Full wwPDB EM Validation Report ⓘ

Jun 8, 2024 – 01:36 PM EDT

PDB ID	:	8EJ3
EMDB ID	:	EMD-28174
Title	:	M. tuberculosis RNAP pause escaped complex with Bacillus subtilis NusG and GMPCPP
Authors	:	Vishwakarma, R.K.; Murakami, K.S.
Deposited on	:	2022-09-16
Resolution	:	3.13 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:

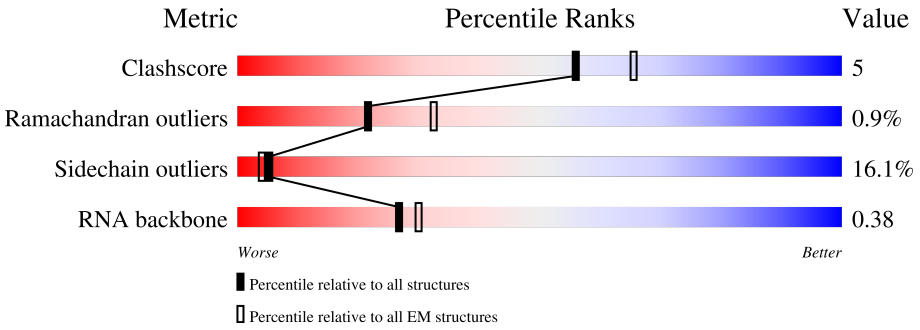
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.13 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	347	44% 18% • 35%
1	B	347	48% 18% • 32%
2	C	1178	71% 21% • 5%
3	D	1316	77% 19% • •
4	E	110	66% 8% • 25%
5	G	177	34% 24% • • 38%
6	N	40	52% 20% 28%

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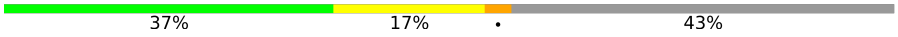
Mol	Chain	Length	Quality of chain
7	R	30	
8	T	40	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 25339 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	226	Total	C	N	O	S	0	0
			1724	1085	297	339	3		
1	B	237	Total	C	N	O	S	0	0
			1765	1115	301	346	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1121	Total	C	N	O	S	0	0
			8672	5423	1527	1683	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1281	Total	C	N	O	S	0	0
			10010	6264	1822	1883	41		

- 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 Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	110	Total	C	N	O	S	1	0
			878	563	147	165	3		

- Molecule 6 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	29	Total	C	N	O	P	0	0
			587	279	99	180	29		

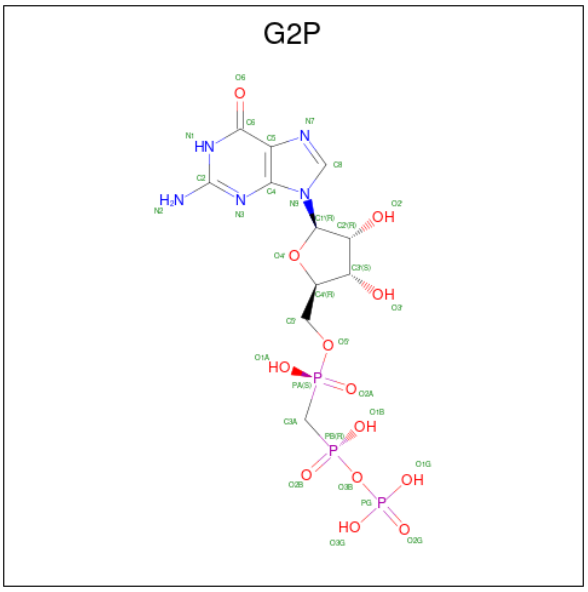
- Molecule 7 is a RNA chain called RNA (5'-R(P*UP*CP*GP*GP*CP*AP*GP*GP*AP*GP *AP*GP*GP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	17	Total	C	N	O	P	0	0
			369	164	70	118	17		

- Molecule 8 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	32	Total	C	N	O	P	0	0
			649	307	119	191	32		

- Molecule 9 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	C	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Mg	0
			2	2	

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

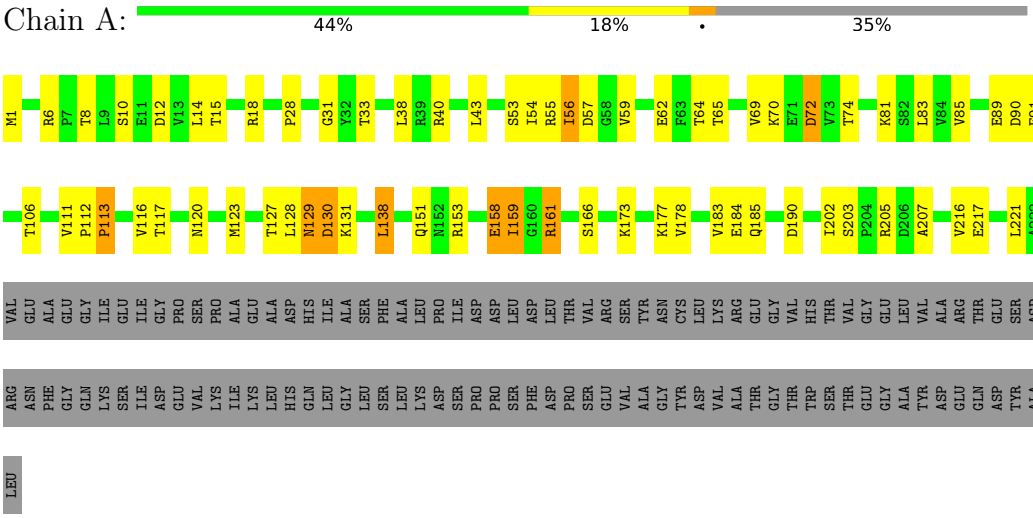
Mol	Chain	Residues	Atoms		AltConf
11	D	2	Total	Zn	0
			2	2	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

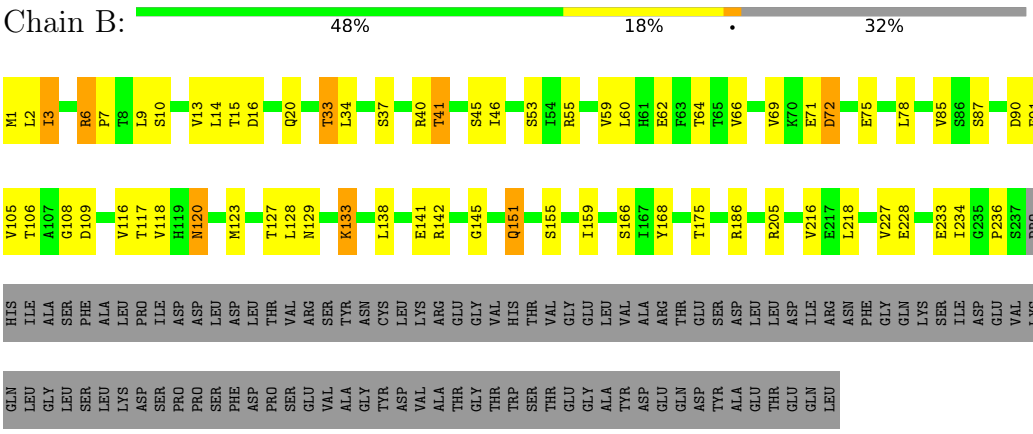
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



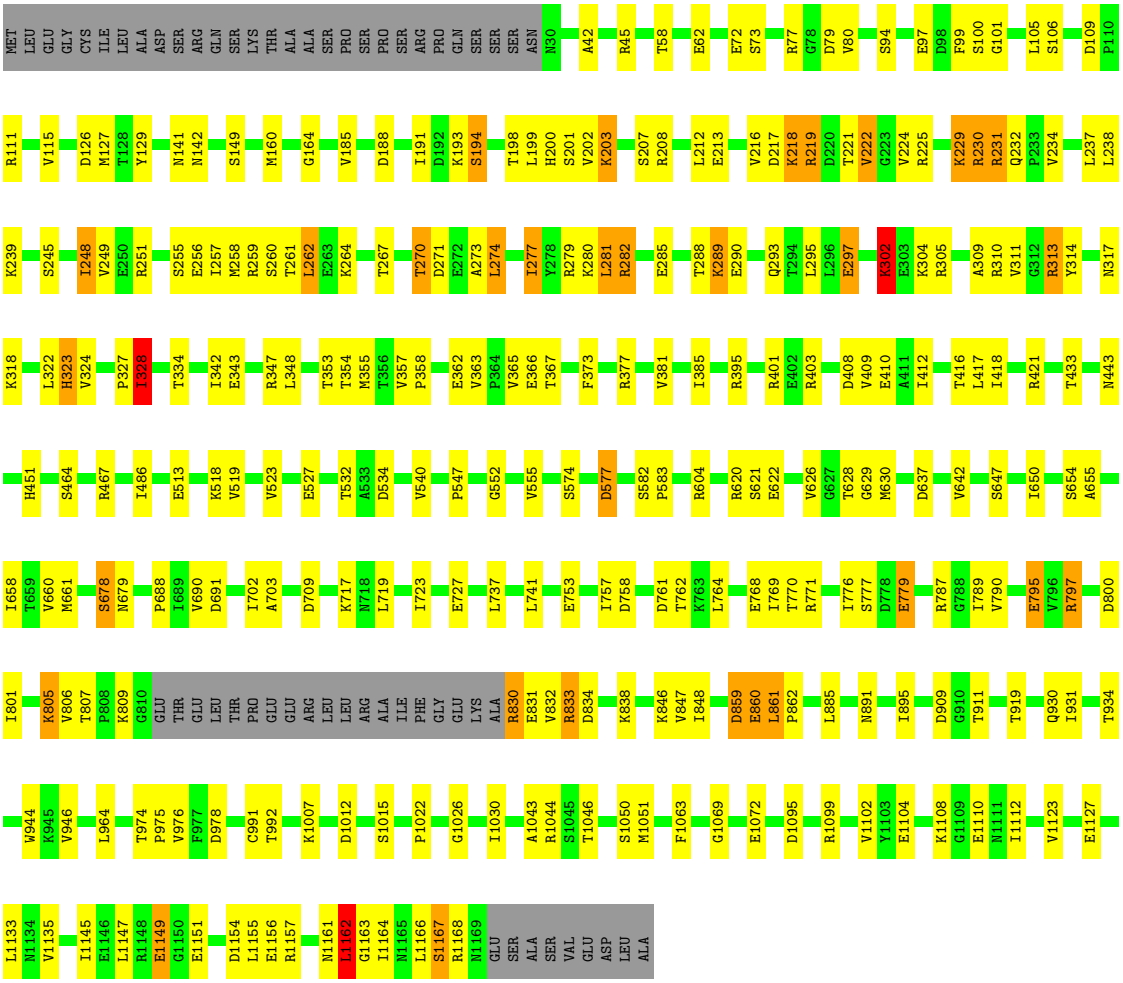
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



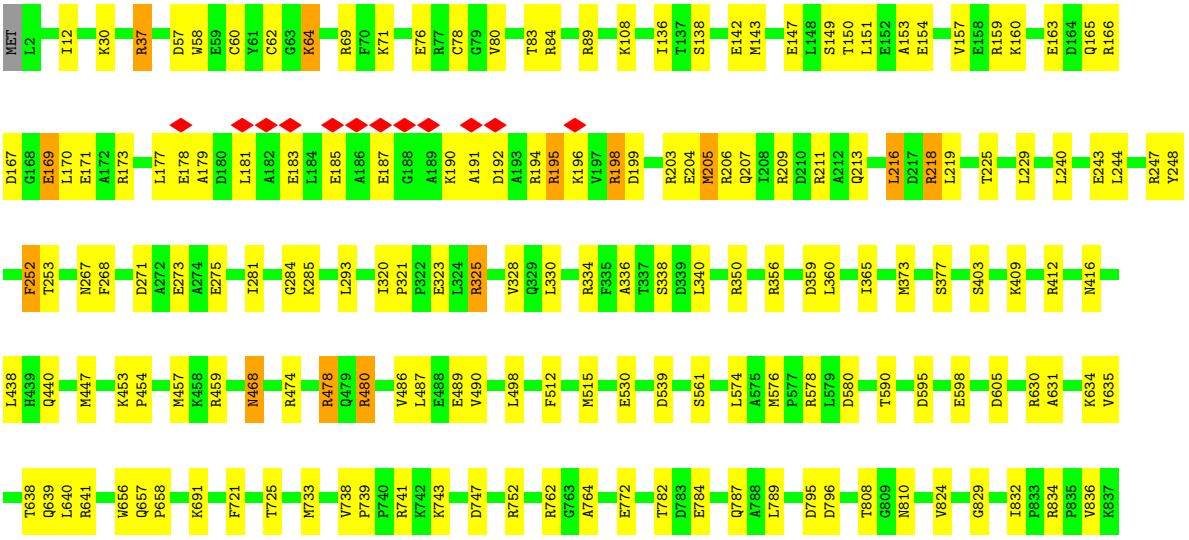
• Molecule 2: DNA-directed RNA polymerase subunit beta

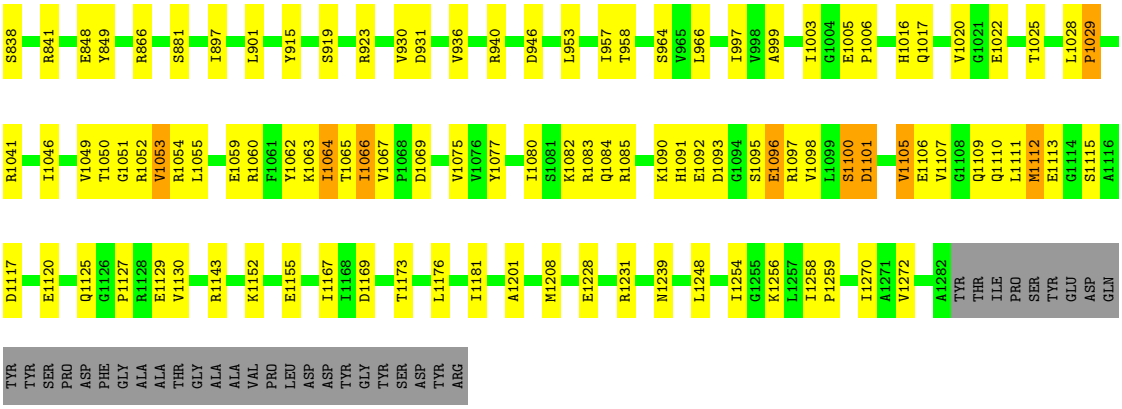
Chain C:



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

Chain D:



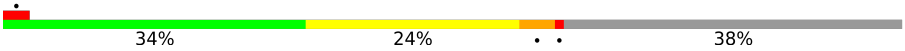


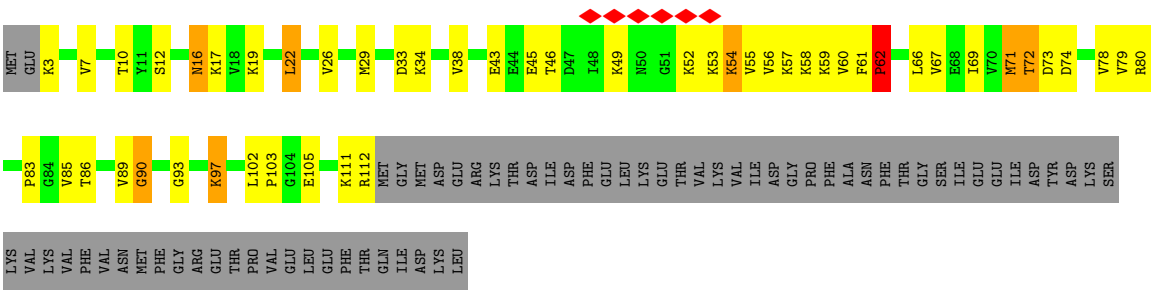
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:

• Molecule 5: Transcription termination/antitermination protein NusG

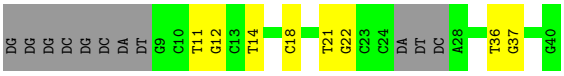
Chain G:





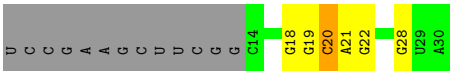
• Molecule 6: DNA (29-MER)

Chain N:



• Molecule 7: RNA (5'-R(P*UP*CP*GP*GP*CP*AP*GP*GP*AP*GP*AP*GP*UP*A)-3')

Chain R:



• Molecule 8: DNA (32-MER)

Chain T:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71839	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.391	Depositor
Minimum map value	-0.765	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.294	Depositor
Map size (Å)	348.0, 348.0, 348.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, G2P

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	0.26	0/1750	0.53	0/2380
1	B	0.26	0/1792	0.52	0/2442
2	C	0.27	0/8828	0.52	1/11968 (0.0%)
3	D	0.26	0/10178	0.53	0/13758
4	E	0.27	0/662	0.49	0/901
5	G	0.26	0/896	0.48	0/1209
6	N	0.52	0/653	0.95	0/1002
7	R	0.30	0/413	0.78	0/643
8	T	0.56	0/726	0.89	0/1116
All	All	0.29	0/25898	0.56	1/35419 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	126	ASP	CB-CG-OD1	5.39	123.15	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1724	0	1768	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1765	0	1794	13	0
2	C	8672	0	8595	97	0
3	D	10010	0	10066	113	0
4	E	649	0	645	5	0
5	G	878	0	896	18	0
6	N	587	0	329	5	0
7	R	369	0	185	1	0
8	T	649	0	358	4	0
9	C	32	0	13	0	0
10	D	2	0	0	0	0
11	D	2	0	0	0	0
All	All	25339	0	24649	258	0

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

All (258) 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:195:ARG:HH22	3:D:198:ARG:HH21	1.23	0.84
1:B:120:ASN:H	1:B:120:ASN:HD22	1.26	0.80
3:D:836:VAL:HG12	3:D:848:GLU:HG2	1.66	0.78
2:C:222:VAL:HG23	2:C:261:THR:HG21	1.69	0.74
2:C:1156:GLU:OE1	2:C:1156:GLU:N	2.23	0.72
5:G:86:THR:HG23	6:N:18:DC:H2'	1.72	0.70
3:D:62:CYS:HB3	3:D:78:CYS:SG	2.33	0.69
2:C:282:ARG:HB2	2:C:285:GLU:HG3	1.75	0.69
2:C:930:GLN:HG3	2:C:931:ILE:HD12	1.74	0.69
3:D:1228:GLU:OE1	3:D:1231:ARG:NH2	2.27	0.68
5:G:38:VAL:HG22	5:G:67:VAL:HG13	1.75	0.67
3:D:320:ILE:O	3:D:325:ARG:NH1	2.27	0.67
3:D:1254:ILE:HD11	3:D:1256:LYS:HD3	1.78	0.66
2:C:1046:THR:HG22	2:C:1163:GLY:HA3	1.76	0.66
2:C:723:ILE:HG22	2:C:919:THR:HG22	1.79	0.65
3:D:739:PRO:HG3	3:D:789:LEU:HD13	1.78	0.64
3:D:1167:ILE:HD11	3:D:1181:ILE:HG13	1.80	0.64
3:D:930:VAL:HG12	3:D:936:VAL:HG12	1.79	0.64
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.80	0.63
5:G:22:LEU:HD21	5:G:79:VAL:HG23	1.79	0.62
2:C:518:LYS:NZ	2:C:527:GLU:OE1	2.32	0.62
2:C:42:ALA:HB2	2:C:975:PRO:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1046:THR:HG21	2:C:1162:LEU:HG	1.82	0.60
3:D:356:ARG:HH12	5:G:62:PRO:HD2	1.67	0.60
3:D:136:ILE:HD12	3:D:252:PHE:HE1	1.66	0.60
5:G:10:THR:HA	5:G:85:VAL:HA	1.84	0.60
3:D:165:GLN:O	3:D:169:GLU:HG3	2.02	0.59
3:D:179:ALA:O	3:D:183:GLU:HG2	2.03	0.59
2:C:256:GLU:HG2	2:C:259:ARG:HH21	1.67	0.59
2:C:313:ARG:HG2	2:C:328:ILE:HG22	1.85	0.59
3:D:459:ARG:NH1	3:D:489:GLU:OE2	2.36	0.58
3:D:1091:HIS:H	3:D:1096:GLU:HA	1.70	0.57
2:C:628:THR:HG22	2:C:629:GLY:H	1.69	0.57
3:D:365:ILE:HD11	5:G:90:GLY:HA2	1.86	0.56
3:D:1270:ILE:HD11	4:E:106:HIS:HD2	1.70	0.56
3:D:1125:GLN:HB3	3:D:1129:GLU:HG3	1.88	0.56
2:C:1012:ASP:OD2	2:C:1015:SER:OG	2.24	0.56
2:C:1044:ARG:NH1	2:C:1063:PHE:O	2.38	0.56
3:D:181:LEU:HG	3:D:185:GLU:HB3	1.87	0.56
2:C:293:GLN:NE2	2:C:297:GLU:OE1	2.39	0.56
2:C:464:SER:HB2	2:C:467:ARG:HB3	1.88	0.56
2:C:809:LYS:HG3	2:C:831:GLU:HG2	1.88	0.56
1:B:106:THR:HG23	1:B:108:GLY:H	1.70	0.55
2:C:547:PRO:HB2	2:C:555:VAL:HB	1.87	0.55
1:A:55:ARG:HH21	1:A:161:ARG:NH1	2.04	0.55
3:D:412:ARG:HD3	3:D:416:ASN:HD22	1.71	0.55
5:G:74:ASP:O	5:G:78:VAL:HG23	2.06	0.55
2:C:202:VAL:HG12	2:C:203:LYS:H	1.72	0.55
1:A:64:THR:OG1	1:A:65:THR:N	2.40	0.55
1:A:202:ILE:HD12	1:A:207:ALA:HB2	1.89	0.54
2:C:200:HIS:H	2:C:216:VAL:HG22	1.72	0.54
2:C:218:LYS:HB2	2:C:219:ARG:HH21	1.72	0.54
2:C:909:ASP:OD1	2:C:911:THR:OG1	2.22	0.54
2:C:248:ILE:HG23	2:C:262:LEU:HD11	1.89	0.54
3:D:881:SER:O	3:D:881:SER:OG	2.24	0.54
1:B:3:ILE:HG12	1:B:234:ILE:HG22	1.90	0.54
3:D:360:LEU:HD11	5:G:61:PHE:HE1	1.73	0.54
2:C:97:GLU:O	2:C:401:ARG:NH1	2.40	0.53
3:D:37:ARG:NH2	6:N:14:DT:OP2	2.41	0.53
2:C:1135:VAL:HG22	3:D:12:ILE:HG13	1.89	0.53
3:D:356:ARG:NH1	5:G:62:PRO:HD2	2.24	0.52
2:C:347:ARG:HD2	2:C:355:MET:HB3	1.91	0.52
3:D:440:GLN:HG2	3:D:515:MET:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:897:ILE:HG12	3:D:964:SER:HB2	1.91	0.52
2:C:642:VAL:HB	2:C:703:ALA:HB3	1.92	0.52
2:C:577:ASP:OD1	2:C:577:ASP:N	2.41	0.51
3:D:1025:THR:O	3:D:1029:PRO:HD2	2.09	0.51
2:C:934:THR:HG23	2:C:1026:GLY:HA3	1.92	0.51
3:D:89:ARG:HB3	3:D:323:GLU:HB2	1.92	0.51
2:C:978:ASP:N	2:C:978:ASP:OD1	2.44	0.51
2:C:249:VAL:HG12	2:C:262:LEU:HD13	1.92	0.51
3:D:163:GLU:HA	3:D:166:ARG:HE	1.75	0.51
3:D:454:PRO:HA	3:D:457:MET:HE2	1.92	0.51
2:C:234:VAL:O	2:C:238:LEU:HD12	2.11	0.51
3:D:218:ARG:HH21	3:D:219:LEU:HD13	1.76	0.51
3:D:205:MET:O	3:D:209:ARG:HD3	2.09	0.50
3:D:1005:GLU:HB3	3:D:1006:PRO:HD3	1.93	0.50
2:C:885:LEU:HG	2:C:895:ILE:HD11	1.92	0.50
1:A:113:PRO:HD2	1:A:116:VAL:HB	1.93	0.50
1:B:120:ASN:HD22	1:B:120:ASN:N	2.02	0.50
3:D:159:ARG:HH22	3:D:216:LEU:HB2	1.77	0.50
3:D:204:GLU:O	3:D:207:GLN:HG3	2.12	0.50
3:D:338:SER:O	3:D:340:LEU:N	2.42	0.50
2:C:737:LEU:HG	2:C:741:LEU:HD12	1.93	0.50
3:D:281:ILE:HD13	3:D:293:LEU:HD23	1.93	0.50
2:C:58:THR:O	2:C:62:GLU:HG2	2.11	0.49
2:C:408:ASP:OD1	2:C:408:ASP:N	2.45	0.49
1:A:72:ASP:OD1	1:A:72:ASP:N	2.44	0.49
1:B:72:ASP:OD1	1:B:72:ASP:N	2.45	0.49
3:D:923:ARG:NH2	3:D:1155:GLU:OE2	2.44	0.49
2:C:94:SER:HB3	2:C:106:SER:HA	1.94	0.49
3:D:487:LEU:HA	3:D:490:VAL:HG22	1.95	0.49
2:C:1007:LYS:HB3	2:C:1022:PRO:HB2	1.95	0.49
2:C:109:ASP:OD2	2:C:111:ARG:NH1	2.43	0.49
2:C:381:VAL:O	2:C:385:ILE:HG22	2.12	0.49
2:C:622:GLU:HG2	2:C:717:LYS:HD3	1.95	0.49
3:D:915:TYR:CE1	3:D:1143:ARG:HD2	2.47	0.49
2:C:1123:VAL:O	2:C:1127:GLU:HG3	2.13	0.48
3:D:1053:VAL:HG22	3:D:1066:ILE:HG12	1.95	0.48
6:N:11:DT:H2"	6:N:12:DG:C8	2.48	0.48
1:B:37:SER:O	1:B:41:THR:OG1	2.20	0.48
2:C:650:ILE:HG12	2:C:660:VAL:HG22	1.95	0.48
2:C:1095:ASP:O	2:C:1099:ARG:HG3	2.13	0.48
1:A:31:GLY:HA3	1:A:178:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:530:GLU:HG2	3:D:574:LEU:HD22	1.95	0.48
3:D:284:GLY:O	3:D:285:LYS:HE2	2.14	0.48
2:C:1069:GLY:N	2:C:1072:GLU:OE1	2.47	0.48
3:D:213:GLN:HA	3:D:216:LEU:HD23	1.95	0.48
3:D:1152:LYS:HA	3:D:1155:GLU:HG3	1.95	0.48
2:C:860:GLU:H	2:C:860:GLU:HG3	1.36	0.48
2:C:946:VAL:HG11	2:C:964:LEU:HD22	1.96	0.48
2:C:654:SER:OG	2:C:655:ALA:N	2.46	0.47
2:C:260:SER:O	2:C:264:LYS:HG2	2.15	0.47
2:C:403:ARG:NH1	2:C:416:THR:O	2.44	0.47
3:D:1248:LEU:HD22	3:D:1258:ILE:HB	1.95	0.47
3:D:412:ARG:HH11	3:D:416:ASN:ND2	2.13	0.47
3:D:1270:ILE:HD11	4:E:106:HIS:CD2	2.50	0.47
4:E:60:ARG:HH11	4:E:63:GLN:HE21	1.61	0.47
5:G:53:LYS:HG2	5:G:55:VAL:HG12	1.96	0.47
4:E:107:THR:O	4:E:107:THR:OG1	2.32	0.47
3:D:1090:LYS:HA	3:D:1096:GLU:HA	1.97	0.46
2:C:833:ARG:HG2	2:C:834:ASP:H	1.80	0.46
3:D:901:LEU:HB3	3:D:958:THR:O	2.15	0.46
1:A:69:VAL:HG22	1:A:128:LEU:HD23	1.98	0.46
3:D:915:TYR:CZ	3:D:1143:ARG:HD2	2.50	0.46
2:C:270:THR:O	2:C:274:LEU:HB2	2.16	0.46
3:D:1064:ILE:HD13	3:D:1111:LEU:HD13	1.96	0.46
2:C:727:GLU:H	3:D:725:THR:HG21	1.81	0.46
3:D:76:GLU:OE1	3:D:76:GLU:N	2.49	0.46
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.81	0.46
2:C:1108:LYS:NZ	2:C:1110:GLU:OE1	2.46	0.46
3:D:1248:LEU:HD23	3:D:1259:PRO:HD2	1.98	0.46
5:G:67:VAL:HG12	5:G:69:ILE:HG23	1.97	0.46
1:A:184:GLU:CD	1:A:185:GLN:H	2.19	0.46
3:D:177:LEU:HD22	3:D:198:ARG:HG2	1.97	0.46
8:T:15:DT:H2'	8:T:16:DA:C8	2.51	0.46
2:C:628:THR:HG22	2:C:629:GLY:N	2.31	0.46
3:D:838:SER:OG	3:D:848:GLU:OE1	2.34	0.46
2:C:273:ALA:O	2:C:277:ILE:HG13	2.16	0.46
2:C:795:GLU:H	2:C:795:GLU:HG2	1.49	0.46
5:G:71:MET:HB2	5:G:72:THR:H	1.58	0.46
2:C:225:ARG:HE	2:C:225:ARG:HB3	1.44	0.45
2:C:160:MET:SD	2:C:164:GLY:HA2	2.56	0.45
3:D:478:ARG:HB3	3:D:480:ARG:HH21	1.81	0.45
2:C:1043:ALA:HB2	3:D:447:MET:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:225:THR:HG21	3:D:240:LEU:HD11	1.99	0.45
3:D:284:GLY:C	3:D:285:LYS:HE2	2.36	0.45
3:D:1127:PRO:O	3:D:1130:VAL:HG12	2.16	0.45
3:D:412:ARG:HH11	3:D:416:ASN:HD22	1.64	0.45
5:G:16:ASN:HA	5:G:19:LYS:HB3	1.99	0.45
5:G:54:LYS:HB3	5:G:54:LYS:HE2	1.45	0.45
3:D:64:LYS:HE3	3:D:64:LYS:HB3	1.84	0.44
1:A:225:LEU:HD12	1:A:225:LEU:HA	1.83	0.44
3:D:598:GLU:HG2	3:D:631:ALA:HB1	2.00	0.44
3:D:641:ARG:HA	3:D:657:GLN:HG3	2.00	0.44
3:D:1064:ILE:O	3:D:1077:TYR:HB2	2.17	0.44
3:D:824:VAL:HG23	3:D:832:ILE:HD12	1.99	0.44
2:C:620:ARG:HH11	2:C:620:ARG:HG3	1.83	0.44
2:C:678:SER:OG	2:C:679:ASN:N	2.50	0.44
3:D:1100:SER:HB2	3:D:1101:ASP:H	1.67	0.44
2:C:727:GLU:H	3:D:725:THR:CG2	2.31	0.44
2:C:1133:LEU:HD13	3:D:12:ILE:HD11	1.99	0.44
2:C:1166:LEU:HB3	2:C:1167:SER:H	1.59	0.44
3:D:1051:GLY:H	3:D:1105:VAL:HG23	1.81	0.44
1:B:133:LYS:HB3	1:B:133:LYS:HE3	1.31	0.44
2:C:805:LYS:HB3	2:C:805:LYS:HE2	1.44	0.44
3:D:177:LEU:HD13	3:D:198:ARG:HH11	1.83	0.44
2:C:518:LYS:HE3	2:C:518:LYS:HB2	1.77	0.44
3:D:1117:ASP:HB3	3:D:1120:GLU:HB2	2.00	0.44
1:A:40:ARG:HE	1:B:33:THR:HG22	1.83	0.44
3:D:590:THR:O	3:D:630:ARG:HB3	2.18	0.44
1:B:3:ILE:H	1:B:3:ILE:HG13	1.47	0.43
3:D:486:VAL:O	3:D:490:VAL:HG13	2.18	0.43
3:D:657:GLN:N	3:D:658:PRO:HD2	2.33	0.43
3:D:733:MET:O	3:D:733:MET:HG2	2.17	0.43
2:C:433:THR:O	2:C:433:THR:OG1	2.28	0.43
2:C:582:SER:OG	2:C:583:PRO:O	2.32	0.43
3:D:330:LEU:HD23	3:D:330:LEU:HA	1.89	0.43
5:G:7:VAL:HB	5:G:89:VAL:HB	2.00	0.43
6:N:21:DT:H2"	6:N:22:DG:O5'	2.18	0.43
2:C:779:GLU:H	2:C:779:GLU:HG3	1.62	0.43
3:D:206:ARG:HG2	3:D:209:ARG:NH2	2.33	0.43
3:D:247:ARG:HG3	3:D:248:TYR:CD1	2.53	0.43
3:D:195:ARG:HH12	3:D:198:ARG:HE	1.66	0.43
3:D:1112:MET:HB3	3:D:1113:GLU:H	1.70	0.43
4:E:49:SER:OG	4:E:50:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:36:DT:H2"	6:N:37:DG:C8	2.53	0.43
3:D:191:ALA:HA	3:D:194:ARG:HB3	1.99	0.43
1:A:129:ASN:HB3	1:A:130:ASP:H	1.62	0.43
3:D:136:ILE:HD12	3:D:252:PHE:CE1	2.51	0.43
3:D:1173:THR:HG21	3:D:1201:ALA:HB2	2.01	0.43
7:R:20:C:O2	7:R:21:A:N6	2.52	0.43
2:C:523:VAL:HA	2:C:552:GLY:O	2.19	0.43
3:D:330:LEU:HG	3:D:336:ALA:HB2	2.01	0.43
2:C:412:ILE:HG23	2:C:417:LEU:HD11	2.00	0.43
3:D:83:THR:OG1	3:D:84:ARG:N	2.51	0.43
5:G:102:LEU:HG	5:G:103:PRO:HD2	2.01	0.43
1:A:56:ILE:HG22	1:A:57:ASP:H	1.83	0.43
1:A:153:ARG:HG3	2:C:795:GLU:HG3	2.00	0.43
2:C:229:LYS:O	2:C:230:ARG:HB2	2.19	0.43
2:C:348:LEU:HD13	2:C:365:VAL:HG12	2.01	0.43
3:D:328:VAL:HG13	3:D:336:ALA:HB3	2.00	0.43
2:C:513:GLU:HG2	2:C:532:THR:HG22	2.00	0.42
2:C:1102:VAL:HG22	2:C:1112:ILE:HG23	2.01	0.42
3:D:320:ILE:HG12	3:D:321:PRO:HD2	1.99	0.42
3:D:468:ASN:OD1	3:D:468:ASN:N	2.50	0.42
3:D:108:LYS:HD2	3:D:108:LYS:HA	1.73	0.42
3:D:498:LEU:HD12	3:D:512:PHE:CD2	2.55	0.42
1:A:112:PRO:HA	1:A:113:PRO:HD3	1.85	0.42
3:D:634:LYS:HB3	3:D:634:LYS:HE3	1.83	0.42
1:A:70:LYS:O	1:A:70:LYS:HG2	2.18	0.42
2:C:302:LYS:HD2	2:C:302:LYS:HA	1.36	0.42
2:C:621:SER:O	2:C:709:ASP:HB2	2.19	0.42
2:C:719:LEU:HD12	2:C:1030:ILE:HG13	2.00	0.42
1:A:158:GLU:HB3	1:A:159:ILE:H	1.69	0.42
1:A:54:ILE:HG22	1:A:138:LEU:HD23	2.02	0.42
2:C:289:LYS:HA	2:C:289:LYS:HD2	1.88	0.42
2:C:313:ARG:HE	2:C:317:ASN:HD21	1.68	0.42
3:D:453:LYS:HB3	3:D:453:LYS:HE2	1.73	0.42
3:D:638:THR:HG22	3:D:639:GLN:HG2	2.02	0.42
5:G:97:LYS:H	5:G:97:LYS:HG2	1.72	0.42
1:B:151:GLN:HE21	1:B:151:GLN:HB3	1.65	0.42
2:C:409:VAL:O	2:C:410:GLU:HB2	2.20	0.42
3:D:409:LYS:HB2	3:D:409:LYS:HE3	1.76	0.42
2:C:944:TRP:HB2	2:C:991:CYS:O	2.20	0.41
2:C:859:ASP:HB3	2:C:861:LEU:HD12	2.01	0.41
3:D:268:PHE:CZ	3:D:273:GLU:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:752:ARG:HE	3:D:752:ARG:HB3	1.61	0.41
3:D:999:ALA:O	3:D:1003:ILE:HG13	2.20	0.41
1:A:153:ARG:HH22	2:C:797:ARG:HE	1.67	0.41
2:C:105:LEU:HD21	2:C:418:ILE:HD11	2.02	0.41
3:D:640:LEU:HD23	3:D:640:LEU:HA	1.89	0.41
3:D:1176:LEU:HD13	3:D:1176:LEU:HA	1.92	0.41
1:B:69:VAL:HG12	1:B:71:GLU:H	1.84	0.41
8:T:8:DC:H2"	8:T:9:DG:C8	2.55	0.41
2:C:281:LEU:HD13	2:C:281:LEU:HA	1.85	0.41
2:C:830:ARG:O	2:C:832:VAL:HG22	2.20	0.41
1:A:56:ILE:HB	1:A:59:VAL:HB	2.02	0.41
1:B:145:GLY:O	1:B:168:TYR:HB2	2.21	0.41
2:C:142:ASN:HD22	2:C:142:ASN:HA	1.62	0.41
3:D:57:ASP:HB3	3:D:58:TRP:CD1	2.55	0.41
3:D:271:ASP:O	3:D:275:GLU:HG3	2.21	0.41
5:G:22:LEU:HD13	5:G:38:VAL:HG11	2.01	0.41
3:D:243:GLU:O	3:D:247:ARG:HG2	2.21	0.41
3:D:953:LEU:HD23	3:D:953:LEU:HA	1.83	0.41
2:C:604:ARG:HA	2:C:604:ARG:HD2	1.78	0.40
3:D:159:ARG:HG2	3:D:219:LEU:HD23	2.03	0.40
8:T:26:DG:H2"	8:T:27:DA:C8	2.56	0.40
2:C:115:VAL:HG11	2:C:129:TYR:CE1	2.56	0.40
2:C:1050:SER:OG	2:C:1051:MET:N	2.54	0.40
3:D:438:LEU:O	3:D:561:SER:OG	2.39	0.40
3:D:931:ASP:HA	3:D:957:ILE:HD11	2.03	0.40
2:C:100:SER:OG	2:C:101:GLY:N	2.52	0.40
2:C:257:ILE:H	2:C:257:ILE:HG13	1.51	0.40
3:D:169:GLU:HG3	3:D:169:GLU:H	1.59	0.40
1:B:6:ARG:HA	1:B:7:PRO:HD3	1.93	0.40
3:D:153:ALA:O	3:D:157:VAL:HG23	2.22	0.40
8:T:31:DG:H2"	8:T:32:DC:O5'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	224/347 (65%)	191 (85%)	31 (14%)	2 (1%)	17 50
1	B	235/347 (68%)	197 (84%)	37 (16%)	1 (0%)	34 67
2	C	1117/1178 (95%)	1016 (91%)	88 (8%)	13 (1%)	13 42
3	D	1279/1316 (97%)	1178 (92%)	94 (7%)	7 (0%)	29 63
4	E	81/110 (74%)	80 (99%)	1 (1%)	0	100 100
5	G	109/177 (62%)	76 (70%)	29 (27%)	4 (4%)	3 17
All	All	3045/3475 (88%)	2738 (90%)	280 (9%)	27 (1%)	21 50

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1149	GLU
3	D	229	LEU
3	D	1066	ILE
1	A	113	PRO
2	C	230	ARG
2	C	231	ARG
2	C	302	LYS
2	C	323	HIS
2	C	1161	ASN
3	D	764	ALA
1	B	236	PRO
2	C	309	ALA
2	C	862	PRO
3	D	1093	ASP
2	C	358	PRO
3	D	192	ASP
5	G	90	GLY
2	C	194	SER
2	C	1162	LEU
5	G	62	PRO
2	C	328	ILE
3	D	829	GLY
3	D	1020	VAL
5	G	93	GLY
1	A	28	PRO
5	G	83	PRO
2	C	327	PRO

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	195/297 (66%)	144 (74%)	51 (26%)	0 1
1	B	195/297 (66%)	136 (70%)	59 (30%)	0 1
2	C	943/998 (94%)	799 (85%)	144 (15%)	2 11
3	D	1059/1095 (97%)	935 (88%)	124 (12%)	5 21
4	E	69/90 (77%)	64 (93%)	5 (7%)	14 41
5	G	98/159 (62%)	68 (69%)	30 (31%)	0 1
All	All	2559/2936 (87%)	2146 (84%)	413 (16%)	5 10

All (413) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	ARG
1	A	8	THR
1	A	10	SER
1	A	12	ASP
1	A	14	LEU
1	A	15	THR
1	A	18	ARG
1	A	33	THR
1	A	38	LEU
1	A	43	LEU
1	A	53	SER
1	A	56	ILE
1	A	62	GLU
1	A	72	ASP
1	A	74	THR
1	A	81	LYS
1	A	83	LEU
1	A	85	VAL
1	A	89	GLU
1	A	90	ASP
1	A	91	GLU

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Mol	Chain	Res	Type
1	A	95	MET
1	A	97	LEU
1	A	106	THR
1	A	111	VAL
1	A	117	THR
1	A	120	ASN
1	A	123	MET
1	A	127	THR
1	A	129	ASN
1	A	130	ASP
1	A	131	LYS
1	A	138	LEU
1	A	151	GLN
1	A	158	GLU
1	A	159	ILE
1	A	161	ARG
1	A	166	SER
1	A	173	LYS
1	A	177	LYS
1	A	183	VAL
1	A	190	ASP
1	A	203	SER
1	A	205	ARG
1	A	216	VAL
1	A	217	GLU
1	A	221	LEU
1	A	223	ARG
1	A	224	GLU
1	A	225	LEU
1	B	1	MET
1	B	2	LEU
1	B	3	ILE
1	B	6	ARG
1	B	9	LEU
1	B	10	SER
1	B	13	VAL
1	B	14	LEU
1	B	15	THR
1	B	16	ASP
1	B	20	GLN
1	B	33	THR
1	B	34	LEU

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Mol	Chain	Res	Type
1	B	40	ARG
1	B	41	THR
1	B	45	SER
1	B	46	ILE
1	B	53	SER
1	B	55	ARG
1	B	59	VAL
1	B	60	LEU
1	B	62	GLU
1	B	64	THR
1	B	66	VAL
1	B	72	ASP
1	B	75	GLU
1	B	78	LEU
1	B	85	VAL
1	B	87	SER
1	B	90	ASP
1	B	91	GLU
1	B	95	MET
1	B	104	GLU
1	B	105	VAL
1	B	109	ASP
1	B	116	VAL
1	B	117	THR
1	B	118	VAL
1	B	120	ASN
1	B	123	MET
1	B	127	THR
1	B	128	LEU
1	B	129	ASN
1	B	133	LYS
1	B	138	LEU
1	B	141	GLU
1	B	142	ARG
1	B	151	GLN
1	B	155	SER
1	B	159	ILE
1	B	166	SER
1	B	175	THR
1	B	186	ARG
1	B	205	ARG
1	B	216	VAL

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Mol	Chain	Res	Type
1	B	218	LEU
1	B	227	VAL
1	B	228	GLU
1	B	233	GLU
2	C	45	ARG
2	C	72	GLU
2	C	73	SER
2	C	77	ARG
2	C	79	ASP
2	C	80	VAL
2	C	99	PHE
2	C	127	MET
2	C	141	ASN
2	C	149	SER
2	C	185	VAL
2	C	188	ASP
2	C	191	ILE
2	C	193	LYS
2	C	194	SER
2	C	198	THR
2	C	199	LEU
2	C	201	SER
2	C	203	LYS
2	C	207	SER
2	C	208	ARG
2	C	212	LEU
2	C	213	GLU
2	C	217	ASP
2	C	218	LYS
2	C	219	ARG
2	C	221	THR
2	C	222	VAL
2	C	224	VAL
2	C	229	LYS
2	C	231	ARG
2	C	232	GLN
2	C	237	LEU
2	C	239	LYS
2	C	245	SER
2	C	248	ILE
2	C	251	ARG
2	C	255	SER

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Mol	Chain	Res	Type
2	C	258	MET
2	C	262	LEU
2	C	267	THR
2	C	270	THR
2	C	271	ASP
2	C	274	LEU
2	C	277	ILE
2	C	279	ARG
2	C	280	LYS
2	C	281	LEU
2	C	282	ARG
2	C	288	THR
2	C	289	LYS
2	C	290	GLU
2	C	295	LEU
2	C	297	GLU
2	C	302	LYS
2	C	304	LYS
2	C	305	ARG
2	C	310	ARG
2	C	311	VAL
2	C	313	ARG
2	C	314	TYR
2	C	318	LYS
2	C	322	LEU
2	C	323	HIS
2	C	324	VAL
2	C	328	ILE
2	C	334	THR
2	C	342	ILE
2	C	343	GLU
2	C	353	THR
2	C	354	THR
2	C	357	VAL
2	C	362	GLU
2	C	363	VAL
2	C	366	GLU
2	C	367	THR
2	C	373	PHE
2	C	377	ARG
2	C	395	ARG
2	C	421	ARG

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Mol	Chain	Res	Type
2	C	443	ASN
2	C	451	HIS
2	C	519	VAL
2	C	534	ASP
2	C	540	VAL
2	C	574	SER
2	C	577	ASP
2	C	626	VAL
2	C	630	MET
2	C	637	ASP
2	C	647	SER
2	C	661	MET
2	C	678	SER
2	C	690	VAL
2	C	691	ASP
2	C	702	ILE
2	C	753	GLU
2	C	757	ILE
2	C	758	ASP
2	C	761	ASP
2	C	762	THR
2	C	764	LEU
2	C	768	GLU
2	C	769	ILE
2	C	770	THR
2	C	771	ARG
2	C	776	ILE
2	C	777	SER
2	C	779	GLU
2	C	787	ARG
2	C	789	ILE
2	C	790	VAL
2	C	795	GLU
2	C	797	ARG
2	C	800	ASP
2	C	801	ILE
2	C	805	LYS
2	C	806	VAL
2	C	807	THR
2	C	830	ARG
2	C	833	ARG
2	C	838	LYS

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Mol	Chain	Res	Type
2	C	846	LYS
2	C	847	VAL
2	C	848	ILE
2	C	859	ASP
2	C	860	GLU
2	C	861	LEU
2	C	891	ASN
2	C	974	THR
2	C	976	VAL
2	C	992	THR
2	C	1104	GLU
2	C	1145	ILE
2	C	1147	LEU
2	C	1149	GLU
2	C	1151	GLU
2	C	1154	ASP
2	C	1155	LEU
2	C	1157	ARG
2	C	1162	LEU
2	C	1164	ILE
2	C	1167	SER
2	C	1168	ARG
3	D	30	LYS
3	D	37	ARG
3	D	60	CYS
3	D	64	LYS
3	D	69	ARG
3	D	71	LYS
3	D	80	VAL
3	D	138	SER
3	D	142	GLU
3	D	143	MET
3	D	147	GLU
3	D	149	SER
3	D	150	THR
3	D	151	LEU
3	D	154	GLU
3	D	160	LYS
3	D	167	ASP
3	D	169	GLU
3	D	170	LEU
3	D	171	GLU

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Mol	Chain	Res	Type
3	D	173	ARG
3	D	178	GLU
3	D	187	GLU
3	D	190	LYS
3	D	195	ARG
3	D	196	LYS
3	D	198	ARG
3	D	199	ASP
3	D	203	ARG
3	D	205	MET
3	D	211	ARG
3	D	216	LEU
3	D	218	ARG
3	D	244	LEU
3	D	252	PHE
3	D	253	THR
3	D	267	ASN
3	D	325	ARG
3	D	334	ARG
3	D	350	ARG
3	D	359	ASP
3	D	373	MET
3	D	377	SER
3	D	403	SER
3	D	468	ASN
3	D	474	ARG
3	D	478	ARG
3	D	480	ARG
3	D	539	ASP
3	D	576	MET
3	D	578	ARG
3	D	580	ASP
3	D	595	ASP
3	D	605	ASP
3	D	635	VAL
3	D	656	TRP
3	D	691	LYS
3	D	721	PHE
3	D	738	VAL
3	D	741	ARG
3	D	743	LYS
3	D	747	ASP

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Mol	Chain	Res	Type
3	D	762	ARG
3	D	772	GLU
3	D	782	THR
3	D	784	GLU
3	D	787	GLN
3	D	795	ASP
3	D	796	ASP
3	D	808	THR
3	D	810	ASN
3	D	834	ARG
3	D	841	ARG
3	D	866	ARG
3	D	919	SER
3	D	940	ARG
3	D	946	ASP
3	D	966	LEU
3	D	997	ILE
3	D	1016	HIS
3	D	1017	GLN
3	D	1022	GLU
3	D	1028	LEU
3	D	1029	PRO
3	D	1041	ARG
3	D	1046	ILE
3	D	1049	VAL
3	D	1050	THR
3	D	1052	ARG
3	D	1053	VAL
3	D	1054	ARG
3	D	1055	LEU
3	D	1059	GLU
3	D	1060	ARG
3	D	1062	TYR
3	D	1063	LYS
3	D	1064	ILE
3	D	1065	THR
3	D	1067	VAL
3	D	1069	ASP
3	D	1075	VAL
3	D	1080	ILE
3	D	1082	LYS
3	D	1083	ARG

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Mol	Chain	Res	Type
3	D	1084	GLN
3	D	1085	ARG
3	D	1092	GLU
3	D	1095	SER
3	D	1096	GLU
3	D	1097	ARG
3	D	1098	VAL
3	D	1100	SER
3	D	1101	ASP
3	D	1105	VAL
3	D	1106	GLU
3	D	1107	VAL
3	D	1109	GLN
3	D	1110	GLN
3	D	1112	MET
3	D	1115	SER
3	D	1169	ASP
3	D	1208	MET
3	D	1239	ASN
3	D	1272	VAL
4	E	33	LEU
4	E	41	ASP
4	E	56	TYR
4	E	68	TYR
4	E	107	THR
5	G	3	LYS
5	G	12	SER
5	G	16	ASN
5	G	17	LYS
5	G	22	LEU
5	G	26	VAL
5	G	29	MET
5	G	33	ASP
5	G	34	LYS
5	G	43	GLU
5	G	45	GLU
5	G	46	THR
5	G	49	LYS
5	G	52	LYS
5	G	54	LYS
5	G	56	VAL
5	G	57	LYS

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Mol	Chain	Res	Type
5	G	58	LYS
5	G	59	LYS
5	G	60	VAL
5	G	62	PRO
5	G	66	LEU
5	G	71	MET
5	G	72	THR
5	G	73	ASP
5	G	80	ARG
5	G	97	LYS
5	G	105	GLU
5	G	111	LYS
5	G	112	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	120	ASN
1	A	129	ASN
1	B	20	GLN
1	B	119	HIS
1	B	120	ASN
1	B	129	ASN
1	B	151	GLN
1	B	200	ASN
2	C	141	ASN
2	C	142	ASN
2	C	169	ASN
2	C	349	HIS
2	C	372	HIS
2	C	386	GLN
2	C	545	ASN
2	C	610	ASN
2	C	612	GLN
2	C	775	ASN
2	C	889	HIS
2	C	1066	GLN
2	C	1077	GLN
2	C	1165	ASN
3	D	22	GLN
3	D	207	GLN

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Mol	Chain	Res	Type
3	D	396	ASN
3	D	416	ASN
3	D	687	GLN
3	D	882	GLN
3	D	935	ASN
3	D	1016	HIS
3	D	1110	GLN
3	D	1139	GLN
3	D	1145	GLN
4	E	63	GLN
4	E	106	HIS
5	G	9	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	R	16/30 (53%)	5 (31%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	R	18	G
7	R	19	G
7	R	20	C
7	R	22	G
7	R	28	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
9	G2P	C	1201	10	27,34,34	5.27	13 (48%)	33,54,54	1.69	6 (18%)

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
9	G2P	C	1201	10	-	6/15/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	G2P	O4'-C1'	14.09	1.60	1.41
9	C	1201	G2P	C2'-C1'	-12.64	1.34	1.53
9	C	1201	G2P	C4-N3	8.92	1.49	1.35
9	C	1201	G2P	C5-C6	8.19	1.55	1.41
9	C	1201	G2P	PB-O3B	7.32	1.66	1.58
9	C	1201	G2P	O4'-C4'	-6.36	1.30	1.45
9	C	1201	G2P	C2-N1	6.22	1.46	1.35
9	C	1201	G2P	C6-N1	5.36	1.42	1.33
9	C	1201	G2P	C2-N2	5.05	1.44	1.33
9	C	1201	G2P	PA-O5'	4.84	1.64	1.57
9	C	1201	G2P	O3'-C3'	-3.17	1.35	1.43
9	C	1201	G2P	C2-N3	2.51	1.46	1.34
9	C	1201	G2P	O2'-C2'	2.01	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	1201	G2P	N3-C2-N1	-5.58	119.78	127.22
9	C	1201	G2P	C2-N3-C4	4.81	120.85	115.36
9	C	1201	G2P	C5-C6-N1	-2.42	120.13	123.43
9	C	1201	G2P	C2-N1-C6	2.36	119.67	115.93
9	C	1201	G2P	PB-O3B-PG	-2.34	124.37	132.62
9	C	1201	G2P	C3'-C2'-C1'	2.33	104.49	100.98

There are no chirality outliers.

All (6) torsion outliers are listed below:

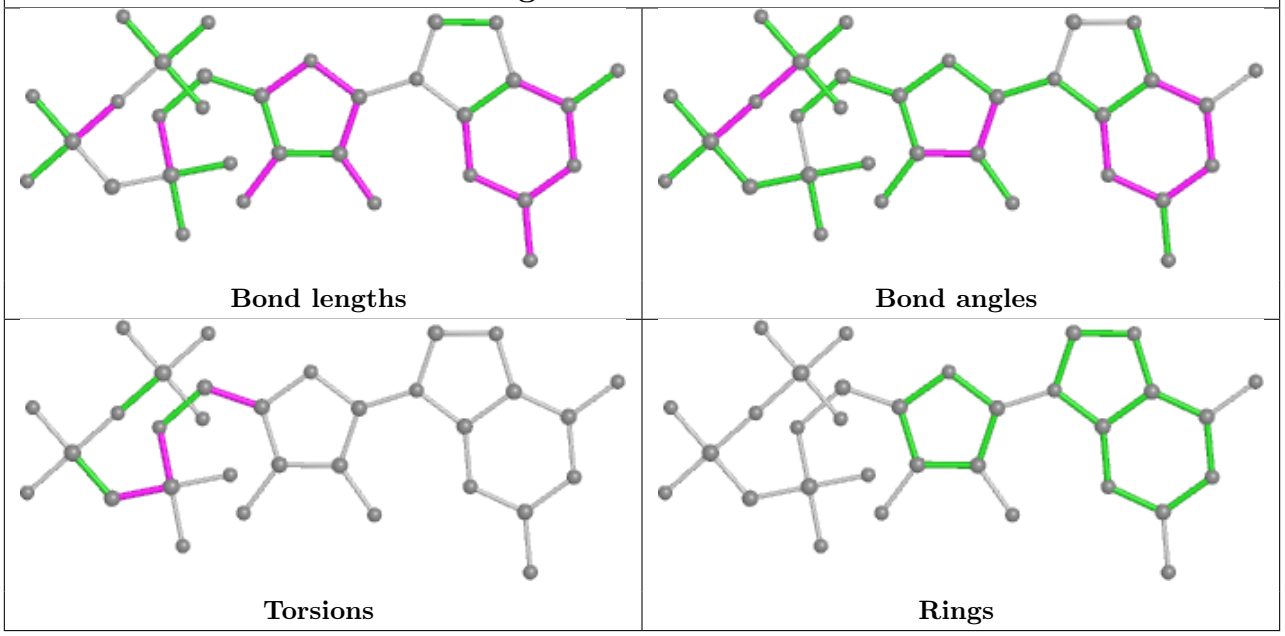
Mol	Chain	Res	Type	Atoms
9	C	1201	G2P	PB-C3A-PA-O1A
9	C	1201	G2P	PB-C3A-PA-O2A
9	C	1201	G2P	PB-C3A-PA-O5'
9	C	1201	G2P	C5'-O5'-PA-O2A
9	C	1201	G2P	C3'-C4'-C5'-O5'
9	C	1201	G2P	O4'-C4'-C5'-O5'

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 then 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.

Ligand G2P C 1201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

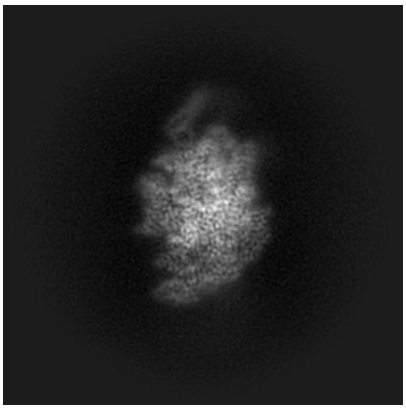
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28174. These allow visual inspection of the internal detail of the map and identification of artifacts.

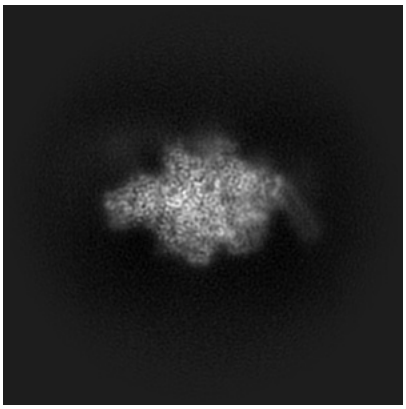
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

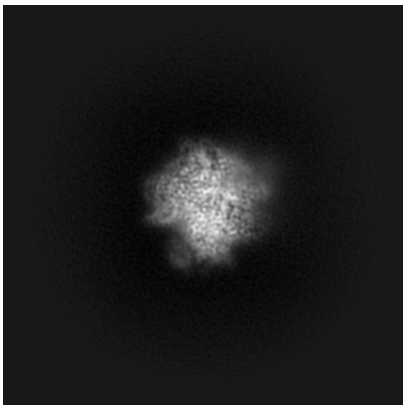
6.1.1 Primary map



X

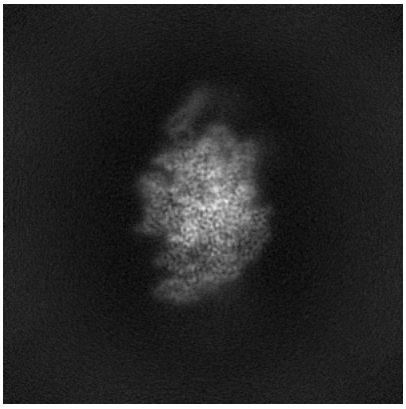


Y

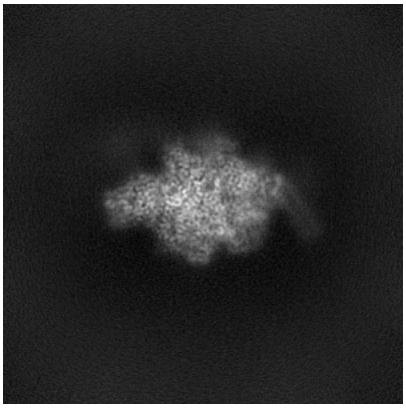


Z

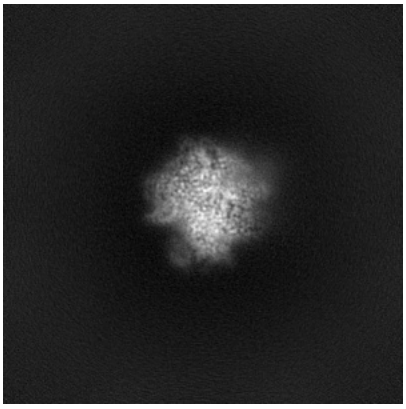
6.1.2 Raw map



X



Y



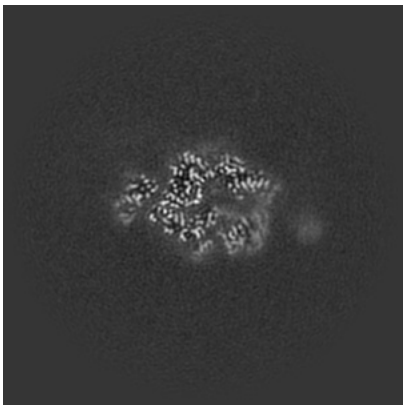
Z

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

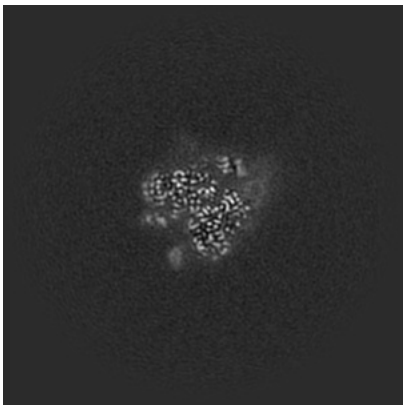
6.2 Central slices (i)

6.2.1 Primary map

X Index: 200



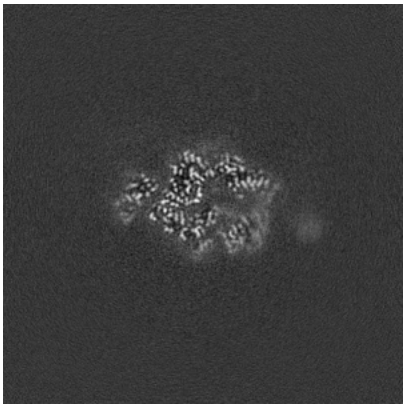
Y Index: 200



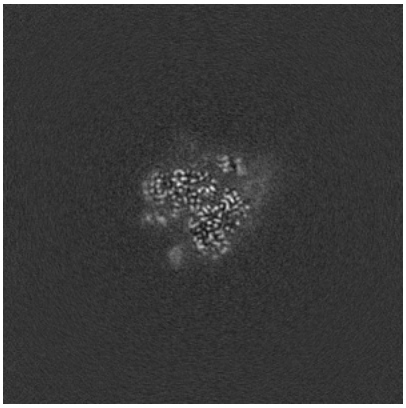
Z Index: 200

6.2.2 Raw map

X Index: 200



Y Index: 200



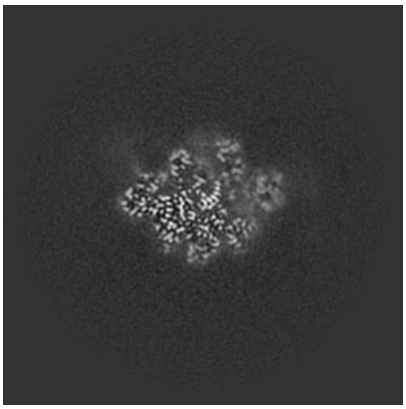
Z Index: 200

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

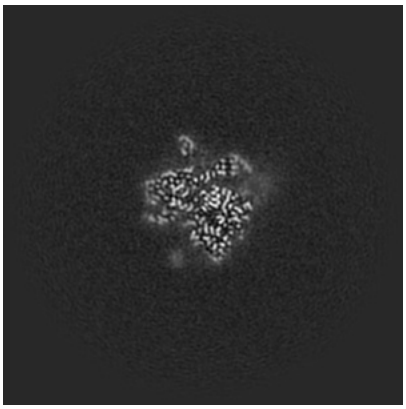
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 200



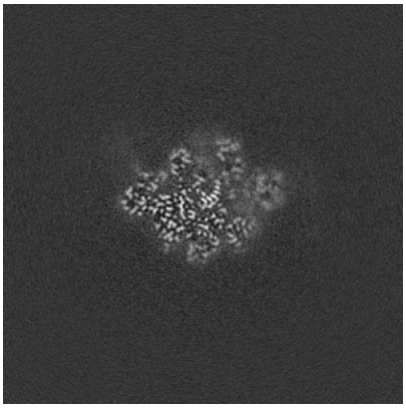
Y Index: 214



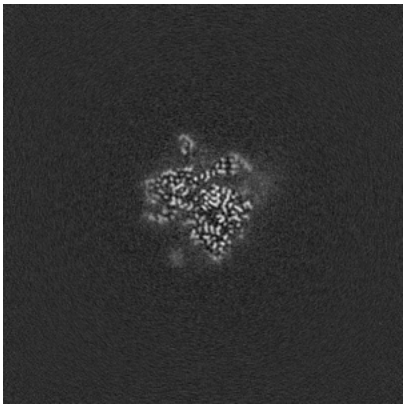
Z Index: 195

6.3.2 Raw map

X Index: 200



Y Index: 214

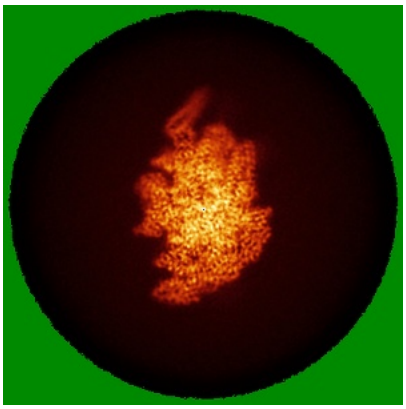


Z Index: 195

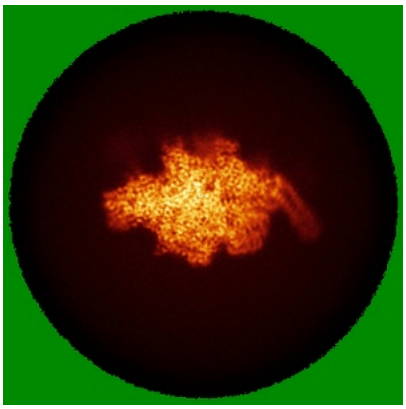
The images above show the largest variance slices of the map in three orthogonal directions.

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

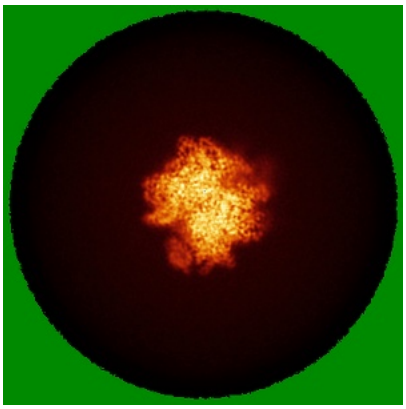
6.4.1 Primary map



X

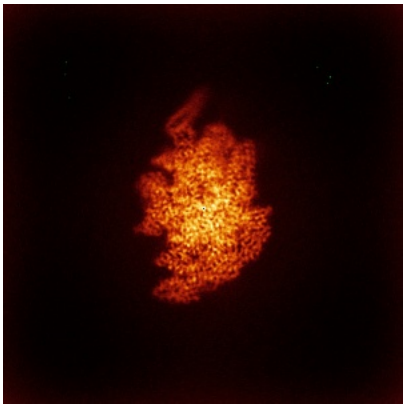


Y

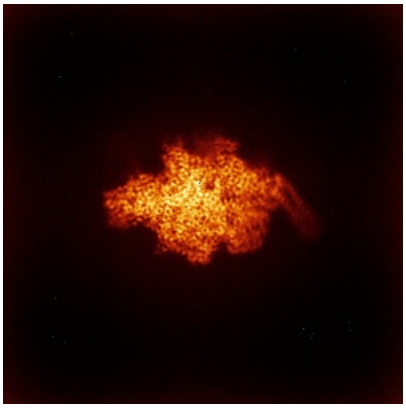


Z

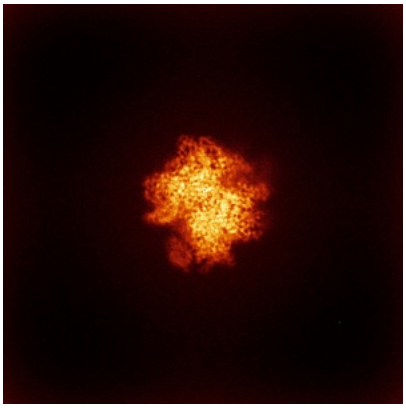
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.294. 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.

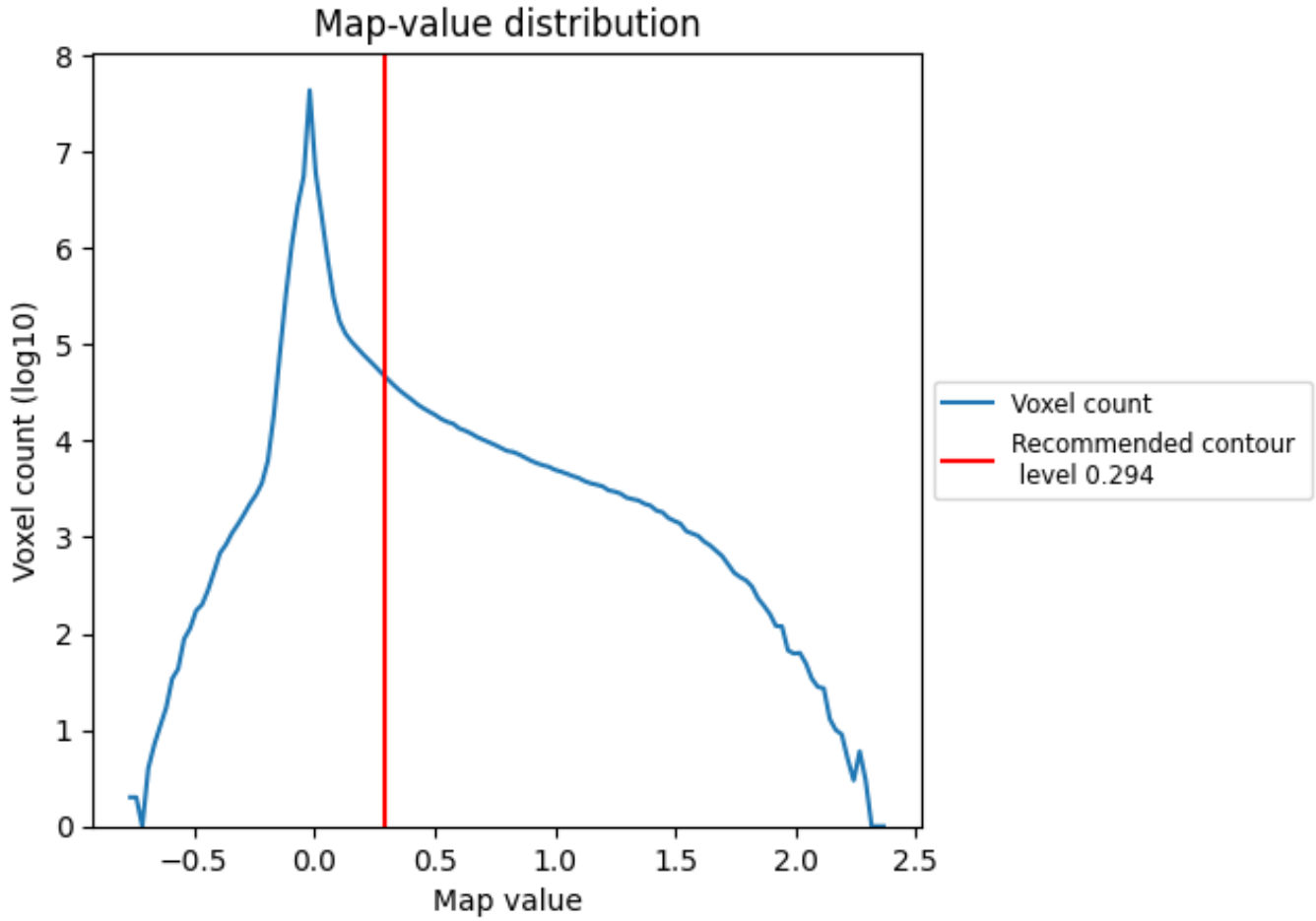
6.6 Mask visualisation (i)

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

7 Map analysis

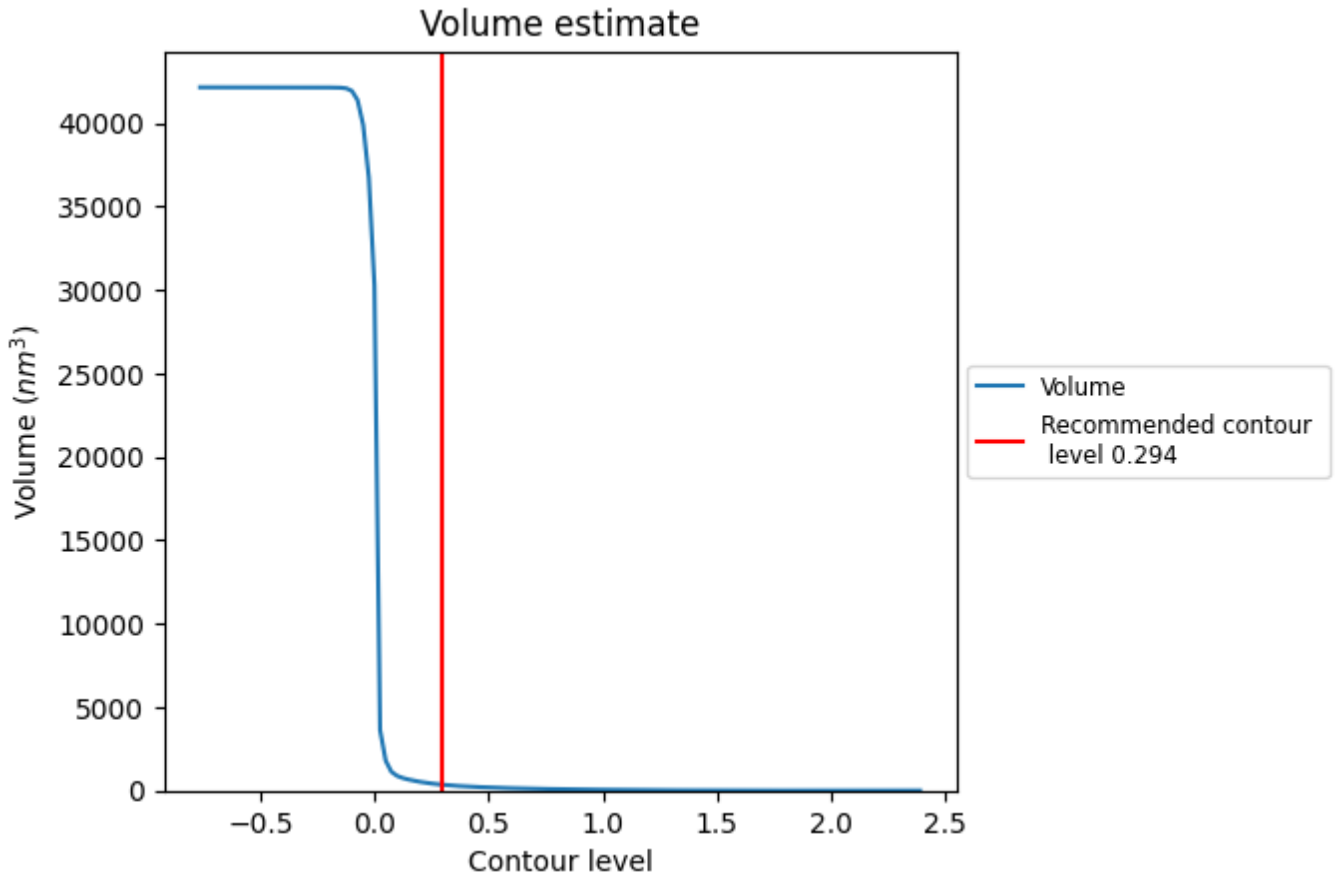
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

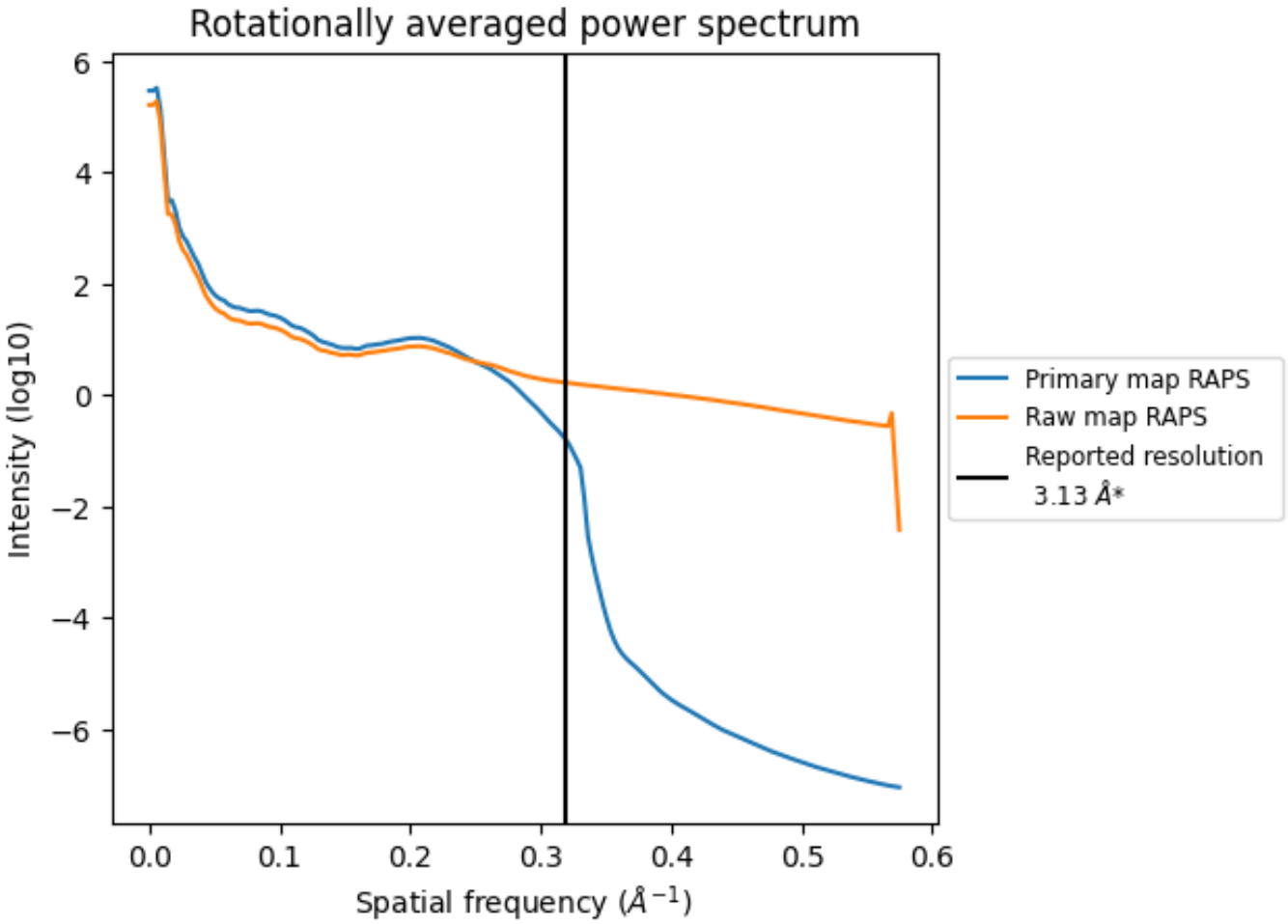
7.2 Volume estimate



The volume at the recommended contour level is 355 nm^3; this corresponds to an approximate mass of 320 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)

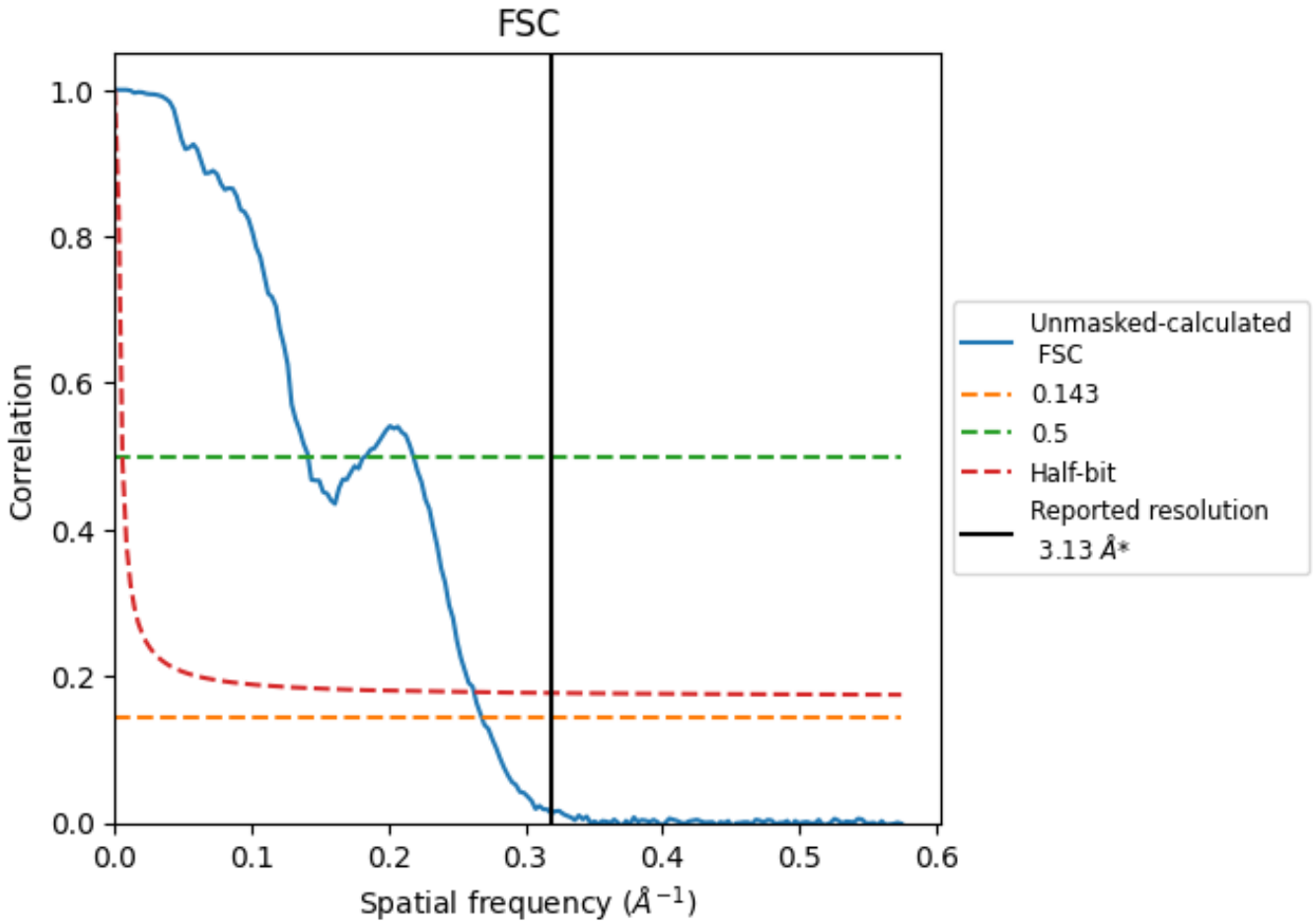


*Reported resolution corresponds to spatial frequency of 0.319 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.319 Å^{-1}

8.2 Resolution estimates (i)

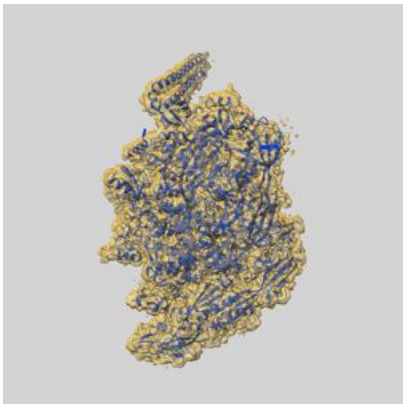
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.73	7.09	3.81

*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 3.73 differs from the reported value 3.13 by more than 10 %

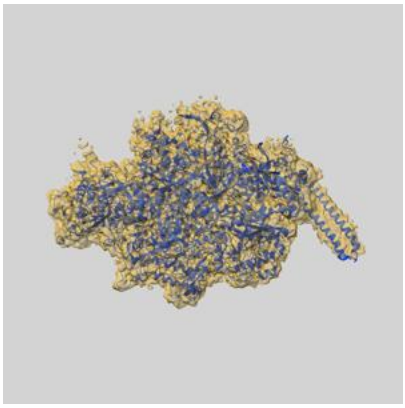
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28174 and PDB model 8EJ3. Per-residue inclusion information can be found in section 3 on page 7.

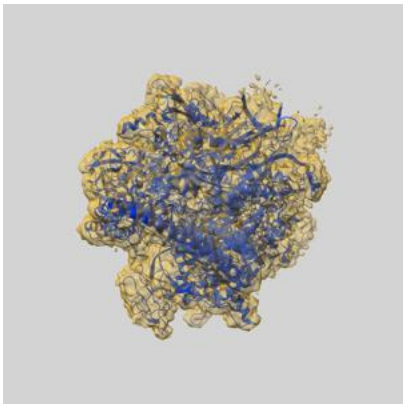
9.1 Map-model overlay



X



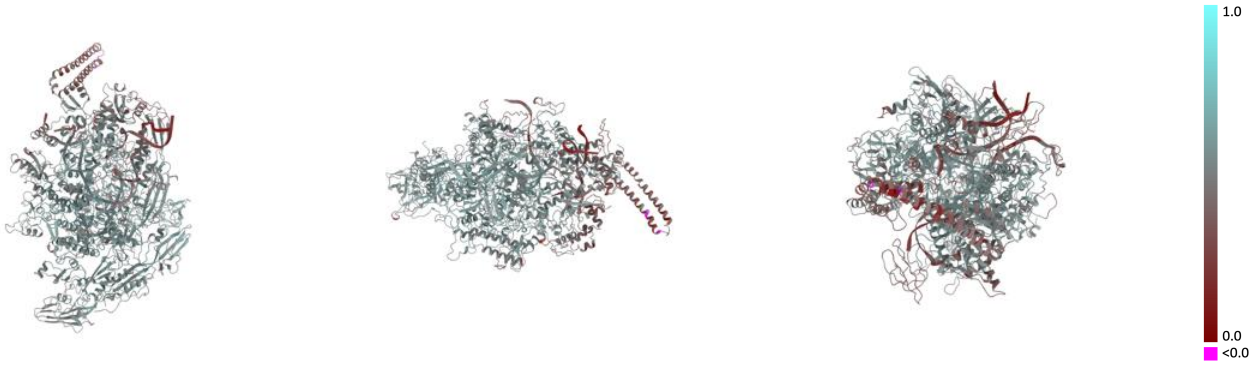
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.294 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.

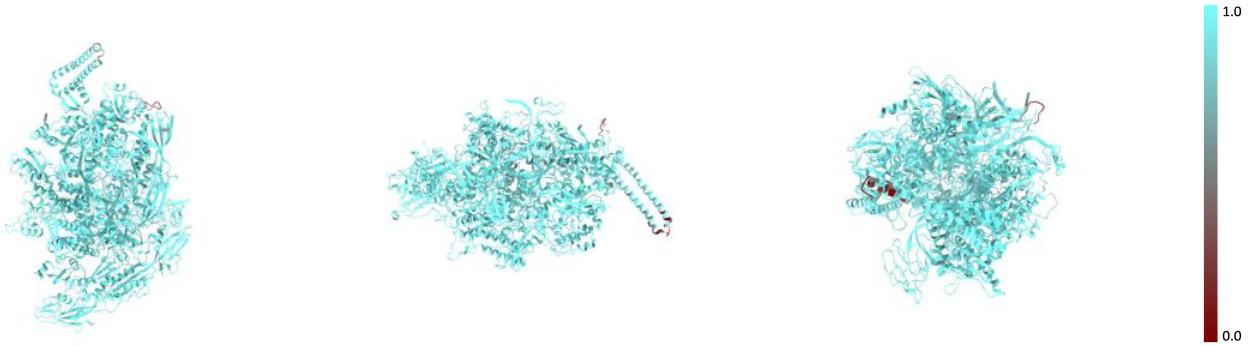
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

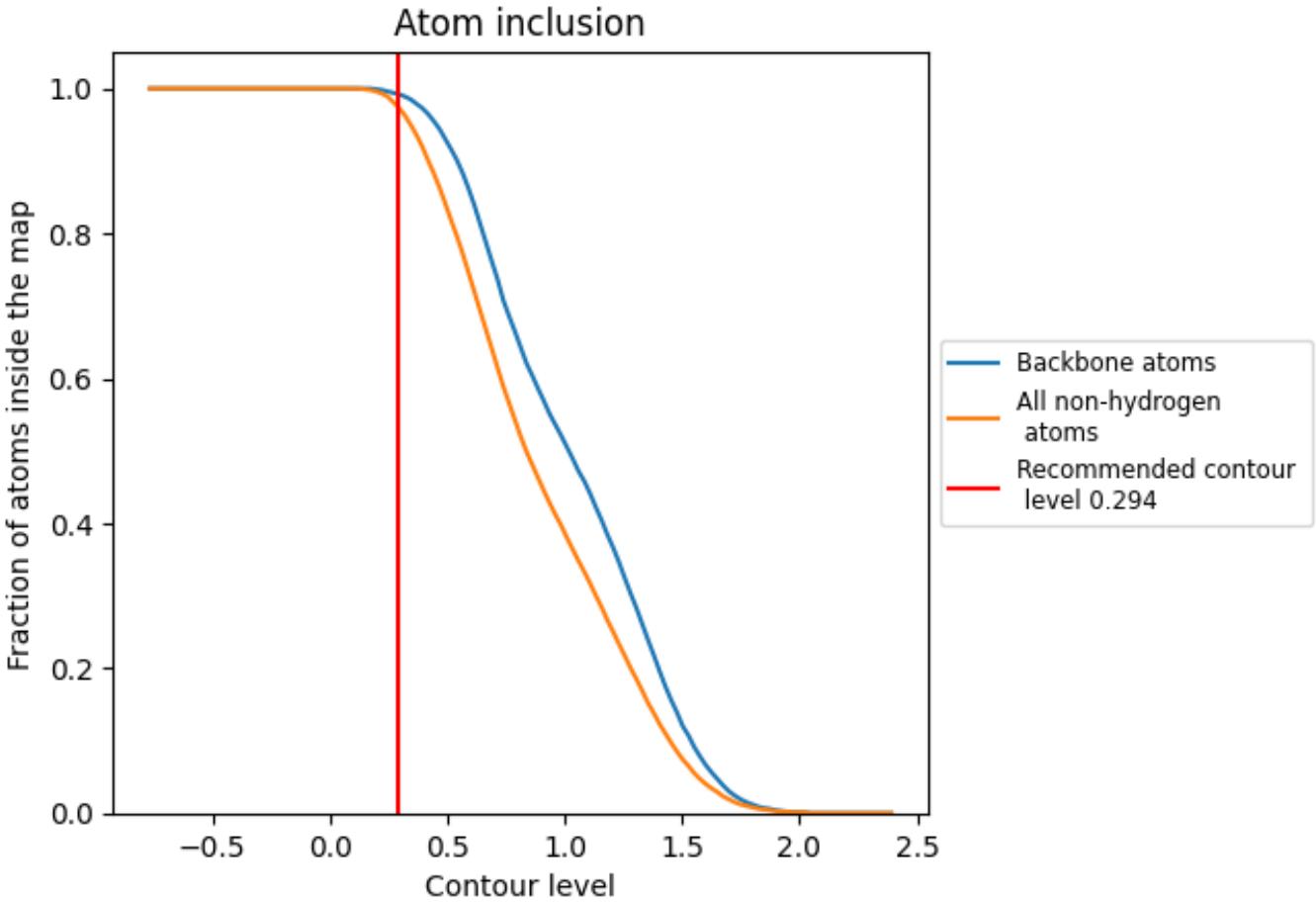
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.294).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.294) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9740	0.5110
A	0.9820	0.5450
B	0.9720	0.5220
C	0.9810	0.5300
D	0.9720	0.5110
E	0.9780	0.5260
G	0.9100	0.4240
N	0.9740	0.3510
R	0.9840	0.4610
T	0.9650	0.4320