Full wwPDB EM Validation Report (i)

Jul 8, 2024 – 02:44 am BST

PDB ID	:	7P5X
EMDB ID	:	EMD-13205
Title	:	Mycobacterial RNAP with transcriptional activator PafBC
Authors	:	Mueller, A.U.; Kummer, E.; Schilling, C.M.; Ban, N.; Weber-Ban, E.
Deposited on	:	2021-07-15
Resolution	:	3.20 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 (i) 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 (i)) were used in the production of this report:

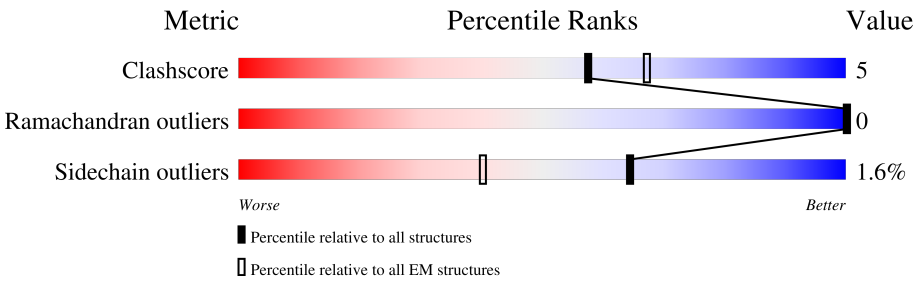
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.20 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

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	AA	350	51% 13% 36%
1	AB	350	54% 13% 33%
2	AC	1169	83% 13%
3	AD	1317	6% 84% 12%
4	AE	107	7% 69% 13% 17%
5	AF	466	58% 11% 32%
6	AJ	114	50% 70% 8% 22%
7	AO	77	51% 5% 44%

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Mol	Chain	Length	Quality of chain
8	AP	77	40% 16% 44%
9	AX	318	16% 29% 8% 62%
10	AY	331	14% 32% 5% 63%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 29465 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
			Total	C	N	O	S		
1	AA	225	1708	1075	295	336	2	0	0
1	AB	236	1790	1125	308	354	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AC	1121	8678	5424	1521	1697	36	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AD	1265	9897	6199	1794	1862	42	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	AE	89	684	433	114	137	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AF	318	2543	1588	461	487	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AJ	89	726	454	132	138	2	0	0

- Molecule 7 is a DNA chain called recA-op non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	AO	43	879	417	159	260	43	0	0

- Molecule 8 is a DNA chain called recA-op template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	AP	43	884	418	173	250	43	0	0

- Molecule 9 is a protein called PafC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	AX	121	808	506	141	158	3	0	0

- Molecule 10 is a protein called Transcriptional regulator-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AY	124	866	534	159	171	2	0	0

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

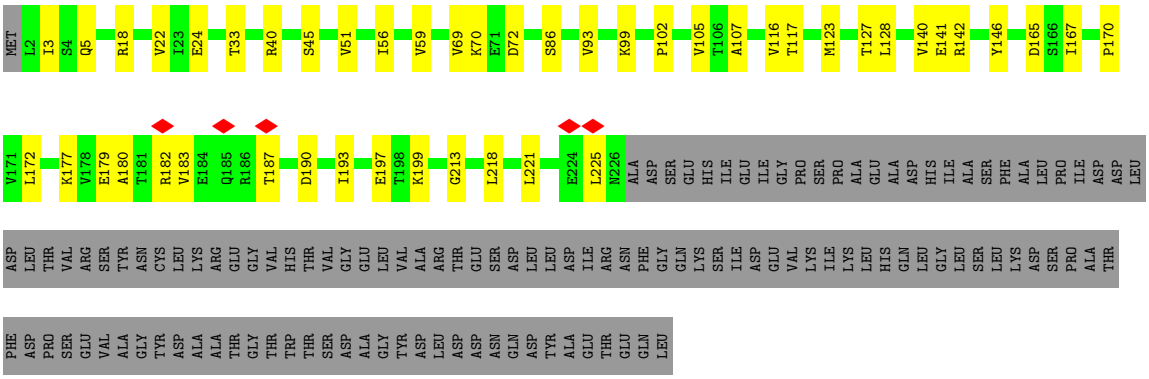
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
11	AD	2	2	2	0

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.

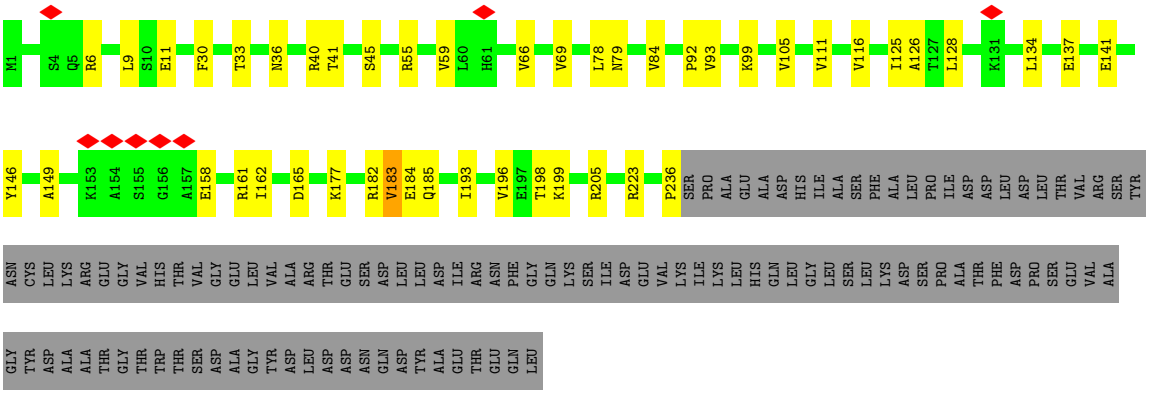
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain AA:



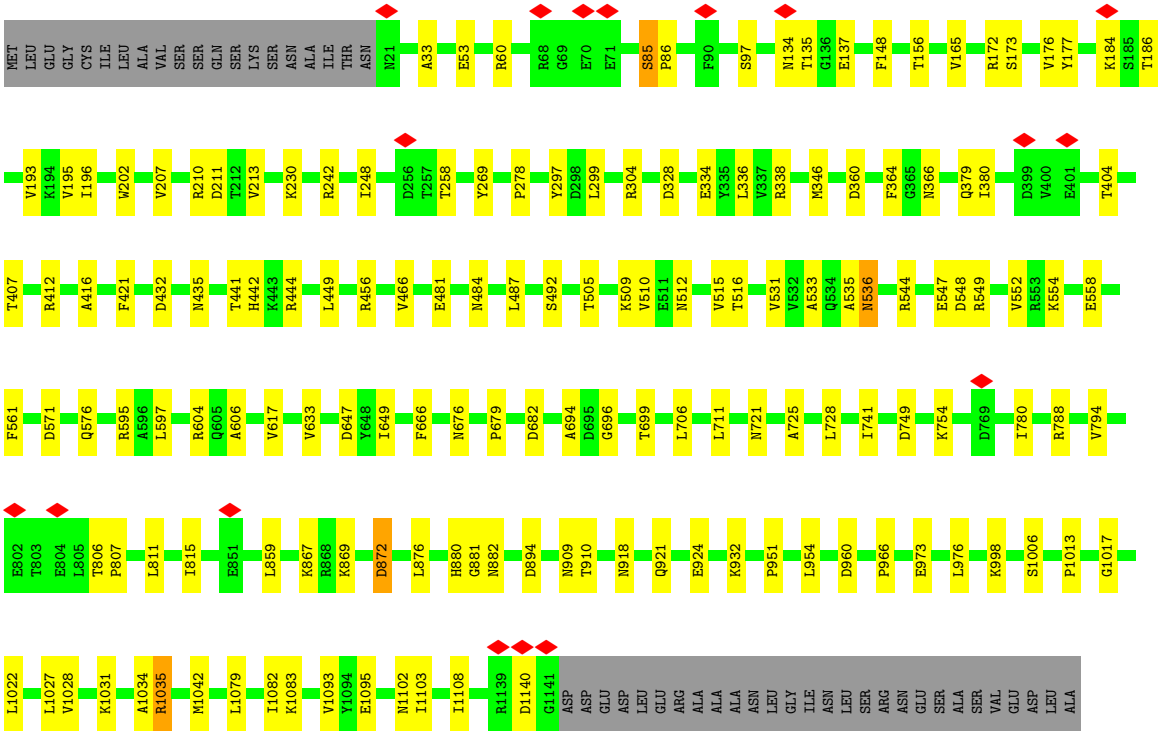
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain AB:



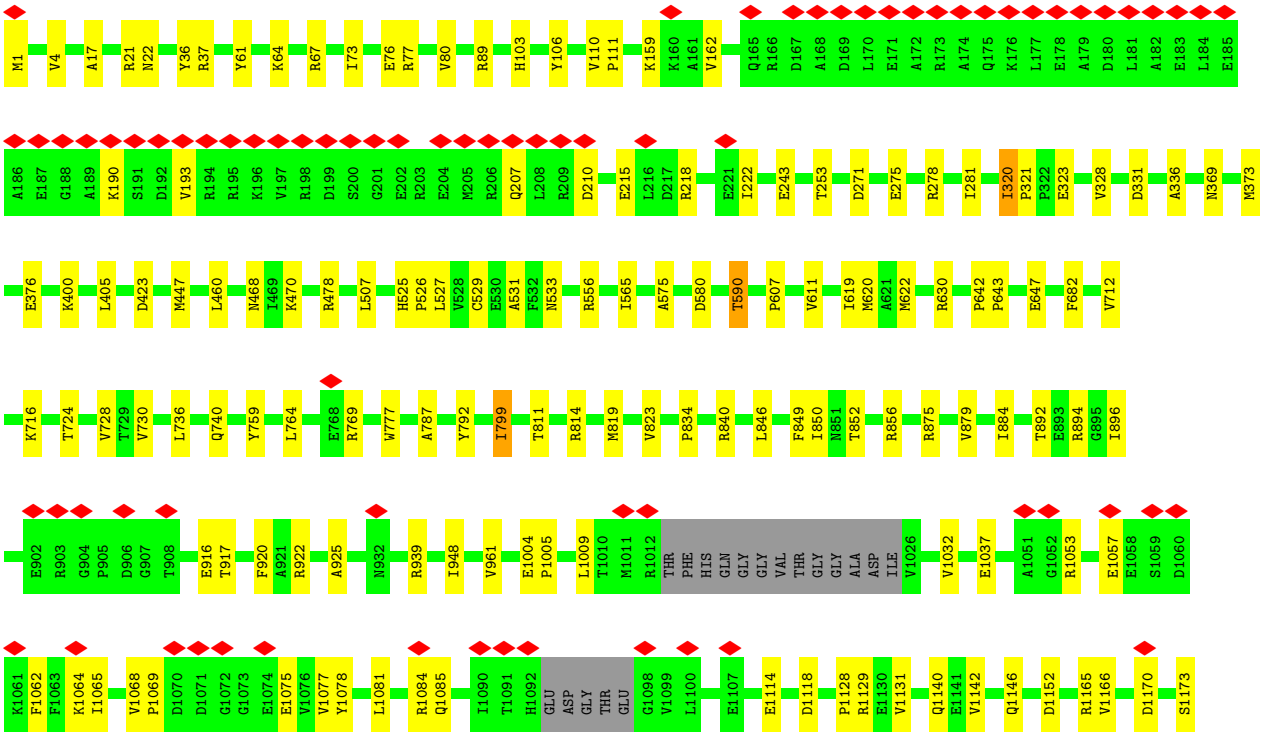
• Molecule 2: DNA-directed RNA polymerase subunit beta

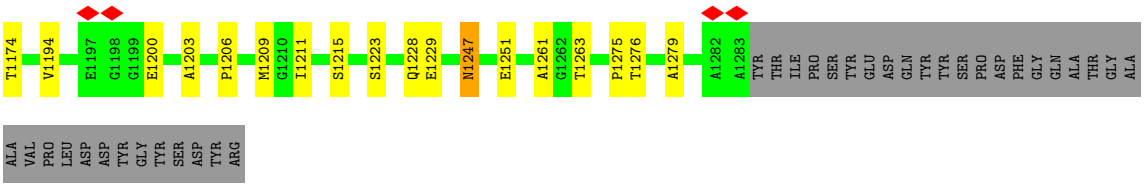
Chain AC:



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

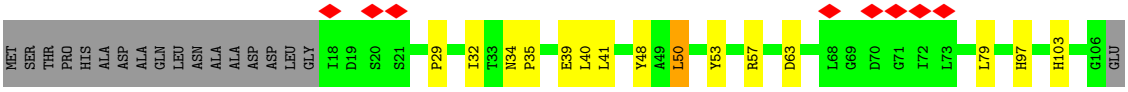
Chain AD:





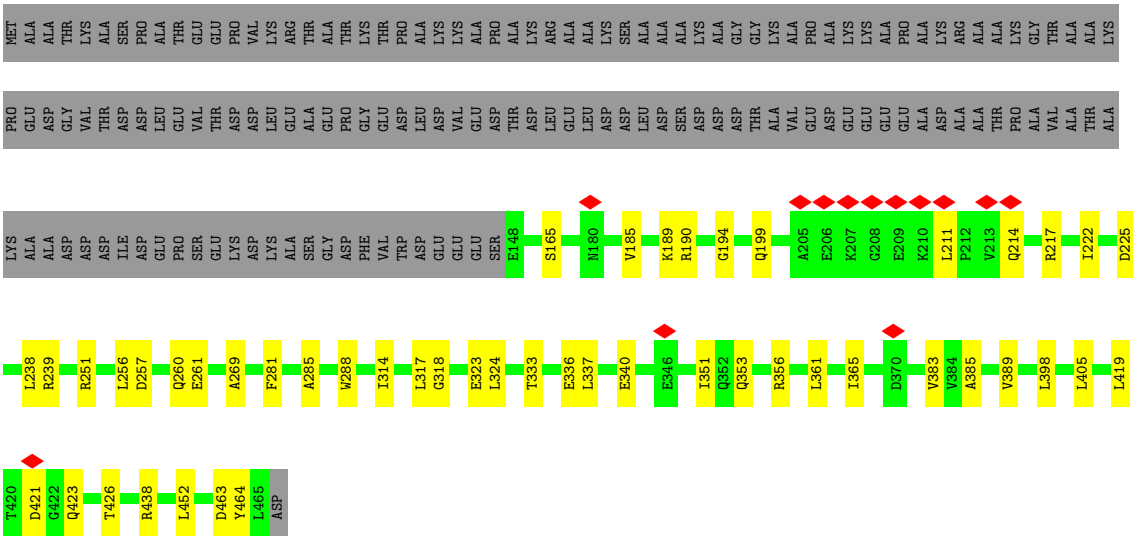
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain AE:



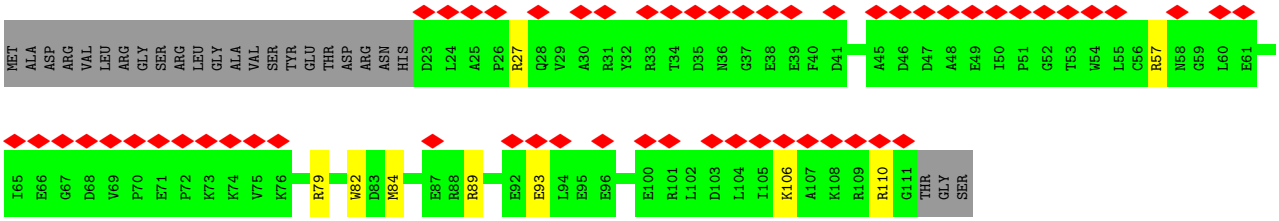
• Molecule 5: RNA polymerase sigma factor SigA

Chain AF:



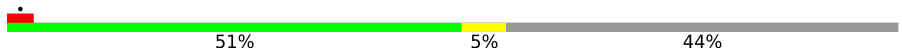
• Molecule 6: RNA polymerase-binding protein RbpA

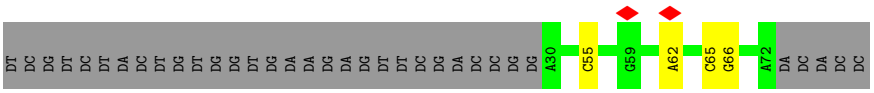
Chain AJ:



• Molecule 7: recA-op non-template strand

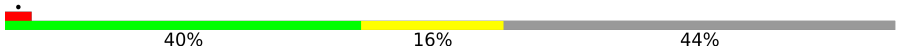
Chain AO:

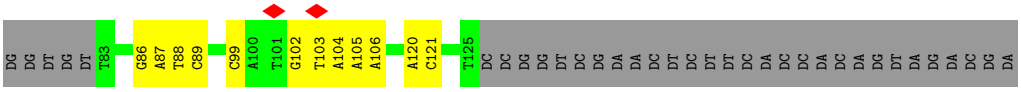




• Molecule 8: recA-op template strand

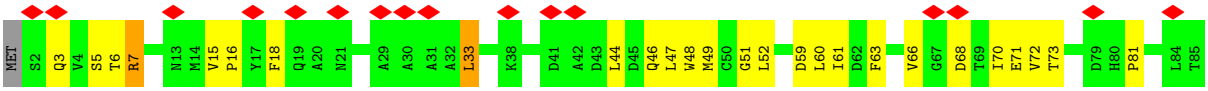
Chain AP:

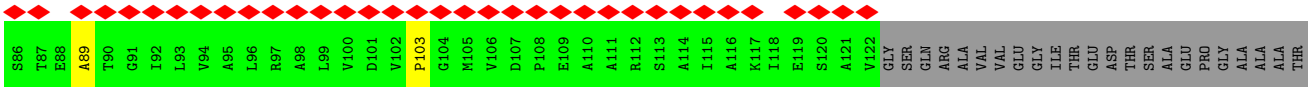




• Molecule 9: PafC

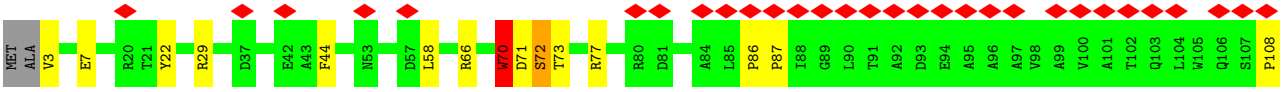
Chain AX:

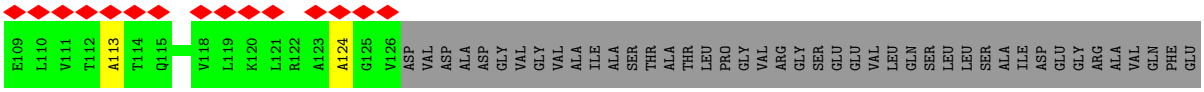


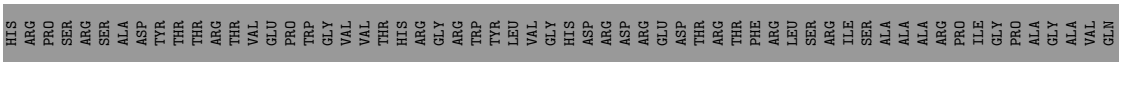


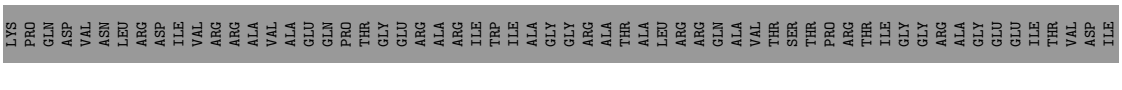
• Molecule 10: Transcriptional regulator-like protein

Chain AY:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128190	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.077	Depositor
Minimum map value	-2.122	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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: 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	AA	0.25	0/1734	0.51	0/2360
1	AB	0.25	0/1818	0.49	0/2474
2	AC	0.25	0/8831	0.50	0/11965
3	AD	0.25	0/10055	0.50	0/13584
4	AE	0.25	0/697	0.46	0/949
5	AF	0.24	0/2574	0.49	0/3468
6	AJ	0.23	0/740	0.51	0/999
7	AO	0.50	0/984	0.85	0/1516
8	AP	0.50	0/994	0.82	0/1531
9	AX	0.35	0/821	0.55	1/1126 (0.1%)
10	AY	0.46	1/876 (0.1%)	0.63	3/1191 (0.3%)
All	All	0.28	1/30124 (0.0%)	0.53	4/41163 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AY	70	TRP	CB-CG	-5.82	1.39	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AX	103	PRO	N-CA-CB	5.91	110.40	103.30
10	AY	87	PRO	N-CA-CB	5.54	109.95	103.30
10	AY	86	PRO	N-CA-CB	5.47	109.86	103.30
10	AY	108	PRO	N-CA-CB	5.39	109.77	103.30

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	AA	1708	0	1747	30	0
1	AB	1790	0	1824	26	0
2	AC	8678	0	8618	92	0
3	AD	9897	0	10037	102	0
4	AE	684	0	677	10	0
5	AF	2543	0	2590	40	0
6	AJ	726	0	723	7	0
7	AO	879	0	484	3	0
8	AP	884	0	480	9	0
9	AX	808	0	696	14	0
10	AY	866	0	769	14	0
11	AD	2	0	0	0	0
All	All	29465	0	28645	286	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 (286) 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:AF:353:GLN:CB	10:AY:70:TRP:HZ2	1.92	0.83
9:AX:5:SER:HB2	10:AY:58:LEU:HD21	1.59	0.81
3:AD:1057:GLU:HB3	3:AD:1064:LYS:HB3	1.69	0.75
1:AA:33:THR:HG21	1:AB:40:ARG:HG3	1.72	0.71
3:AD:1228:GLN:HG2	3:AD:1229:GLU:HG3	1.73	0.70
5:AF:353:GLN:HB3	10:AY:70:TRP:HZ2	1.55	0.70
3:AD:73:ILE:HG22	6:AJ:27:ARG:HD3	1.74	0.70
9:AX:89:ALA:HA	10:AY:113:ALA:HB1	1.74	0.68
3:AD:879:VAL:HG21	3:AD:1211:ILE:HB	1.74	0.68
3:AD:37:ARG:NE	10:AY:72:SER:OG	2.21	0.68
3:AD:892:THR:HG22	3:AD:894:ARG:H	1.58	0.67
2:AC:554:LYS:HB2	2:AC:558:GLU:HB2	1.77	0.67
2:AC:910:THR:HG23	3:AD:730:VAL:HG23	1.76	0.66
1:AA:93:VAL:HG21	1:AA:116:VAL:HG21	1.76	0.66
2:AC:951:PRO:HD2	2:AC:954:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:225:LEU:HD23	1:AB:9:LEU:H	1.62	0.65
2:AC:360:ASP:O	2:AC:366:ASN:ND2	2.30	0.65
5:AF:251:ARG:NH1	8:AP:105:DA:OP2	2.31	0.64
2:AC:811:LEU:HD13	5:AF:419:LEU:HD11	1.80	0.64
2:AC:666:PHE:H	2:AC:676:ASN:HB3	1.62	0.64
3:AD:369:ASN:ND2	5:AF:260:GLN:OE1	2.32	0.63
4:AE:39:GLU:OE1	4:AE:97:HIS:NE2	2.31	0.63
3:AD:1053:ARG:HB3	3:AD:1068:VAL:HB	1.79	0.63
2:AC:33:ALA:HB2	2:AC:966:PRO:HG2	1.81	0.62
4:AE:40:LEU:HB3	4:AE:50:LEU:HD11	1.80	0.62
3:AD:1140:GLN:NE2	3:AD:1152:ASP:OD1	2.33	0.62
2:AC:456:ARG:NH1	2:AC:484:ASN:OD1	2.33	0.62
3:AD:468:ASN:HD21	5:AF:463:ASP:HB2	1.63	0.62
3:AD:89:ARG:HB3	3:AD:323:GLU:HB2	1.83	0.61
2:AC:230:LYS:NZ	2:AC:258:THR:O	2.33	0.61
5:AF:353:GLN:HB3	10:AY:70:TRP:CZ2	2.36	0.61
2:AC:882:ASN:ND2	2:AC:921:GLN:OE1	2.34	0.60
2:AC:932:LYS:NZ	2:AC:960:ASP:OD1	2.30	0.59
2:AC:416:ALA:HB1	8:AP:102:DG:H2"	1.82	0.59
2:AC:1102:ASN:ND2	4:AE:63:ASP:OD1	2.35	0.59
2:AC:435:ASN:HD22	2:AC:706:LEU:HD22	1.67	0.59
3:AD:525:HIS:HE1	3:AD:527:LEU:HD12	1.67	0.58
3:AD:590:THR:HG23	3:AD:630:ARG:HD2	1.84	0.58
4:AE:29:PRO:HB2	4:AE:34:ASN:HA	1.84	0.58
1:AA:213:GLY:HA2	1:AB:223:ARG:HD3	1.86	0.58
5:AF:333:THR:OG1	5:AF:336:GLU:OE1	2.21	0.58
2:AC:973:GLU:OE1	3:AD:840:ARG:NH1	2.37	0.57
2:AC:176:VAL:HG12	2:AC:195:VAL:HG22	1.85	0.57
3:AD:37:ARG:HE	10:AY:72:SER:HG	1.46	0.57
3:AD:565:ILE:HG23	3:AD:575:ALA:HB3	1.87	0.57
5:AF:239:ARG:HG2	7:AO:55:DC:H5'	1.87	0.57
1:AB:99:LYS:HG2	1:AB:105:VAL:HG22	1.86	0.57
9:AX:46:GLN:NE2	10:AY:7:GLU:OE2	2.35	0.57
3:AD:556:ARG:HG2	4:AE:32:ILE:HD11	1.86	0.57
5:AF:365:ILE:HD12	8:AP:99:DC:H1'	1.86	0.57
1:AA:22:VAL:HG12	1:AA:193:ILE:HG12	1.87	0.56
3:AD:792:TYR:HD2	3:AD:799:ILE:HG12	1.69	0.56
1:AA:24:GLU:OE1	1:AA:182:ARG:NH1	2.38	0.56
3:AD:1247:ASN:O	3:AD:1247:ASN:ND2	2.39	0.56
1:AA:177:LYS:NZ	1:AA:179:GLU:OE2	2.39	0.56
2:AC:172:ARG:HH22	2:AC:196:ILE:HD13	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:146:TYR:OH	2:AC:869:LYS:NZ	2.40	0.55
3:AD:740:GLN:HE21	3:AD:787:ALA:HB1	1.71	0.55
10:AY:22:TYR:HA	10:AY:77:ARG:HG3	1.89	0.55
1:AB:59:VAL:HG21	1:AB:66:VAL:HG22	1.88	0.55
1:AA:40:ARG:NH1	2:AC:894:ASP:OD1	2.34	0.55
3:AD:222:ILE:HD13	3:AD:243:GLU:HG2	1.89	0.55
6:AJ:89:ARG:HH21	6:AJ:93:GLU:HB3	1.72	0.54
6:AJ:89:ARG:NE	6:AJ:93:GLU:OE1	2.40	0.54
1:AB:41:THR:O	1:AB:45:SER:HB3	2.08	0.54
3:AD:849:PHE:O	3:AD:852:THR:OG1	2.23	0.54
2:AC:505:THR:OG1	2:AC:576:GLN:NE2	2.40	0.54
3:AD:1275:PRO:HB3	4:AE:79:LEU:HD11	1.90	0.54
3:AD:400:LYS:HE2	3:AD:405:LEU:HD23	1.88	0.54
1:AB:92:PRO:HB3	1:AB:141:GLU:HG2	1.89	0.54
1:AA:172:LEU:HG	1:AA:199:LYS:HG2	1.89	0.54
3:AD:376:GLU:OE2	5:AF:165:SER:OG	2.25	0.53
5:AF:194:GLY:HA2	5:AF:222:ILE:HG22	1.90	0.53
2:AC:547:GLU:OE1	2:AC:549:ARG:N	2.40	0.53
1:AA:180:ALA:HA	1:AA:190:ASP:HA	1.90	0.53
1:AB:93:VAL:HG11	1:AB:116:VAL:HG21	1.90	0.53
3:AD:759:TYR:HA	3:AD:764:LEU:HB2	1.90	0.53
2:AC:449:LEU:HD21	2:AC:487:LEU:HD13	1.91	0.52
1:AA:72:ASP:OD1	1:AA:72:ASP:N	2.41	0.52
1:AB:162:ILE:HG23	3:AD:607:PRO:HG2	1.90	0.52
2:AC:595:ARG:NH2	2:AC:881:GLY:O	2.43	0.52
2:AC:1034:ALA:HB2	3:AD:447:MET:HG3	1.91	0.52
3:AD:1170:ASP:HB2	3:AD:1203:ALA:HB3	1.91	0.52
1:AA:102:PRO:HA	1:AA:128:LEU:O	2.09	0.52
2:AC:1079:LEU:HD23	2:AC:1083:LYS:HD2	1.91	0.52
1:AA:99:LYS:HD3	1:AA:105:VAL:HG22	1.91	0.52
3:AD:1174:THR:HG22	3:AD:1194:VAL:HG21	1.91	0.51
3:AD:1064:LYS:HE2	3:AD:1077:VAL:HG13	1.91	0.51
3:AD:925:ALA:O	3:AD:939:ARG:NH1	2.34	0.51
2:AC:1108:ILE:HG12	3:AD:4:VAL:HG22	1.93	0.51
5:AF:438:ARG:HH12	9:AX:49:MET:HG3	1.76	0.51
5:AF:318:GLY:HA3	8:AP:104:DA:H62	1.76	0.51
9:AX:51:GLY:HA3	9:AX:60:LEU:HA	1.91	0.51
2:AC:536:ASN:ND2	2:AC:536:ASN:O	2.42	0.51
3:AD:1166:VAL:HG12	3:AD:1206:PRO:HA	1.91	0.51
3:AD:814:ARG:NH1	3:AD:819:MET:O	2.44	0.51
2:AC:135:THR:HG23	2:AC:137:GLU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AD:162:VAL:HG21	3:AD:215:GLU:HG2	1.92	0.50
3:AD:879:VAL:HG22	3:AD:1215:SER:HB3	1.92	0.50
4:AE:41:LEU:HD12	4:AE:50:LEU:HD12	1.93	0.50
9:AX:47:LEU:HB3	9:AX:61:ILE:HD11	1.93	0.50
3:AD:1173:SER:OG	3:AD:1200:GLU:O	2.23	0.50
3:AD:643:PRO:HG3	3:AD:682:PHE:HB3	1.93	0.50
3:AD:507:LEU:HB3	3:AD:531:ALA:HB1	1.93	0.50
3:AD:470:LYS:HD3	5:AF:464:TYR:HA	1.94	0.50
3:AD:642:PRO:HB2	3:AD:647:GLU:HB2	1.93	0.50
1:AB:198:THR:OG1	1:AB:199:LYS:N	2.45	0.49
3:AD:875:ARG:NH1	3:AD:1037:GLU:OE2	2.45	0.49
1:AA:45:SER:HG	1:AB:30:PHE:HZ	1.61	0.49
2:AC:807:PRO:HB2	5:AF:419:LEU:HD23	1.95	0.49
5:AF:353:GLN:HG3	10:AY:70:TRP:CZ2	2.48	0.49
2:AC:444:ARG:NH2	2:AC:492:SER:O	2.45	0.49
4:AE:34:ASN:HB3	4:AE:35:PRO:HD3	1.95	0.49
5:AF:317:LEU:HD11	5:AF:337:LEU:HD13	1.94	0.48
1:AA:3:ILE:HG22	1:AA:5:GLN:H	1.78	0.48
3:AD:619:ILE:HA	3:AD:622:MET:HG2	1.96	0.48
3:AD:916:GLU:HG3	3:AD:917:THR:HG23	1.95	0.48
1:AB:69:VAL:HG21	1:AB:126:ALA:HB1	1.95	0.48
3:AD:736:LEU:HB2	3:AD:792:TYR:CE1	2.49	0.48
8:AP:120:DA:H2"	8:AP:121:DC:H5'	1.96	0.48
2:AC:207:VAL:HG22	2:AC:213:VAL:HG12	1.96	0.48
2:AC:1082:ILE:HD12	2:AC:1093:VAL:HG21	1.94	0.48
3:AD:1263:THR:HG22	4:AE:48:TYR:HB3	1.96	0.47
1:AB:6:ARG:HD2	1:AB:236:PRO:HD2	1.95	0.47
9:AX:7:ARG:HE	9:AX:7:ARG:HB2	1.59	0.47
2:AC:1095:GLU:HG2	5:AF:389:VAL:HB	1.96	0.47
5:AF:199:GLN:HG2	6:AJ:82:TRP:CZ2	2.50	0.47
1:AA:51:VAL:HG12	1:AA:140:VAL:HG22	1.96	0.47
1:AA:69:VAL:HG22	1:AA:128:LEU:HD22	1.97	0.47
2:AC:338:ARG:HD2	2:AC:346:MET:HG3	1.97	0.47
2:AC:880:HIS:NE2	2:AC:924:GLU:OE1	2.44	0.47
3:AD:215:GLU:OE2	3:AD:218:ARG:NH1	2.48	0.47
3:AD:373:MET:SD	5:AF:256:LEU:HB3	2.55	0.47
9:AX:63:PHE:CE1	9:AX:72:VAL:HG22	2.49	0.47
3:AD:759:TYR:CG	3:AD:769:ARG:HD3	2.50	0.47
1:AB:36:ASN:ND2	2:AC:1006:SER:O	2.48	0.47
2:AC:53:GLU:OE2	2:AC:60:ARG:NH1	2.47	0.47
2:AC:998:LYS:HB3	2:AC:1013:PRO:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:79:ASN:ND2	1:AB:125:ILE:O	2.45	0.47
5:AF:314:ILE:HG12	5:AF:351:ILE:HG23	1.96	0.46
9:AX:15:VAL:HB	9:AX:16:PRO:HD3	1.97	0.46
1:AA:165:ASP:OD2	2:AC:869:LYS:NZ	2.40	0.46
1:AB:128:LEU:HD21	1:AB:134:LEU:HB2	1.96	0.46
2:AC:749:ASP:HB3	2:AC:859:LEU:HD13	1.97	0.46
3:AD:922:ARG:HD3	3:AD:961:VAL:HG21	1.97	0.46
5:AF:211:LEU:HD12	5:AF:211:LEU:H	1.81	0.46
3:AD:1065:ILE:HB	3:AD:1078:TYR:HD2	1.81	0.46
5:AF:405:LEU:HD11	5:AF:452:LEU:HD11	1.96	0.46
2:AC:535:ALA:HB2	2:AC:571:ASP:HB2	1.97	0.46
3:AD:525:HIS:CE1	3:AD:527:LEU:HD12	2.49	0.46
3:AD:527:LEU:HD13	3:AD:712:VAL:HG12	1.97	0.45
3:AD:527:LEU:HD11	3:AD:716:LYS:HB2	1.99	0.45
3:AD:1069:PRO:HD3	3:AD:1075:GLU:HA	1.98	0.45
2:AC:509:LYS:O	2:AC:516:THR:OG1	2.22	0.45
2:AC:1035:ARG:NH2	3:AD:423:ASP:OD1	2.48	0.45
3:AD:529:CYS:O	3:AD:533:ASN:N	2.49	0.45
3:AD:64:LYS:NZ	3:AD:76:GLU:OE2	2.40	0.45
3:AD:1223:SER:OG	3:AD:1251:GLU:OE2	2.23	0.45
1:AA:18:ARG:HG2	1:AA:197:GLU:HB2	1.99	0.45
1:AA:170:PRO:HA	1:AA:199:LYS:HE2	1.98	0.45
2:AC:404:THR:O	2:AC:407:THR:HG22	2.17	0.45
3:AD:103:HIS:HB3	3:AD:106:TYR:HD2	1.82	0.45
3:AD:36:TYR:OH	3:AD:37:ARG:NH1	2.49	0.45
5:AF:353:GLN:CG	10:AY:70:TRP:HZ2	2.29	0.45
1:AA:107:ALA:HB2	1:AA:123:MET:HG2	1.99	0.44
2:AC:512:ASN:O	2:AC:544:ARG:NH1	2.50	0.44
3:AD:190:LYS:HG3	3:AD:193:VAL:HG12	1.99	0.44
5:AF:190:ARG:NH2	5:AF:225:ASP:OD1	2.49	0.44
1:AB:78:LEU:HD21	3:AD:611:VAL:HG12	2.00	0.44
2:AC:134:ASN:OD1	2:AC:135:THR:N	2.51	0.44
2:AC:1093:VAL:HG22	2:AC:1103:ILE:HG23	2.00	0.44
1:AA:86:SER:HB3	1:AA:117:THR:HG23	1.99	0.44
2:AC:412:ARG:HE	8:AP:103:DT:H5”	1.82	0.44
3:AD:17:ALA:O	3:AD:21:ARG:HG2	2.17	0.44
3:AD:336:ALA:HB1	5:AF:361:LEU:HG	1.99	0.44
2:AC:815:ILE:HD11	5:AF:452:LEU:HD23	2.00	0.44
2:AC:297:TYR:HE1	2:AC:299:LEU:HG	1.82	0.44
3:AD:61:TYR:HB2	3:AD:80:VAL:HG21	1.99	0.44
1:AA:218:LEU:O	1:AA:221:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AD:320:ILE:HG12	3:AD:321:PRO:HD2	1.99	0.44
3:AD:331:ASP:OD1	3:AD:331:ASP:N	2.51	0.44
5:AF:324:LEU:HD21	5:AF:340:GLU:HG2	2.00	0.44
9:AX:33:LEU:H	9:AX:33:LEU:HG	1.73	0.44
3:AD:846:LEU:O	3:AD:850:ILE:HG13	2.18	0.43
2:AC:85:SER:O	2:AC:97:SER:HA	2.18	0.43
2:AC:304:ARG:NH2	2:AC:328:ASP:OD2	2.31	0.43
2:AC:441:THR:HG21	2:AC:604:ARG:HD3	2.00	0.43
5:AF:185:VAL:HG12	5:AF:189:LYS:HE2	1.99	0.43
2:AC:184:LYS:NZ	3:AD:1084:ARG:HH22	2.15	0.43
2:AC:872:ASP:OD1	2:AC:872:ASP:N	2.51	0.43
3:AD:1085:GLN:NE2	3:AD:1114:GLU:O	2.47	0.43
9:AX:3:GLN:N	9:AX:3:GLN:OE1	2.51	0.43
2:AC:811:LEU:HD22	5:AF:398:LEU:HD21	1.99	0.43
3:AD:1165:ARG:HD2	3:AD:1209:MET:SD	2.58	0.43
1:AB:55:ARG:NH1	1:AB:137:GLU:OE1	2.41	0.43
2:AC:156:THR:HG22	2:AC:165:VAL:HG22	2.00	0.43
9:AX:18:PHE:HE2	9:AX:44:LEU:HD21	1.84	0.43
2:AC:432:ASP:H	2:AC:442:HIS:HD2	1.66	0.43
2:AC:711:LEU:HD12	2:AC:1017:GLY:O	2.19	0.43
1:AA:141:GLU:HG2	1:AA:142:ARG:H	1.84	0.43
1:AA:183:VAL:HG22	1:AA:187:THR:HA	2.00	0.43
2:AC:148:PHE:HE1	2:AC:380:ILE:HD11	1.84	0.43
2:AC:647:ASP:OD1	2:AC:647:ASP:N	2.52	0.43
2:AC:754:LYS:HE3	2:AC:754:LYS:HB2	1.87	0.43
3:AD:1009:LEU:HD12	3:AD:1146:GLN:HG3	2.01	0.43
5:AF:214:GLN:HA	5:AF:217:ARG:HE	1.84	0.43
1:AB:182:ARG:HH11	1:AB:185:GLN:H	1.67	0.42
2:AC:211:ASP:HB3	2:AC:248:ILE:HG22	2.01	0.42
2:AC:780:ILE:HG23	2:AC:794:VAL:HG22	2.01	0.42
2:AC:1042:MET:SD	3:AD:328:VAL:HG11	2.59	0.42
3:AD:920:PHE:HE1	3:AD:948:ILE:HG13	1.83	0.42
3:AD:1276:THR:HG23	3:AD:1279:ALA:H	1.83	0.42
5:AF:383:VAL:HG12	5:AF:385:ALA:H	1.83	0.42
8:AP:86:DG:H2"	8:AP:87:DA:H5'	2.01	0.42
9:AX:52:LEU:HB2	9:AX:59:ASP:HB3	2.01	0.42
1:AA:56:ILE:HB	1:AA:59:VAL:HG22	2.01	0.42
3:AD:278:ARG:HA	3:AD:281:ILE:HG22	2.01	0.42
1:AB:11:GLU:OE1	1:AB:205:ARG:NH2	2.51	0.42
1:AB:84:VAL:HG12	1:AB:199:LYS:HD3	2.01	0.42
1:AB:183:VAL:HG23	1:AB:184:GLU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AC:728:LEU:HD11	2:AC:876:LEU:HD11	2.00	0.42
1:AA:24:GLU:HB2	1:AA:182:ARG:HD2	2.01	0.42
1:AB:146:TYR:HB2	3:AD:620:MET:HE2	2.02	0.42
3:AD:159:LYS:O	3:AD:162:VAL:HG12	2.20	0.42
3:AD:1118:ASP:OD1	3:AD:1118:ASP:N	2.51	0.42
5:AF:281:PHE:CE2	5:AF:285:ALA:HB2	2.54	0.42
3:AD:811:THR:HG23	3:AD:814:ARG:HH21	1.84	0.42
3:AD:884:ILE:HD13	3:AD:1261:ALA:HB2	2.01	0.42
2:AC:788:ARG:HH21	3:AD:478:ARG:HH21	1.66	0.42
3:AD:207:GLN:HA	3:AD:210:ASP:OD2	2.20	0.42
3:AD:875:ARG:O	3:AD:879:VAL:HG23	2.19	0.42
5:AF:421:ASP:OD1	5:AF:421:ASP:N	2.52	0.42
4:AE:57:ARG:HA	4:AE:57:ARG:HD2	1.86	0.42
8:AP:105:DA:H4'	8:AP:106:DA:OP2	2.18	0.42
2:AC:533:ALA:HA	2:AC:552:VAL:HG12	2.02	0.42
3:AD:110:VAL:HA	3:AD:111:PRO:HA	1.91	0.42
10:AY:29:ARG:HB2	10:AY:44:PHE:CZ	2.54	0.42
2:AC:481:GLU:HB3	2:AC:597:LEU:HD21	2.01	0.41
1:AB:149:ALA:N	1:AB:165:ASP:OD1	2.54	0.41
2:AC:85:SER:OG	2:AC:86:PRO:HD3	2.20	0.41
3:AD:22:ASN:O	6:AJ:57:ARG:NH2	2.53	0.41
1:AA:146:TYR:HD1	1:AA:167:ILE:HG13	1.85	0.41
2:AC:242:ARG:NH1	2:AC:334:GLU:OE1	2.37	0.41
2:AC:549:ARG:HB3	2:AC:561:PHE:CD1	2.55	0.41
2:AC:649:ILE:HD11	2:AC:679:PRO:HB3	2.02	0.41
1:AB:158:GLU:HG2	1:AB:161:ARG:HG2	2.02	0.41
2:AC:696:GLY:H	2:AC:699:THR:HB	1.85	0.41
3:AD:1004:GLU:HB3	3:AD:1005:PRO:HD3	2.03	0.41
6:AJ:106:LYS:HG3	6:AJ:110:ARG:NE	2.36	0.41
5:AF:257:ASP:O	5:AF:261:GLU:HG2	2.20	0.41
2:AC:741:ILE:HG12	2:AC:867:LYS:HG2	2.03	0.41
1:AA:70:LYS:NZ	2:AC:682:ASP:OD1	2.53	0.41
2:AC:173:SER:O	2:AC:177:TYR:OH	2.21	0.41
2:AC:909:ASN:OD1	2:AC:910:THR:N	2.54	0.41
3:AD:525:HIS:CD2	3:AD:526:PRO:HD2	2.56	0.41
5:AF:234:LEU:O	5:AF:238:LEU:HG	2.21	0.41
5:AF:353:GLN:CB	10:AY:70:TRP:CZ2	2.85	0.41
6:AJ:79:ARG:HH21	6:AJ:84:MET:HG2	1.85	0.41
8:AP:88:DT:H2"	8:AP:89:DC:H5'	2.03	0.41
2:AC:510:VAL:HG12	2:AC:515:VAL:HG13	2.03	0.41
2:AC:606:ALA:HB2	2:AC:1022:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AC:749:ASP:OD1	2:AC:749:ASP:N	2.50	0.41
2:AC:918:ASN:O	2:AC:921:GLN:HG2	2.20	0.41
2:AC:1140:ASP:HB2	3:AD:1:MET:HB2	2.03	0.41
3:AD:271:ASP:O	3:AD:275:GLU:HG2	2.21	0.41
3:AD:1062:PHE:HA	3:AD:1081:LEU:O	2.20	0.41
3:AD:1128:PRO:HA	3:AD:1131:VAL:HG12	2.03	0.41
9:AX:81:PRO:HG3	10:AY:124:ALA:HB2	2.03	0.41
2:AC:202:TRP:HH2	7:AO:62:DA:H8	1.68	0.41
2:AC:547:GLU:OE1	2:AC:548:ASP:N	2.53	0.40
2:AC:633:VAL:HB	2:AC:694:ALA:HB3	2.03	0.40
3:AD:64:LYS:HD2	3:AD:77:ARG:HH22	1.86	0.40
3:AD:777:TRP:CD2	3:AD:834:PRO:HG3	2.56	0.40
3:AD:1032:VAL:HG23	3:AD:1142:VAL:HG11	2.02	0.40
2:AC:193:VAL:HG12	2:AC:336:LEU:HD22	2.01	0.40
7:AO:65:DC:H2'	7:AO:66:DG:C8	2.56	0.40
2:AC:269:TYR:CD1	2:AC:278:PRO:HB3	2.57	0.40
2:AC:379:GLN:HG3	2:AC:421:PHE:HB2	2.03	0.40
3:AD:896:ILE:HD12	3:AD:1129:ARG:CZ	2.52	0.40
5:AF:269:ALA:HB2	5:AF:288:TRP:HB2	2.02	0.40
2:AC:466:VAL:HG23	3:AD:856:ARG:HD2	2.03	0.40
2:AC:721:ASN:HA	2:AC:725:ALA:HB3	2.04	0.40
2:AC:1027:LEU:O	2:AC:1031:LYS:HG2	2.21	0.40
3:AD:67:ARG:HD2	5:AF:423:GLN:HB3	2.02	0.40
1:AB:177:LYS:HE3	1:AB:193:ILE:HD12	2.03	0.40
3:AD:190:LYS:HZ3	3:AD:193:VAL:H	1.70	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	AA	223/350 (64%)	215 (96%)	8 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	234/350 (67%)	226 (97%)	8 (3%)	0	100	100
2	AC	1119/1169 (96%)	1079 (96%)	40 (4%)	0	100	100
3	AD	1259/1317 (96%)	1225 (97%)	34 (3%)	0	100	100
4	AE	87/107 (81%)	86 (99%)	1 (1%)	0	100	100
5	AF	316/466 (68%)	301 (95%)	15 (5%)	0	100	100
6	AJ	87/114 (76%)	81 (93%)	6 (7%)	0	100	100
9	AX	119/318 (37%)	112 (94%)	7 (6%)	0	100	100
10	AY	122/331 (37%)	119 (98%)	3 (2%)	0	100	100
All	All	3566/4522 (79%)	3444 (97%)	122 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AA	192/297 (65%)	191 (100%)	1 (0%)	88	95
1	AB	201/297 (68%)	197 (98%)	4 (2%)	55	80
2	AC	945/984 (96%)	933 (99%)	12 (1%)	69	87
3	AD	1055/1095 (96%)	1045 (99%)	10 (1%)	78	91
4	AE	73/86 (85%)	70 (96%)	3 (4%)	30	66
5	AF	270/379 (71%)	267 (99%)	3 (1%)	73	88
6	AJ	78/98 (80%)	78 (100%)	0	100	100
9	AX	65/248 (26%)	56 (86%)	9 (14%)	3	16
10	AY	72/261 (28%)	66 (92%)	6 (8%)	11	40
All	All	2951/3745 (79%)	2903 (98%)	48 (2%)	64	84

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	127	THR
1	AB	33	THR
1	AB	111	VAL
1	AB	183	VAL
1	AB	196	VAL
2	AC	85	SER
2	AC	186	THR
2	AC	210	ARG
2	AC	364	PHE
2	AC	531	VAL
2	AC	536	ASN
2	AC	617	VAL
2	AC	806	THR
2	AC	872	ASP
2	AC	976	LEU
2	AC	1028	VAL
2	AC	1035	ARG
3	AD	253	THR
3	AD	320	ILE
3	AD	460	LEU
3	AD	580	ASP
3	AD	590	THR
3	AD	724	THR
3	AD	728	VAL
3	AD	799	ILE
3	AD	823	VAL
3	AD	1247	ASN
4	AE	50	LEU
4	AE	53	TYR
4	AE	103	HIS
5	AF	323	GLU
5	AF	356	ARG
5	AF	426	THR
9	AX	6	THR
9	AX	7	ARG
9	AX	33	LEU
9	AX	48	TRP
9	AX	66	VAL
9	AX	68	ASP
9	AX	70	ILE
9	AX	71	GLU
9	AX	73	THR
10	AY	3	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	AY	66	ARG
10	AY	70	TRP
10	AY	71	ASP
10	AY	72	SER
10	AY	73	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	AD	369	ASN
5	AF	260	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 2 ligands modelled in this entry, 2 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

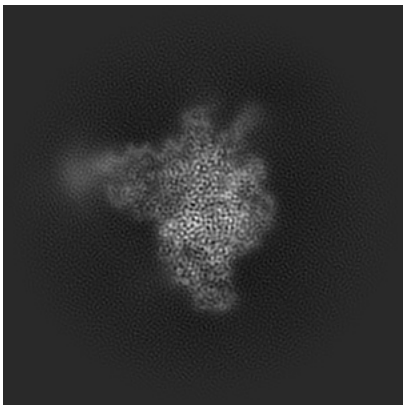
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13205. These allow visual inspection of the internal detail of the map and identification of artifacts.

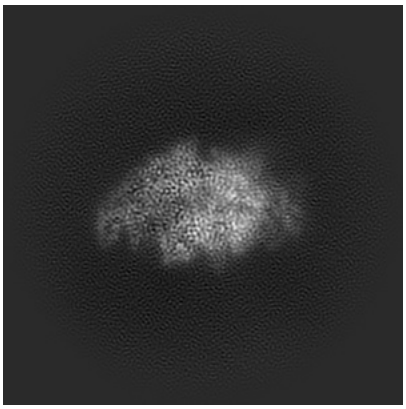
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

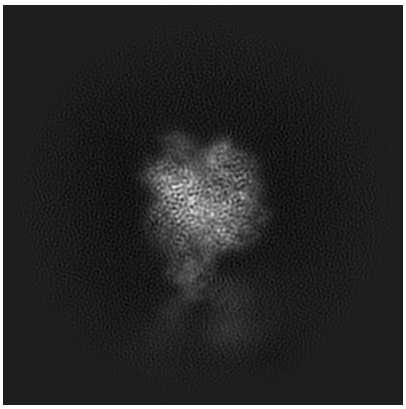
6.1.1 Primary map



X

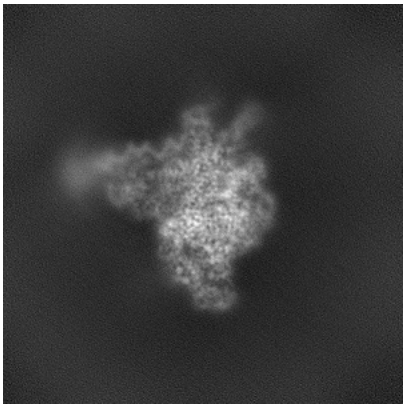


Y

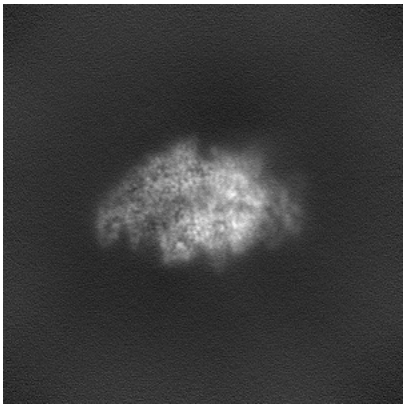


Z

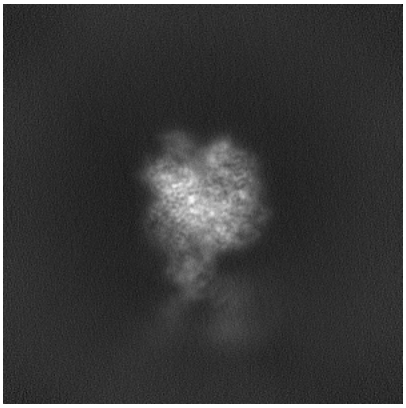
6.1.2 Raw map



X



Y

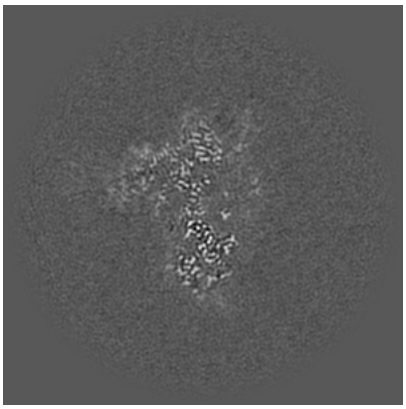


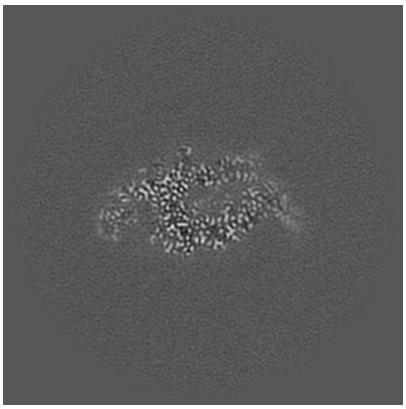
Z

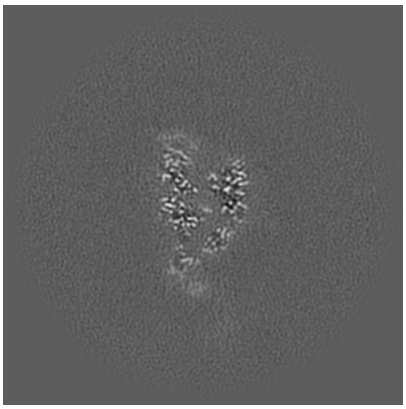
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

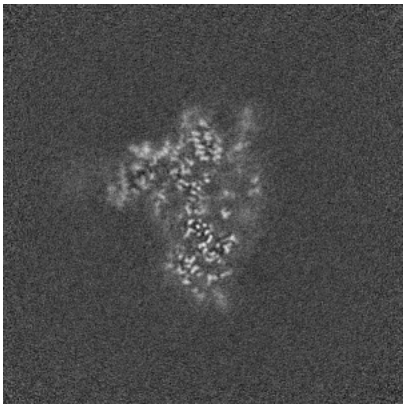
6.2.1 Primary map

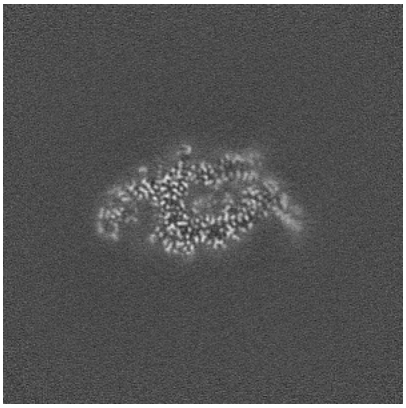

X Index: 200

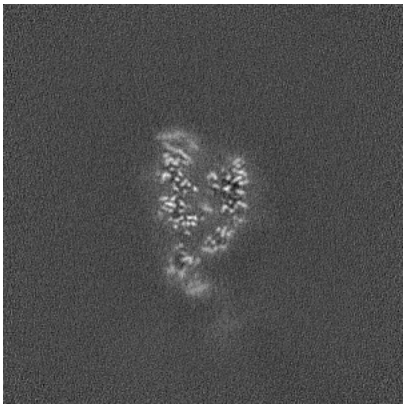

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

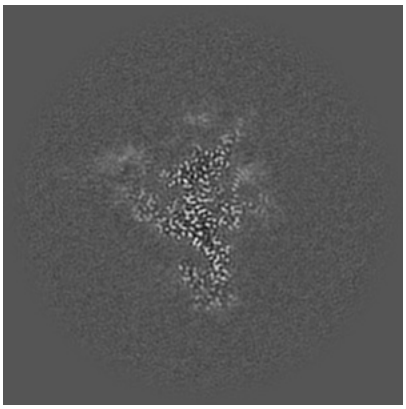

Y Index: 200

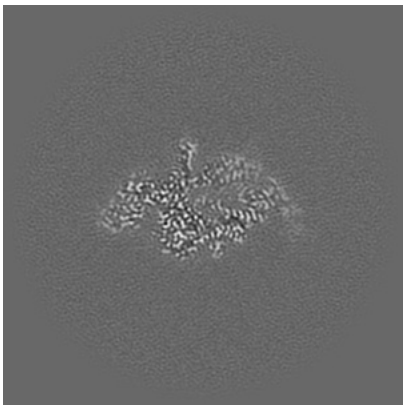

Z Index: 200

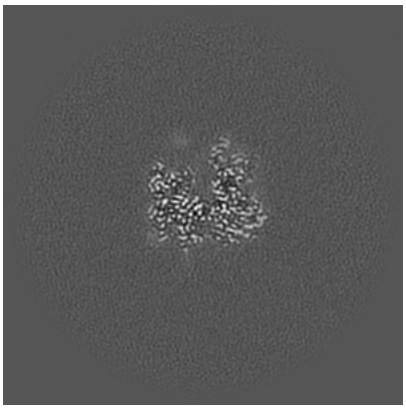
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

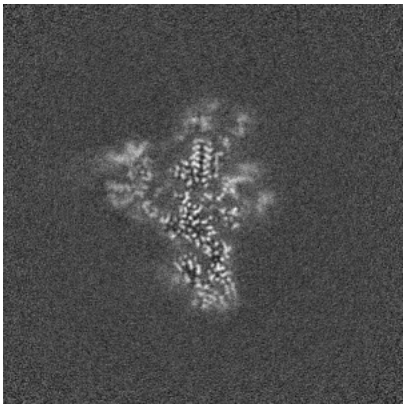
6.3.1 Primary map

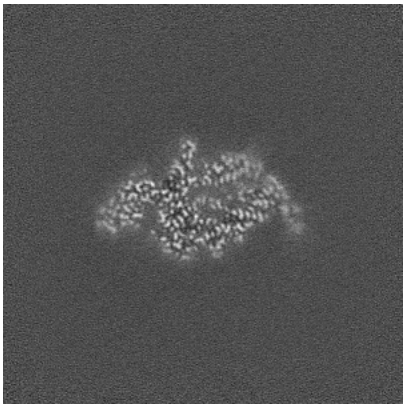

X Index: 183

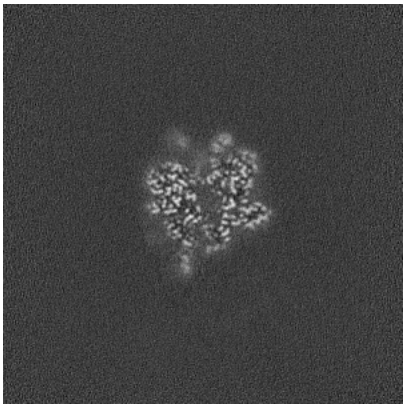

Y Index: 194


Z Index: 180

6.3.2 Raw map


X Index: 188

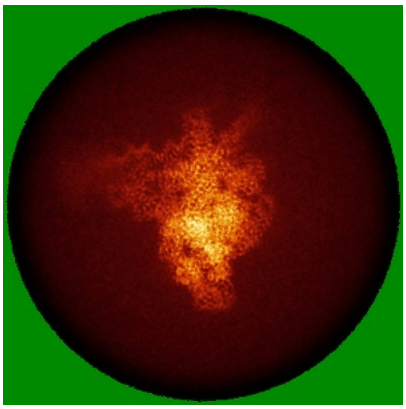

Y Index: 195

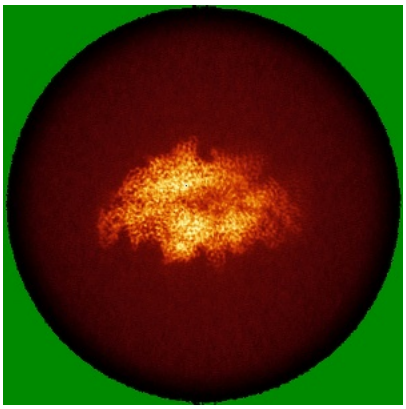

Z Index: 186

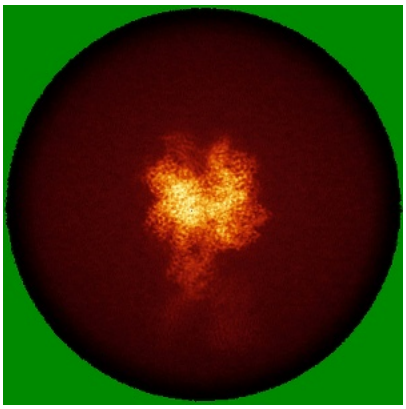
The images above show the largest variance slices of the map in three orthogonal directions.

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

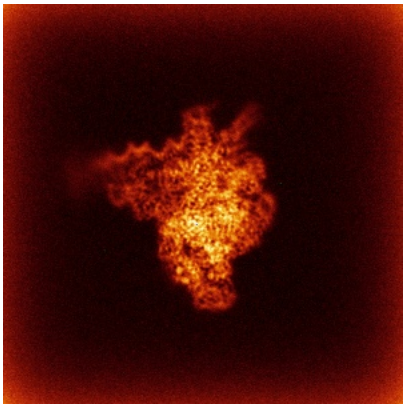
6.4.1 Primary map

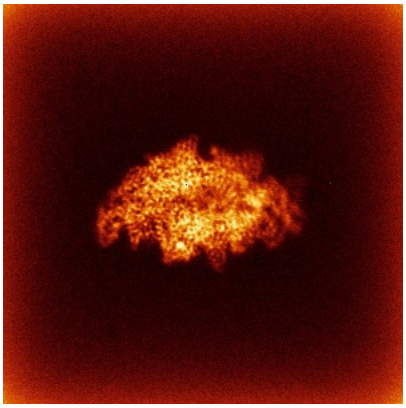

X

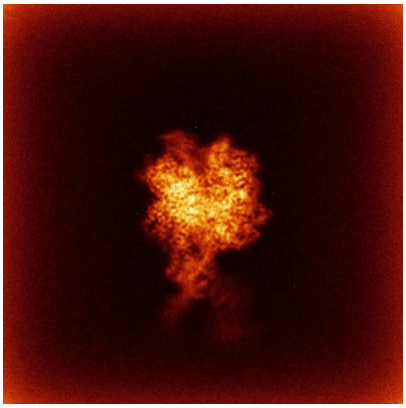

Y


Z

6.4.2 Raw map


X

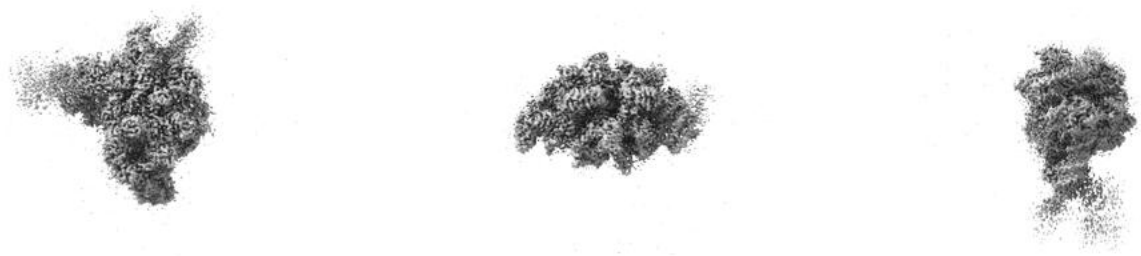

Y


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 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

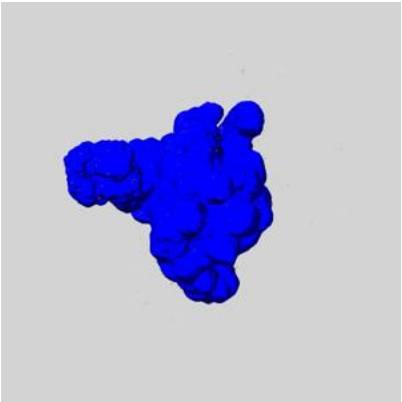
6.6 Mask visualisation (i)

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

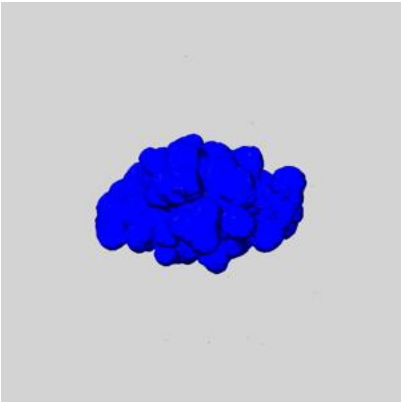
A mask typically either:

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

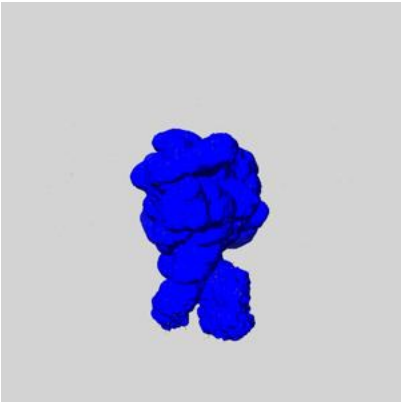
6.6.1 emd_13205_msk_1.map (i)



X



Y

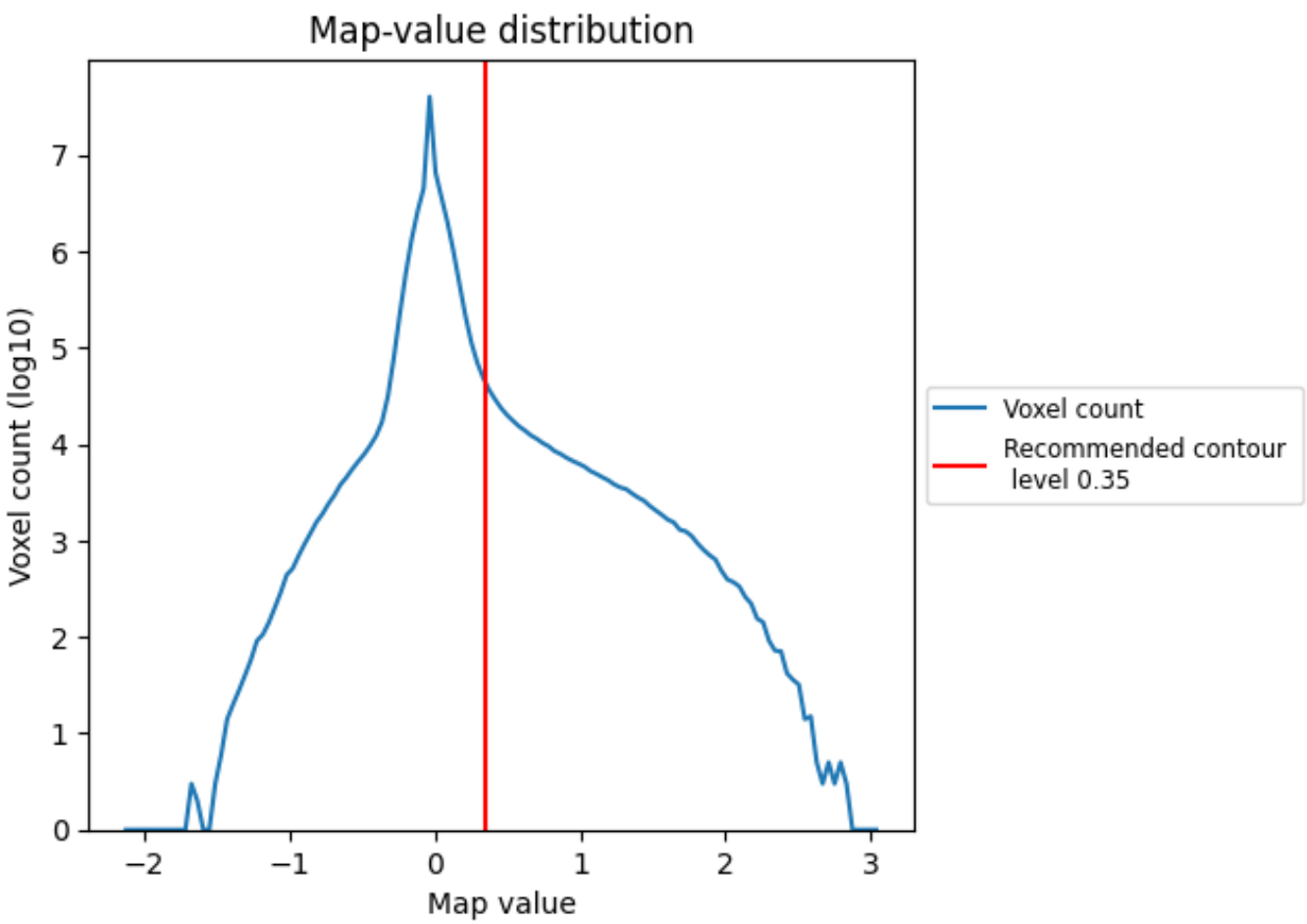


Z

7 Map analysis (i)

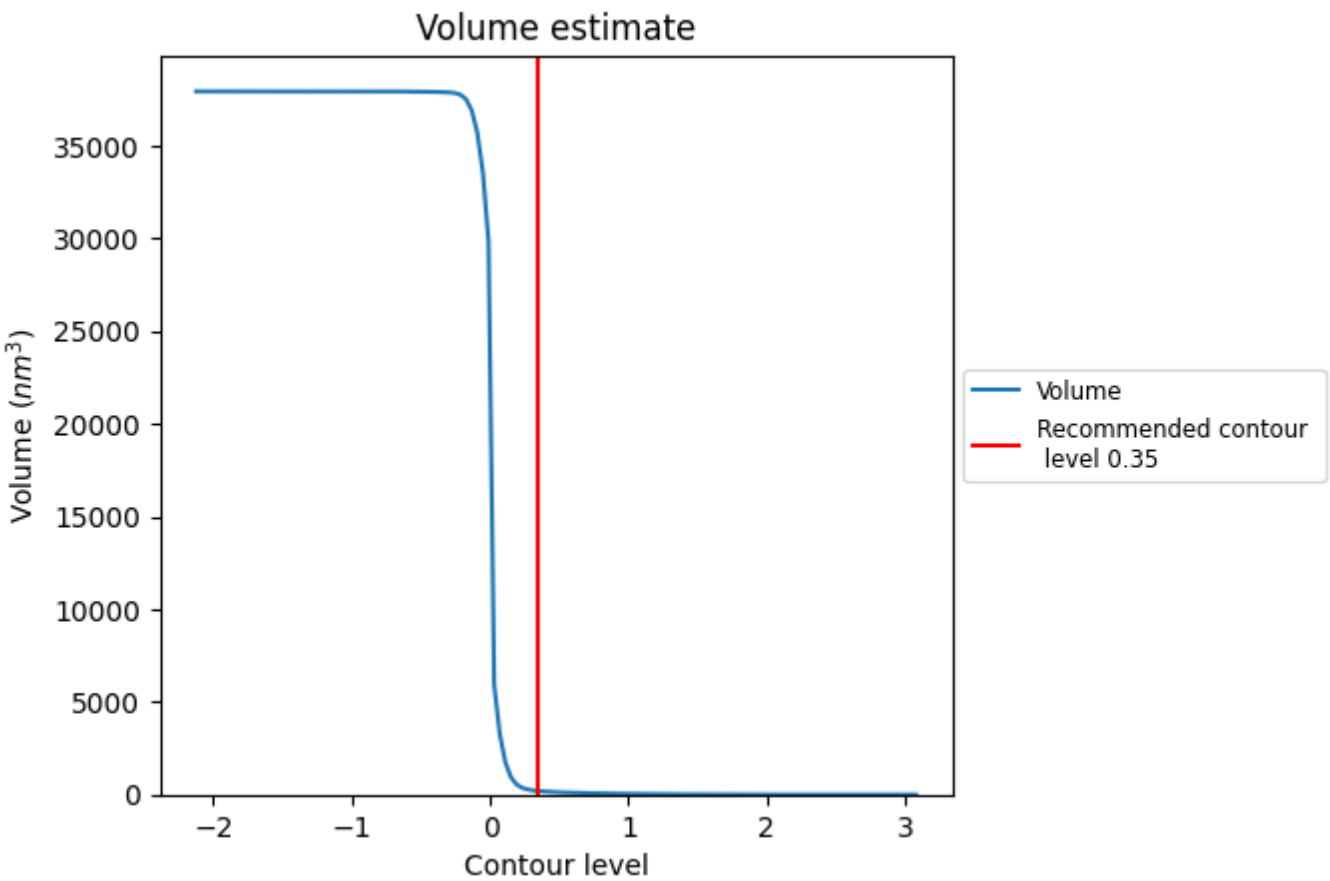
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

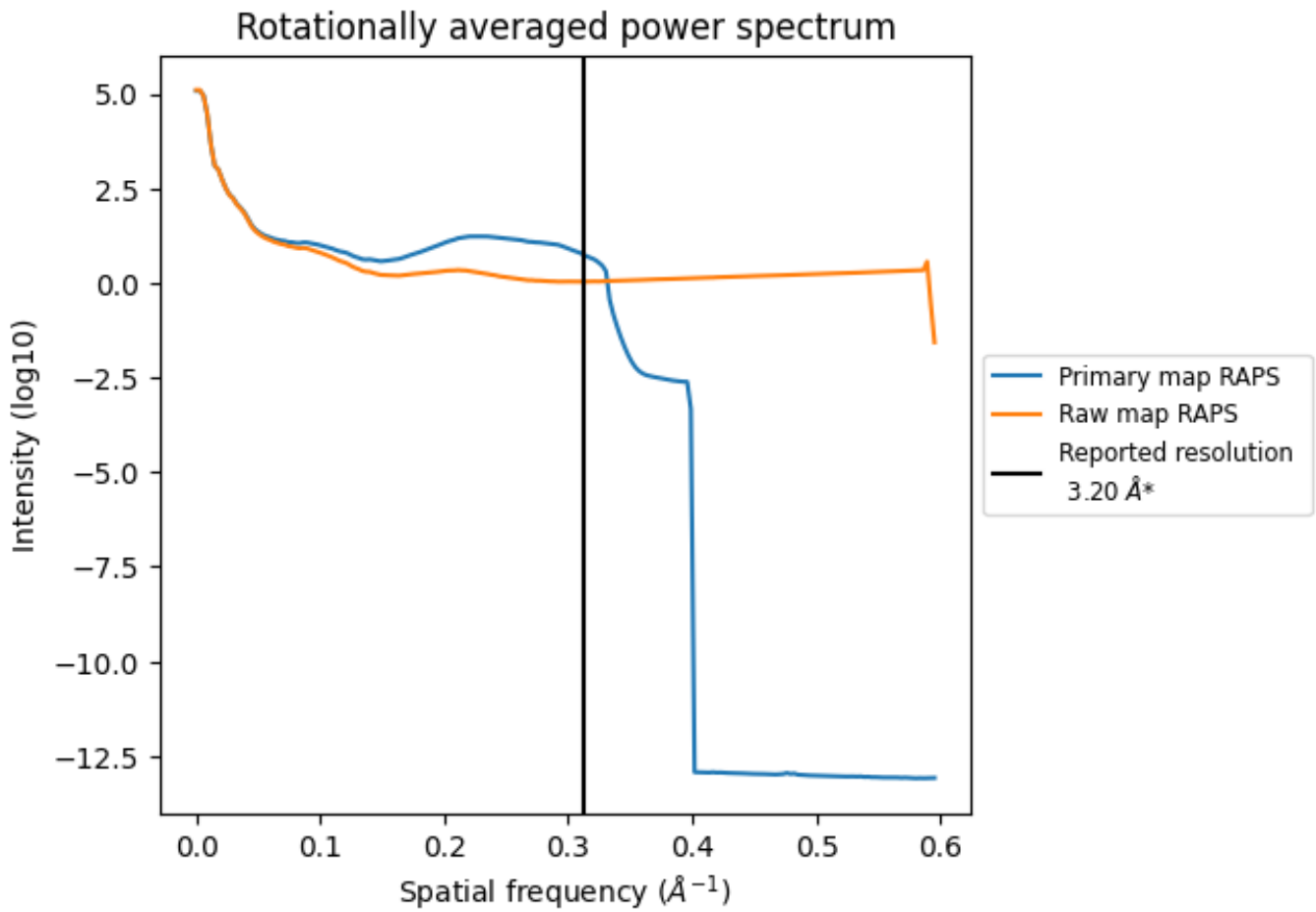
7.2 Volume estimate (i)



The volume at the recommended contour level is 194 nm^3; this corresponds to an approximate mass of 175 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)

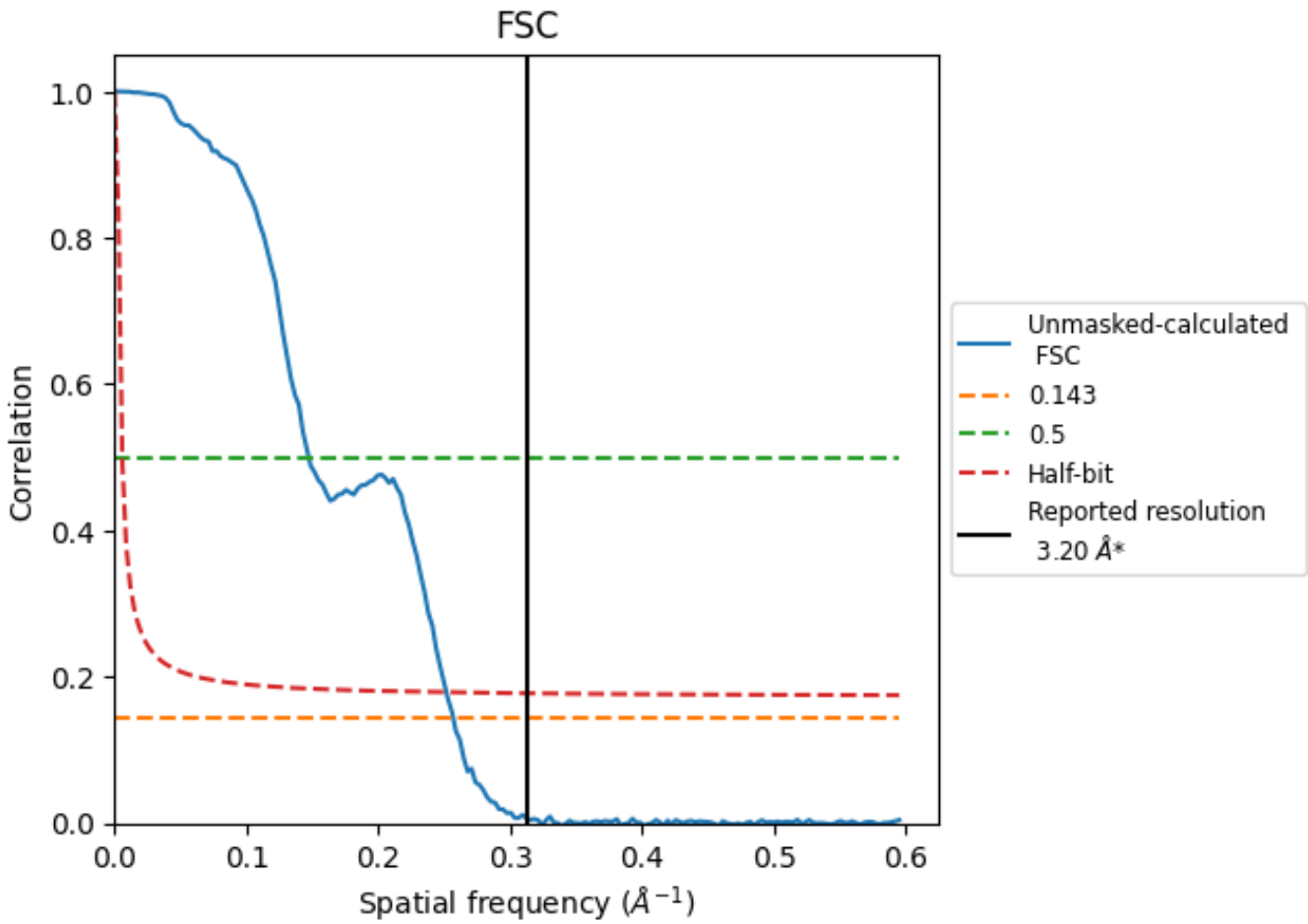


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

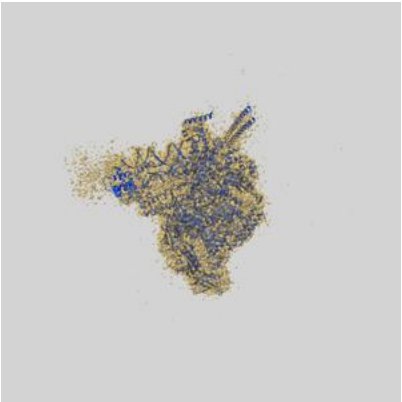
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.89	6.79	3.97

*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 3.89 differs from the reported value 3.2 by more than 10 %

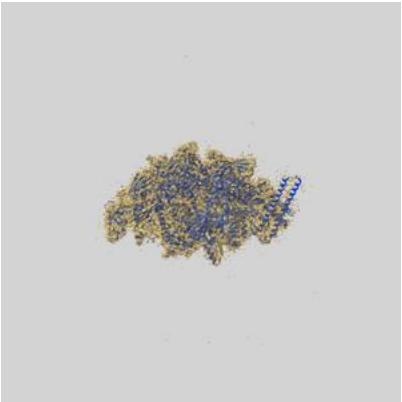
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13205 and PDB model 7P5X. Per-residue inclusion information can be found in section 3 on page 6.

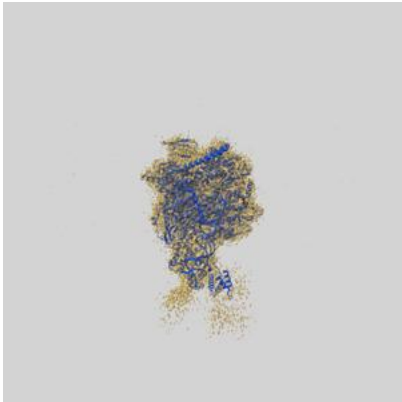
9.1 Map-model overlay (i)



X



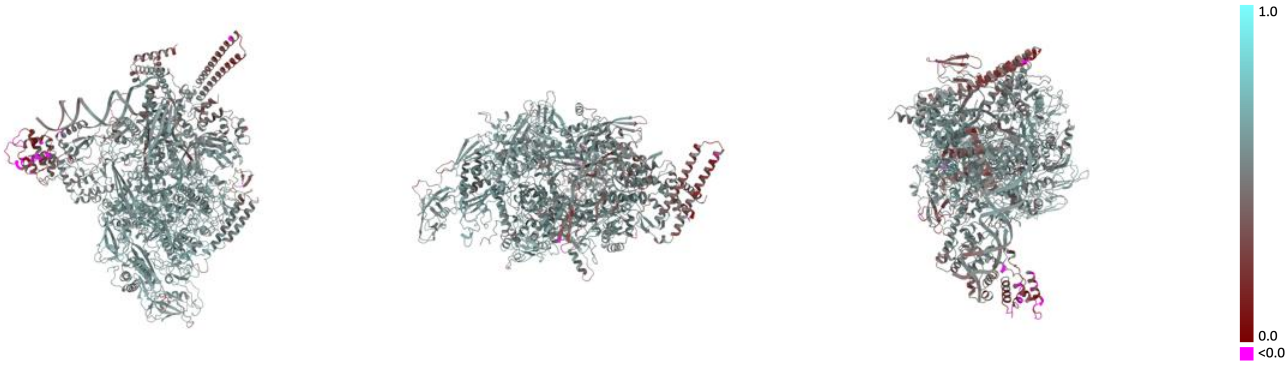
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

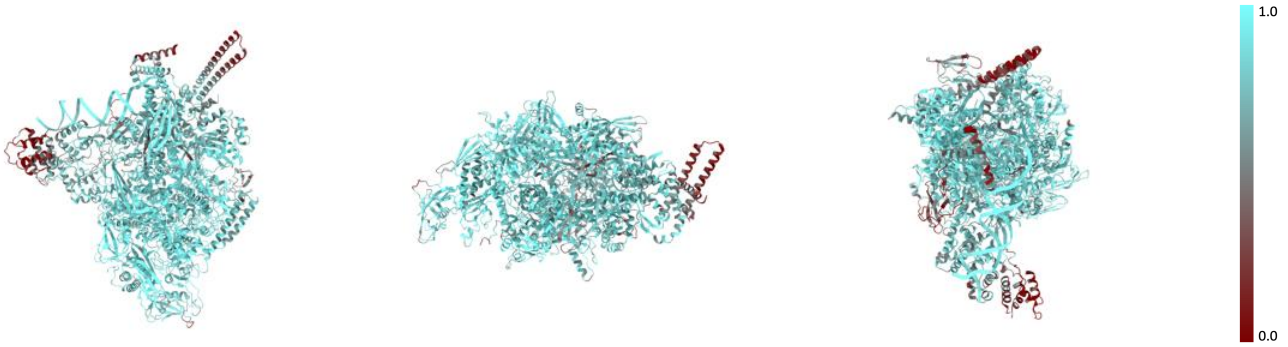
9.2 Q-score mapped to coordinate model (i)



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.

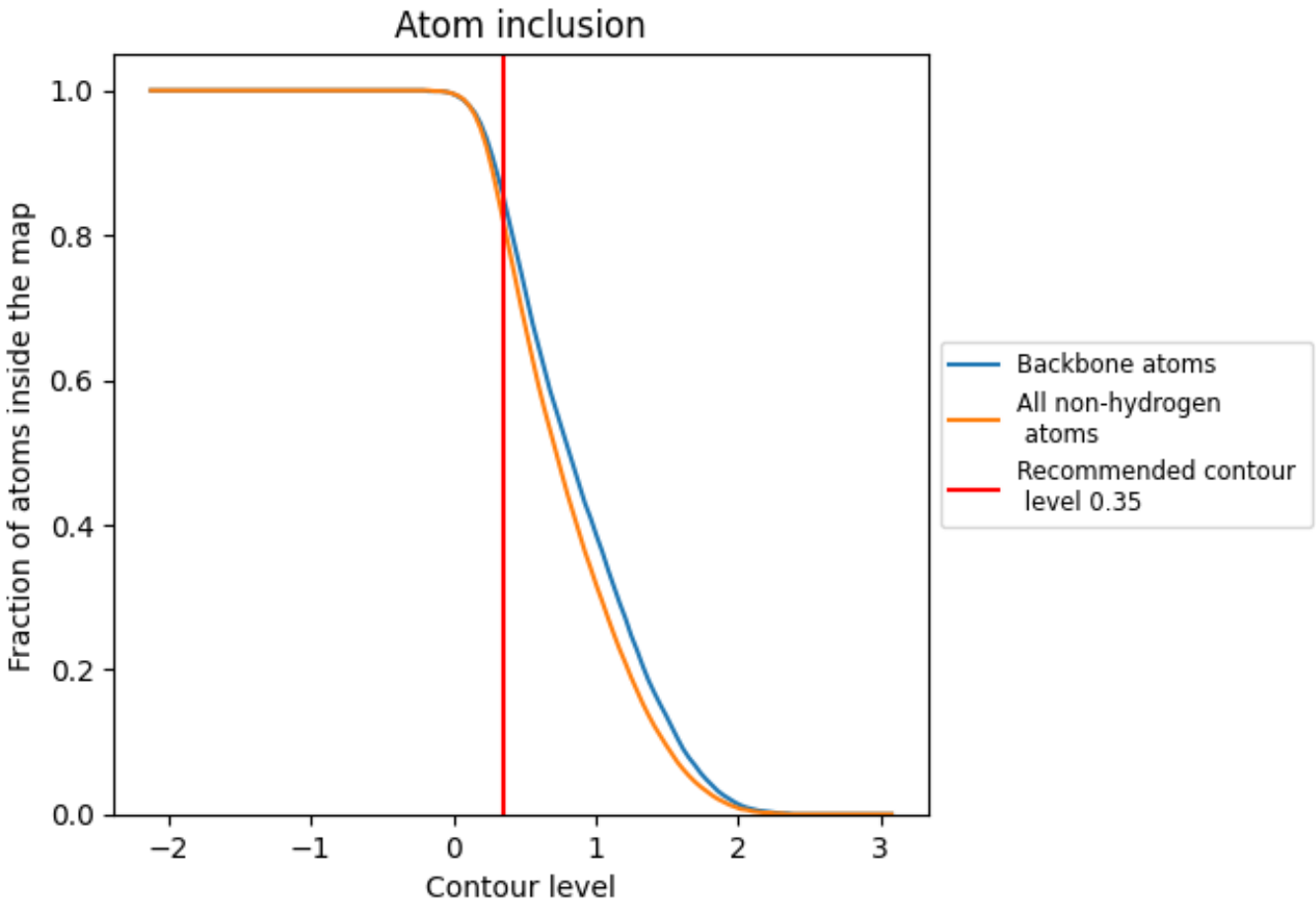
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8220	0.5320
AA	0.8840	0.5580
AB	0.8390	0.5440
AC	0.8760	0.5620
AD	0.8470	0.5460
AE	0.8270	0.5520
AF	0.7880	0.4950
AJ	0.3440	0.3830
AO	0.8460	0.5050
AP	0.8300	0.4830
AX	0.5160	0.3840
AY	0.5850	0.4170