:356:THR:HG21	4:C:362:ALA:HB2	1.88	0.55
4:C:436:ARG:HD2	4:C:436:ARG:O	2.06	0.55
4:C:633:LEU:HB3	4:C:644:LEU:HD12	1.88	0.55
4:C:533:LEU:HD21	4:C:571:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:161:LYS:HB3	4:C:163:LYS:HZ2	1.71	0.55
4:C:1314:MET:HG3	4:C:1316:PRO:HD3	1.88	0.55
5:D:396:ALA:O	5:D:400:MET:HG3	2.06	0.55
4:C:297:SER:HB2	4:C:317:ILE:HD11	1.89	0.55
4:C:411:ARG:NH1	4:C:424:ASP:OD1	2.39	0.55
3:A:159:ARG:HH11	3:A:173:LEU:HD12	1.71	0.55
7:F:503:ARG:O	7:F:507:LYS:HG3	2.07	0.55
1:T:2:DC:OP1	4:C:1261:LYS:N	2.33	0.54
1:T:12:DC:H2'	1:T:13:DT:H71	1.89	0.54
4:C:177:ILE:HG22	4:C:183:TRP:CE2	2.41	0.54
5:D:1156:LEU:HD13	5:D:1222:LEU:HD12	1.88	0.54
4:C:724:ILE:HD13	4:C:734:VAL:HG22	1.89	0.54
4:C:1008:GLN:O	4:C:1012:GLU:HG3	2.07	0.54
4:C:1081:PRO:HG3	3:B:33:ARG:HH11	1.71	0.54
3:B:67:GLU:OE1	3:B:67:GLU:N	2.31	0.54
4:C:189:ASP:OD1	4:C:193:ASN:N	2.29	0.54
2:N:7:DA:H2''	2:N:8:DA:C8	2.42	0.54
4:C:292:ILE:HG21	4:C:322:LEU:HD21	1.88	0.54
4:C:530:ILE:HD11	4:C:575:LEU:HD13	1.90	0.54
4:C:1306:ASN:HB3	4:C:1311:ASN:O	2.08	0.54
5:D:224:VAL:O	5:D:228:VAL:HG23	2.08	0.54
4:C:1242:MET:HE3	5:D:372:MET:HG3	1.90	0.54
4:C:88:ARG:HG3	4:C:88:ARG:HH11	1.72	0.54
3:B:103:LEU:HB2	3:B:116:ILE:HG12	1.90	0.54
4:C:589:THR:OG1	4:C:659:GLN:NE2	2.37	0.54
4:C:1102:GLY:O	4:C:1106:ARG:HG3	2.07	0.54
7:F:593:GLU:HG3	7:F:596:ARG:HH12	1.73	0.54
4:C:750:ILE:HD12	4:C:963:GLU:HG2	1.89	0.54
4:C:1142:ARG:NH1	4:C:1160:ILE:O	2.41	0.54
6:E:68:GLU:O	6:E:72:GLN:HG2	2.09	0.53
4:C:739:GLU:OE1	4:C:739:GLU:N	2.40	0.53
4:C:1255:GLN:NE2	7:F:533:ASP:OD2	2.40	0.53
7:F:594:ARG:HH11	7:F:597:GLN:HG3	1.73	0.53
2:N:-15:DG:OP1	7:F:459:ARG:NH2	2.39	0.53
5:D:144:TYR:CD1	5:D:180:MET:HE3	2.43	0.53
1:T:2:DC:H2''	1:T:3:DT:O4'	2.08	0.53
3:G:263:LEU:HD13	3:G:268:ALA:HB2	1.89	0.53
7:F:168:VAL:HB	7:F:266:GLU:HA	1.90	0.53
4:C:746:ALA:HB1	4:C:967:LEU:HB2	1.91	0.53
7:F:111:GLU:H	7:F:111:GLU:CD	2.17	0.53
7:F:368:ASP:OD2	7:F:372:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:818:VAL:HG22	4:C:1096:ILE:HG12	1.90	0.53
1:T:-4:DC:H2'	1:T:-3:DG:C8	2.43	0.53
4:C:459:MET:HE1	4:C:511:LEU:HD13	1.90	0.53
4:C:591:TYR:OH	4:C:637:ARG:NH2	2.39	0.53
5:D:123:ARG:NH1	5:D:1333:GLU:OE1	2.42	0.52
2:N:-3:DT:H2'	2:N:-2:DC:H2'	1.90	0.52
6:E:30:MET:HE1	6:E:49:ILE:HB	1.91	0.52
4:C:256:GLU:HG3	4:C:257:ALA:H	1.73	0.52
4:C:303:ASN:HB2	4:C:310:ILE:HD11	1.89	0.52
3:B:46:ILE:HD11	3:B:225:LEU:HD13	1.91	0.52
2:N:-37:DA:H3'	7:F:594:ARG:HH21	1.74	0.52
5:D:53:ARG:NH1	5:D:88:CYS:O	2.36	0.52
4:C:1247:THR:HG21	7:F:539:PRO:HG3	1.91	0.52
3:B:44:ARG:HA	3:B:184:ILE:HD13	1.92	0.52
4:C:68:LEU:HD13	4:C:102:LEU:HD13	1.91	0.52
4:C:444:ASP:O	4:C:450:ASN:ND2	2.36	0.52
4:C:808:ASN:H	5:D:633:ALA:HB2	1.73	0.51
5:D:513:MET:HE1	5:D:627:THR:HG22	1.91	0.51
5:D:85:CYS:HB3	5:D:88:CYS:SG	2.51	0.51
4:C:864:LYS:NZ	4:C:876:GLU:O	2.40	0.51
5:D:252:LEU:HD13	5:D:262:THR:HB	1.93	0.51
4:C:298:ALA:HB3	4:C:334:GLU:HG3	1.92	0.51
4:C:1156:GLN:HG2	4:C:1158:VAL:HG23	1.93	0.51
7:F:338:VAL:O	7:F:342:GLU:N	2.42	0.51
4:C:177:ILE:HG22	4:C:183:TRP:CD2	2.46	0.51
4:C:498:ILE:O	4:C:502:VAL:HG22	2.10	0.51
3:A:191:ALA:HB2	3:A:201:LYS:HB2	1.92	0.51
3:B:67:GLU:H	3:B:67:GLU:CD	2.18	0.51
2:N:-4:DG:H2''	2:N:-3:DT:H5''	1.93	0.51
4:C:106:ASP:HB3	4:C:109:ALA:HB3	1.93	0.51
5:D:530:PRO:HB2	5:D:581:GLN:HG3	1.93	0.51
4:C:720:ARG:NH2	4:C:745:GLU:OE1	2.44	0.50
5:D:1220:LEU:HD22	5:D:1305:LEU:HB2	1.93	0.50
2:N:-8:DA:O3'	7:F:434:LYS:NZ	2.42	0.50
4:C:88:ARG:NH2	4:C:1035:LYS:O	2.44	0.50
5:D:370:LYS:HE2	5:D:443:GLU:HG2	1.93	0.50
1:T:8:DA:H2''	1:T:9:DA:C8	2.46	0.50
4:C:20:GLN:OE1	4:C:1155:ARG:NH1	2.44	0.50
5:D:510:LEU:HD11	5:D:624:ILE:HG23	1.92	0.50
4:C:350:THR:HA	4:C:353:VAL:HG12	1.94	0.50
4:C:370:MET:HE2	4:C:370:MET:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:90:VAL:HG13	3:A:122:VAL:HG13	1.93	0.50
2:N:-1:DT:H2''	2:N:0:DC:C5	2.46	0.50
5:D:596:LEU:HD22	5:D:600:GLN:HB3	1.93	0.50
3:G:256:ARG:O	3:G:278:TYR:HA	2.12	0.50
4:C:1183:THR:O	4:C:1183:THR:OG1	2.30	0.50
4:C:733:VAL:HG22	4:C:750:ILE:HG12	1.94	0.50
3:A:215:GLU:O	3:A:219:ARG:HG3	2.11	0.50
7:F:403:THR:HG22	7:F:404:ASN:OD1	2.12	0.50
4:C:195:TYR:CD1	4:C:205:PRO:HA	2.47	0.49
4:C:631:ASP:OD1	4:C:632:GLU:N	2.45	0.49
2:N:-35:DT:H2'	2:N:-34:DA:H8	1.77	0.49
2:N:-28:DT:H2''	2:N:-27:DA:C8	2.47	0.49
4:C:103:VAL:HG12	4:C:117:ILE:HG12	1.95	0.49
4:C:242:VAL:HB	4:C:245:ARG:HD2	1.94	0.49
5:D:22:ILE:HG21	5:D:1334:ALA:HB1	1.94	0.49
3:B:90:VAL:HG23	3:B:122:VAL:HG13	1.94	0.49
7:F:594:ARG:HD2	7:F:597:GLN:HE21	1.77	0.49
5:D:572:THR:OG1	5:D:573:THR:N	2.45	0.49
7:F:340:GLU:O	7:F:343:GLU:HB3	2.12	0.49
4:C:575:LEU:HG	4:C:579:ALA:HB3	1.94	0.49
5:D:660:GLU:OE2	5:D:685:ILE:HG21	2.12	0.49
4:C:905:ILE:HD11	7:F:606:LEU:HD23	1.95	0.49
7:F:296:MET:HE2	7:F:296:MET:HA	1.94	0.49
4:C:238:MET:HE1	4:C:283:ASN:O	2.12	0.49
7:F:431:ARG:HB3	7:F:433:TYR:CD2	2.48	0.49
4:C:417:GLN:HG3	4:C:419:THR:H	1.78	0.49
5:D:126:LEU:HD23	5:D:223:LEU:HD22	1.94	0.49
5:D:613:GLY:O	5:D:617:THR:OG1	2.28	0.49
4:C:260:LYS:HZ3	4:C:282:VAL:HG13	1.78	0.48
5:D:384:LYS:O	5:D:388:ARG:HG3	2.14	0.48
5:D:823:THR:HG22	5:D:879:GLN:HB2	1.94	0.48
1:T:18:DA:H2''	1:T:19:DA:C8	2.48	0.48
1:T:36:DG:H2'	1:T:37:DT:H71	1.96	0.48
5:D:1163:VAL:HG13	5:D:1175:LEU:HD21	1.96	0.48
7:F:285:MET:HG2	7:F:370:SER:HB2	1.95	0.48
7:F:346:ARG:HA	7:F:349:ILE:HG12	1.95	0.48
4:C:1072:ASN:ND2	4:C:1111:GLN:OE1	2.46	0.48
5:D:362:ARG:HG3	5:D:362:ARG:HH11	1.79	0.48
1:T:30:DC:H2''	1:T:31:DA:C8	2.49	0.48
4:C:367:TYR:OH	4:C:374:GLU:OE1	2.26	0.48
4:C:1151:LEU:HD13	4:C:1197:MET:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:47:LEU:O	3:B:179:SER:OG	2.30	0.48
4:C:37:LYS:HB3	4:C:37:LYS:NZ	2.29	0.47
4:C:672:GLU:HG2	4:C:673:HIS:CD2	2.49	0.47
5:D:710:GLN:N	5:D:710:GLN:OE1	2.47	0.47
5:D:1334:ALA:HA	5:D:1339:LYS:HG3	1.96	0.47
5:D:475:GLU:OE2	6:E:28:ARG:NH1	2.45	0.47
5:D:533:ALA:HB1	5:D:574:VAL:HG13	1.95	0.47
5:D:615:LYS:O	5:D:619:ILE:HG13	2.15	0.47
1:T:6:DG:H2''	1:T:7:DA:O5'	2.14	0.47
4:C:89:GLY:HA2	4:C:140:GLY:HA3	1.97	0.47
4:C:1305:LYS:HZ1	7:F:542:SER:CB	2.27	0.47
5:D:370:LYS:HE3	5:D:370:LYS:HB2	1.62	0.47
4:C:898:GLU:OE1	4:C:898:GLU:N	2.47	0.47
5:D:298:MET:SD	7:F:410:LEU:HB3	2.55	0.47
5:D:1308:ILE:O	5:D:1312:SER:OG	2.24	0.47
5:D:1332:THR:O	5:D:1336:VAL:HG22	2.14	0.47
7:F:411:ASP:OD1	7:F:411:ASP:N	2.48	0.47
5:D:1322:ALA:HB1	5:D:1327:THR:HG23	1.97	0.47
3:A:9:LEU:HD12	3:A:199:LEU:HD11	1.96	0.47
7:F:115:ARG:O	7:F:119:ILE:HG12	2.14	0.47
7:F:282:ARG:NH2	7:F:377:GLU:OE2	2.48	0.47
4:C:1119:LEU:HG	4:C:1203:LEU:HD13	1.96	0.47
3:A:188:VAL:HG12	3:A:200:ASP:OD2	2.14	0.47
7:F:307:LYS:N	7:F:307:LYS:HD2	2.30	0.47
7:F:332:LYS:HB2	7:F:335:VAL:HG23	1.96	0.47
4:C:1048:LYS:HB2	4:C:1048:LYS:HE3	1.55	0.46
5:D:744:ARG:HB2	5:D:759:ILE:HB	1.96	0.46
5:D:926:PRO:HG2	5:D:1247:ILE:HD11	1.96	0.46
3:A:13:LEU:HD21	3:A:16:ILE:CD1	2.45	0.46
3:A:101:ILE:HD12	3:A:116:ILE:HG21	1.97	0.46
4:C:61:SER:HB3	4:C:479:LEU:HB3	1.97	0.46
4:C:538:LEU:HD21	4:C:547:VAL:HG21	1.96	0.46
5:D:518:ILE:HB	5:D:706:VAL:HG21	1.96	0.46
5:D:1263:CYS:HB2	5:D:1301:PHE:HB2	1.97	0.46
3:A:67:GLU:HG2	3:A:172:LEU:HD22	1.96	0.46
2:N:-6:DG:C8	7:F:112:LEU:HD11	2.51	0.46
4:C:1107:MET:HE3	5:D:763:PHE:HE2	1.80	0.46
5:D:1286:ILE:HG23	5:D:1289:ARG:HH21	1.81	0.46
4:C:347:MET:HE1	4:C:429:MET:HE2	1.97	0.46
4:C:903:ARG:HD3	4:C:909:LYS:HG3	1.98	0.46
5:D:1005:LYS:HB3	5:D:1009:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:272:LYS:HD3	3:G:272:LYS:HA	1.56	0.46
4:C:323:ALA:O	4:C:327:GLN:HG3	2.16	0.46
5:D:91:GLU:OE1	5:D:101:ARG:NH2	2.49	0.46
4:C:39:ILE:O	4:C:73:TYR:OH	2.32	0.46
4:C:346:PHE:O	4:C:350:THR:HG22	2.16	0.46
4:C:565:GLU:HB2	4:C:680:LEU:HD21	1.97	0.46
3:A:229:LEU:O	3:A:233:VAL:HG23	2.15	0.46
3:G:253:ILE:HG13	3:G:279:ILE:HG21	1.97	0.46
5:D:833:VAL:HG21	5:D:838:LEU:HD21	1.96	0.46
2:N:9:DT:H2'	2:N:10:DG:C8	2.51	0.45
4:C:151:ARG:HD2	4:C:156:PHE:HE2	1.80	0.45
5:D:523:GLU:OE2	5:D:547:ARG:NH1	2.48	0.45
7:F:99:PRO:HB2	7:F:410:LEU:HD11	1.98	0.45
5:D:418:GLU:CD	6:E:48:VAL:HG21	2.41	0.45
5:D:1231:TYR:O	5:D:1235:GLU:HG2	2.17	0.45
5:D:425:ARG:HD2	5:D:459:ALA:HB2	1.97	0.45
7:F:351:LYS:HA	7:F:354:MET:HE2	1.98	0.45
5:D:654:ILE:HD11	5:D:743:MET:SD	2.56	0.45
1:T:9:DA:H4'	1:T:10:DA:C6	2.51	0.45
5:D:681:LYS:O	5:D:685:ILE:HG23	2.17	0.45
3:A:105:LYS:HD3	3:A:111:VAL:HG22	1.98	0.45
7:F:285:MET:HE3	7:F:285:MET:O	2.16	0.45
7:F:426:LYS:HD2	7:F:442:TRP:CZ2	2.51	0.45
1:T:30:DC:H2''	1:T:31:DA:H8	1.82	0.45
5:D:750:PRO:HA	5:D:781:LYS:NZ	2.31	0.45
1:T:37:DT:H2''	1:T:38:DA:C8	2.52	0.45
4:C:354:ASP:OD1	4:C:356:THR:N	2.34	0.45
4:C:1024:ASP:OD1	4:C:1025:PHE:N	2.50	0.45
5:D:822:MET:HG3	5:D:882:VAL:HG22	1.99	0.45
5:D:1156:LEU:HD11	5:D:1223:ARG:HH21	1.81	0.45
5:D:1214:GLU:HB3	5:D:1219:ILE:HD11	1.99	0.45
7:F:295:VAL:HG13	7:F:345:ILE:HG12	1.99	0.45
7:F:428:GLU:OE1	7:F:431:ARG:NH1	2.49	0.45
7:F:482:MET:HE2	7:F:482:MET:HB3	1.74	0.45
2:N:-35:DT:H71	7:F:597:GLN:HE22	1.82	0.45
5:D:93:THR:OG1	5:D:94:GLN:N	2.50	0.45
3:A:52:PRO:HB3	3:B:5:VAL:HB	1.98	0.45
3:A:224:ILE:O	3:A:228:GLN:HG2	2.16	0.45
7:F:145:TYR:O	7:F:148:GLU:HG3	2.17	0.45
7:F:434:LYS:HB3	7:F:434:LYS:HE2	1.59	0.45
2:N:-35:DT:H2'	2:N:-34:DA:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:209:ILE:HA	4:C:212:VAL:HG12	1.99	0.45
4:C:823:VAL:HG22	4:C:1060:ILE:HG22	1.98	0.45
5:D:205:LEU:HD23	5:D:208:THR:HG21	1.99	0.45
2:N:-23:DG:H2''	2:N:-22:DA:C8	2.52	0.45
4:C:803:ALA:HB2	4:C:1094:VAL:HG11	1.98	0.45
3:B:192:ARG:HB3	3:B:197:THR:HA	1.99	0.45
7:F:573:ILE:HG22	7:F:574:ASP:OD1	2.17	0.45
3:A:46:ILE:HD11	3:A:225:LEU:HD13	1.99	0.44
5:D:222:LYS:HD3	5:D:222:LYS:HA	1.74	0.44
3:B:101:ILE:HD12	3:B:116:ILE:HG21	1.99	0.44
7:F:287:ARG:HH11	7:F:355:ILE:HD11	1.82	0.44
4:C:705:GLU:HB3	4:C:794:LEU:H	1.81	0.44
7:F:152:ARG:HB3	7:F:158:LEU:HD23	1.98	0.44
7:F:345:ILE:O	7:F:349:ILE:HG12	2.18	0.44
4:C:970:GLY:O	4:C:974:ARG:HG3	2.18	0.44
5:D:518:ILE:HG12	5:D:547:ARG:NH2	2.31	0.44
4:C:225:PHE:HE2	4:C:347:MET:HB3	1.83	0.44
5:D:751:ASP:OD1	5:D:751:ASP:N	2.51	0.44
7:F:379:LYS:NZ	7:F:379:LYS:HB3	2.33	0.44
7:F:522:ASP:OD1	7:F:523:GLU:N	2.49	0.44
4:C:813:GLU:OE1	5:D:504:GLN:NE2	2.51	0.44
5:D:353:SER:OG	5:D:445:LYS:O	2.34	0.44
5:D:863:LEU:HD21	5:D:901:ARG:HB2	2.00	0.44
4:C:378:LYS:HE2	4:C:382:GLU:CD	2.42	0.44
5:D:114:ILE:HD12	5:D:304:ASP:HB3	2.00	0.44
5:D:857:LEU:HD22	5:D:875:ASN:ND2	2.22	0.44
4:C:295:LYS:HA	4:C:295:LYS:HD3	1.83	0.44
5:D:291:ILE:HD13	7:F:417:ASN:HB3	2.00	0.44
5:D:832:LYS:HD3	5:D:832:LYS:HA	1.76	0.44
5:D:992:LYS:HB3	5:D:992:LYS:HE2	1.61	0.44
5:D:1174:ARG:HG2	5:D:1188:MET:SD	2.58	0.44
5:D:1197:VAL:HG12	5:D:1203:ILE:HG21	2.00	0.44
2:N:-32:DC:H2''	2:N:-31:DT:H5'	2.00	0.44
4:C:253:PHE:CE2	4:C:287:VAL:HG12	2.52	0.44
4:C:1065:LYS:HE2	4:C:1234:LEU:HD12	1.98	0.43
7:F:108:GLY:HA2	7:F:393:ARG:HH12	1.83	0.43
7:F:444:ARG:HH11	7:F:444:ARG:HG3	1.83	0.43
4:C:245:ARG:HD3	4:C:337:PHE:HE2	1.83	0.43
5:D:203:GLU:O	5:D:207:THR:HG22	2.18	0.43
5:D:822:MET:HE1	5:D:838:LEU:C	2.43	0.43
5:D:385:LEU:HD23	5:D:390:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:261:LEU:HB3	3:G:307:VAL:HG11	2.01	0.43
4:C:445:ILE:HG23	4:C:446:ASP:OD1	2.18	0.43
5:D:923:ILE:O	5:D:1240:TYR:OH	2.33	0.43
3:A:181:VAL:HA	3:A:208:THR:HG22	2.00	0.43
3:B:23:HIS:HD2	3:B:207:GLU:OE1	2.00	0.43
7:F:580:THR:HG22	7:F:583:GLU:OE2	2.18	0.43
4:C:221:LEU:HD11	4:C:314:ASN:HB2	2.00	0.43
7:F:470:LYS:HG3	7:F:474:ILE:HD12	2.01	0.43
4:C:648:GLU:H	4:C:648:GLU:CD	2.26	0.43
4:C:964:PHE:HA	4:C:967:LEU:HG	2.00	0.43
4:C:971:LEU:O	4:C:975:VAL:HG23	2.18	0.43
6:E:63:VAL:HG12	6:E:67:ARG:HH21	1.84	0.43
5:D:143:MET:HG3	5:D:159:MET:HE3	2.00	0.43
5:D:215:LYS:O	5:D:218:THR:HG22	2.18	0.43
5:D:368:LEU:HD23	5:D:373:ALA:HB2	2.01	0.43
6:E:5:THR:O	6:E:7:GLN:N	2.51	0.43
4:C:611:GLU:OE2	4:C:637:ARG:NH2	2.52	0.43
4:C:733:VAL:HG11	4:C:966:ILE:HG21	2.00	0.43
4:C:1181:VAL:HG11	4:C:1197:MET:HE1	2.01	0.43
4:C:1245:ARG:NH1	4:C:1264:PHE:O	2.50	0.43
5:D:475:GLU:CD	6:E:28:ARG:HH12	2.26	0.43
1:T:27:DT:H2''	1:T:28:DA:C8	2.53	0.43
4:C:733:VAL:HG21	4:C:966:ILE:HD13	2.01	0.43
1:T:-10:DC:H2''	1:T:-9:DA:C8	2.53	0.43
2:N:-8:DA:H4'	2:N:-7:DA:OP1	2.19	0.43
2:N:4:DG:H2''	2:N:5:DA:C8	2.54	0.43
4:C:50:GLU:O	4:C:54:ARG:HG3	2.18	0.43
4:C:466:VAL:O	4:C:470:ARG:HG3	2.19	0.43
4:C:629:PHE:HB2	4:C:647:ARG:HG3	2.00	0.43
4:C:638:GLN:HG2	4:C:639:LYS:HG3	2.01	0.43
4:C:1151:LEU:HD11	4:C:1200:LEU:HD12	2.01	0.43
7:F:127:ASP:OD1	7:F:127:ASP:C	2.62	0.43
4:C:1033:ARG:HB3	4:C:1033:ARG:CZ	2.49	0.42
6:E:7:GLN:O	6:E:10:VAL:HG22	2.18	0.42
3:A:51:MET:HB3	3:A:51:MET:HE3	1.76	0.42
7:F:273:GLN:O	7:F:277:LEU:HG	2.19	0.42
3:G:285:ARG:NE	3:G:289:GLU:OE1	2.43	0.42
4:C:1252:LEU:HD21	5:D:253:VAL:HG11	2.00	0.42
4:C:916:THR:O	4:C:916:THR:OG1	2.29	0.42
5:D:422:LEU:O	5:D:468:VAL:HA	2.19	0.42
5:D:925:GLU:HB3	5:D:926:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:404:LYS:HE3	4:C:404:LYS:HB3	1.85	0.42
5:D:825:HIS:CE1	5:D:827:GLU:CG	3.03	0.42
7:F:601:LYS:HA	7:F:604:ARG:NH1	2.34	0.42
4:C:1258:LEU:HD11	7:F:532:GLU:HG2	2.01	0.42
5:D:245:LEU:HG	5:D:246:PRO:HD2	2.01	0.42
5:D:511:TYR:O	5:D:515:ARG:HG2	2.20	0.42
7:F:338:VAL:HA	7:F:341:GLN:OE1	2.20	0.42
7:F:583:GLU:HA	7:F:586:LYS:HE2	2.00	0.42
2:N:-28:DT:H2''	2:N:-27:DA:H8	1.83	0.42
4:C:1166:GLU:H	4:C:1166:GLU:CD	2.20	0.42
5:D:611:LYS:HE3	5:D:611:LYS:HB3	1.70	0.42
7:F:478:MET:O	7:F:482:MET:HG2	2.18	0.42
3:G:318:ARG:HH12	3:G:320:GLU:HG2	1.85	0.42
4:C:230:PHE:CZ	4:C:239:MET:HE2	2.55	0.42
4:C:820:GLU:O	4:C:824:GLN:HG3	2.20	0.42
3:B:47:LEU:HB3	3:B:181:VAL:HG21	2.01	0.42
3:B:137:ASP:OD1	3:B:137:ASP:N	2.52	0.42
7:F:139:TYR:CZ	7:F:281:LEU:HD13	2.55	0.42
7:F:328:LEU:HD23	7:F:339:ARG:HG2	2.02	0.42
7:F:594:ARG:HA	7:F:597:GLN:NE2	2.35	0.42
4:C:452:ARG:HH22	4:C:458:GLU:CD	2.27	0.42
2:N:-20:DC:H2''	2:N:-19:DT:C6	2.55	0.42
4:C:898:GLU:HB3	7:F:548:LEU:HG	2.02	0.42
7:F:274:PHE:CD1	7:F:274:PHE:C	2.98	0.42
7:F:570:ARG:HG2	7:F:584:VAL:HG21	2.00	0.42
4:C:273:HIS:ND1	4:C:274:ILE:HG12	2.35	0.42
5:D:264:ASP:OD1	5:D:264:ASP:N	2.53	0.42
5:D:639:VAL:HG13	5:D:725:MET:HE1	2.02	0.42
5:D:853:THR:HG22	5:D:855:GLU:H	1.85	0.42
3:G:286:THR:HG22	3:G:316:GLY:HA2	2.01	0.41
3:G:304:ILE:HG22	3:G:315:LEU:HD11	2.02	0.41
4:C:101:ARG:HA	4:C:118:LYS:O	2.20	0.41
4:C:972:LEU:HD13	4:C:994:ARG:HH12	1.85	0.41
5:D:364:HIS:HB2	5:D:485:MET:HE3	2.02	0.41
5:D:505:ASP:HB2	5:D:629:PHE:HE1	1.85	0.41
3:A:31:LEU:O	3:A:200:ASP:N	2.48	0.41
7:F:431:ARG:HB3	7:F:433:TYR:HD2	1.85	0.41
7:F:460:ILE:HG22	7:F:464:MET:HB3	2.01	0.41
7:F:504:LYS:O	7:F:508:ILE:HG23	2.20	0.41
1:T:4:DG:H4'	7:F:519:ILE:HD12	2.02	0.41
4:C:203:LYS:HE3	4:C:203:LYS:HB3	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:225:PHE:CE2	4:C:347:MET:HB3	2.55	0.41
4:C:448:LEU:HD23	4:C:448:LEU:HA	1.87	0.41
4:C:498:ILE:H	4:C:498:ILE:HG13	1.68	0.41
1:T:37:DT:H2"	1:T:38:DA:H8	1.84	0.41
2:N:-11:DT:OP2	7:F:438:TYR:OH	2.27	0.41
5:D:786:THR:HA	5:D:789:LYS:HG2	2.01	0.41
5:D:912:GLY:O	5:D:1359:GLY:N	2.53	0.41
4:C:468:LEU:HD23	4:C:468:LEU:HA	1.84	0.41
4:C:722:GLY:HA2	4:C:737:ASN:OD1	2.20	0.41
5:D:423:LEU:HD23	5:D:423:LEU:HA	1.90	0.41
4:C:615:VAL:HG22	4:C:638:GLN:HB2	2.03	0.41
5:D:268:LEU:HD13	5:D:306:LEU:HA	2.02	0.41
5:D:1318:PHE:CE1	5:D:1341:ASP:HB2	2.55	0.41
3:B:115:ASP:OD1	3:B:115:ASP:N	2.53	0.41
4:C:1021:LEU:HD23	4:C:1021:LEU:HA	1.93	0.41
1:T:-5:DT:H5"	5:D:1326:GLU:HG2	2.03	0.41
4:C:265:LYS:HE3	4:C:265:LYS:HB3	1.84	0.41
4:C:759:SER:HG	4:C:763:THR:HG1	1.55	0.41
5:D:822:MET:HB3	5:D:822:MET:HE3	1.68	0.41
5:D:951:GLN:HE21	5:D:1014:GLY:HA2	1.85	0.41
5:D:1138:LEU:HB3	5:D:1139:PRO:HD3	2.01	0.41
6:E:5:THR:O	6:E:5:THR:OG1	2.34	0.41
3:A:85:LEU:HD11	3:A:143:MET:HE1	2.03	0.41
7:F:501:LYS:HE3	7:F:501:LYS:HB2	1.76	0.41
5:D:152:THR:HG23	5:D:172:TRP:CE2	2.56	0.41
3:A:13:LEU:HD21	3:A:16:ILE:HD11	2.03	0.41
3:B:47:LEU:HA	3:B:51:MET:HG3	2.03	0.41
7:F:508:ILE:HA	7:F:510:LYS:NZ	2.36	0.41
4:C:230:PHE:HE2	4:C:287:VAL:HG21	1.86	0.41
4:C:299:LYS:NZ	4:C:334:GLU:OE2	2.53	0.41
4:C:436:ARG:HD2	4:C:436:ARG:C	2.46	0.41
5:D:86:GLU:CD	5:D:86:GLU:H	2.28	0.41
5:D:116:PHE:HB3	5:D:237:MET:HE2	2.03	0.41
5:D:1252:ILE:O	5:D:1256:VAL:HG23	2.21	0.41
3:A:205:ASP:OD1	3:A:205:ASP:C	2.63	0.41
3:B:229:LEU:O	3:B:233:VAL:HG23	2.21	0.41
3:G:270:CYS:SG	3:G:295:ASN:HB3	2.60	0.41
3:G:285:ARG:HD2	3:G:285:ARG:HA	1.76	0.41
4:C:195:TYR:HD2	4:C:203:LYS:HD2	1.86	0.41
5:D:246:PRO:HA	5:D:247:PRO:HD3	1.97	0.41
5:D:848:ILE:HD12	5:D:858:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:39:DA:H2''	1:T:40:DA:C8	2.56	0.40
4:C:178:PRO:HG3	4:C:395:TYR:CE1	2.56	0.40
4:C:309:LEU:HD23	4:C:312:THR:HG22	2.02	0.40
4:C:359:ARG:HH11	4:C:359:ARG:HG2	1.86	0.40
5:D:606:ASN:O	5:D:610:ARG:HG2	2.21	0.40
6:E:51:LEU:HD23	6:E:51:LEU:HA	1.93	0.40
3:A:171:ARG:HE	3:A:171:ARG:HB2	1.79	0.40
5:D:362:ARG:HG3	5:D:362:ARG:NH1	2.36	0.40
5:D:997:LEU:HD23	5:D:997:LEU:HA	1.87	0.40
7:F:274:PHE:C	7:F:274:PHE:HD1	2.30	0.40
7:F:391:ASN:HB2	7:F:420:LEU:HD21	2.03	0.40
3:G:287:GLU:HA	3:G:290:LEU:HB2	2.03	0.40
5:D:1260:LEU:O	5:D:1303:ARG:NH2	2.51	0.40
4:C:699:LEU:HD23	4:C:699:LEU:HA	1.89	0.40
5:D:364:HIS:HB3	5:D:487:THR:HG23	2.03	0.40
3:A:126:ASN:OD1	3:A:126:ASN:N	2.54	0.40
3:A:149:ARG:HG2	3:B:5:VAL:HG11	2.04	0.40
7:F:113:LEU:HD22	7:F:117:GLY:HA3	2.03	0.40
1:T:5:DT:OP2	1:T:5:DT:H6	2.05	0.40
1:T:40:DA:H2''	1:T:41:DA:C8	2.56	0.40
4:C:194:LEU:HD12	4:C:194:LEU:HA	1.88	0.40
4:C:245:ARG:CD	4:C:337:PHE:HE2	2.35	0.40
4:C:300:ASP:HB3	4:C:309:LEU:HD11	2.04	0.40
4:C:405:PHE:O	4:C:409:ILE:HG12	2.22	0.40
4:C:1032:LYS:HE2	4:C:1032:LYS:HB2	1.85	0.40
5:D:499:ILE:HD12	5:D:499:ILE:HA	1.96	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	
3	A	228/330 (69%)	223 (98%)	5 (2%)	0	100	100
3	B	218/330 (66%)	217 (100%)	1 (0%)	0	100	100
3	G	67/330 (20%)	58 (87%)	8 (12%)	1 (2%)	8	35
4	C	1323/1341 (99%)	1297 (98%)	26 (2%)	0	100	100
5	D	1195/1401 (85%)	1180 (99%)	15 (1%)	0	100	100
6	E	79/90 (88%)	76 (96%)	3 (4%)	0	100	100
7	F	462/621 (74%)	459 (99%)	3 (1%)	0	100	100
All	All	3572/4443 (80%)	3510 (98%)	61 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	278	TYR

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	
3	A	196/283 (69%)	192 (98%)	4 (2%)	48	76
3	B	186/283 (66%)	181 (97%)	5 (3%)	39	71
3	G	61/283 (22%)	56 (92%)	5 (8%)	10	37
4	C	1135/1144 (99%)	1126 (99%)	9 (1%)	73	86
5	D	1015/1168 (87%)	1003 (99%)	12 (1%)	63	82
6	E	65/74 (88%)	65 (100%)	0	100	100
7	F	417/544 (77%)	413 (99%)	4 (1%)	68	84
All	All	3075/3779 (81%)	3036 (99%)	39 (1%)	59	81

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	261	LEU

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Mol	Chain	Res	Type
3	G	263	LEU
3	G	272	LYS
3	G	279	ILE
3	G	314	SER
4	C	326	SER
4	C	366	ILE
4	C	388	LEU
4	C	417	GLN
4	C	609	ILE
4	C	811	ASN
4	C	946	LEU
4	C	984	TYR
4	C	1000	GLN
5	D	78	LEU
5	D	197	GLU
5	D	421	VAL
5	D	581	GLN
5	D	688	SER
5	D	781	LYS
5	D	865	ASP
5	D	1003	LEU
5	D	1011	VAL
5	D	1159	HIS
5	D	1238	GLU
5	D	1323	SER
3	A	14	VAL
3	A	79	LEU
3	A	99	VAL
3	A	179	SER
3	B	49	SER
3	B	90	VAL
3	B	111	VAL
3	B	199	LEU
3	B	200	ASP
7	F	525	SER
7	F	540	LEU
7	F	599	GLU
7	F	610	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	808	ASN
4	C	824	GLN
4	C	894	GLN
4	C	1208	GLN
4	C	1323	ASN
5	D	277	ASN
5	D	465	GLN
5	D	469	HIS
5	D	606	ASN
5	D	720	ASN
5	D	739	GLN
5	D	825	HIS
5	D	875	ASN
5	D	910	ASN
5	D	911	GLN
5	D	1258	GLN
6	E	72	GLN
3	A	66	HIS
3	B	23	HIS
3	B	37	HIS
3	B	118	HIS
3	B	133	HIS
7	F	154	GLN
7	F	251	HIS
7	F	353	GLN
7	F	463	HIS
7	F	597	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

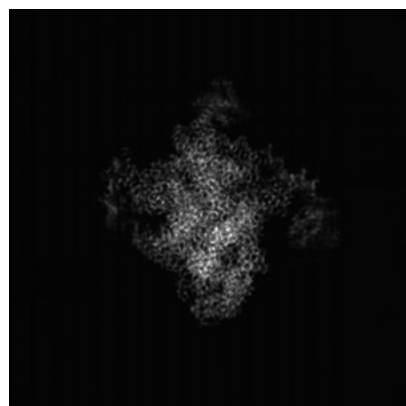
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51273. These allow visual inspection of the internal detail of the map and identification of artifacts.

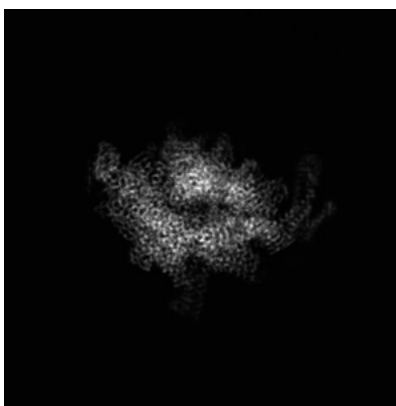
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

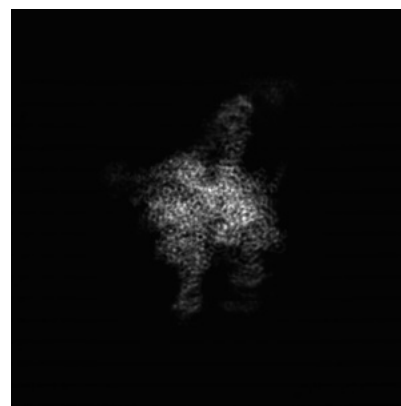
6.1.1 Primary map



X

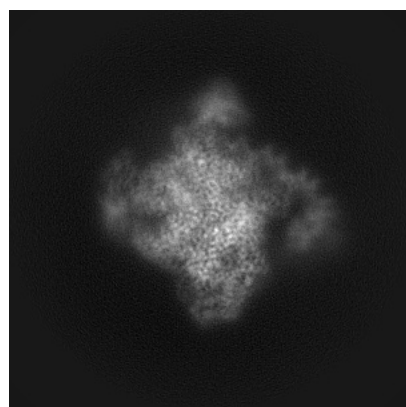


Y

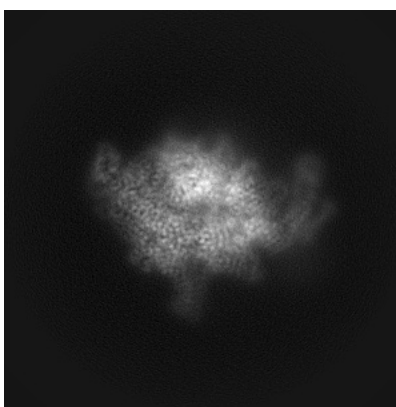


Z

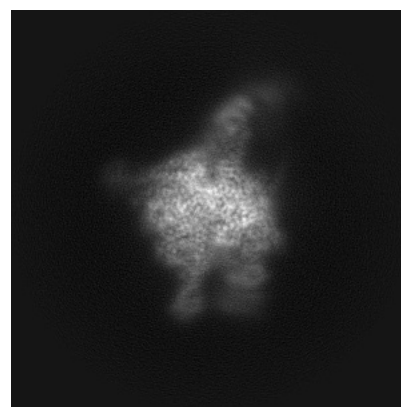
6.1.2 Raw map



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: 180

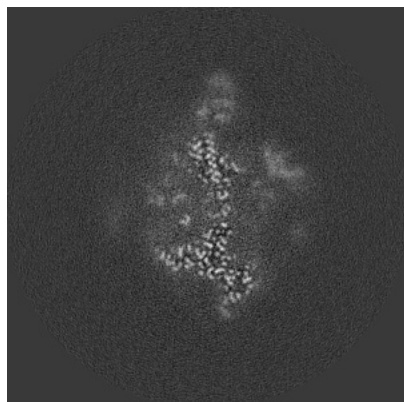


Y Index: 180

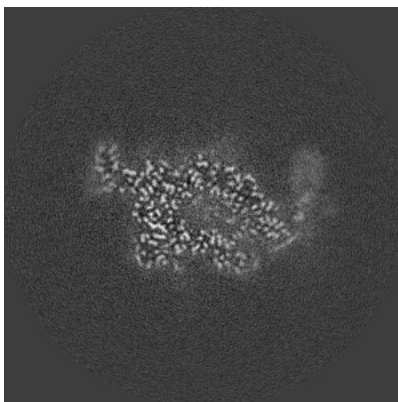


Z Index: 180

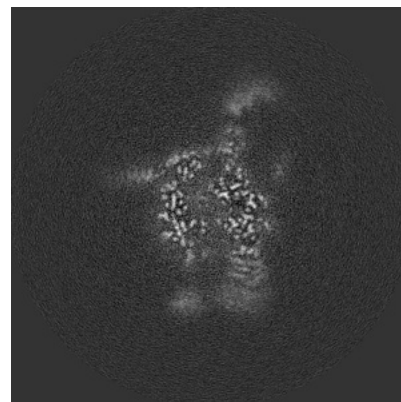
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

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: 199

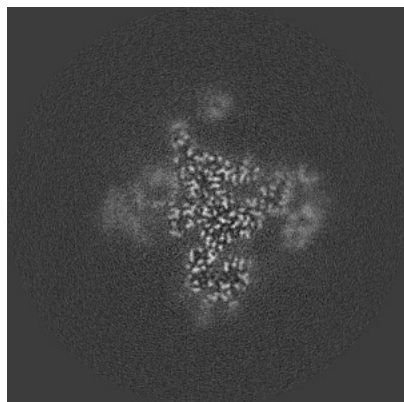


Y Index: 182

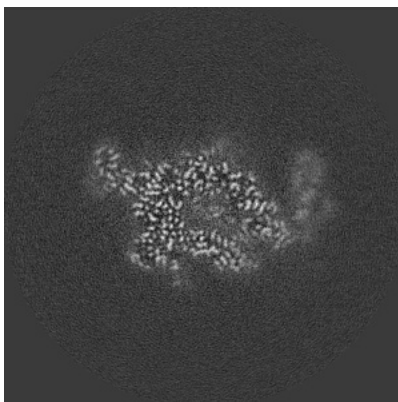


Z Index: 156

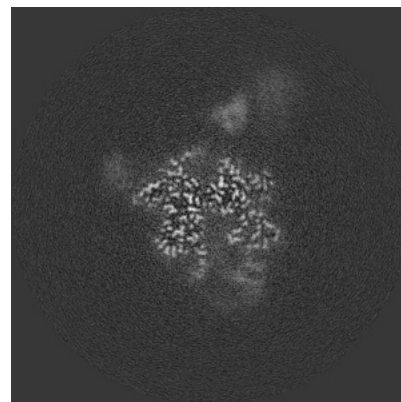
6.3.2 Raw map



X Index: 198



Y Index: 182

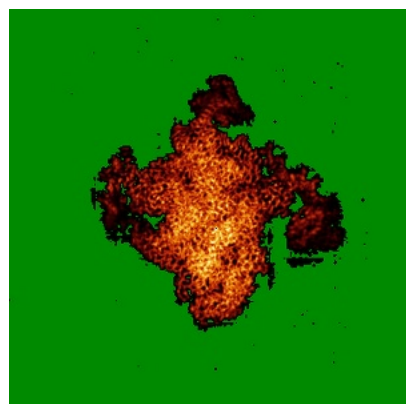


Z Index: 156

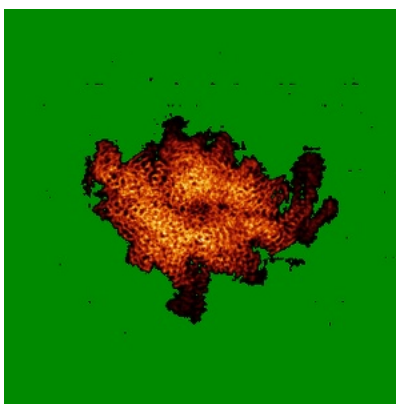
The images above show the largest variance slices of the map in three orthogonal directions.

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

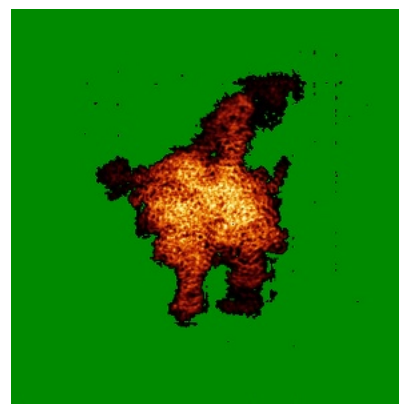
6.4.1 Primary map



X

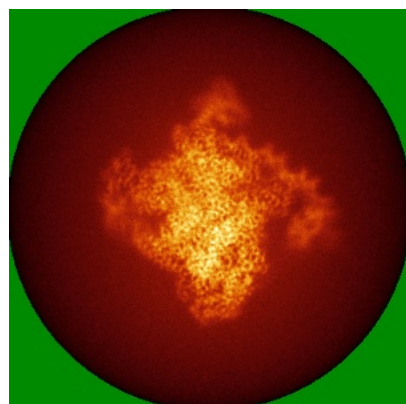


Y

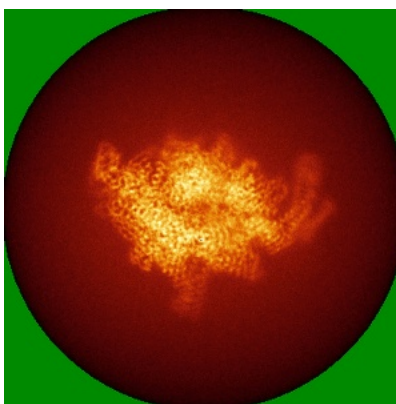


Z

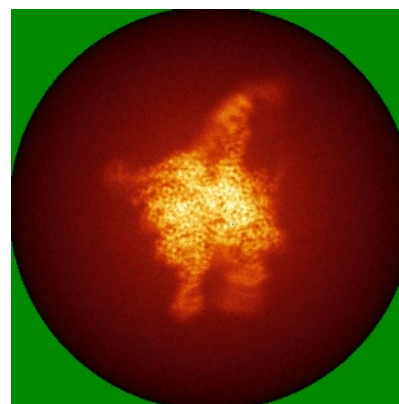
6.4.2 Raw map



X



Y

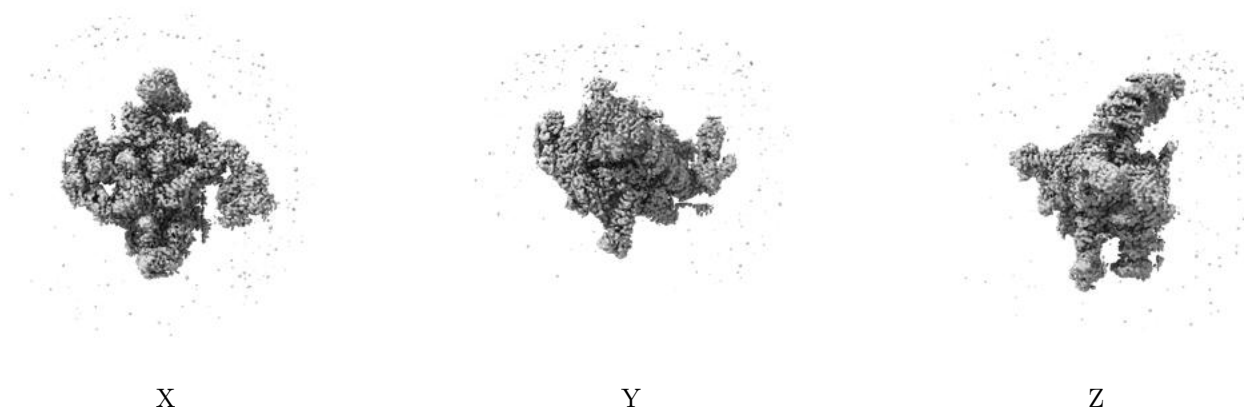


Z

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.

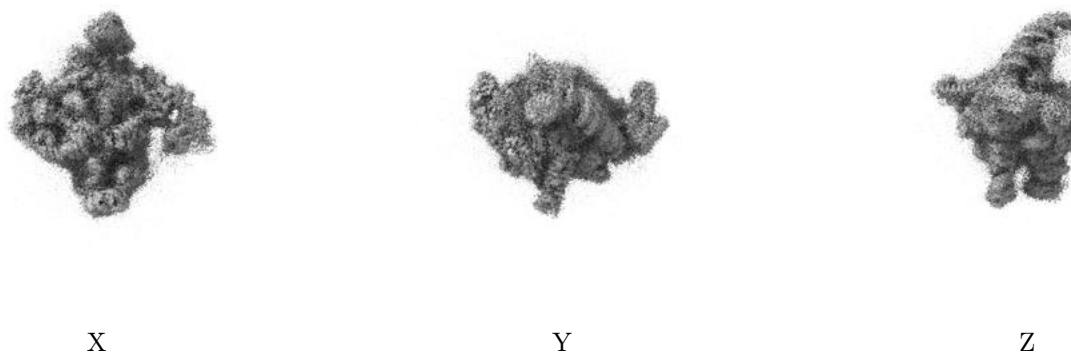
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00455. 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.

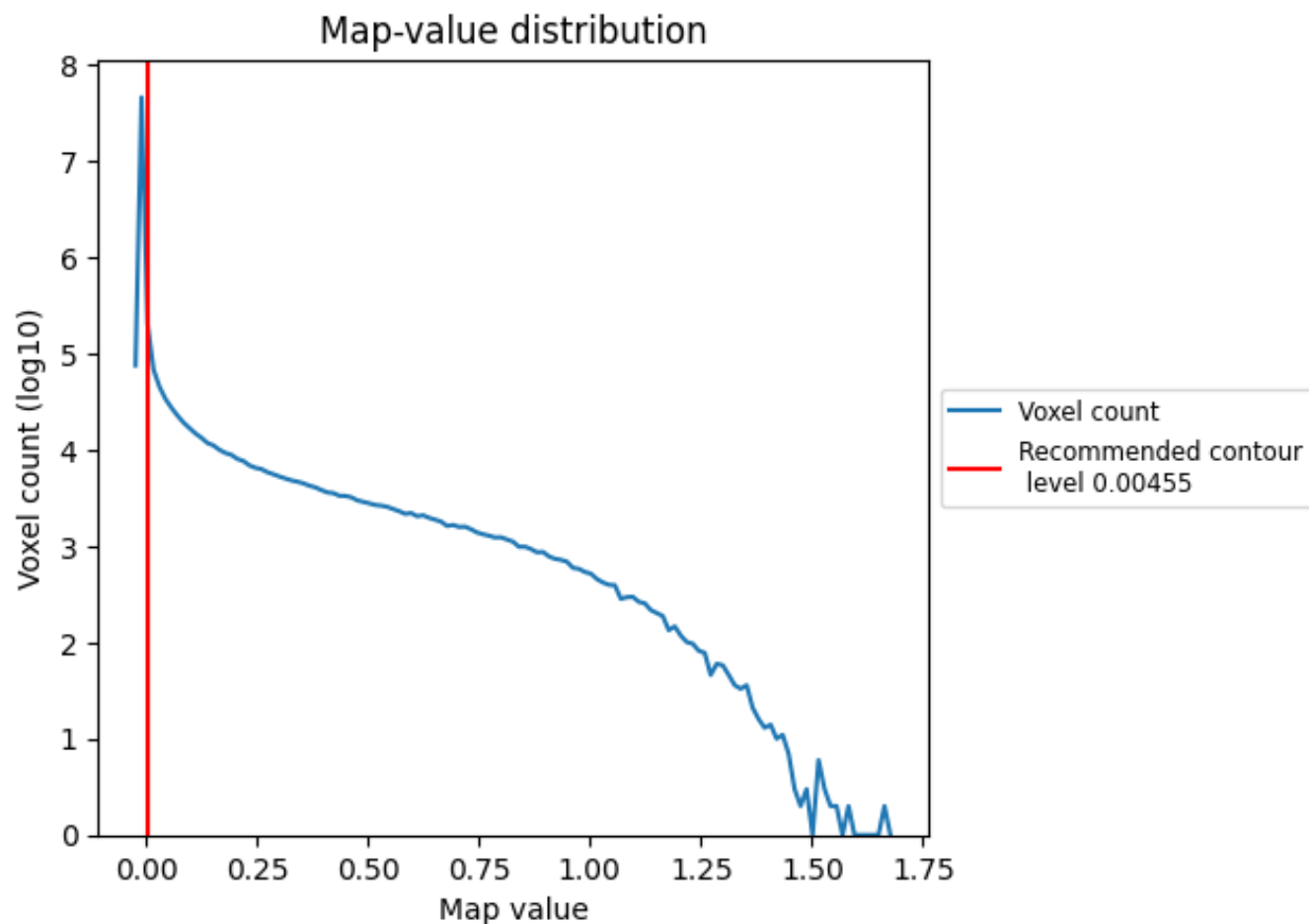
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

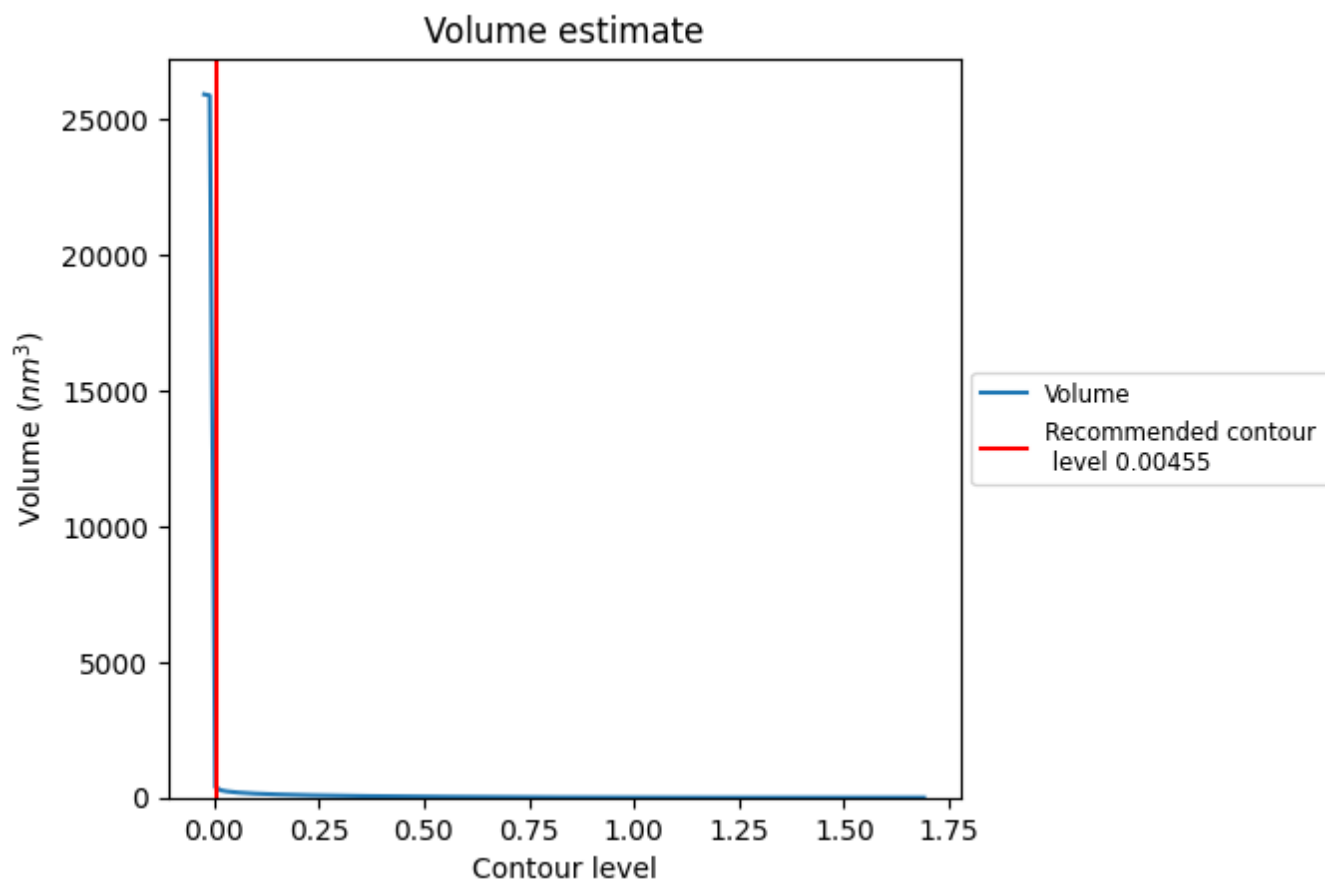
This section contains the results of statistical analysis of the map.

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.

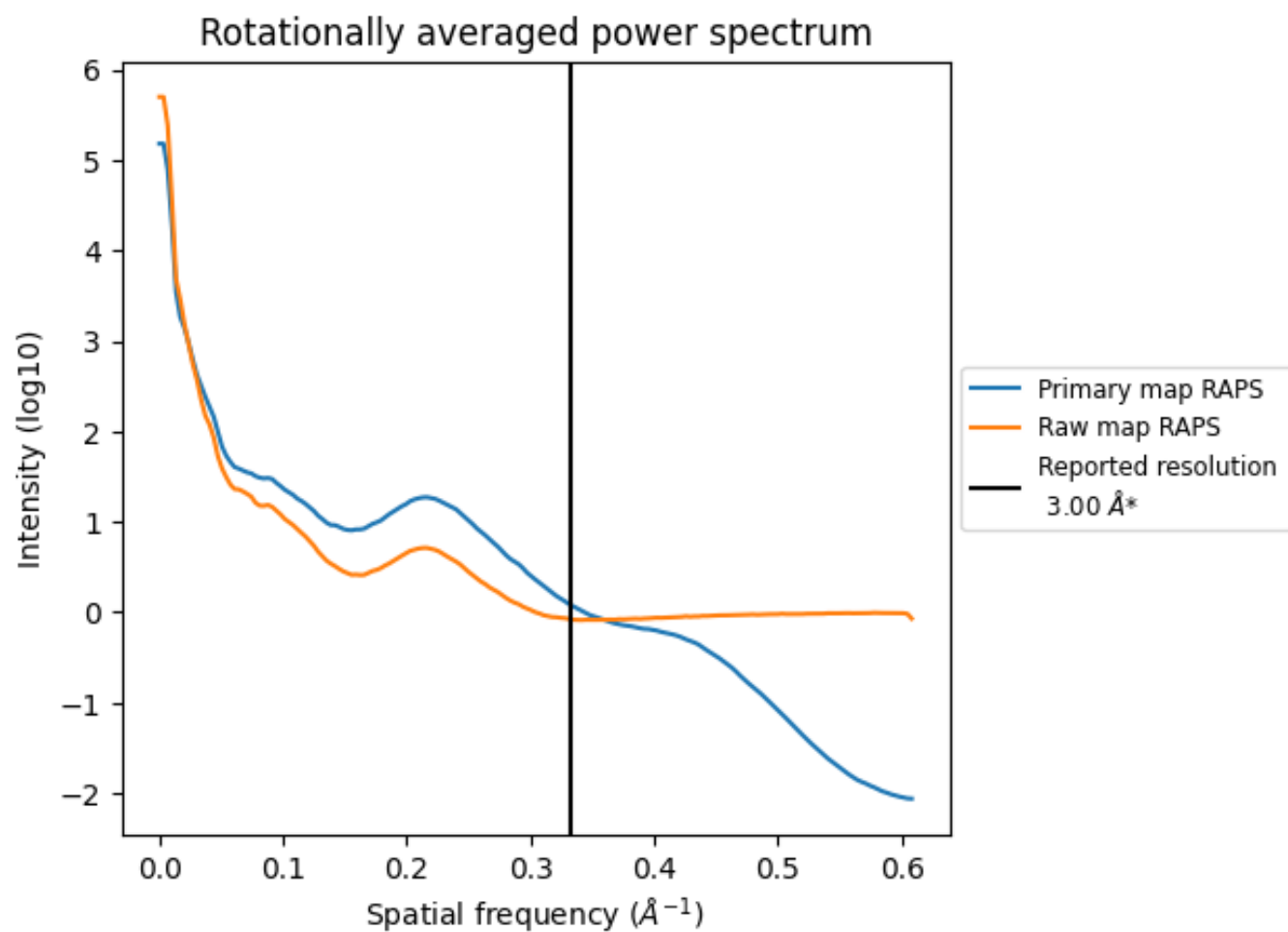
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 376 nm³; this corresponds to an approximate mass of 340 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 ⓘ

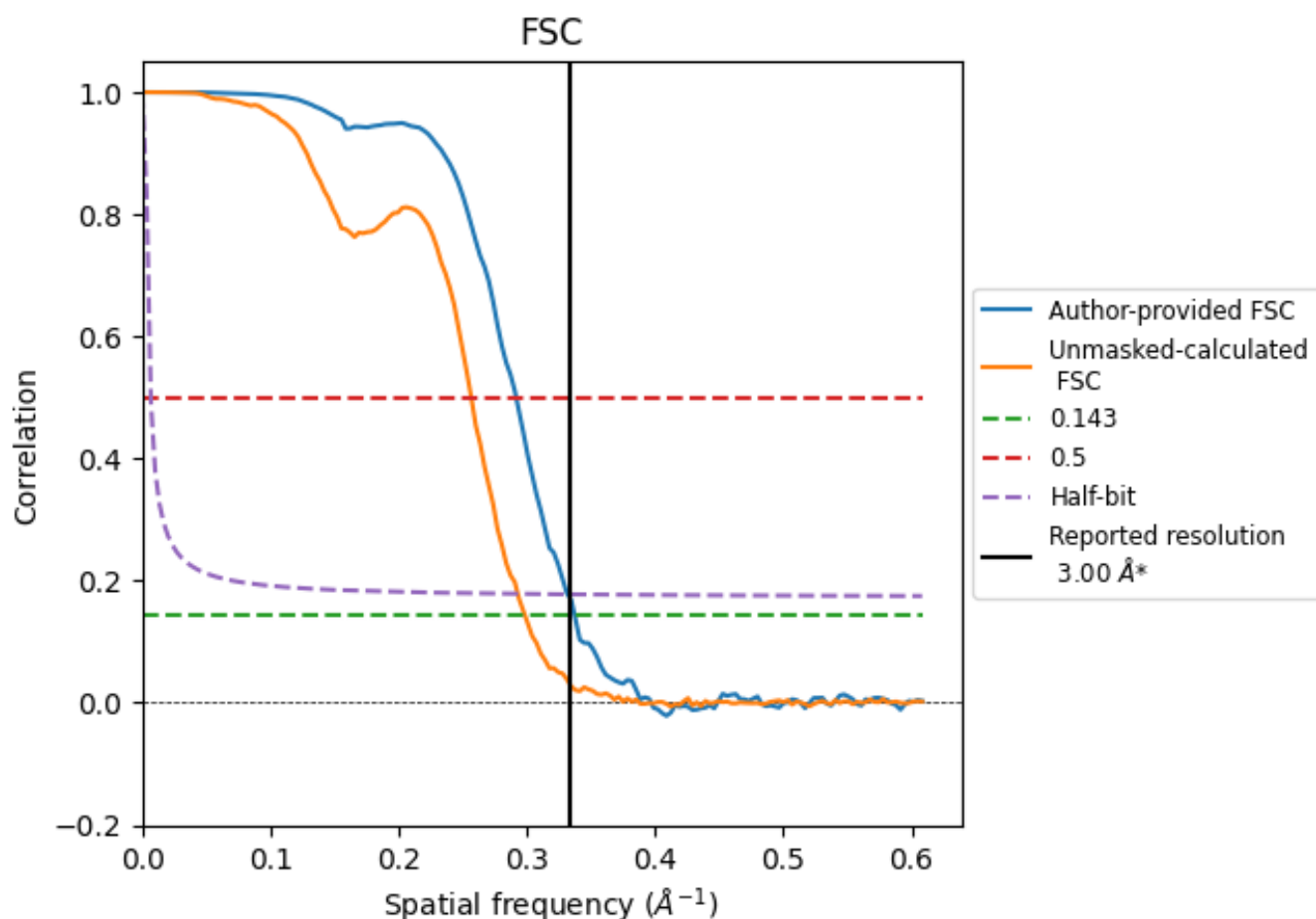


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.96	3.43	3.01
Unmasked-calculated*	3.35	3.90	3.41

*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 3.35 differs from the reported value 3.0 by more than 10 %

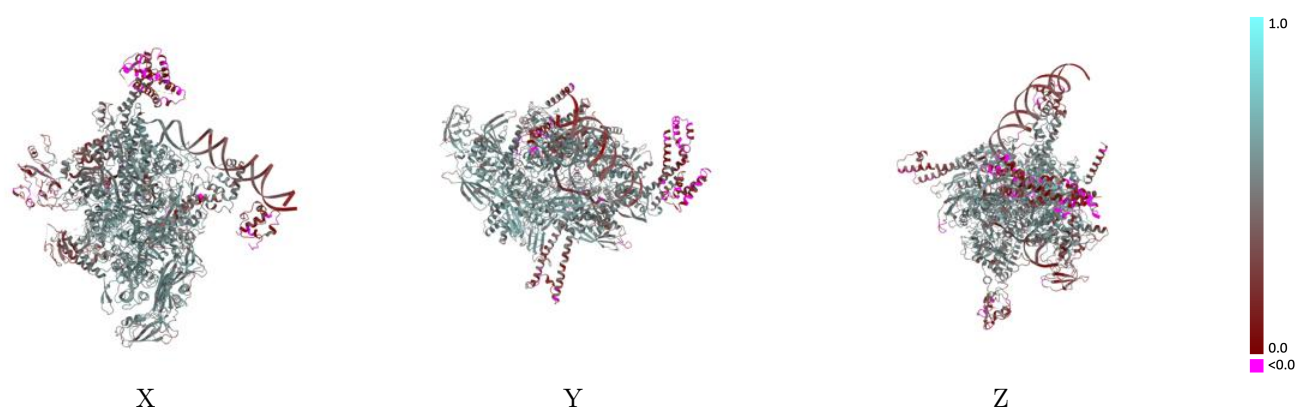
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51273 and PDB model 9GDO. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)

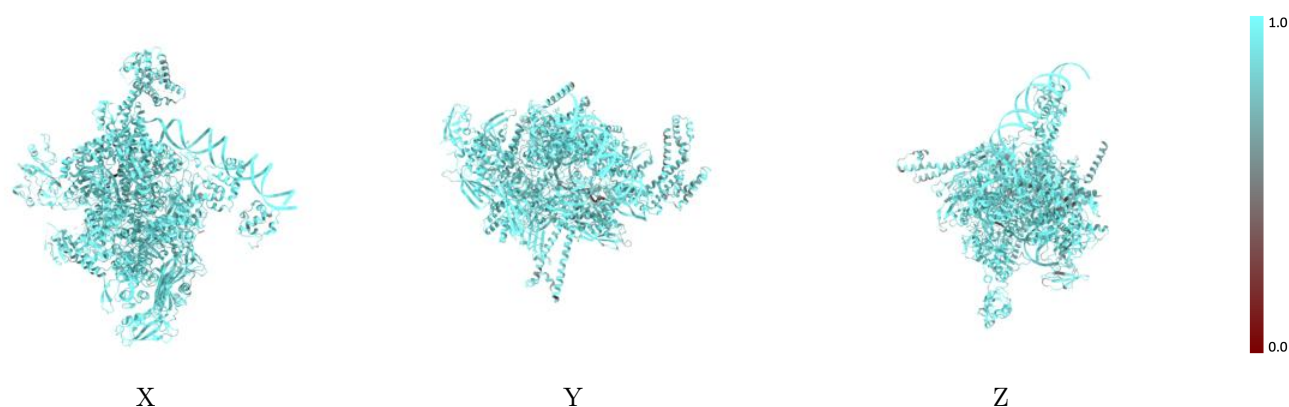
This section was not generated.

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



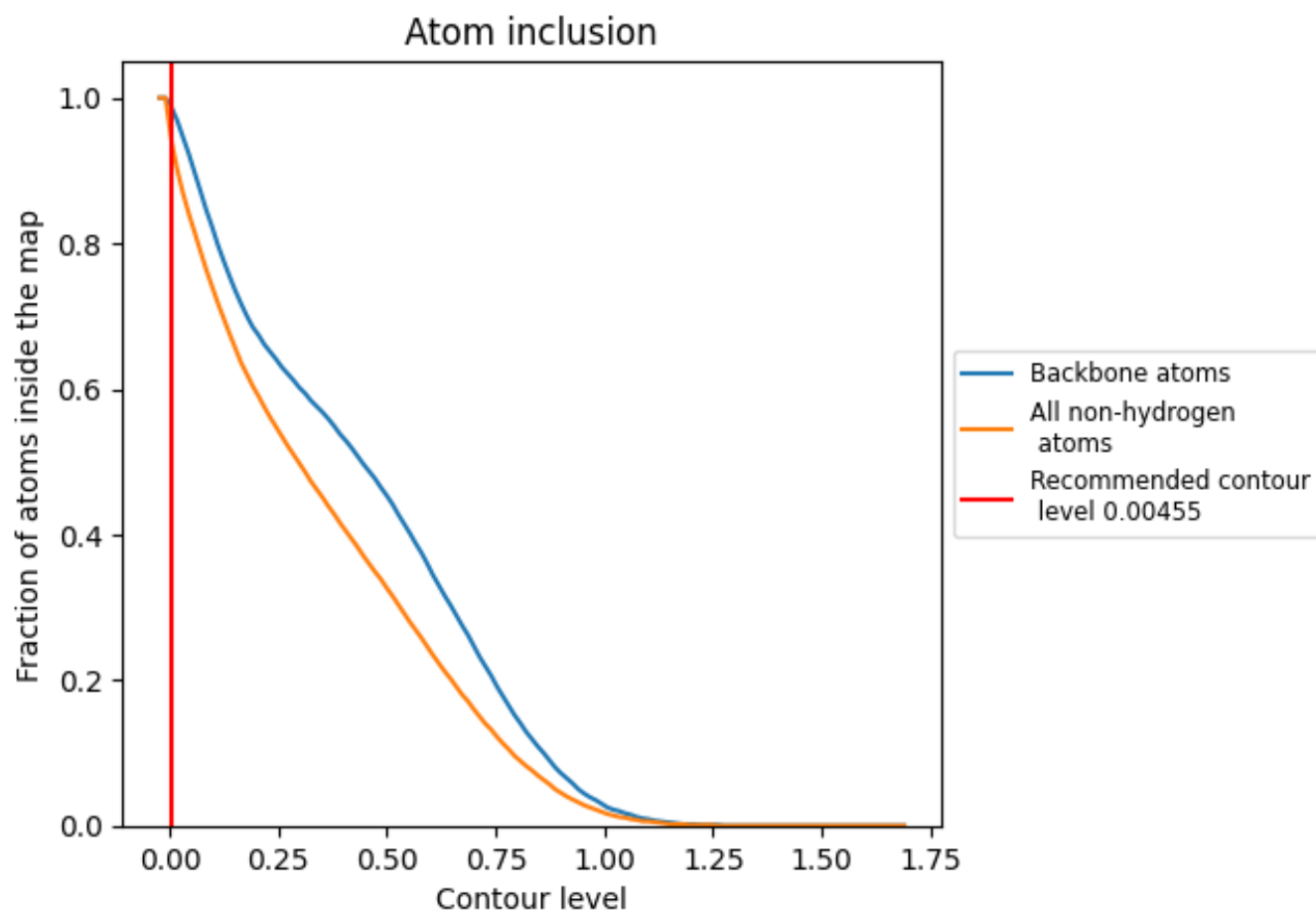
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00455).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (0.00455) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9380	<div><div></div></div> 0.4740
A	<div><div></div></div> 0.9510	<div><div></div></div> 0.5440
B	<div><div></div></div> 0.9500	<div><div></div></div> 0.5130
C	<div><div></div></div> 0.9480	<div><div></div></div> 0.5090
D	<div><div></div></div> 0.9550	<div><div></div></div> 0.5180
E	<div><div></div></div> 0.8910	<div><div></div></div> 0.4400
F	<div><div></div></div> 0.8920	<div><div></div></div> 0.3460
G	<div><div></div></div> 0.8630	<div><div></div></div> 0.1300
N	<div><div></div></div> 0.8960	<div><div></div></div> 0.3640
T	<div><div></div></div> 0.9350	<div><div></div></div> 0.3540

1.0

0.0

<0.0