Full wwPDB EM Validation Report ⓘ

Feb 14, 2023 – 10:29 AM EST

PDB ID	:	8EOT
EMDB ID	:	EMD-28467
Title	:	M. tuberculosis RNAP elongation complex with NusG
Authors	:	Vishwakarma, R.K.; Murakami, K.S.
Deposited on	:	2022-10-04
Resolution	:	3.30 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:

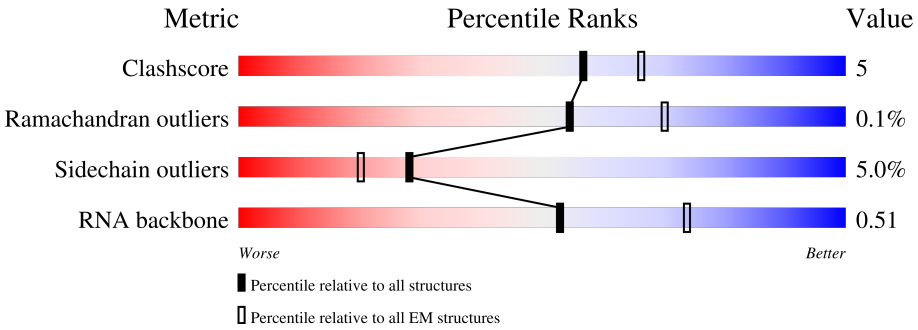
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.30 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.



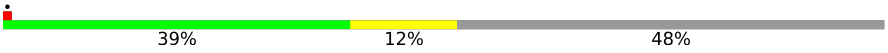
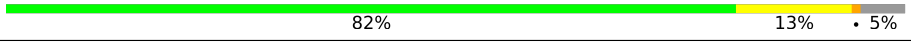
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	55% 9% • 35%
1	B	347	59% 8% • 32%
2	D	1316	80% 16% • •
3	E	110	65% 10% • 25%
4	T	40	50% 32% 18%
5	N	40	45% 32% 22%
6	R	20	40% 20% 5% 35%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	G	238	
8	C	1178	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 25299 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	D	1269	Total	C	N	O	S	0	0
			9919	6209	1804	1865	41		

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

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

- Molecule 4 is a DNA chain called DNA (33-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	33	Total	C	N	O	P	0	0
			672	318	123	198	33		

- Molecule 5 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	31	Total	C	N	O	P	0	0
			634	300	117	186	31		

- Molecule 6 is a RNA chain called RNA (5'-R(P*AP*AP*GP*CP*GP*GP*AP*GP*AP*GP *GP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	13	Total	C	N	O	P	0	0
			288	128	60	87	13		

- Molecule 7 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	124	Total	C	N	O	S	0	0
			968	614	170	183	1		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	1122	Total	C	N	O	S	0	0
			8677	5426	1528	1684	39		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

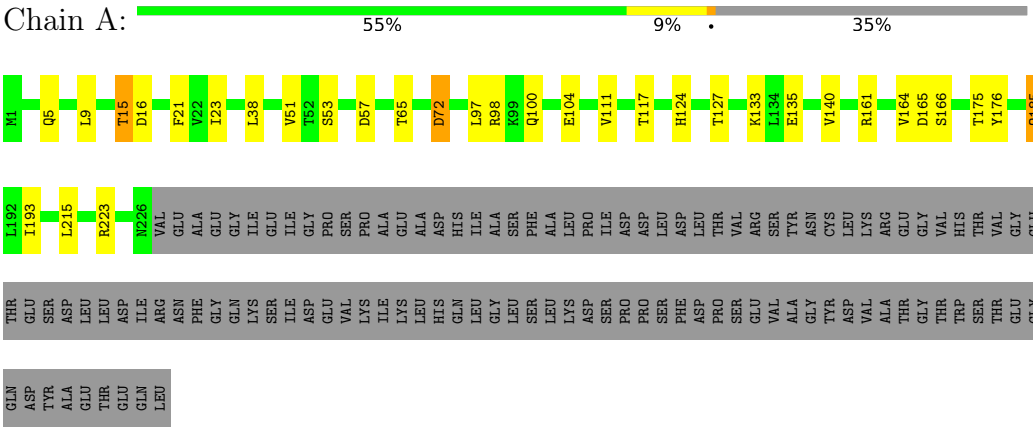
Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	

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.

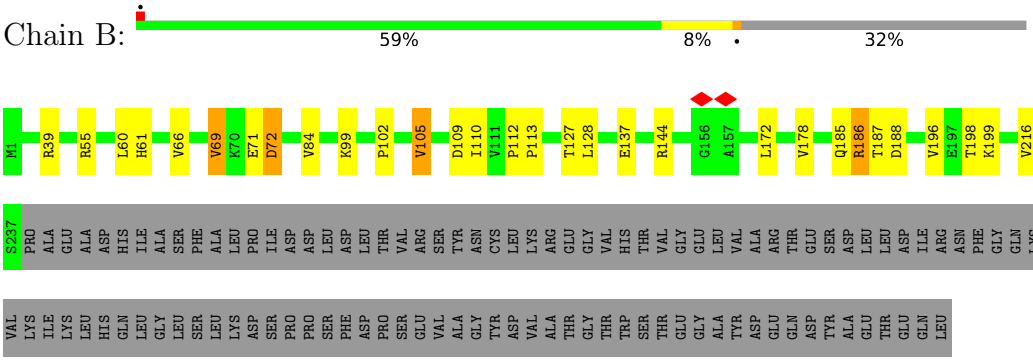
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



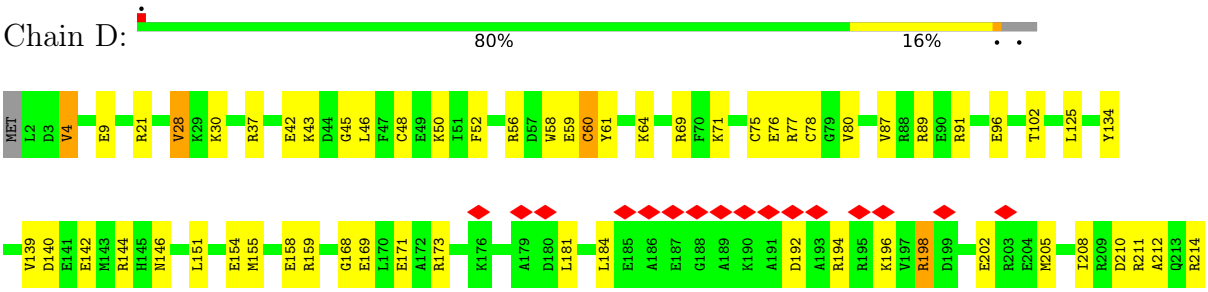
• Molecule 1: DNA-directed RNA polymerase subunit alpha

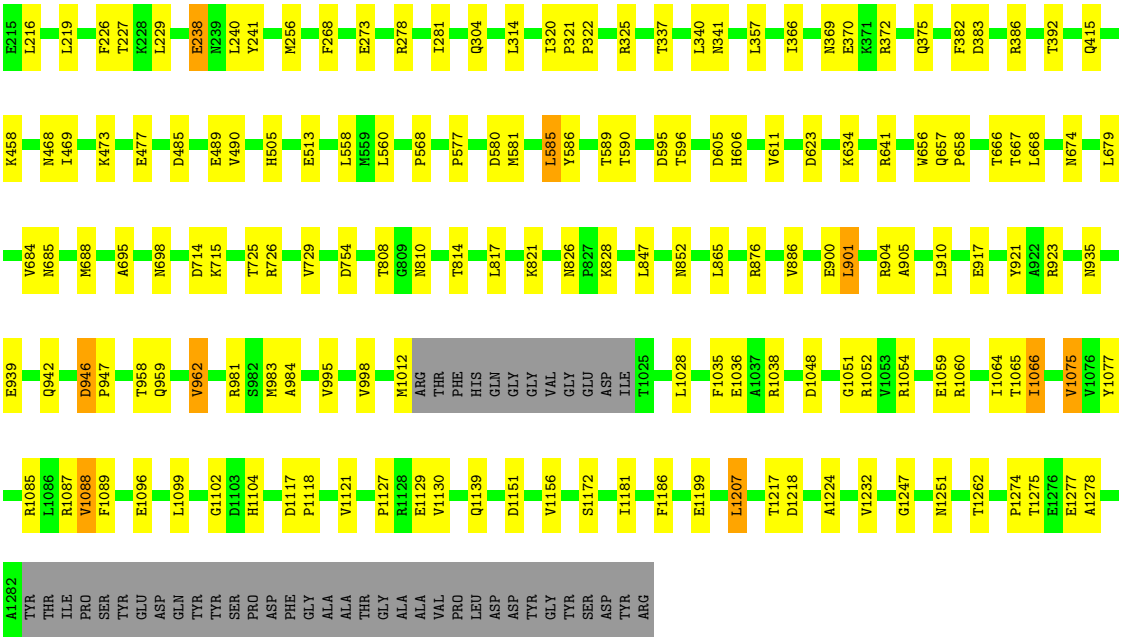
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta'

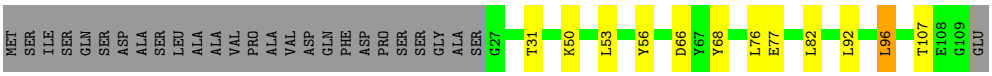
Chain D:





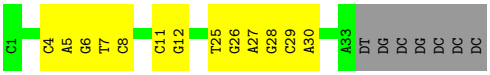
• Molecule 3: DNA-directed RNA polymerase subunit omega

Chain E:



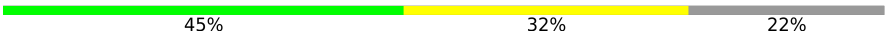
• Molecule 4: DNA (33-MER)

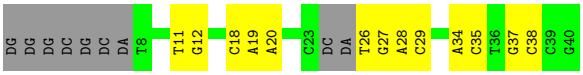
Chain T:



• Molecule 5: DNA (31-MER)

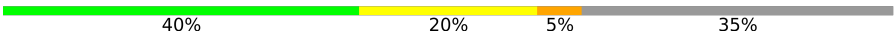
Chain N:

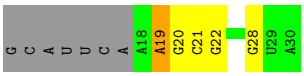




• Molecule 6: RNA (5'-R(P*AP*AP*GP*CP*GP*GP*AP*GP*AP*GP*GP*UP*A)-3')

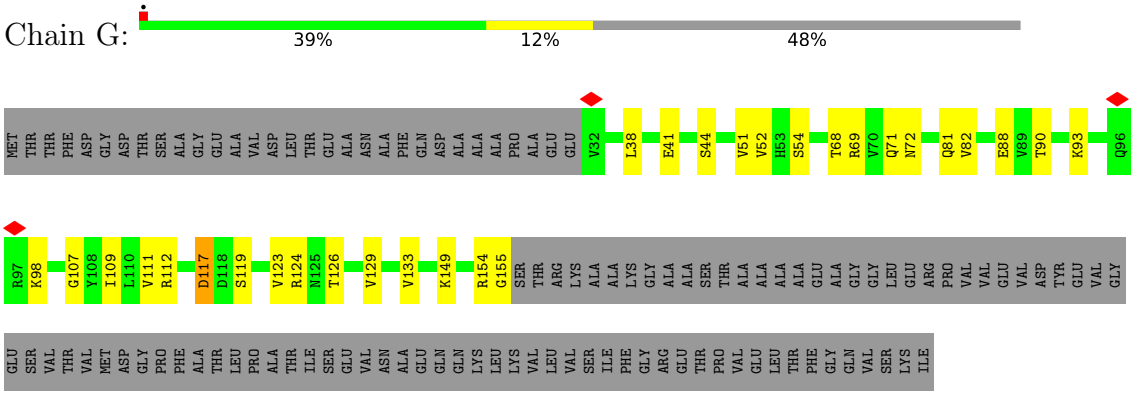
Chain R:





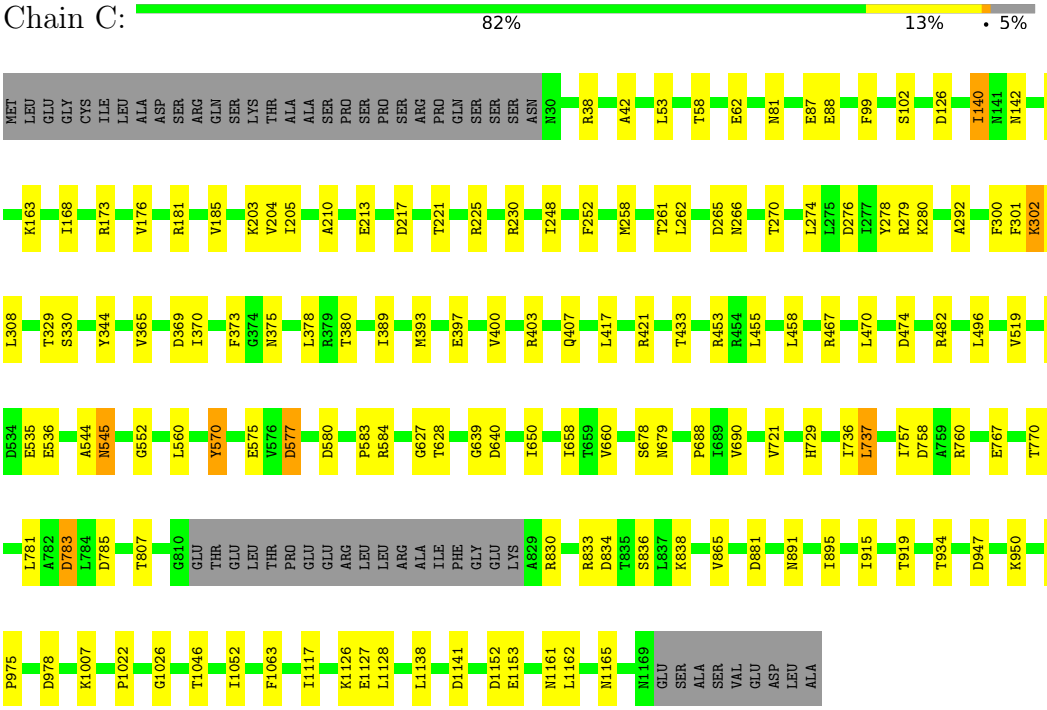
• Molecule 7: Transcription termination/antitermination protein NusG

Chain G:



• Molecule 8: DNA-directed RNA polymerase subunit beta

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46900	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	2.054	Depositor
Minimum map value	-0.693	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.304	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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/1750	0.54	0/2380
1	B	0.29	0/1792	0.53	0/2442
2	D	0.27	0/10085	0.52	0/13633
3	E	0.27	0/662	0.49	0/901
4	T	0.58	0/752	0.89	0/1157
5	N	0.51	0/709	0.92	0/1089
6	R	0.36	0/324	0.82	0/505
7	G	0.25	0/987	0.46	0/1343
8	C	0.28	0/8833	0.52	0/11975
All	All	0.30	0/25894	0.56	0/35425

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

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	16	0
1	B	1765	0	1794	13	0
2	D	9919	0	9985	111	0
3	E	649	0	645	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	T	672	0	370	9	0
5	N	634	0	349	8	0
6	R	288	0	142	1	0
7	G	968	0	973	14	0
8	C	8677	0	8600	87	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	25299	0	24626	252	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 (252) 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)
8:C:934:THR:HG23	8:C:1026:GLY:HA3	1.65	0.78
2:D:60:CYS:SG	2:D:61:TYR:N	2.62	0.72
2:D:821:LYS:NZ	2:D:852:ASN:OD1	2.24	0.71
2:D:89:ARG:NH2	8:C:1052:ILE:O	2.25	0.70
2:D:876:ARG:NH1	2:D:1036:GLU:OE2	2.24	0.69
2:D:847:LEU:HD11	8:C:560:LEU:HD13	1.74	0.69
8:C:403:ARG:O	8:C:407:GLN:NE2	2.26	0.69
5:N:18:DC:H4'	5:N:19:DA:H5'	1.75	0.68
2:D:1247:GLY:O	2:D:1251:ASN:ND2	2.23	0.67
2:D:641:ARG:HA	2:D:657:GLN:HG3	1.74	0.66
8:C:276:ASP:HA	8:C:279:ARG:HE	1.61	0.66
2:D:674:ASN:HD21	2:D:684:VAL:HG22	1.62	0.64
6:R:19:A:N1	8:C:1165:ASN:ND2	2.44	0.64
8:C:400:VAL:HG23	8:C:417:LEU:HB3	1.80	0.64
2:D:568:PRO:HB3	2:D:984:ALA:HB2	1.79	0.63
1:A:98:ARG:HG2	1:A:135:GLU:HG3	1.79	0.63
8:C:774:PRO:HD2	8:C:834:ASP:HB2	1.80	0.63
7:G:69:ARG:NH1	7:G:126:THR:OG1	2.32	0.63
8:C:163:LYS:HE2	8:C:639:GLY:HA3	1.81	0.62
2:D:64:LYS:NZ	2:D:75:CYS:SG	2.68	0.62
2:D:1088:VAL:HB	2:D:1096:GLU:HB3	1.80	0.62
7:G:81:GLN:OE1	7:G:112:ARG:NH1	2.28	0.62
8:C:42:ALA:HB2	8:C:975:PRO:HG2	1.80	0.62
8:C:369:ASP:O	8:C:375:ASN:ND2	2.32	0.61
1:B:55:ARG:NE	1:B:137:GLU:OE2	2.30	0.61
8:C:760:ARG:HD3	8:C:865:VAL:HG12	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:ARG:HB3	2:D:59:GLU:HG3	1.83	0.60
8:C:771:ARG:NH2	8:C:781:LEU:O	2.33	0.60
1:A:104:GLU:OE2	1:A:124:HIS:ND1	2.34	0.59
2:D:923:ARG:HD3	2:D:962:VAL:HG11	1.84	0.59
2:D:939:GLU:OE2	2:D:942:GLN:NE2	2.35	0.59
1:A:165:ASP:OD1	1:A:166:SER:N	2.36	0.58
7:G:82:VAL:HG22	7:G:111:VAL:HG12	1.86	0.58
8:C:185:VAL:HG12	8:C:204:VAL:HG22	1.86	0.58
2:D:45:GLY:H	2:D:48:CYS:HB2	1.69	0.57
8:C:658:ILE:HD11	8:C:688:PRO:HB3	1.85	0.57
8:C:783:ASP:OD1	8:C:783:ASP:N	2.31	0.57
8:C:378:LEU:HD11	8:C:455:LEU:HD22	1.88	0.56
8:C:140:ILE:HB	8:C:147:ILE:HG12	1.87	0.56
1:B:69:VAL:HG13	1:B:71:GLU:H	1.69	0.56
8:C:577:ASP:OD1	8:C:577:ASP:N	2.36	0.56
2:D:473:LYS:NZ	2:D:477:GLU:OE2	2.40	0.54
8:C:181:ARG:HG3	8:C:370:ILE:HD11	1.90	0.54
2:D:9:GLU:HB2	8:C:1138:LEU:HB2	1.90	0.54
2:D:139:VAL:HG21	2:D:144:ARG:HH21	1.73	0.54
7:G:149:LYS:O	7:G:154:ARG:NH1	2.40	0.54
2:D:144:ARG:NH1	2:D:226:PHE:O	2.41	0.54
8:C:721:VAL:HG22	8:C:915:ILE:HG23	1.90	0.54
2:D:585:LEU:O	2:D:589:THR:HG22	2.07	0.54
8:C:785:ASP:N	8:C:785:ASP:OD1	2.40	0.54
2:D:1172:SER:N	2:D:1199:GLU:OE1	2.38	0.53
7:G:71:GLN:NE2	7:G:72:ASN:OD1	2.41	0.53
8:C:248:ILE:HD11	8:C:262:LEU:HD22	1.90	0.53
2:D:1052:ARG:NH2	2:D:1102:GLY:O	2.42	0.53
8:C:628:THR:HG23	8:C:975:PRO:HA	1.91	0.53
8:C:678:SER:OG	8:C:679:ASN:N	2.42	0.53
2:D:325:ARG:NH1	2:D:341:ASN:OD1	2.41	0.53
2:D:320:ILE:HG12	2:D:321:PRO:HD2	1.91	0.53
8:C:523:VAL:HG23	8:C:552:GLY:HA3	1.90	0.53
2:D:369:ASN:OD1	2:D:372:ARG:NH1	2.42	0.52
2:D:210:ASP:O	2:D:214:ARG:HD3	2.09	0.52
8:C:265:ASP:OD1	8:C:266:ASN:N	2.42	0.52
1:A:100:GLN:HE21	1:A:133:LYS:HD3	1.75	0.52
4:T:4:DC:H2"	4:T:5:DA:N7	2.23	0.52
8:C:252:PHE:HB3	8:C:258:MET:HG3	1.91	0.52
2:D:589:THR:HG21	2:D:688:MET:HG2	1.91	0.52
8:C:274:LEU:HB3	8:C:292:ALA:HB1	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:LYS:HE3	2:D:50:LYS:HG3	1.93	0.51
2:D:1118:PRO:HA	2:D:1121:VAL:HG12	1.93	0.51
1:A:51:VAL:HG12	1:A:140:VAL:HG12	1.92	0.51
2:D:21:ARG:NE	2:D:96:GLU:OE2	2.37	0.51
2:D:383:ASP:OD2	2:D:386:ARG:NH1	2.44	0.50
8:C:221:THR:HA	8:C:261:THR:HG22	1.93	0.50
2:D:169:GLU:HB3	2:D:208:ILE:HG21	1.93	0.50
2:D:485:ASP:OD1	2:D:485:ASP:N	2.44	0.50
2:D:1181:ILE:HD11	2:D:1186:PHE:HD1	1.75	0.50
2:D:142:GLU:O	2:D:146:ASN:ND2	2.44	0.50
8:C:38:ARG:HG2	8:C:973:SER:HB2	1.93	0.50
8:C:545:ASN:O	8:C:545:ASN:ND2	2.44	0.50
1:B:198:THR:OG1	1:B:199:LYS:N	2.45	0.50
7:G:88:GLU:H	7:G:155:GLY:HA3	1.77	0.50
2:D:144:ARG:HH22	2:D:229:LEU:HB2	1.77	0.49
2:D:151:LEU:O	2:D:155:MET:HG2	2.12	0.49
2:D:1127:PRO:HA	2:D:1130:VAL:HG13	1.93	0.49
8:C:81:ASN:OD1	8:C:81:ASN:N	2.45	0.49
2:D:865:LEU:HD22	8:C:470:LEU:HD13	1.94	0.49
8:C:1046:THR:HG21	8:C:1162:LEU:HG	1.95	0.49
8:C:1152:ASP:OD1	8:C:1153:GLU:N	2.39	0.49
8:C:203:LYS:O	8:C:205:ILE:HG13	2.12	0.49
1:B:39:ARG:NH2	2:D:623:ASP:OD2	2.45	0.49
2:D:28:VAL:HG21	2:D:46:LEU:HD23	1.95	0.49
2:D:168:GLY:O	2:D:171:GLU:HG3	2.12	0.49
8:C:102:SER:HA	8:C:142:ASN:HB2	1.95	0.49
2:D:4:VAL:HG13	8:C:1117:ILE:HG12	1.95	0.49
2:D:1277:GLU:OE1	2:D:1277:GLU:N	2.36	0.49
3:E:76:LEU:HG	3:E:77:GLU:H	1.77	0.49
1:A:53:SER:OG	1:A:161:ARG:NH1	2.45	0.48
2:D:1036:GLU:OE1	2:D:1038:ARG:NH2	2.46	0.48
5:N:34:DA:H1'	5:N:35:DC:H5'	1.94	0.48
2:D:173:ARG:HD2	2:D:205:MET:HB3	1.95	0.48
2:D:586:TYR:O	2:D:590:THR:OG1	2.30	0.48
2:D:684:VAL:HG23	2:D:685:ASN:H	1.79	0.48
2:D:238:GLU:O	2:D:241:TYR:N	2.47	0.48
2:D:1129:GLU:N	2:D:1129:GLU:OE1	2.47	0.47
8:C:535:GLU:OE1	8:C:535:GLU:N	2.46	0.47
8:C:210:ALA:HB3	8:C:300:PHE:HE1	1.79	0.47
1:B:72:ASP:OD1	1:B:72:ASP:N	2.38	0.47
8:C:544:ALA:HA	8:C:580:ASP:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1117:ASP:OD1	2:D:1117:ASP:N	2.48	0.47
1:B:102:PRO:HA	1:B:128:LEU:O	2.15	0.47
2:D:935:ASN:H	2:D:935:ASN:HD22	1.61	0.47
2:D:901:LEU:HB3	2:D:958:THR:O	2.14	0.47
1:A:191:LYS:HE2	1:A:193:ILE:HD11	1.95	0.47
2:D:154:GLU:O	2:D:158:GLU:HG2	2.15	0.47
2:D:1224:ALA:HA	2:D:1232:VAL:HG21	1.97	0.47
8:C:102:SER:O	8:C:142:ASN:N	2.35	0.47
4:T:7:DT:H2"	4:T:8:DC:C6	2.50	0.47
2:D:1054:ARG:HB2	2:D:1065:THR:HG22	1.97	0.47
4:T:26:DG:H2"	4:T:27:DA:C8	2.50	0.46
2:D:1048:ASP:OD1	2:D:1077:TYR:OH	2.25	0.46
8:C:369:ASP:OD1	8:C:370:ILE:N	2.48	0.46
8:C:213:GLU:HB3	8:C:225:ARG:HB2	1.98	0.46
8:C:1161:ASN:HD21	8:C:1165:ASN:HD22	1.63	0.46
8:C:482:ARG:NH2	8:C:536:GLU:OE1	2.44	0.46
8:C:640:ASP:OD1	8:C:640:ASP:N	2.44	0.46
2:D:198:ARG:O	2:D:202:GLU:HG2	2.16	0.46
7:G:54:SER:N	7:G:107:GLY:O	2.43	0.46
2:D:904:ARG:HG3	2:D:910:LEU:HD13	1.97	0.45
1:A:15:THR:HG22	1:A:16:ASP:H	1.81	0.45
2:D:78:CYS:SG	2:D:80:VAL:HG12	2.56	0.45
4:T:25:DT:H2"	4:T:26:DG:C8	2.51	0.45
2:D:134:TYR:HD1	2:D:256:MET:HB2	1.81	0.45
2:D:140:ASP:OD1	2:D:140:ASP:N	2.39	0.45
2:D:580:ASP:OD1	2:D:580:ASP:N	2.50	0.45
2:D:1217:THR:OG1	2:D:1218:ASP:N	2.49	0.45
2:D:58:TRP:HZ3	2:D:71:LYS:HB3	1.81	0.45
2:D:192:ASP:O	2:D:196:LYS:HG2	2.17	0.45
1:A:65:THR:HG22	1:A:72:ASP:HB3	1.98	0.45
2:D:102:THR:OG1	2:D:375:GLN:NE2	2.49	0.45
2:D:212:ALA:O	2:D:216:LEU:HG	2.16	0.45
2:D:357:LEU:HD23	2:D:370:GLU:HG3	1.99	0.45
2:D:595:ASP:OD1	2:D:596:THR:N	2.37	0.45
2:D:904:ARG:HG2	2:D:905:ALA:H	1.81	0.45
3:E:96:LEU:HD13	3:E:96:LEU:HA	1.84	0.45
4:T:11:DC:H2'	4:T:12:DG:C8	2.52	0.45
8:C:458:LEU:HD21	8:C:496:LEU:HD13	1.99	0.45
2:D:181:LEU:HB2	2:D:198:ARG:HH22	1.82	0.45
2:D:656:TRP:CE2	2:D:658:PRO:HG2	2.52	0.45
4:T:27:DA:H2"	4:T:28:DG:H8	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:836:SER:OG	8:C:838:LYS:NZ	2.46	0.45
8:C:729:HIS:HB2	8:C:736:ILE:HD11	1.98	0.44
2:D:611:VAL:HG12	2:D:634:LYS:HB2	1.98	0.44
8:C:650:ILE:HG12	8:C:660:VAL:HG22	1.98	0.44
8:C:947:ASP:OD1	8:C:947:ASP:N	2.48	0.44
1:A:9:LEU:HD23	1:A:23:ILE:HG12	1.98	0.44
2:D:52:PHE:CD1	2:D:322:PRO:HD3	2.53	0.44
5:N:37:DG:H1'	5:N:38:DC:H5'	1.99	0.44
8:C:757:ILE:HG12	8:C:758:ASP:H	1.83	0.44
2:D:1012:MET:SD	2:D:1012:MET:N	2.91	0.44
2:D:1064:ILE:HG23	2:D:1077:TYR:HD1	1.82	0.44
8:C:583:PRO:O	8:C:584:ARG:HG2	2.18	0.44
2:D:917:GLU:HA	2:D:921:TYR:CD1	2.53	0.44
2:D:946:ASP:CG	2:D:947:PRO:HD3	2.38	0.44
5:N:28:DA:H4'	5:N:29:DC:OP1	2.16	0.44
8:C:58:THR:O	8:C:62:GLU:HG2	2.17	0.44
2:D:1139:GLN:NE2	2:D:1151:ASP:OD1	2.51	0.44
8:C:770:THR:OG1	8:C:771:ARG:N	2.51	0.44
2:D:314:LEU:HD11	2:D:382:PHE:HE2	1.82	0.44
8:C:278:TYR:CD1	8:C:292:ALA:HA	2.53	0.43
8:C:329:THR:OG1	8:C:330:SER:N	2.51	0.43
8:C:1141:ASP:OD1	8:C:1141:ASP:N	2.51	0.43
8:C:217:ASP:OD1	8:C:221:THR:OG1	2.30	0.43
1:B:228:GLU:N	1:B:228:GLU:OE1	2.51	0.43
2:D:1051:GLY:O	2:D:1104:HIS:ND1	2.49	0.43
5:N:28:DA:N1	8:C:467:ARG:HD2	2.33	0.43
1:A:57:ASP:OD1	1:A:57:ASP:N	2.50	0.43
2:D:30:LYS:HE3	2:D:30:LYS:HB2	1.86	0.43
2:D:64:LYS:HD3	2:D:77:ARG:HH12	1.83	0.43
2:D:469:ILE:H	2:D:469:ILE:HG13	1.71	0.43
8:C:389:ILE:O	8:C:393:MET:HG2	2.19	0.43
8:C:560:LEU:HG	8:C:570:TYR:CE1	2.53	0.43
8:C:1007:LYS:HB3	8:C:1022:PRO:HB2	2.01	0.43
1:B:186:ARG:HD3	1:B:188:ASP:HB3	2.00	0.43
8:C:767:GLU:HG2	8:C:807:THR:HA	2.00	0.43
2:D:58:TRP:CZ3	2:D:71:LYS:HB3	2.54	0.43
8:C:230:ARG:HB2	8:C:280:LYS:HZ2	1.83	0.43
1:B:112:PRO:HA	1:B:113:PRO:HD3	1.86	0.43
2:D:695:ALA:HA	2:D:698:ASN:ND2	2.34	0.43
1:B:172:LEU:HG	1:B:199:LYS:HG3	1.99	0.43
2:D:268:PHE:CZ	2:D:273:GLU:HG3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:26:DT:H4'	5:N:27:DG:OP2	2.19	0.43
7:G:119:SER:O	7:G:123:VAL:HG12	2.19	0.43
2:D:208:ILE:O	2:D:211:ARG:HG3	2.19	0.42
2:D:657:GLN:N	2:D:658:PRO:HD2	2.34	0.42
2:D:666:THR:OG1	2:D:667:THR:N	2.52	0.42
8:C:397:GLU:HA	8:C:400:VAL:HG12	2.01	0.42
2:D:76:GLU:OE1	2:D:76:GLU:N	2.52	0.42
1:A:9:LEU:HD21	1:A:21:PHE:HB3	1.99	0.42
2:D:184:LEU:HA	2:D:194:ARG:HG2	2.00	0.42
7:G:52:VAL:HB	7:G:109:ILE:HG12	2.01	0.42
8:C:575:GLU:OE1	8:C:575:GLU:N	2.52	0.42
2:D:1118:PRO:HB2	2:D:1207:LEU:HD12	2.01	0.42
4:T:29:DC:H2"	4:T:30:DA:C8	2.55	0.42
7:G:124:ARG:HH11	7:G:129:VAL:HG12	1.84	0.42
8:C:126:ASP:OD1	8:C:126:ASP:N	2.52	0.42
2:D:826:ASN:ND2	2:D:828:LYS:H	2.18	0.42
8:C:305:ARG:HD2	8:C:305:ARG:HA	1.76	0.42
2:D:558:LEU:HD23	3:E:50:LYS:HE2	2.01	0.42
2:D:1274:PRO:HB3	3:E:82:LEU:HD11	2.02	0.42
7:G:68:THR:O	7:G:71:GLN:HG3	2.19	0.42
8:C:168:ILE:HD11	8:C:173:ARG:HH11	1.85	0.42
2:D:577:PRO:HB3	2:D:581:MET:HB2	2.00	0.42
8:C:230:ARG:HB2	8:C:280:LYS:NZ	2.35	0.42
8:C:304:LYS:HB3	8:C:304:LYS:HE2	1.58	0.42
1:B:99:LYS:HG2	1:B:105:VAL:HB	2.02	0.41
2:D:1059:GLU:HG2	2:D:1060:ARG:HG3	2.01	0.41
4:T:5:DA:H2"	4:T:6:DG:C8	2.55	0.41
8:C:532:THR:HG22	8:C:533:ALA:H	1.85	0.41
8:C:978:ASP:N	8:C:978:ASP:OD1	2.53	0.41
2:D:278:ARG:HA	2:D:281:ILE:HG12	2.02	0.41
2:D:935:ASN:H	2:D:935:ASN:ND2	2.18	0.41
2:D:1099:LEU:HD13	2:D:1099:LEU:HA	1.94	0.41
7:G:41:GLU:O	7:G:44:SER:OG	2.31	0.41
2:D:1066:ILE:HG23	2:D:1075:VAL:HG23	2.02	0.41
5:N:19:DA:H2"	5:N:20:DA:H5"	2.01	0.41
2:D:605:ASP:OD1	2:D:605:ASP:N	2.54	0.41
8:C:308:LEU:HD23	8:C:308:LEU:HA	1.84	0.41
8:C:737:LEU:HD22	8:C:895:ILE:HD13	2.02	0.41
2:D:42:GLU:OE1	2:D:42:GLU:N	2.48	0.41
8:C:1126:LYS:HD3	8:C:1126:LYS:HA	1.85	0.41
1:B:84:VAL:HG12	1:B:199:LYS:HE3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:ARG:HA	2:D:198:ARG:HD2	1.90	0.41
2:D:340:LEU:HD23	2:D:340:LEU:HA	1.90	0.41
2:D:900:GLU:OE1	2:D:959:GLN:NE2	2.53	0.41
2:D:1275:THR:HG23	2:D:1278:ALA:H	1.86	0.41
8:C:433:THR:O	8:C:433:THR:OG1	2.34	0.41
8:C:1128:LEU:HD23	8:C:1128:LEU:HA	1.93	0.40
1:A:223:ARG:HH11	1:B:216:VAL:HG21	1.85	0.40
4:T:4:DC:H2"	4:T:5:DA:C8	2.57	0.40
8:C:53:LEU:O	8:C:453:ARG:HD2	2.22	0.40
8:C:274:LEU:HD13	8:C:274:LEU:HA	1.97	0.40
2:D:357:LEU:HD21	2:D:366:ILE:HG22	2.02	0.40
5:N:11:DT:H2"	5:N:12:DG:C8	2.56	0.40
7:G:38:LEU:O	7:G:41:GLU:HG3	2.21	0.40
8:C:344:TYR:OH	8:C:365:VAL:HA	2.21	0.40
8:C:950:LYS:HE2	8:C:950:LYS:HB2	1.89	0.40
7:G:117:ASP:OD1	7:G:117:ASP:N	2.54	0.40
8:C:627:GLY:O	8:C:973:SER:HA	2.21	0.40
1:A:5:GLN:OE1	1:A:5:GLN:N	2.50	0.40
1:A:175:THR:OG1	1:A:176:TYR:N	2.55	0.40
1:A:185:GLN:HE21	1:A:185:GLN:HB2	1.63	0.40
2:D:159:ARG:HD2	2:D:216:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	224/347 (65%)	216 (96%)	8 (4%)	0	100 100
1	B	235/347 (68%)	222 (94%)	13 (6%)	0	100 100
2	D	1265/1316 (96%)	1191 (94%)	72 (6%)	2 (0%)	47 77
3	E	81/110 (74%)	78 (96%)	3 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	G	122/238 (51%)	120 (98%)	2 (2%)	0	100 100
8	C	1118/1178 (95%)	1048 (94%)	68 (6%)	2 (0%)	47 77
All	All	3045/3536 (86%)	2875 (94%)	166 (6%)	4 (0%)	54 81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	1066	ILE
8	C	302	LYS
8	C	303	GLU
2	D	337	THR

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%)	184 (94%)	11 (6%)	21 52
1	B	195/297 (66%)	179 (92%)	16 (8%)	11 36
2	D	1050/1095 (96%)	995 (95%)	55 (5%)	23 54
3	E	69/90 (77%)	61 (88%)	8 (12%)	5 22
7	G	104/189 (55%)	98 (94%)	6 (6%)	20 50
8	C	943/998 (94%)	911 (97%)	32 (3%)	37 65
All	All	2556/2966 (86%)	2428 (95%)	128 (5%)	28 55

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	38	LEU
1	A	72	ASP
1	A	97	LEU
1	A	111	VAL
1	A	117	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	127	THR
1	A	164	VAL
1	A	185	GLN
1	A	187	THR
1	A	215	LEU
1	B	60	LEU
1	B	61	HIS
1	B	66	VAL
1	B	69	VAL
1	B	72	ASP
1	B	105	VAL
1	B	109	ASP
1	B	110	ILE
1	B	127	THR
1	B	144	ARG
1	B	178	VAL
1	B	185	GLN
1	B	186	ARG
1	B	187	THR
1	B	196	VAL
1	B	218	LEU
2	D	4	VAL
2	D	28	VAL
2	D	37	ARG
2	D	60	CYS
2	D	69	ARG
2	D	87	VAL
2	D	91	ARG
2	D	125	LEU
2	D	198	ARG
2	D	219	LEU
2	D	227	THR
2	D	238	GLU
2	D	240	LEU
2	D	304	GLN
2	D	392	THR
2	D	415	GLN
2	D	458	LYS
2	D	468	ASN
2	D	489	GLU
2	D	490	VAL
2	D	505	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	513	GLU
2	D	560	LEU
2	D	585	LEU
2	D	606	HIS
2	D	668	LEU
2	D	679	LEU
2	D	714	ASP
2	D	715	LYS
2	D	725	THR
2	D	726	ARG
2	D	729	VAL
2	D	754	ASP
2	D	808	THR
2	D	810	ASN
2	D	814	THR
2	D	817	LEU
2	D	886	VAL
2	D	901	LEU
2	D	946	ASP
2	D	962	VAL
2	D	981	ARG
2	D	983	MET
2	D	995	VAL
2	D	998	VAL
2	D	1028	LEU
2	D	1035	PHE
2	D	1075	VAL
2	D	1085	ARG
2	D	1087	ARG
2	D	1088	VAL
2	D	1089	PHE
2	D	1156	VAL
2	D	1207	LEU
2	D	1262	THR
3	E	31	THR
3	E	53	LEU
3	E	56	TYR
3	E	66	ASP
3	E	68	TYR
3	E	92	LEU
3	E	96	LEU
3	E	107	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	51	VAL
7	G	90	THR
7	G	93	LYS
7	G	98	LYS
7	G	117	ASP
7	G	133	VAL
8	C	87	GLU
8	C	88	GLU
8	C	99	PHE
8	C	140	ILE
8	C	146	GLU
8	C	151	THR
8	C	176	VAL
8	C	270	THR
8	C	301	PHE
8	C	302	LYS
8	C	304	LYS
8	C	305	ARG
8	C	373	PHE
8	C	380	THR
8	C	421	ARG
8	C	474	ASP
8	C	519	VAL
8	C	545	ASN
8	C	570	TYR
8	C	577	ASP
8	C	690	VAL
8	C	737	LEU
8	C	772	ASP
8	C	783	ASP
8	C	830	ARG
8	C	833	ARG
8	C	881	ASP
8	C	891	ASN
8	C	919	THR
8	C	962	GLU
8	C	1063	PHE
8	C	1127	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	36	ASN
1	A	100	GLN
1	A	185	GLN
2	D	146	ASN
2	D	262	GLN
2	D	375	GLN
2	D	505	HIS
2	D	552	GLN
2	D	563	ASN
2	D	653	HIS
2	D	674	ASN
2	D	693	GLN
2	D	826	ASN
2	D	935	ASN
2	D	1032	GLN
2	D	1239	ASN
7	G	71	GLN
8	C	178	GLN
8	C	435	GLN
8	C	443	ASN
8	C	543	GLN
8	C	610	ASN
8	C	875	GLN
8	C	1055	GLN
8	C	1165	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	12/20 (60%)	5 (41%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	R	19	A
6	R	20	G
6	R	21	C
6	R	22	G
6	R	28	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no monosaccharides 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.

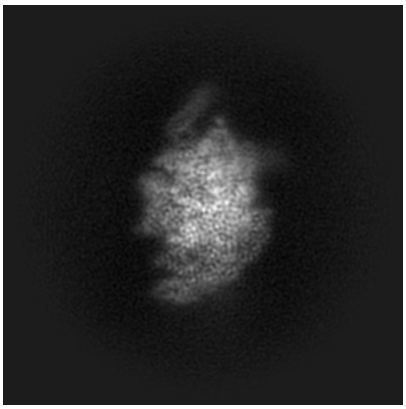
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28467. These allow visual inspection of the internal detail of the map and identification of artifacts.

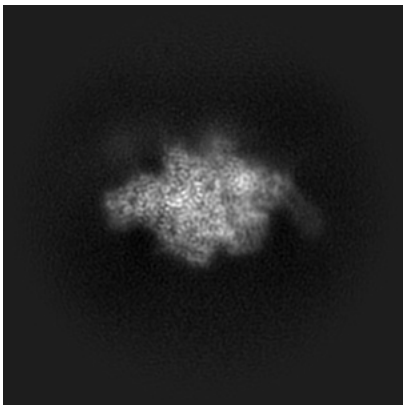
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

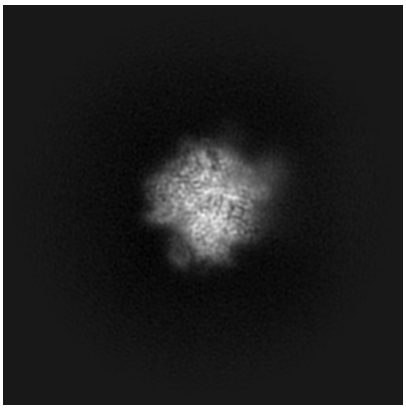
6.1.1 Primary map



X

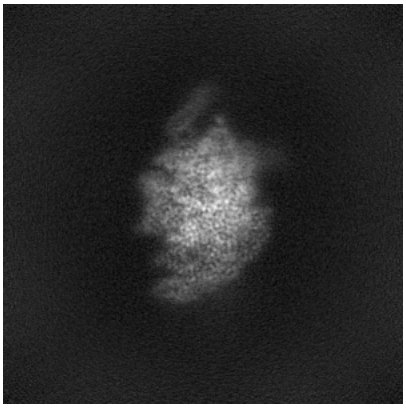


Y

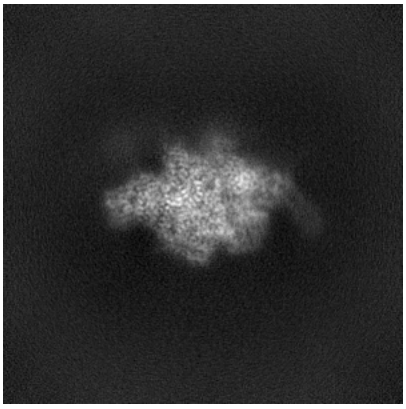


Z

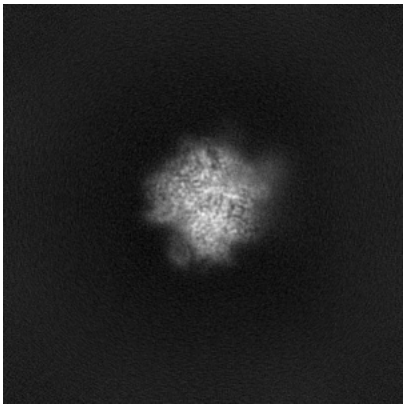
6.1.2 Raw map



X



Y

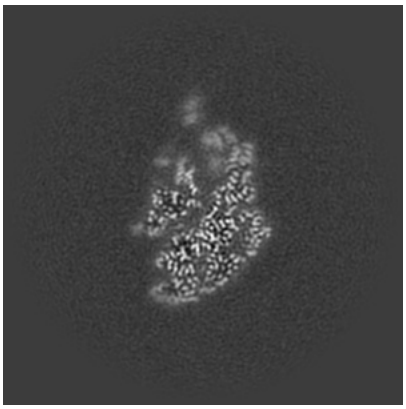


Z

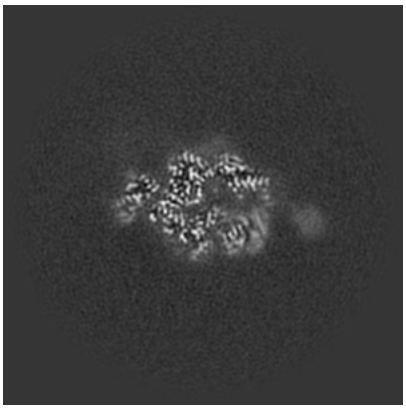
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

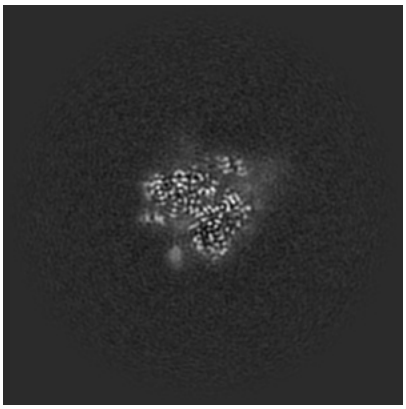
6.2.1 Primary map



X Index: 200

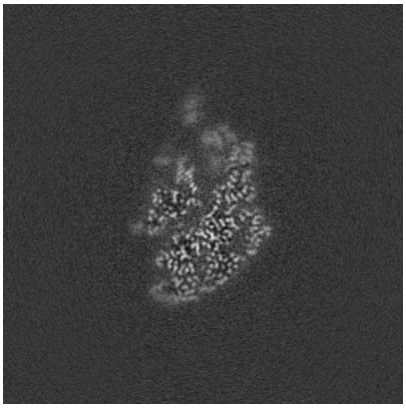


Y Index: 200

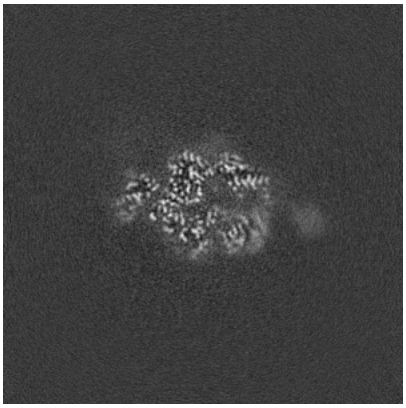


Z Index: 200

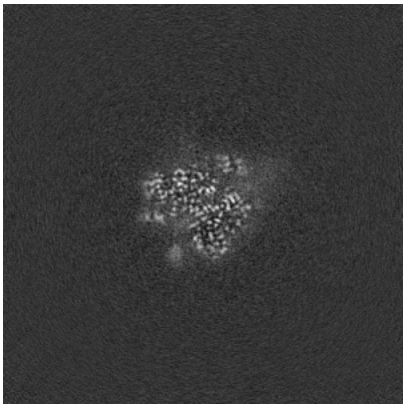
6.2.2 Raw map



X Index: 200



Y Index: 200

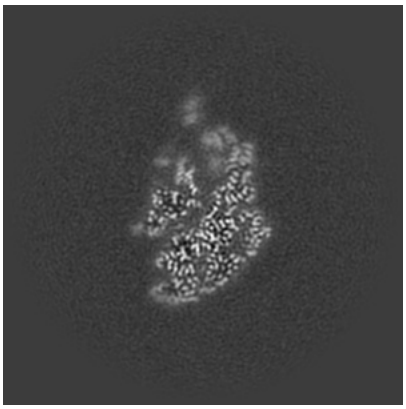


Z Index: 200

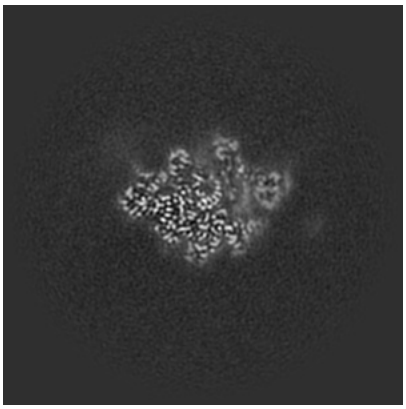
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

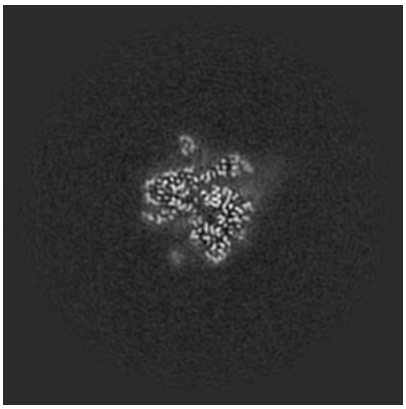
6.3.1 Primary map



X Index: 200

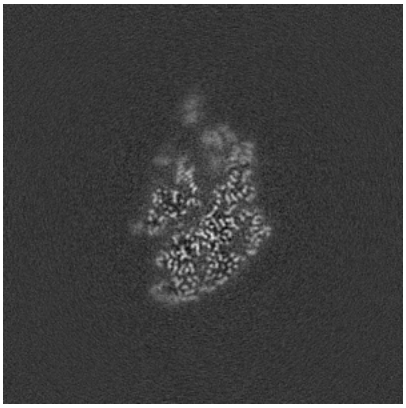


Y Index: 213

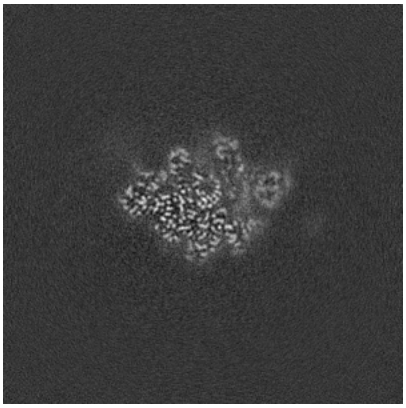


Z Index: 195

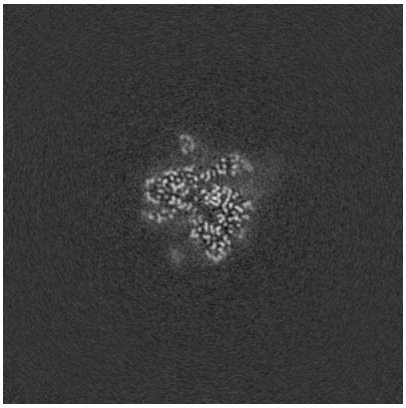
6.3.2 Raw map



X Index: 200



Y Index: 213

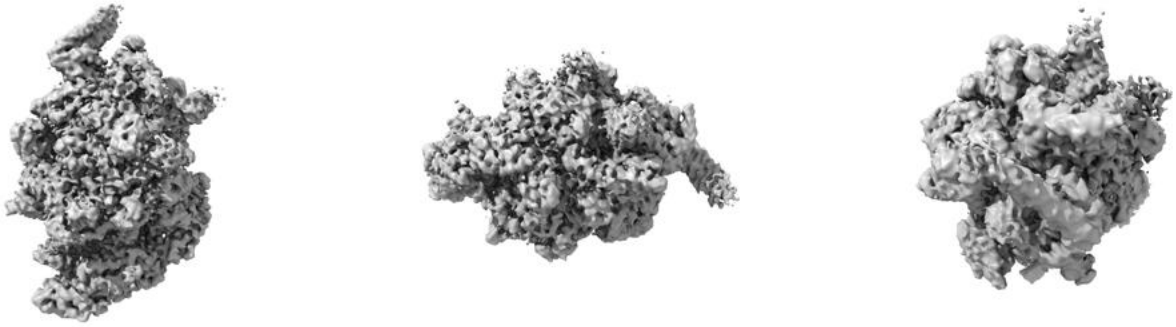


Z Index: 195

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.304. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

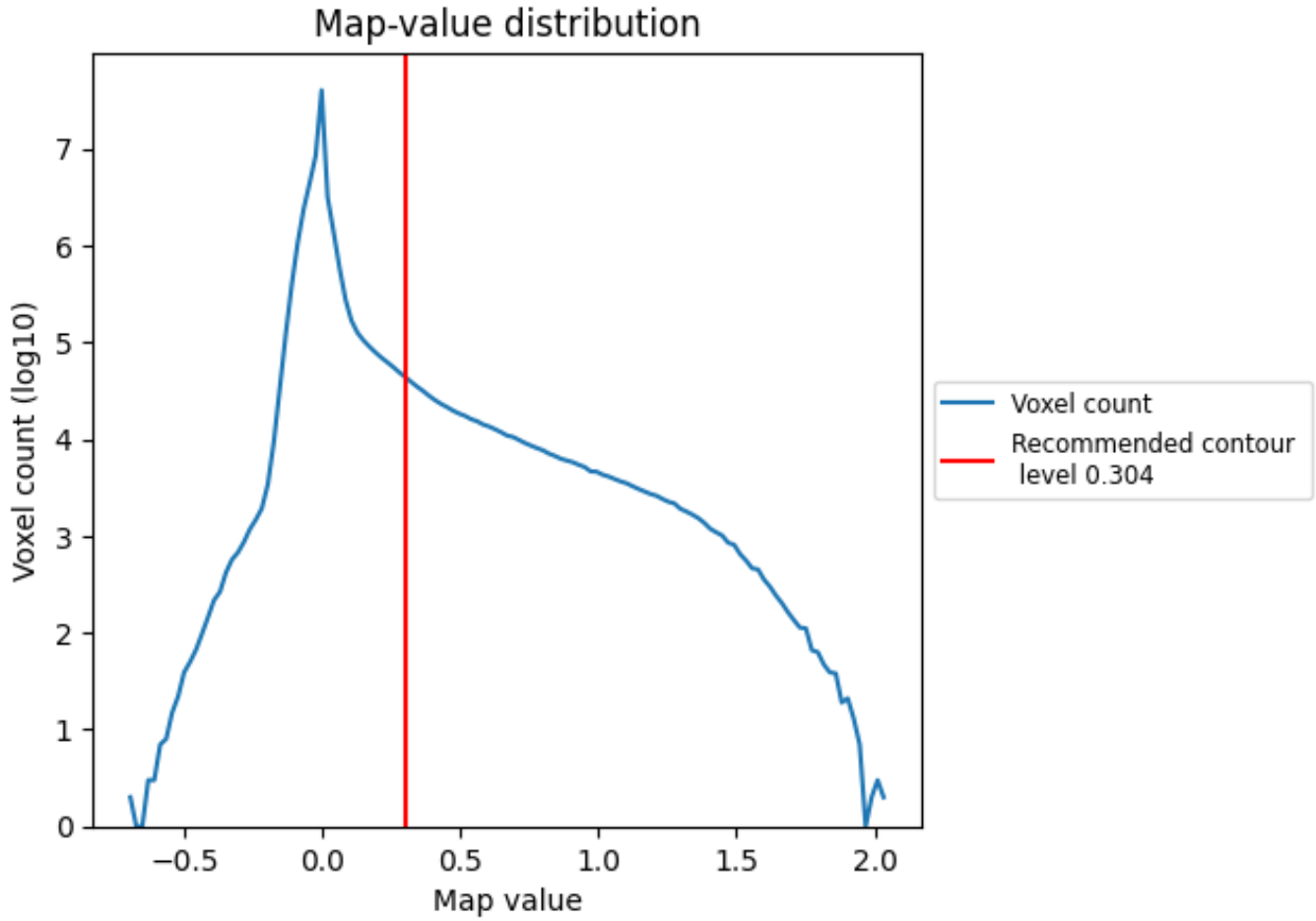
6.5 Mask visualisation (i)

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

7 Map analysis

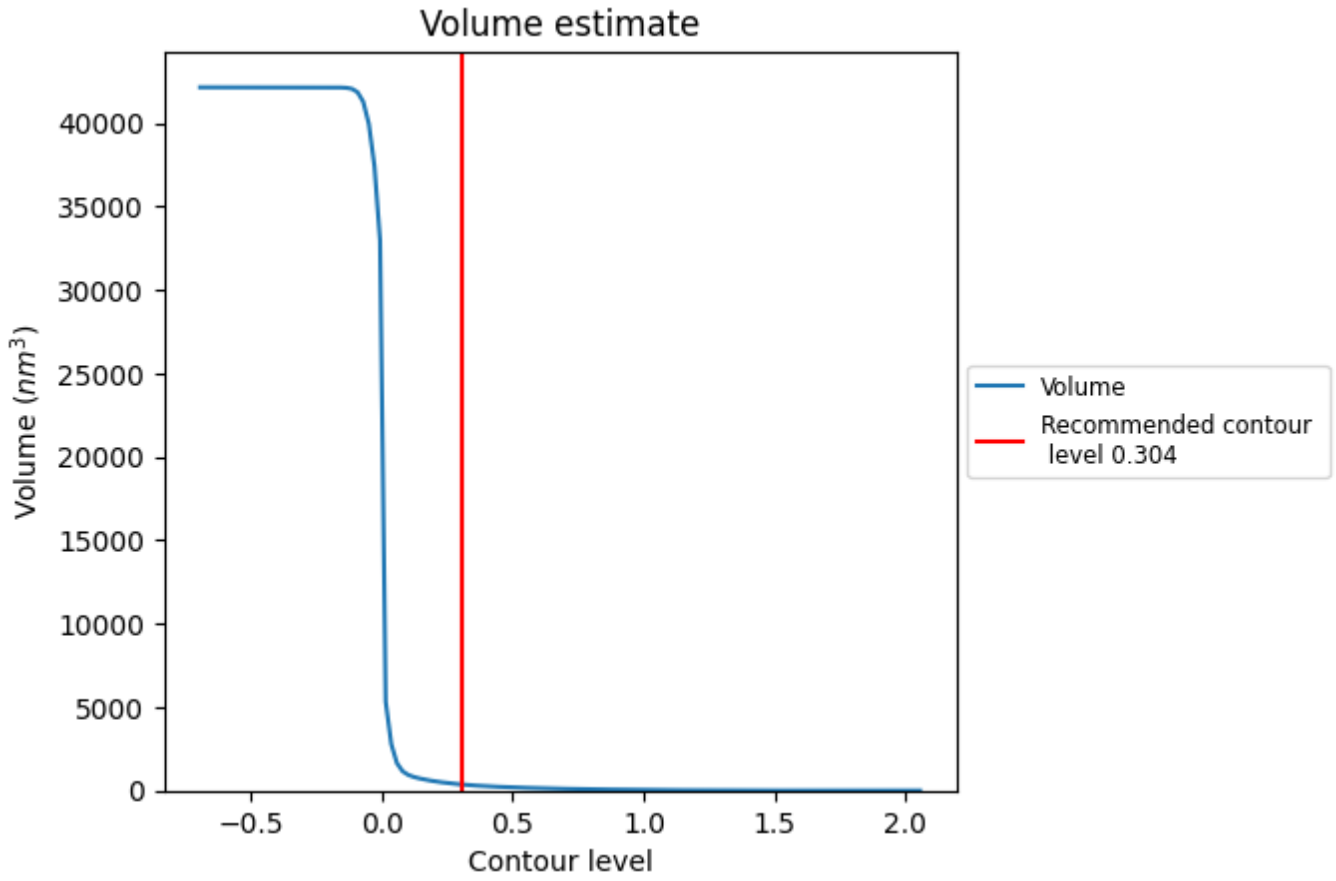
This section contains the results of statistical analysis of the map.

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.

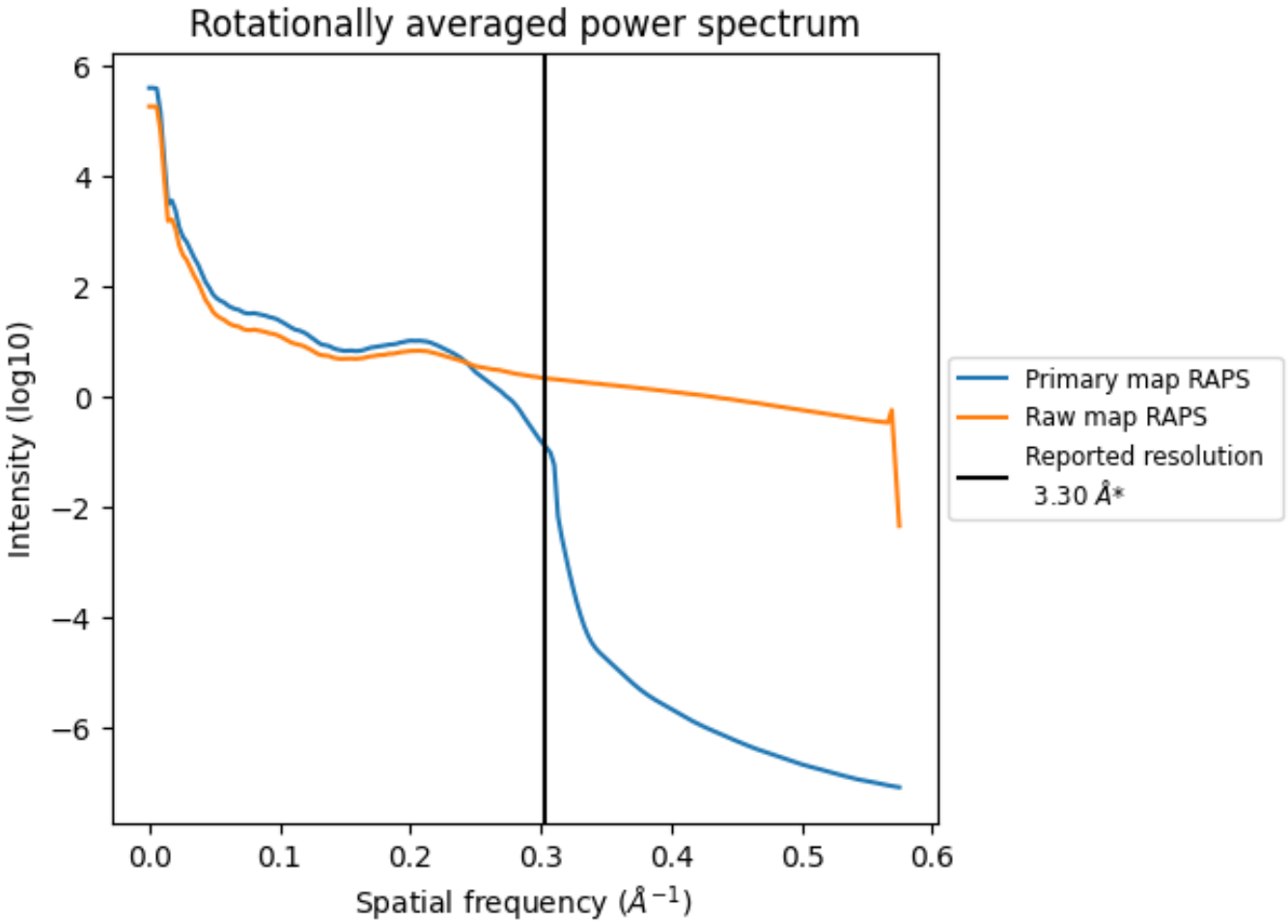
7.2 Volume estimate (i)



The volume at the recommended contour level is 366 nm^3; this corresponds to an approximate mass of 331 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)

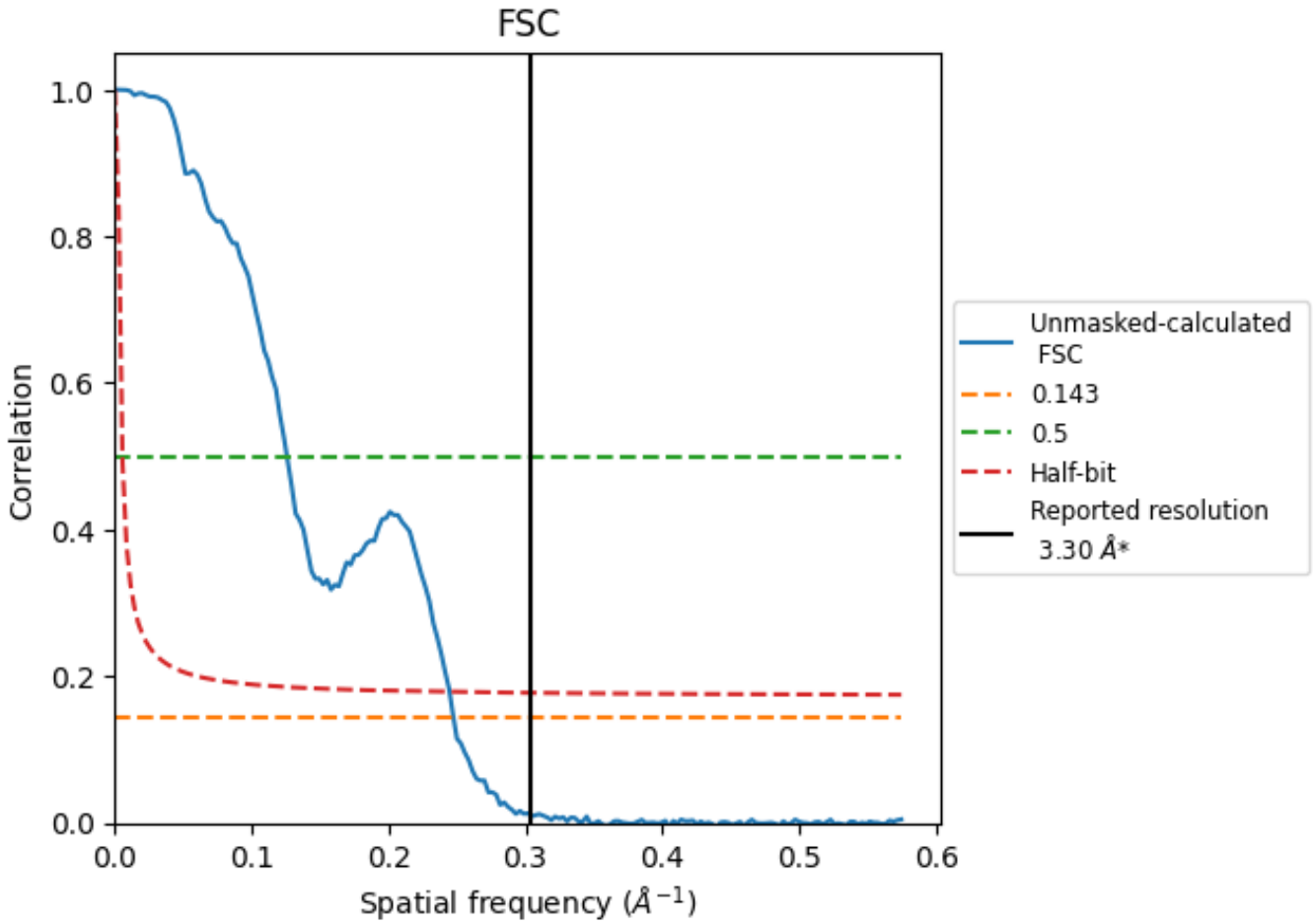


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

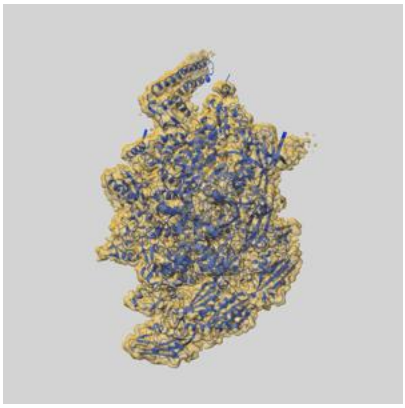
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.04	7.95	4.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.04 differs from the reported value 3.3 by more than 10 %

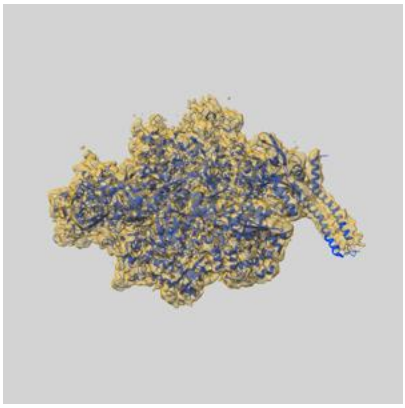
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28467 and PDB model 8EOT. Per-residue inclusion information can be found in section 3 on page 6.

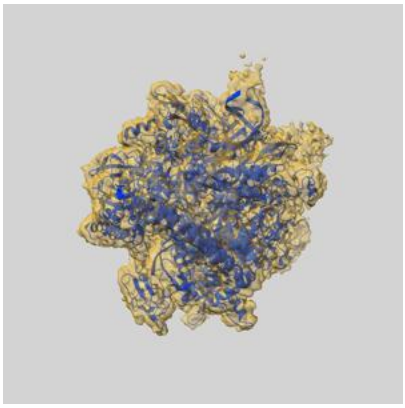
9.1 Map-model overlay



X



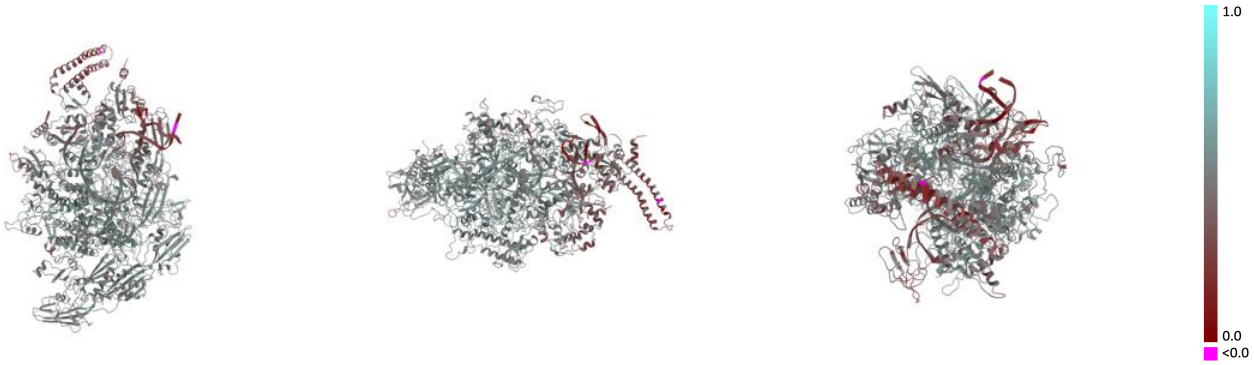
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.304 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.

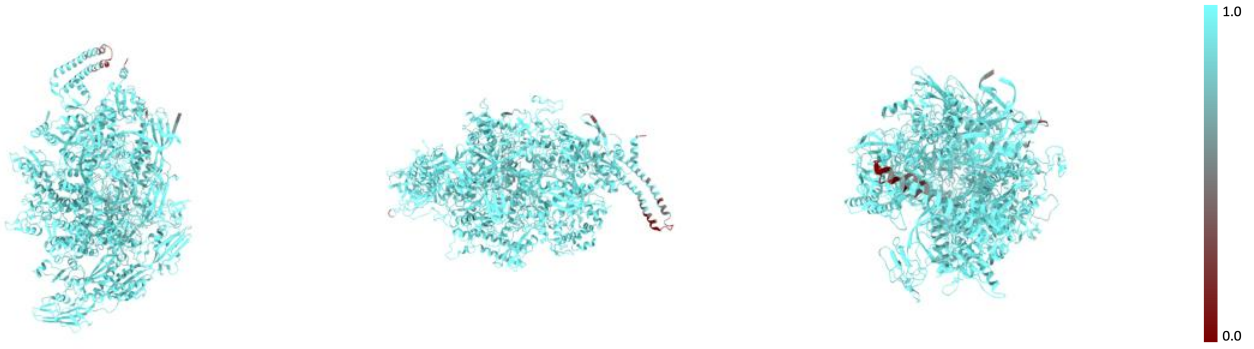
9.2 Q-score mapped to coordinate model



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.

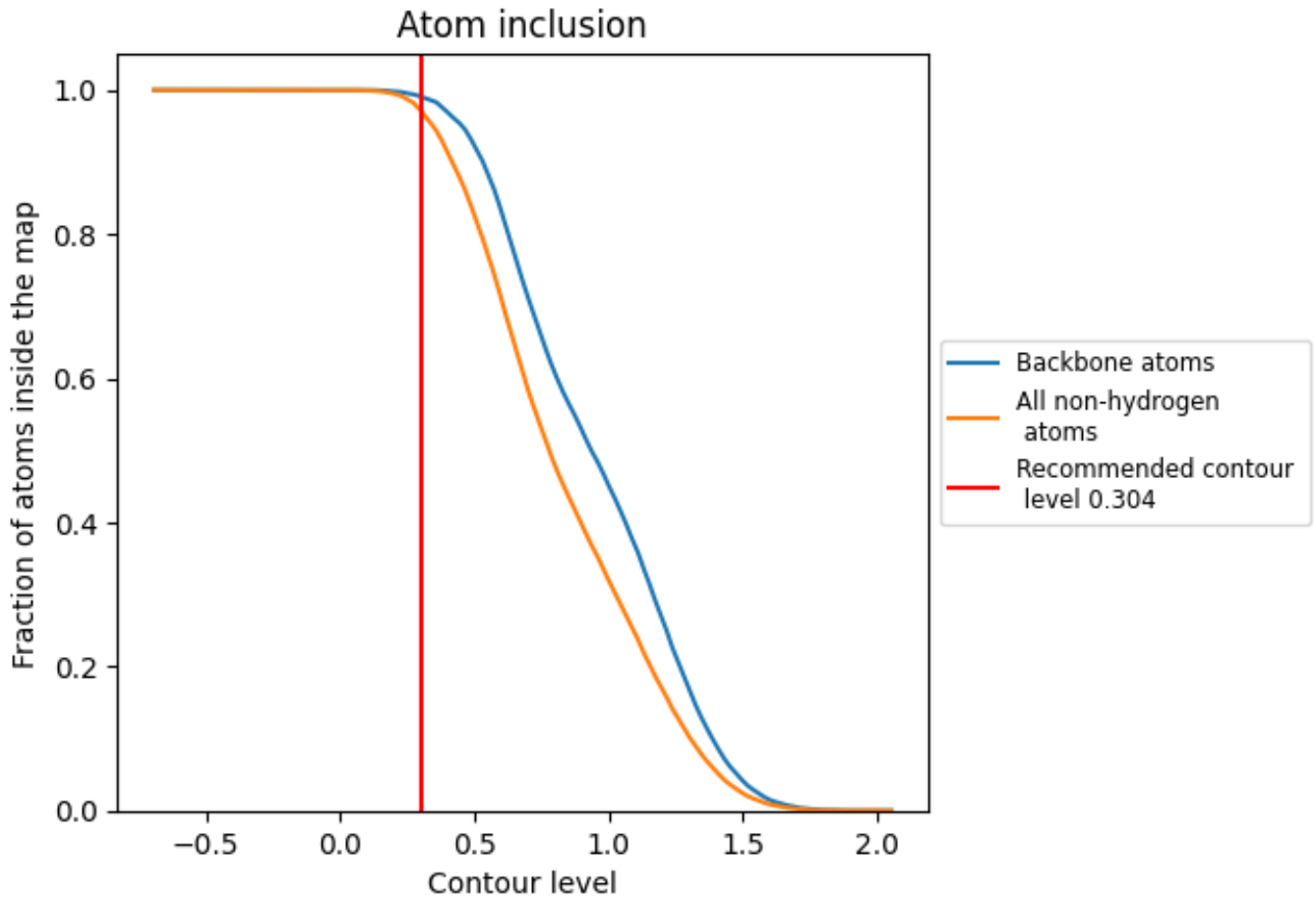
9.3 Atom inclusion mapped to coordinate model



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 (0.304).

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 (0.304) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9697	0.4840
A	0.9746	0.5150
B	0.9660	0.4930
C	0.9768	0.5060
D	0.9683	0.4860
E	0.9622	0.4980
G	0.9122	0.3670
N	0.9653	0.3140
R	0.9965	0.4560
T	0.9762	0.3990