Full wwPDB EM Validation Report (i)

Aug 26, 2026 – 07:49 pm BST

PDB ID	:	6S2F / pdb_00006s2f
EMDB ID	:	EMD-10089
Title	:	Cryo-EM structure of Ctf18-1-8 in complex with the catalytic domain of DNA polymerase epsilon (Class 2)
Authors	:	Grabarczyk, D.B.; Song, B.
Deposited on	:	2019-06-20
Resolution	:	5.80 Å(reported)
Based on initial models	:	4M8O, 5OKC

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 (1)) were used in the production of this report:

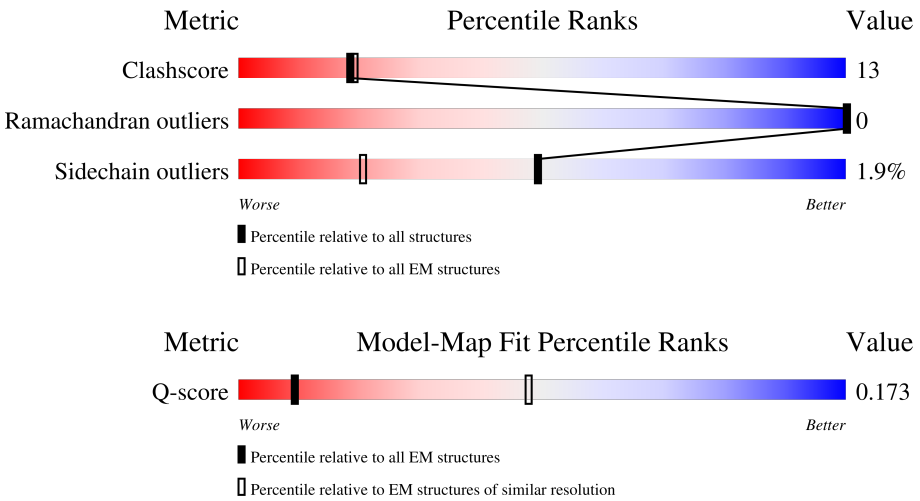
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 5.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	511 (5.30 - 6.30)

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	1219	24% 57% 24% • 17%
2	D	133	15% 58% 38% • •
3	E	33	9% 42% 36% 21%
4	B	380	8% 66% 31% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SF4	A	1401	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12459 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 polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1006	8154	5224	1358	1529	43	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	initiating methionine	UNP P21951
A	-25	LYS	-	expression tag	UNP P21951
A	-24	HIS	-	expression tag	UNP P21951
A	-23	HIS	-	expression tag	UNP P21951
A	-22	HIS	-	expression tag	UNP P21951
A	-21	HIS	-	expression tag	UNP P21951
A	-20	HIS	-	expression tag	UNP P21951
A	-19	HIS	-	expression tag	UNP P21951
A	-18	SER	-	expression tag	UNP P21951
A	-17	ALA	-	expression tag	UNP P21951
A	-16	GLY	-	expression tag	UNP P21951
A	-15	LEU	-	expression tag	UNP P21951
A	-14	GLU	-	expression tag	UNP P21951
A	-13	VAL	-	expression tag	UNP P21951
A	-12	LEU	-	expression tag	UNP P21951
A	-11	PHE	-	expression tag	UNP P21951
A	-10	GLN	-	expression tag	UNP P21951
A	-9	GLY	-	expression tag	UNP P21951
A	-8	PRO	-	expression tag	UNP P21951
A	-7	GLY	-	expression tag	UNP P21951
A	-6	THR	-	expression tag	UNP P21951
A	-5	GLY	-	expression tag	UNP P21951
A	-4	SER	-	expression tag	UNP P21951
A	-3	GLU	-	expression tag	UNP P21951
A	-2	PHE	-	expression tag	UNP P21951
A	-1	GLU	-	expression tag	UNP P21951
A	0	LEU	-	expression tag	UNP P21951
A	290	ALA	ASP	conflict	UNP P21951

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	ALA	GLU	conflict	UNP P21951

- Molecule 2 is a protein called Chromosome transmission fidelity protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	132	1031	653	176	195	7	0	0

- Molecule 3 is a protein called Chromosome transmission fidelity protein 18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	26	225	148	40	37	0	0

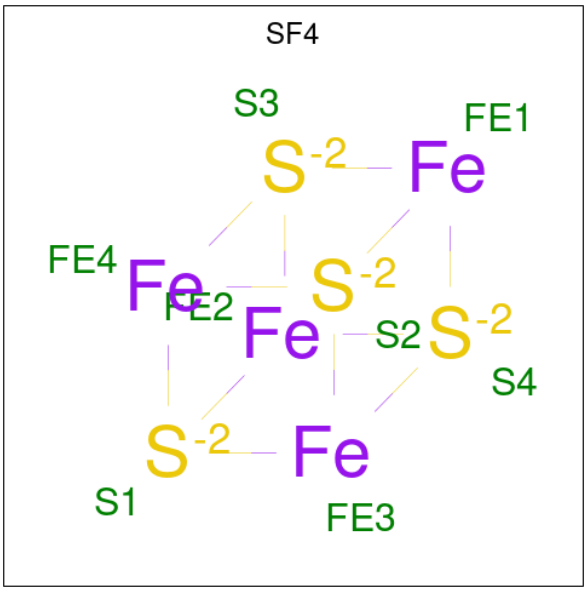
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	709	GLY	-	expression tag	UNP P49956
E	710	ALA	-	expression tag	UNP P49956
E	711	MET	-	expression tag	UNP P49956
E	712	GLY	-	expression tag	UNP P49956

- Molecule 4 is a protein called Sister chromatid cohesion protein DCC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	375	3041	1959	505	563	14	0	0

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



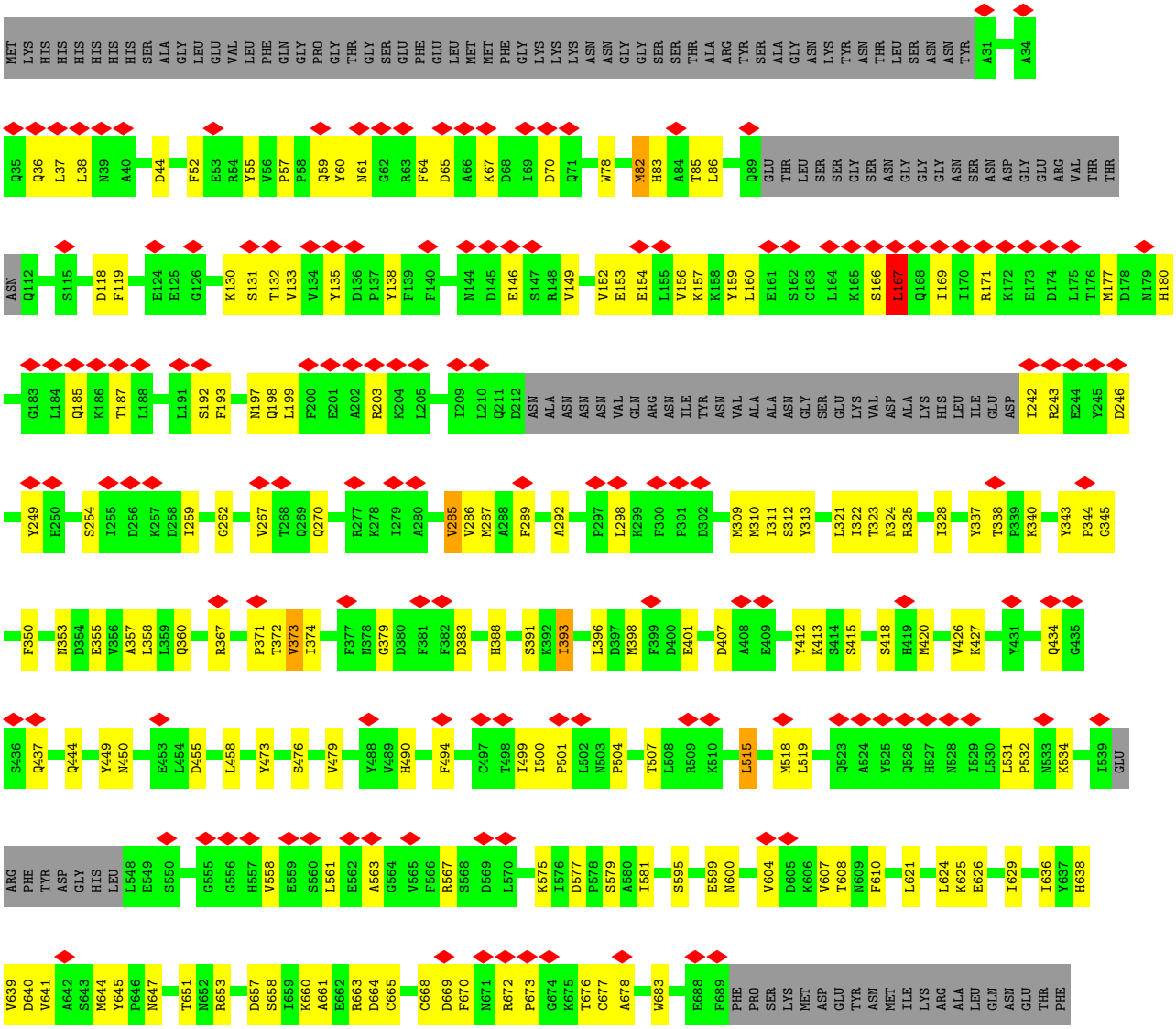
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
5	A	1	8	4	4	0

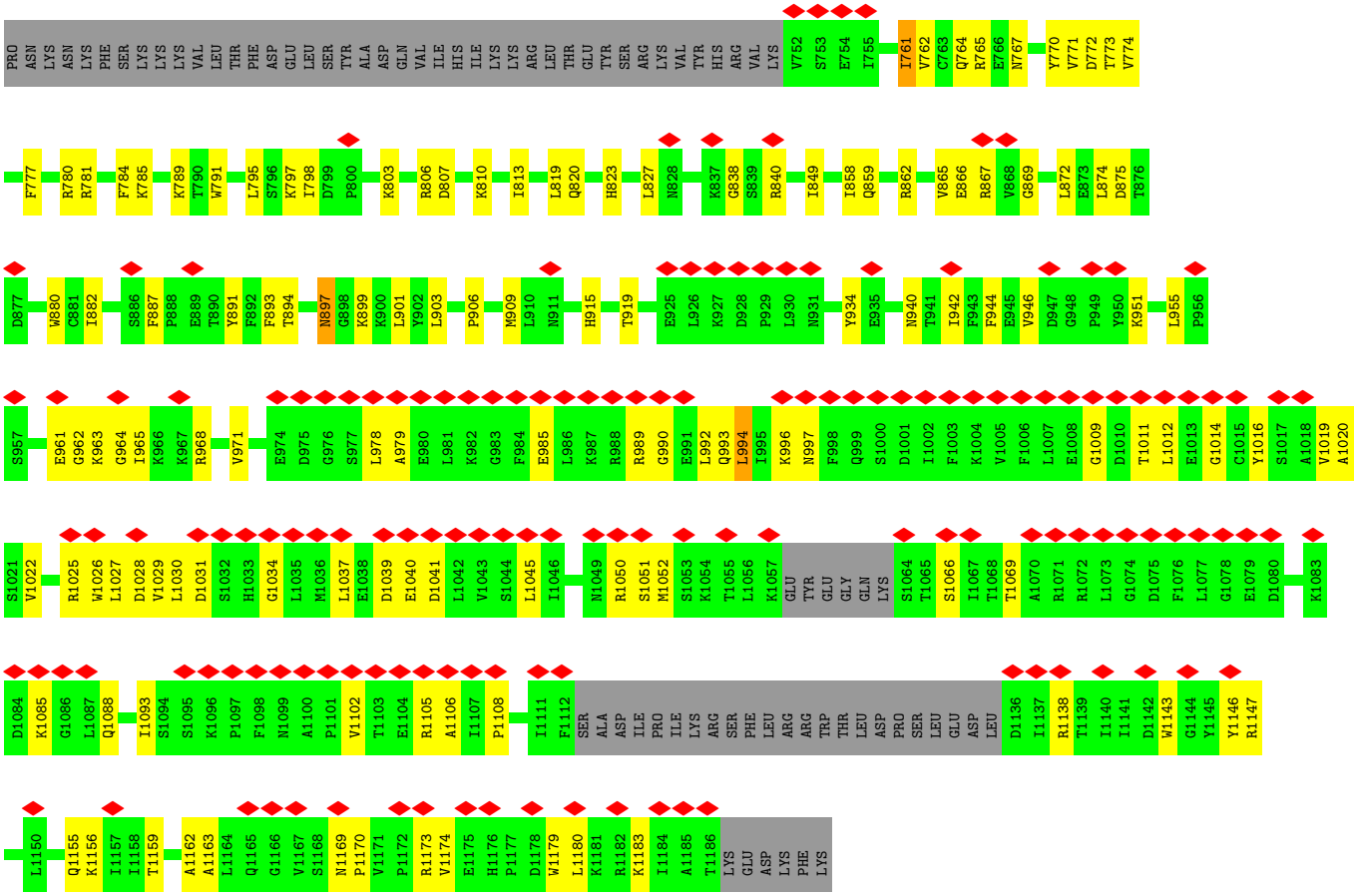
3 Residue-property plots (i)

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 polymerase epsilon catalytic subunit A

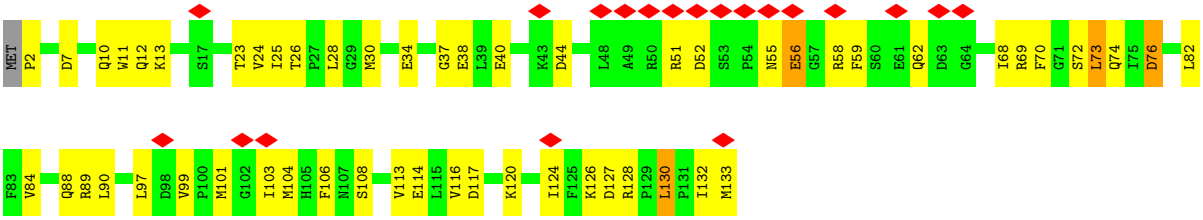
Chain A:





• Molecule 2: Chromosome transmission fidelity protein 8

Chain D:

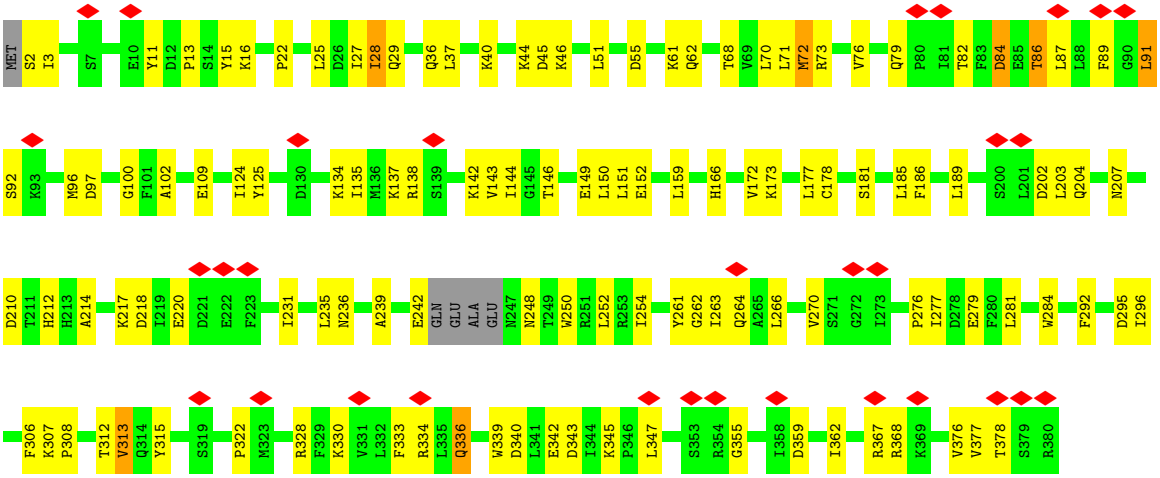


• Molecule 3: Chromosome transmission fidelity protein 18

Chain E:

• Molecule 4: Sister chromatid cohesion protein DCC1

Chain B:


MET S2 I3 S7 E10 Y11 D12 P13 S14 Y15 K16 P22 L25 D26 I27 I28 Q29 Q36 L37 K40 K44 D45 K46 L51 D55 K61 Q62 T68 V69 L70 L71 M72 R73 V76 Q79 P80 I81 T82 F83 D84 E85 T86 L87 L88 F89 G90 L91
S92 K93 M96 D97 G100 F101 A102 E109 I124 Y125 D130 K134 I135 M136 K137 R138 S139 K142 V143 I144 G145 T146 E149 L150 L151 E152 L159 H166 V172 K173 L177 C178 S181 L185 F186 L189 S200 L201 D202 L203 Q204 N207
D210 T211 H212 H213 A214 K217 D218 T219 E220 D221 E222 F223 I231 L235 N236 A239 E242 GLN GLU ALA GLU N247 N248 T249 W250 R251 L252 R253 I254 Y261 G262 I263 Q264 A265 L266 V270 S271 G272 I273 P276 I277 D278 E279 F280 L281 W284 F292 D295 I296
F306 K307 P308 T312 V313 Q314 Y315 S319 P322 M323 R328 F329 K330 V331 L332 F333 R334 L335 Q336 W339 D340 L341 E342 D343 I344 K345 P346 L347 S353 R354 G355 I358 D359 I362 R367 R368 K369 V376 V377 T378 S379 R380

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24967	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.190	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	308.415, 308.415, 308.415	wwPDB
Map dimensions	290, 290, 290	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	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: SF4

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	0.44	0/8338	1.02	9/11267 (0.1%)
2	D	0.44	0/1047	1.00	3/1407 (0.2%)
3	E	0.48	0/232	1.01	0/316
4	B	0.45	0/3110	0.98	8/4204 (0.2%)
All	All	0.45	0/12727	1.01	20/17194 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	84	ASP	CA-C-N	-6.82	113.09	122.30
4	B	84	ASP	C-N-CA	-6.82	113.09	122.30
4	B	91	LEU	CA-C-N	6.17	134.43	122.03
4	B	91	LEU	C-N-CA	6.17	134.43	122.03
1	A	246	ASP	CA-C-N	-6.08	118.22	122.59
1	A	246	ASP	C-N-CA	-6.08	118.22	122.59
4	B	336	GLN	CA-CB-CG	5.76	125.62	114.10
1	A	661	ALA	CA-C-N	5.73	135.02	124.82
1	A	661	ALA	C-N-CA	5.73	135.02	124.82
4	B	36	GLN	CA-C-N	-5.52	114.93	122.93
4	B	36	GLN	C-N-CA	-5.52	114.93	122.93
1	A	167	LEU	CA-CB-CG	5.51	135.58	116.30
1	A	515	LEU	CA-CB-CG	5.46	135.40	116.30
1	A	1106	ALA	N-CA-C	5.33	116.94	108.67
1	A	499	ILE	CA-C-N	-5.32	118.15	123.04
1	A	499	ILE	C-N-CA	-5.32	118.15	123.04
2	D	56	GLU	CA-C-N	5.32	128.14	120.11
2	D	56	GLU	C-N-CA	5.32	128.14	120.11
4	B	86	THR	OG1-CB-CG2	-5.27	98.75	109.30
2	D	130	LEU	N-CA-C	-5.01	102.89	110.50

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	A	8154	0	8067	196	0
2	D	1031	0	1044	53	0
3	E	225	0	220	16	0
4	B	3041	0	3052	92	0
5	A	8	0	0	3	0
All	All	12459	0	12383	325	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 13.

All (325) 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)
4:B:266:LEU:HB3	4:B:315:TYR:HB2	1.68	0.76
4:B:2:SER:N	4:B:92:SER:HG	1.83	0.75
4:B:368:ARG:HA	4:B:377:VAL:HA	1.68	0.73
1:A:434:GLN:HA	1:A:437:GLN:HG2	1.71	0.71
1:A:64:PHE:HB2	1:A:270:GLN:HG2	1.75	0.69
1:A:1030:LEU:HD12	1:A:1147:ARG:HH11	1.57	0.69
3:E:732:LYS:HB2	4:B:62:GLN:HG3	1.74	0.68
1:A:1020:ALA:HB2	1:A:1170:PRO:HB2	1.75	0.67
1:A:771:VAL:HA	1:A:774:VAL:HG22	1.75	0.67
2:D:34:GLU:HG2	2:D:124:ILE:HD13	1.77	0.67
2:D:56:GLU:HA	4:B:84:ASP:HB2	1.77	0.66
1:A:311:ILE:HG23	1:A:322:ILE:HB	1.79	0.65
1:A:962:GLY:HA2	1:A:1183:LYS:HE3	1.78	0.65
4:B:262:GLY:HA2	4:B:284:TRP:HE1	1.61	0.64
1:A:891:TYR:HB2	1:A:903:LEU:HD23	1.79	0.64
1:A:59:GLN:HE21	1:A:61:ASN:HD21	1.46	0.64
1:A:563:ALA:HA	1:A:955:LEU:HB2	1.79	0.63
1:A:608:THR:HB	1:A:894:THR:HG23	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:ARG:HH21	2:D:130:LEU:HD23	1.64	0.62
1:A:338:THR:HG22	1:A:345:GLY:H	1.65	0.62
2:D:12:GLN:NE2	4:B:28:ILE:O	2.33	0.61
1:A:1138:ARG:O	1:A:1143:TRP:NE1	2.31	0.61
4:B:277:ILE:HG12	4:B:313:VAL:HG13	1.81	0.61
1:A:60:TYR:O	1:A:270:GLN:NE2	2.34	0.61
1:A:819:LEU:O	1:A:823:HIS:ND1	2.26	0.61
1:A:672:ARG:HH12	1:A:934:TYR:HB2	1.65	0.61
1:A:177:MET:O	1:A:180:HIS:ND1	2.25	0.60
1:A:57:PRO:HG3	1:A:267:VAL:HG22	1.84	0.60
4:B:11:TYR:HB3	4:B:102:ALA:HA	1.84	0.60
4:B:342:GLU:HA	4:B:345:LYS:HD3	1.83	0.60
1:A:985:GLU:OE2	1:A:1156:LYS:NZ	2.35	0.60
4:B:125:TYR:O	4:B:181:SER:N	2.31	0.60
1:A:407:ASP:OD2	1:A:413:LYS:NZ	2.35	0.60
1:A:625:LYS:NZ	1:A:626:GLU:OE2	2.35	0.60
2:D:76:ASP:OD1	2:D:76:ASP:N	2.35	0.59
1:A:581:ILE:HG23	1:A:621:LEU:HB2	1.84	0.59
1:A:388:HIS:ND1	1:A:412:TYR:OH	2.36	0.58
1:A:1169:ASN:ND2	1:A:1174:VAL:O	2.36	0.58
2:D:26:THR:HG22	2:D:30:MET:H	1.68	0.58
4:B:125:TYR:OH	4:B:173:LYS:NZ	2.37	0.58
1:A:289:PHE:HD1	1:A:374:ILE:HD11	1.68	0.58
2:D:56:GLU:O	2:D:69:ARG:NH2	2.36	0.58
1:A:243:ARG:NH2	1:A:531:LEU:O	2.36	0.57
1:A:337:TYR:HE2	1:A:479:VAL:HG11	1.69	0.57
4:B:45:ASP:OD1	4:B:46:LYS:NZ	2.36	0.57
1:A:624:LEU:HD11	1:A:887:PHE:HA	1.84	0.57
1:A:1050:ARG:NH1	1:A:1066:SER:OG	2.32	0.57
1:A:641:VAL:HA	1:A:944:PHE:HA	1.86	0.57
4:B:359:ASP:OD2	4:B:368:ARG:NH1	2.37	0.57
2:D:108:SER:HA	3:E:740:TRP:HE1	1.69	0.57
2:D:38:GLU:O	3:E:721:LYS:N	2.33	0.57
1:A:1179:TRP:O	1:A:1183:LYS:HB2	2.05	0.56
1:A:309:MET:HG3	1:A:310:MET:HG2	1.87	0.56
1:A:153:GLU:HG2	1:A:157:LYS:HE2	1.87	0.56
2:D:103:ILE:HD11	4:B:15:TYR:HB3	1.87	0.56
1:A:669:ASP:OD1	1:A:669:ASP:N	2.36	0.56
1:A:1026:TRP:HB3	1:A:1147:ARG:HH12	1.69	0.56
1:A:1102:VAL:HA	1:A:1105:ARG:HG3	1.86	0.56
2:D:104:MET:HA	2:D:116:VAL:H	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:LEU:HD11	1:A:874:LEU:HD23	1.88	0.55
4:B:96:MET:HE3	4:B:97:ASP:H	1.71	0.55
4:B:261:TYR:OH	4:B:284:TRP:O	2.23	0.55
2:D:11:TRP:CD1	2:D:117:ASP:HA	2.42	0.55
1:A:418:SER:HB2	1:A:420:MET:HE3	1.89	0.55
2:D:58:ARG:NH2	4:B:86:THR:OG1	2.40	0.55
4:B:266:LEU:HA	4:B:270:VAL:HG12	1.88	0.55
1:A:138:TYR:HA	1:A:192:SER:HA	1.89	0.55
1:A:1011:THR:HG23	1:A:1014:GLY:H	1.72	0.55
2:D:23:THR:OG1	2:D:24:VAL:N	2.40	0.55
4:B:214:ALA:O	4:B:217:LYS:NZ	2.40	0.55
1:A:810:LYS:HA	1:A:813:ILE:HD12	1.89	0.54
4:B:307:LYS:H	4:B:336:GLN:NE2	2.05	0.54
1:A:579:SER:OG	1:A:867:ARG:NH2	2.40	0.54
2:D:97:LEU:N	2:D:120:LYS:O	2.35	0.54
1:A:322:ILE:HG12	1:A:350:PHE:HB2	1.90	0.54
1:A:773:THR:O	1:A:777:PHE:HB2	2.06	0.54
1:A:1069:THR:HA	1:A:1108:PRO:HD3	1.89	0.54
4:B:339:TRP:H	4:B:376:VAL:HG13	1.72	0.54
1:A:639:VAL:HG22	1:A:946:VAL:HG12	1.88	0.54
2:D:74:GLN:HG2	4:B:91:LEU:HA	1.89	0.54
3:E:733:ASN:OD1	4:B:61:LYS:NZ	2.35	0.54
4:B:263:ILE:HA	4:B:266:LEU:HD12	1.90	0.54
1:A:455:ASP:HB3	1:A:458:LEU:HD13	1.90	0.54
1:A:678:ALA:HB1	1:A:761:ILE:HB	1.90	0.54
1:A:1031:ASP:OD1	1:A:1173:ARG:NH1	2.41	0.54
1:A:990:GLY:HA3	1:A:1050:ARG:HD3	1.90	0.53
2:D:11:TRP:HH2	4:B:29:GLN:HE21	1.54	0.53
1:A:193:PHE:HB3	1:A:198:GLN:HB2	1.90	0.53
1:A:501:PRO:HD2	1:A:518:MET:HE1	1.91	0.53
1:A:289:PHE:HA	1:A:313:TYR:HA	1.89	0.53
1:A:357:ALA:O	1:A:360:GLN:NE2	2.38	0.53
1:A:657:ASP:N	1:A:657:ASP:OD1	2.39	0.53
1:A:83:HIS:O	1:A:118:ASP:N	2.39	0.53
1:A:595:SER:O	1:A:600:ASN:ND2	2.36	0.53
1:A:1025:ARG:NH1	2:D:133:MET:OXT	2.42	0.53
1:A:665:CYS:HB3	1:A:670:PHE:HB3	1.90	0.53
1:A:653:ARG:NH1	1:A:764:GLN:O	2.41	0.52
2:D:2:PRO:HG3	4:B:44:LYS:HG2	1.91	0.52
1:A:777:PHE:HA	1:A:780:ARG:HG2	1.90	0.52
1:A:325:ARG:NH1	1:A:328:ILE:O	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ASN:OD1	1:A:450:ASN:N	2.39	0.52
2:D:133:MET:HA	4:B:89:PHE:HE1	1.75	0.52
4:B:239:ALA:HB2	4:B:252:LEU:HD23	1.92	0.52
4:B:135:ILE:HD12	4:B:138:ARG:HD2	1.92	0.52
1:A:668:CYS:HB2	1:A:765:ARG:HH12	1.75	0.52
4:B:13:PRO:O	4:B:16:LYS:NZ	2.37	0.52
4:B:40:LYS:NZ	4:B:152:GLU:O	2.43	0.51
4:B:146:THR:HG23	4:B:149:GLU:H	1.75	0.51
1:A:532:PRO:O	1:A:840:ARG:NH1	2.38	0.51
4:B:322:PRO:HD2	4:B:328:ARG:HA	1.92	0.51
1:A:658:SER:HB2	1:A:762:VAL:HG23	1.93	0.51
1:A:1039:ASP:N	1:A:1039:ASP:OD1	2.40	0.51
1:A:338:THR:HG22	1:A:344:PRO:HA	1.91	0.51
2:D:7:ASP:HB3	2:D:114:GLU:HA	1.92	0.51
2:D:126:LYS:O	3:E:722:TYR:OH	2.27	0.51
1:A:171:ARG:NH1	1:A:185:GLN:O	2.43	0.51
1:A:169:ILE:HD11	1:A:187:THR:HG23	1.93	0.51
1:A:254:SER:OG	1:A:259:ILE:O	2.28	0.51
1:A:961:GLU:HA	1:A:1179:TRP:CE3	2.46	0.51
2:D:106:PHE:CG	3:E:739:LEU:HD21	2.46	0.51
1:A:285:VAL:HG23	1:A:372:THR:H	1.76	0.50
1:A:154:GLU:HA	1:A:157:LYS:HE3	1.94	0.50
4:B:172:VAL:HA	4:B:177:LEU:HA	1.93	0.50
4:B:367:ARG:O	4:B:378:THR:N	2.43	0.50
4:B:142:LYS:NZ	4:B:143:VAL:O	2.38	0.50
1:A:55:TYR:O	1:A:131:SER:OG	2.28	0.50
1:A:567:ARG:NH2	1:A:1009:GLY:O	2.34	0.50
1:A:798:ILE:HD12	1:A:806:ARG:HD2	1.94	0.50
1:A:286:VAL:HA	1:A:373:VAL:HG13	1.92	0.50
4:B:203:LEU:HB3	4:B:252:LEU:HD12	1.94	0.50
1:A:36:GLN:HE22	1:A:197:ASN:HD21	1.60	0.50
1:A:65:ASP:OD2	1:A:67:LYS:NZ	2.37	0.50
1:A:118:ASP:OD2	1:A:132:THR:OG1	2.29	0.49
1:A:651:THR:HG22	1:A:940:ASN:HA	1.93	0.49
1:A:444:GLN:HE22	1:A:450:ASN:HA	1.77	0.49
2:D:68:ILE:HG13	2:D:70:PHE:HB3	1.93	0.49
4:B:202:ASP:OD1	4:B:202:ASP:N	2.44	0.49
1:A:915:HIS:O	1:A:919:THR:OG1	2.27	0.49
1:A:772:ASP:N	1:A:772:ASP:OD1	2.44	0.49
1:A:1041:ASP:HB2	2:D:128:ARG:HH21	1.77	0.49
2:D:58:ARG:O	2:D:69:ARG:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:724:GLU:OE1	3:E:724:GLU:N	2.44	0.49
1:A:989:ARG:HD3	1:A:1051:SER:HB3	1.95	0.48
1:A:993:GLN:O	1:A:997:ASN:ND2	2.46	0.48
2:D:38:GLU:HB3	3:E:721:LYS:HB3	1.95	0.48
4:B:27:ILE:HG22	4:B:37:LEU:HD21	1.95	0.48
1:A:500:ILE:HG12	1:A:519:LEU:HD21	1.95	0.48
1:A:795:LEU:HD22	1:A:813:ILE:HD13	1.95	0.48
1:A:156:VAL:HB	1:A:160:LEU:HD23	1.95	0.48
1:A:994:LEU:HD12	1:A:1045:LEU:HD13	1.94	0.48
4:B:186:PHE:CG	4:B:264:GLN:HG3	2.48	0.48
4:B:306:PHE:HB2	4:B:336:GLN:HE21	1.78	0.48
1:A:367:ARG:NH1	1:A:401:GLU:O	2.41	0.48
1:A:166:SER:OG	1:A:167:LEU:N	2.46	0.48
1:A:193:PHE:HB2	1:A:199:LEU:HD22	1.95	0.48
1:A:770:TYR:O	1:A:773:THR:OG1	2.23	0.48
1:A:865:VAL:O	1:A:869:GLY:N	2.47	0.48
1:A:1025:ARG:NH2	1:A:1028:ASP:OD2	2.46	0.48
2:D:10:GLN:HA	2:D:13:LYS:HE2	1.95	0.48
2:D:89:ARG:N	2:D:130:LEU:O	2.46	0.48
3:E:734:VAL:HG22	4:B:62:GLN:HG2	1.96	0.48
1:A:1016:TYR:HA	1:A:1019:VAL:HG12	1.95	0.47
2:D:72:SER:HG	4:B:2:SER:HG	1.52	0.47
1:A:292:ALA:O	1:A:309:MET:N	2.46	0.47
1:A:83:HIS:NE2	1:A:415:SER:O	2.42	0.47
1:A:670:PHE:HA	1:A:677:CYS:HB2	1.95	0.47
4:B:218:ASP:OD1	4:B:218:ASP:N	2.46	0.47
1:A:490:HIS:O	1:A:494:PHE:HB2	2.14	0.47
4:B:55:ASP:HB3	4:B:159:LEU:HD12	1.96	0.47
4:B:134:LYS:HA	4:B:137:LYS:HD3	1.97	0.47
1:A:52:PHE:HB3	1:A:130:LYS:HB3	1.95	0.47
1:A:862:ARG:HA	1:A:865:VAL:HG12	1.96	0.47
4:B:333:PHE:HZ	4:B:377:VAL:HB	1.79	0.47
1:A:353:ASN:OD1	1:A:353:ASN:N	2.46	0.47
1:A:636:ILE:HG13	1:A:882:ILE:HG22	1.95	0.47
4:B:308:PRO:HD2	4:B:312:THR:HG23	1.96	0.47
1:A:357:ALA:HA	1:A:360:GLN:HG3	1.97	0.47
2:D:58:ARG:HA	2:D:69:ARG:HB3	1.95	0.47
2:D:73:LEU:HG	4:B:3:ILE:HB	1.96	0.47
4:B:212:HIS:HB2	4:B:231:ILE:HG13	1.97	0.47
1:A:70:ASP:OD1	1:A:70:ASP:N	2.44	0.47
1:A:135:TYR:O	1:A:249:TYR:OH	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:LEU:HD22	1:A:1173:ARG:HH11	1.79	0.47
4:B:144:ILE:HG12	4:B:150:LEU:HD13	1.97	0.47
1:A:534:LYS:NZ	1:A:838:GLY:O	2.40	0.46
1:A:1034:GLY:HA2	1:A:1037:LEU:HD13	1.97	0.46
1:A:82:MET:HE3	1:A:82:MET:HB3	1.84	0.46
1:A:777:PHE:HD2	1:A:827:LEU:HG	1.80	0.46
4:B:61:LYS:O	4:B:109:GLU:N	2.41	0.46
4:B:276:PRO:HA	4:B:312:THR:HA	1.96	0.46
1:A:803:LYS:NZ	4:B:355:GLY:O	2.46	0.46
1:A:595:SER:HA	1:A:599:GLU:HB2	1.97	0.46
1:A:324:ASN:HB2	1:A:358:LEU:HD23	1.97	0.46
1:A:37:LEU:HG	1:A:86:LEU:HD23	1.98	0.46
1:A:577:ASP:HB3	1:A:867:ARG:HB3	1.97	0.46
4:B:281:LEU:HD22	4:B:296:ILE:HG12	1.97	0.46
1:A:156:VAL:HA	1:A:159:TYR:HB2	1.98	0.46
1:A:784:PHE:HB2	1:A:820:GLN:HB3	1.98	0.46
1:A:1040:GLU:CD	3:E:719:TRP:HE1	2.24	0.46
1:A:575:LYS:HG2	1:A:629:ILE:HD12	1.98	0.45
1:A:807:ASP:HA	1:A:810:LYS:HD2	1.98	0.45
2:D:62:GLN:HE22	4:B:79:GLN:H	1.63	0.45
1:A:859:GLN:HA	1:A:862:ARG:HG3	1.97	0.45
2:D:82:LEU:O	2:D:90:LEU:N	2.37	0.45
4:B:242:GLU:HB3	4:B:248:ASN:HA	1.97	0.45
1:A:647:ASN:HB3	1:A:942:ILE:HG12	1.98	0.45
2:D:40:GLU:N	3:E:719:TRP:O	2.48	0.45
1:A:858:ILE:HD12	1:A:858:ILE:HA	1.79	0.45
1:A:1027:LEU:HD22	1:A:1173:ARG:HD3	1.99	0.45
1:A:203:ARG:HG2	1:A:242:ILE:HD11	1.99	0.45
1:A:781:ARG:NE	1:A:820:GLN:OE1	2.49	0.45
1:A:781:ARG:HG3	1:A:820:GLN:HB2	1.98	0.45
1:A:1019:VAL:HA	1:A:1022:VAL:HG12	1.98	0.45
4:B:22:PRO:HA	4:B:25:LEU:HD12	2.00	0.44
1:A:1155:GLN:HA	1:A:1159:THR:OG1	2.17	0.44
1:A:965:ILE:HG21	1:A:968:ARG:HD2	1.99	0.44
4:B:328:ARG:NH1	4:B:347:LEU:O	2.50	0.44
1:A:665:CYS:N	5:A:1401:SF4:S1	2.73	0.44
1:A:797:LYS:HE2	1:A:797:LYS:HB3	1.75	0.44
1:A:1052:MET:O	1:A:1085:LYS:NZ	2.50	0.44
1:A:287:MET:HB3	1:A:374:ILE:HD13	1.99	0.44
1:A:473:TYR:O	1:A:476:SER:OG	2.31	0.44
1:A:899:LYS:HB3	1:A:899:LYS:HE2	1.71	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:127:ASP:OD1	2:D:127:ASP:N	2.46	0.44
4:B:254:ILE:HG23	4:B:292:PHE:CZ	2.53	0.44
1:A:149:VAL:HA	1:A:152:VAL:HG22	1.98	0.44
2:D:101:MET:HE3	2:D:101:MET:HB3	1.86	0.44
1:A:379:GLY:HA2	1:A:383:ASP:HB3	2.00	0.43
1:A:393:ILE:HD13	1:A:393:ILE:HA	1.77	0.43
1:A:767:ASN:OD1	1:A:767:ASN:N	2.50	0.43
1:A:862:ARG:O	1:A:866:GLU:HB2	2.18	0.43
2:D:37:GLY:HA2	3:E:723:ASN:H	1.83	0.43
4:B:72:MET:SD	4:B:72:MET:N	2.91	0.43
1:A:807:ASP:OD1	1:A:810:LYS:NZ	2.41	0.43
1:A:119:PHE:HE2	1:A:133:VAL:HB	1.83	0.43
2:D:89:ARG:NH1	2:D:132:ILE:O	2.51	0.43
1:A:660:LYS:HB2	1:A:761:ILE:HG13	2.00	0.43
1:A:992:LEU:HG	1:A:994:LEU:HB3	1.99	0.43
1:A:1026:TRP:HA	1:A:1029:VAL:HG12	1.99	0.43
2:D:52:ASP:HB2	2:D:59:PHE:HB2	2.00	0.43
4:B:295:ASP:OD1	4:B:295:ASP:N	2.47	0.43
1:A:36:GLN:NE2	1:A:197:ASN:HD21	2.16	0.43
1:A:391:SER:O	1:A:396:LEU:N	2.39	0.43
1:A:971:VAL:HG23	1:A:979:ALA:HB3	2.01	0.43
2:D:44:ASP:OD1	2:D:44:ASP:N	2.49	0.43
2:D:72:SER:HB3	4:B:91:LEU:HD11	2.01	0.43
4:B:71:LEU:HB2	4:B:102:ALA:HB3	2.01	0.43
4:B:125:TYR:HB2	4:B:178:CYS:SG	2.58	0.43
1:A:310:MET:HE3	1:A:310:MET:HB3	1.83	0.43
1:A:1012:LEU:HD23	1:A:1012:LEU:H	1.84	0.43
4:B:2:SER:N	4:B:92:SER:OG	2.49	0.43
1:A:78:TRP:NE1	1:A:262:GLY:O	2.48	0.43
4:B:166:HIS:CG	4:B:236:ASN:HB3	2.54	0.43
1:A:427:LYS:HA	1:A:437:GLN:HE21	1.82	0.43
1:A:638:HIS:HB2	1:A:880:TRP:CZ3	2.54	0.43
4:B:2:SER:OG	4:B:3:ILE:N	2.52	0.43
4:B:342:GLU:OE1	4:B:345:LYS:NZ	2.35	0.43
1:A:963:LYS:NZ	1:A:964:GLY:O	2.37	0.42
1:A:781:ARG:O	1:A:785:LYS:HG3	2.19	0.42
4:B:45:ASP:OD1	4:B:45:ASP:N	2.51	0.42
4:B:340:ASP:HB3	4:B:343:ASP:HB2	2.01	0.42
1:A:285:VAL:HB	1:A:371:PRO:HA	2.00	0.42
2:D:34:GLU:N	2:D:34:GLU:OE1	2.52	0.42
1:A:644:MET:HG2	1:A:645:TYR:CD1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:LYS:HA	1:A:789:LYS:HD2	1.80	0.42
2:D:72:SER:OG	4:B:2:SER:OG	2.27	0.42
4:B:28:ILE:HD13	4:B:28:ILE:HA	1.83	0.42
1:A:44:ASP:OD1	1:A:130:LYS:NZ	2.50	0.42
1:A:298:LEU:O	1:A:1088:GLN:NE2	2.52	0.42
4:B:330:LYS:HA	4:B:330:LYS:HD2	1.76	0.42
1:A:340:LYS:HB2	1:A:343:TYR:CD2	2.55	0.42
1:A:791:TRP:HB3	1:A:813:ILE:HG12	2.01	0.42
1:A:1016:TYR:CZ	1:A:1162:ALA:HB2	2.55	0.42
2:D:26:THR:HG23	2:D:28:LEU:H	1.84	0.42
4:B:276:PRO:HB2	4:B:279:GLU:OE1	2.20	0.42
1:A:638:HIS:CE1	1:A:640:ASP:HB2	2.54	0.42
2:D:55:ASN:HA	4:B:82:THR:HG23	2.02	0.42
1:A:312:SER:HB3	1:A:321:LEU:HD13	2.01	0.42
1:A:683:TRP:HB3	1:A:849:ILE:HG12	2.02	0.42
1:A:1093:ILE:H	1:A:1146:TYR:HH	1.60	0.42
4:B:70:LEU:HD11	4:B:100:GLY:HA3	2.01	0.42
1:A:993:GLN:HA	1:A:996:LYS:HE3	2.01	0.42
2:D:104:MET:HB2	2:D:104:MET:HE2	1.71	0.42
2:D:104:MET:HE1	2:D:113:VAL:HB	2.01	0.42
1:A:893:PHE:HB2	1:A:901:LEU:HG	2.01	0.41
1:A:644:MET:HE3	1:A:644:MET:H	1.84	0.41
4:B:202:ASP:HB2	4:B:204:GLN:HE22	1.84	0.41
1:A:558:VAL:HG13	1:A:875:ASP:HA	2.03	0.41
1:A:897:ASN:OD1	1:A:897:ASN:N	2.47	0.41
4:B:207:ASN:ND2	4:B:210:ASP:H	2.19	0.41
2:D:51:ARG:HG3	3:E:715:THR:HG22	2.02	0.41
2:D:88:GLN:CD	3:E:720:VAL:H	2.28	0.41
3:E:733:ASN:O	4:B:62:GLN:NE2	2.54	0.41
4:B:159:LEU:HD23	4:B:159:LEU:HA	1.86	0.41
1:A:504:PRO:O	1:A:507:THR:OG1	2.24	0.41
2:D:24:VAL:HG13	2:D:25:ILE:HG12	2.01	0.41
1:A:765:ARG:NH1	5:A:1401:SF4:S3	2.94	0.41
1:A:607:VAL:HG13	1:A:610:PHE:HB2	2.02	0.41
2:D:30:MET:SD	4:B:73:ARG:HB2	2.61	0.41
3:E:739:LEU:HD13	3:E:740:TRP:CZ3	2.56	0.41
4:B:86:THR:HG22	4:B:87:LEU:H	1.85	0.41
4:B:186:PHE:HZ	4:B:261:TYR:HD1	1.68	0.41
1:A:146:GLU:HA	1:A:149:VAL:HG23	2.02	0.41
1:A:289:PHE:CD1	1:A:374:ILE:HD11	2.52	0.41
1:A:398:MET:HE2	1:A:398:MET:HB3	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:GLN:NE2	1:A:449:TYR:O	2.52	0.41
1:A:765:ARG:HB2	5:A:1401:SF4:S4	2.60	0.41
1:A:887:PHE:HE2	1:A:906:PRO:HG3	1.86	0.41
4:B:281:LEU:HD23	4:B:281:LEU:HA	1.84	0.41
1:A:355:GLU:O	1:A:358:LEU:HG	2.20	0.41
1:A:604:VAL:O	1:A:607:VAL:HG12	2.21	0.41
1:A:663:ARG:NH2	1:A:664:ASP:O	2.42	0.41
1:A:906:PRO:O	1:A:909:MET:HG2	2.21	0.41
1:A:1163:ALA:HB1	1:A:1180:LEU:HD13	2.03	0.41
1:A:638:HIS:HB2	1:A:880:TRP:CE3	2.56	0.40
1:A:951:LYS:HE2	1:A:951:LYS:HB2	1.94	0.40
4:B:186:PHE:CD1	4:B:189:LEU:HD23	2.56	0.40
4:B:235:LEU:HB3	4:B:250:TRP:CD1	2.56	0.40
4:B:362:ILE:HD13	4:B:377:VAL:HG21	2.02	0.40
1:A:426:VAL:O	1:A:437:GLN:NE2	2.54	0.40
4:B:330:LYS:O	4:B:334:ARG:HG2	2.22	0.40
4:B:124:ILE:HD11	4:B:181:SER:HA	2.03	0.40
2:D:84:VAL:HB	2:D:88:GLN:HB2	2.03	0.40
4:B:51:LEU:HD23	4:B:51:LEU:HA	1.90	0.40
1:A:670:PHE:O	1:A:673:PRO:HD2	2.22	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	992/1219 (81%)	949 (96%)	43 (4%)	0	100	100
2	D	130/133 (98%)	126 (97%)	4 (3%)	0	100	100
3	E	24/33 (73%)	23 (96%)	1 (4%)	0	100	100
4	B	371/380 (98%)	353 (95%)	18 (5%)	0	100	100
All	All	1517/1765 (86%)	1451 (96%)	66 (4%)	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	A	903/1090 (83%)	888 (98%)	15 (2%)	53	68
2	D	114/120 (95%)	111 (97%)	3 (3%)	40	61
3	E	24/28 (86%)	24 (100%)	0	100	100
4	B	343/352 (97%)	335 (98%)	8 (2%)	44	63
All	All	1384/1590 (87%)	1358 (98%)	26 (2%)	49	66

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	82	MET
1	A	85	THR
1	A	167	LEU
1	A	285	VAL
1	A	323	THR
1	A	373	VAL
1	A	393	ILE
1	A	515	LEU
1	A	676	THR
1	A	761	ILE
1	A	872	LEU
1	A	897	ASN
1	A	978	LEU
1	A	994	LEU
2	D	73	LEU
2	D	76	ASP
2	D	99	VAL
4	B	28	ILE
4	B	68	THR
4	B	72	MET
4	B	76	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	151	LEU
4	B	185	LEU
4	B	220	GLU
4	B	313	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	185	GLN
1	A	197	ASN
1	A	250	HIS
1	A	437	GLN
1	A	468	GLN
1	A	526	GLN
1	A	916	GLN
1	A	931	ASN
1	A	973	ASN
1	A	997	ASN
1	A	1033	HIS
1	A	1049	ASN
2	D	62	GLN
4	B	29	GLN
4	B	120	ASN
4	B	126	ASN
4	B	264	GLN
4	B	305	HIS
4	B	336	GLN
4	B	352	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
5	SF4	A	1401	1	0,12,12	-	-	-		

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
5	SF4	A	1401	1	-	-	0/6/5/5

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1401	SF4	3	0

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.

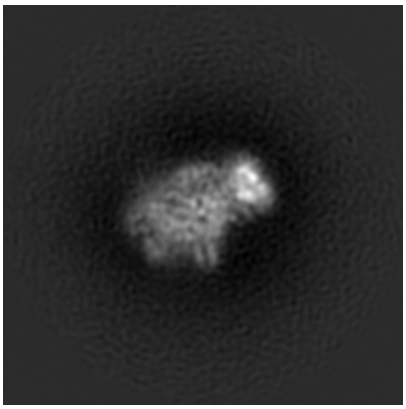
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10089. These allow visual inspection of the internal detail of the map and identification of artifacts.

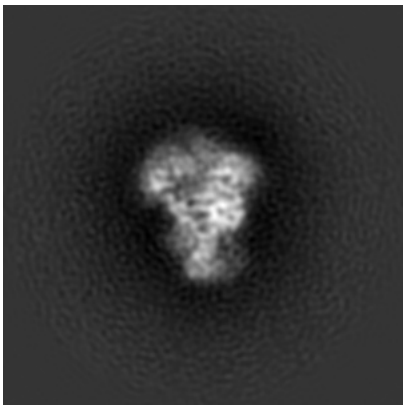
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

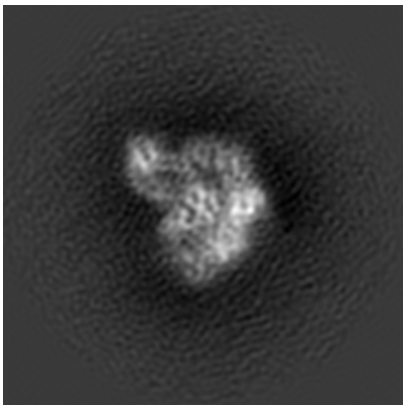
6.1.1 Primary map



X

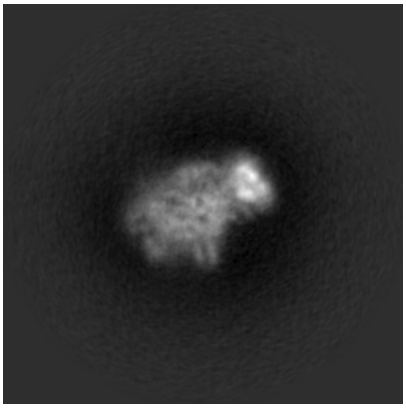


Y

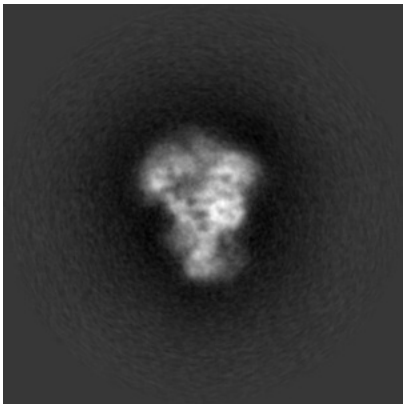


Z

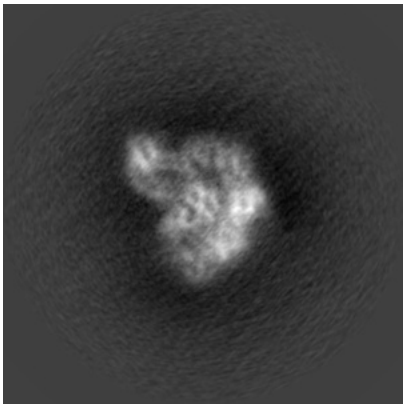
6.1.2 Raw map



X



Y

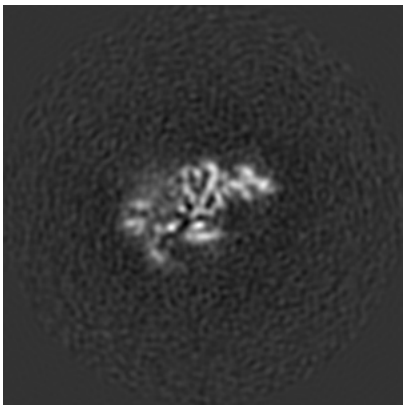


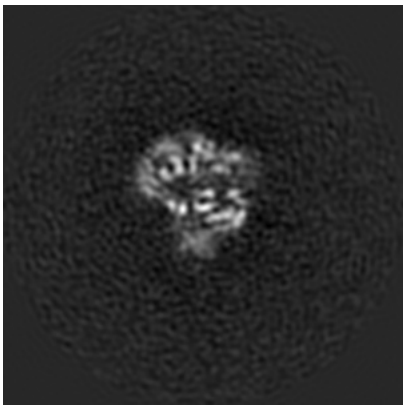
Z

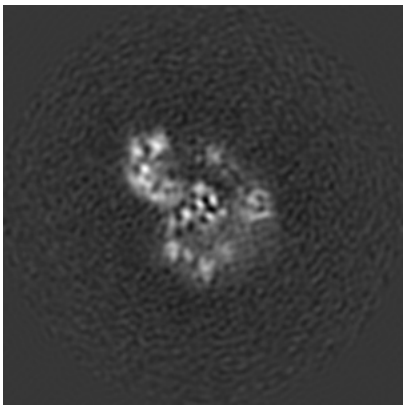
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

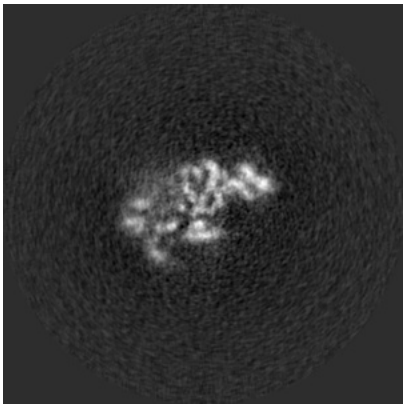
6.2.1 Primary map

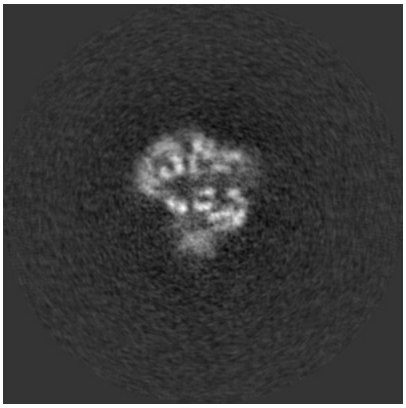

X Index: 145

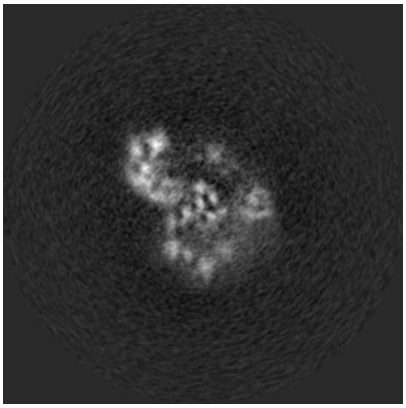

Y Index: 145


Z Index: 145

6.2.2 Raw map


X Index: 145

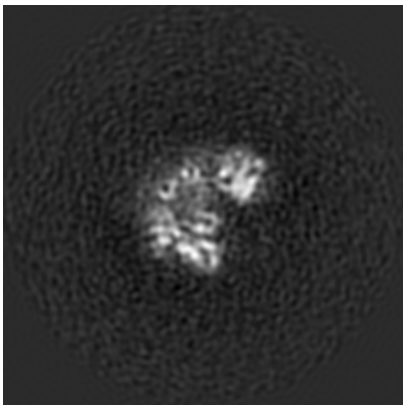

Y Index: 145

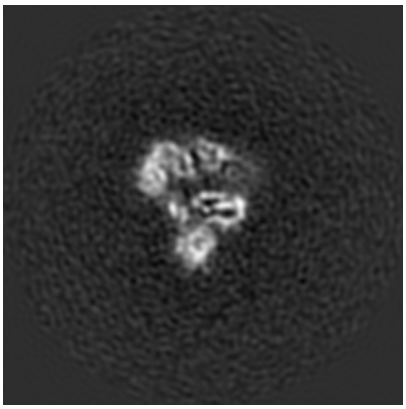

Z Index: 145

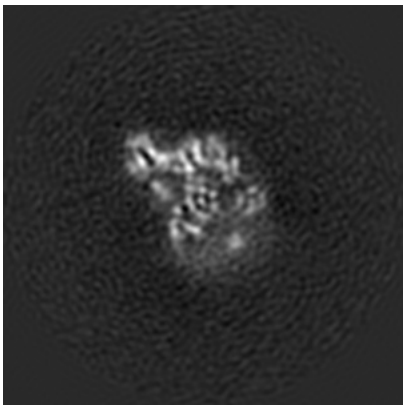
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

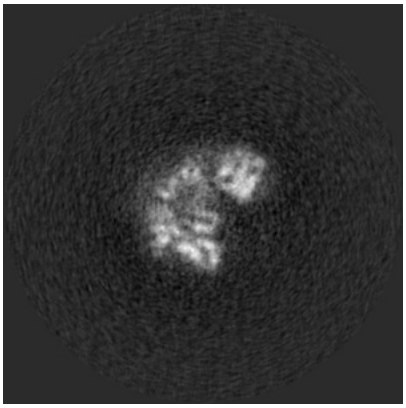
6.3.1 Primary map

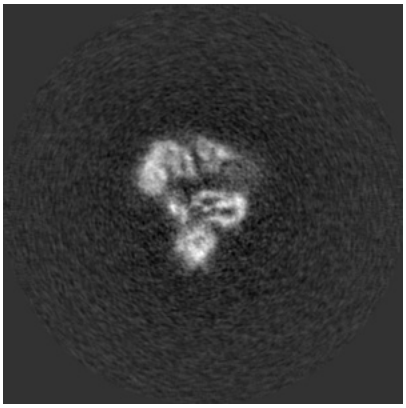

X Index: 168

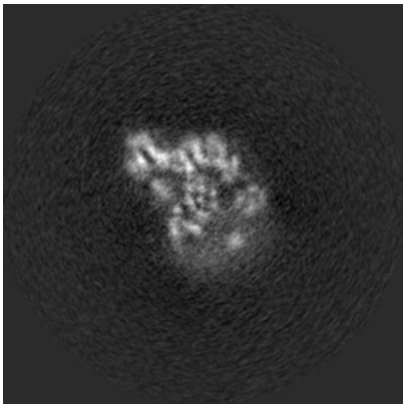

Y Index: 151


Z Index: 152

6.3.2 Raw map


X Index: 168

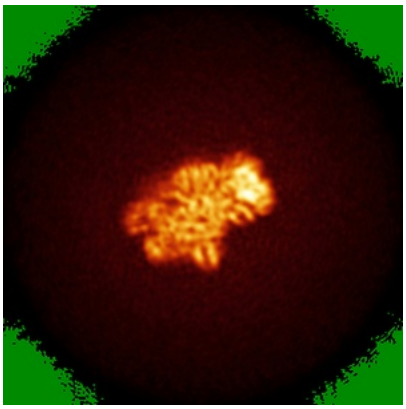

Y Index: 151

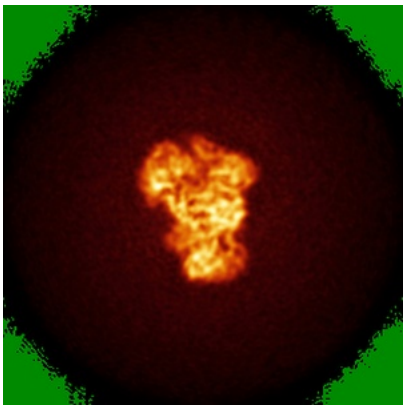

Z Index: 152

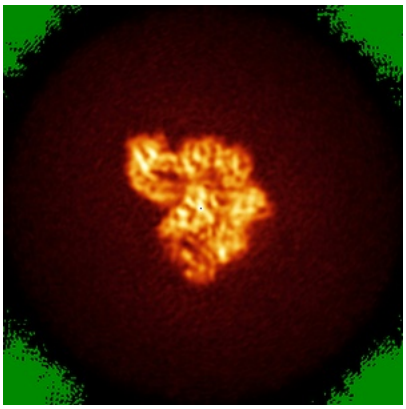
The images above show the largest variance slices of the map in three orthogonal directions.

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

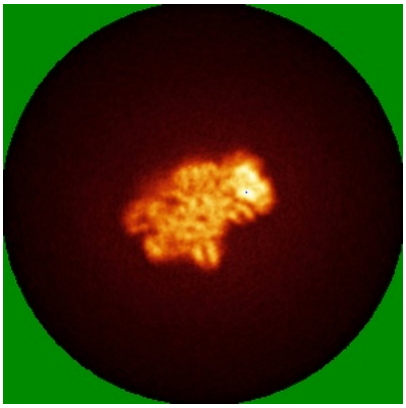
6.4.1 Primary map

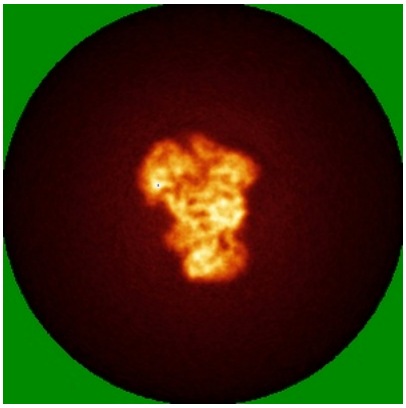

X

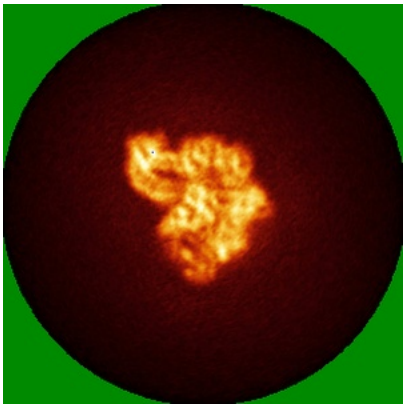

Y


Z

6.4.2 Raw map


X

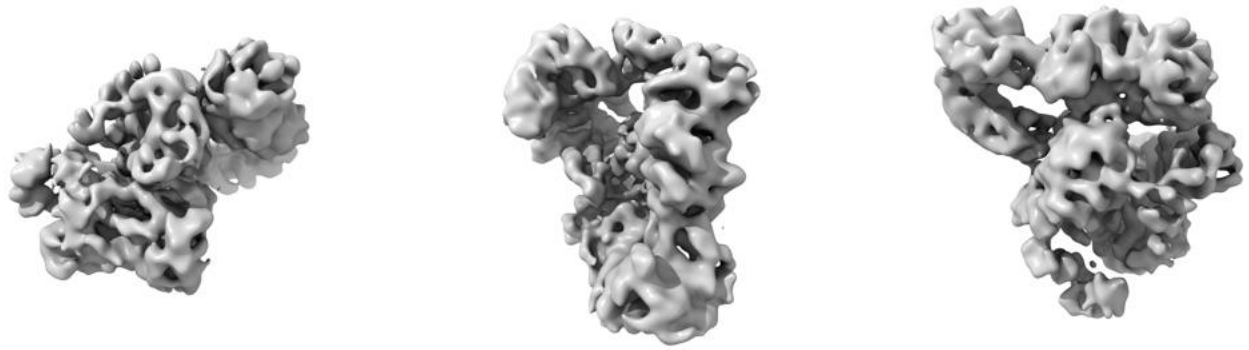

Y


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)

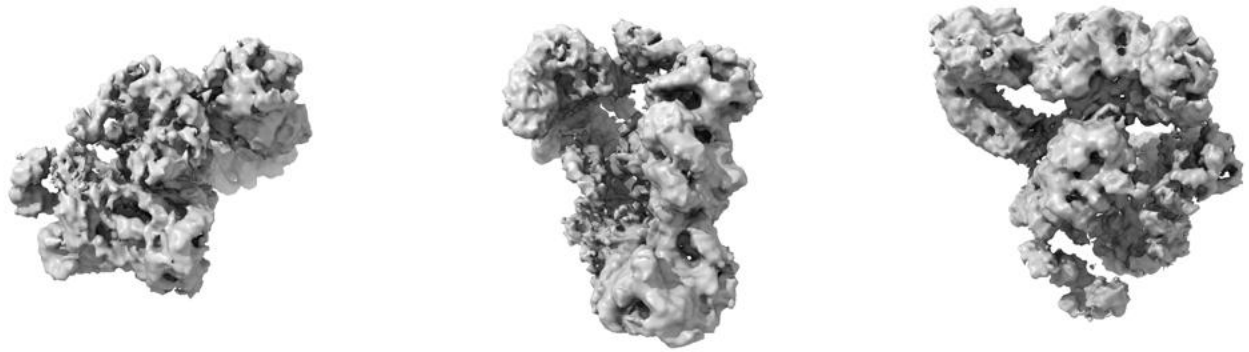
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

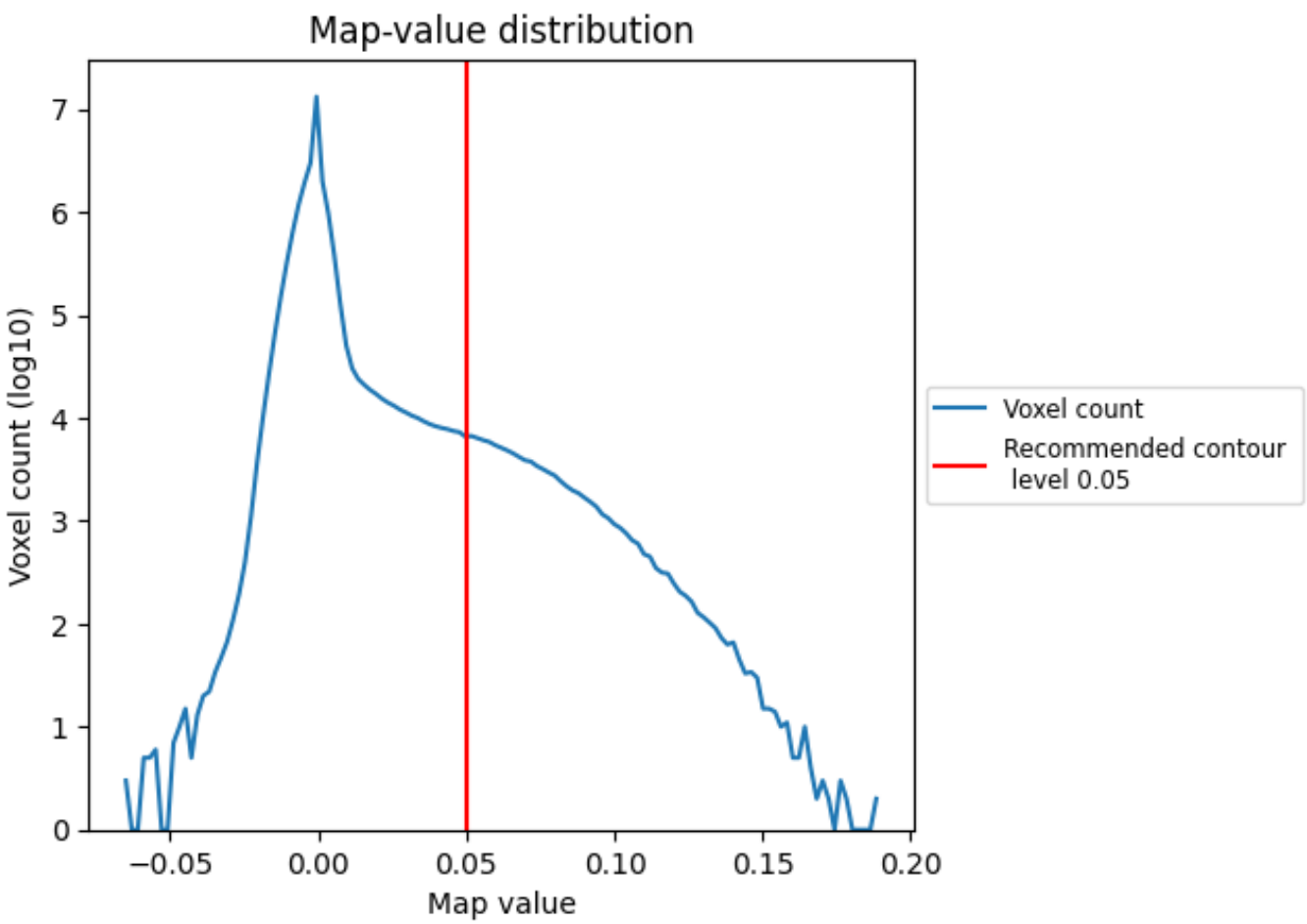
6.6 Mask visualisation (i)

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

7 Map analysis (i)

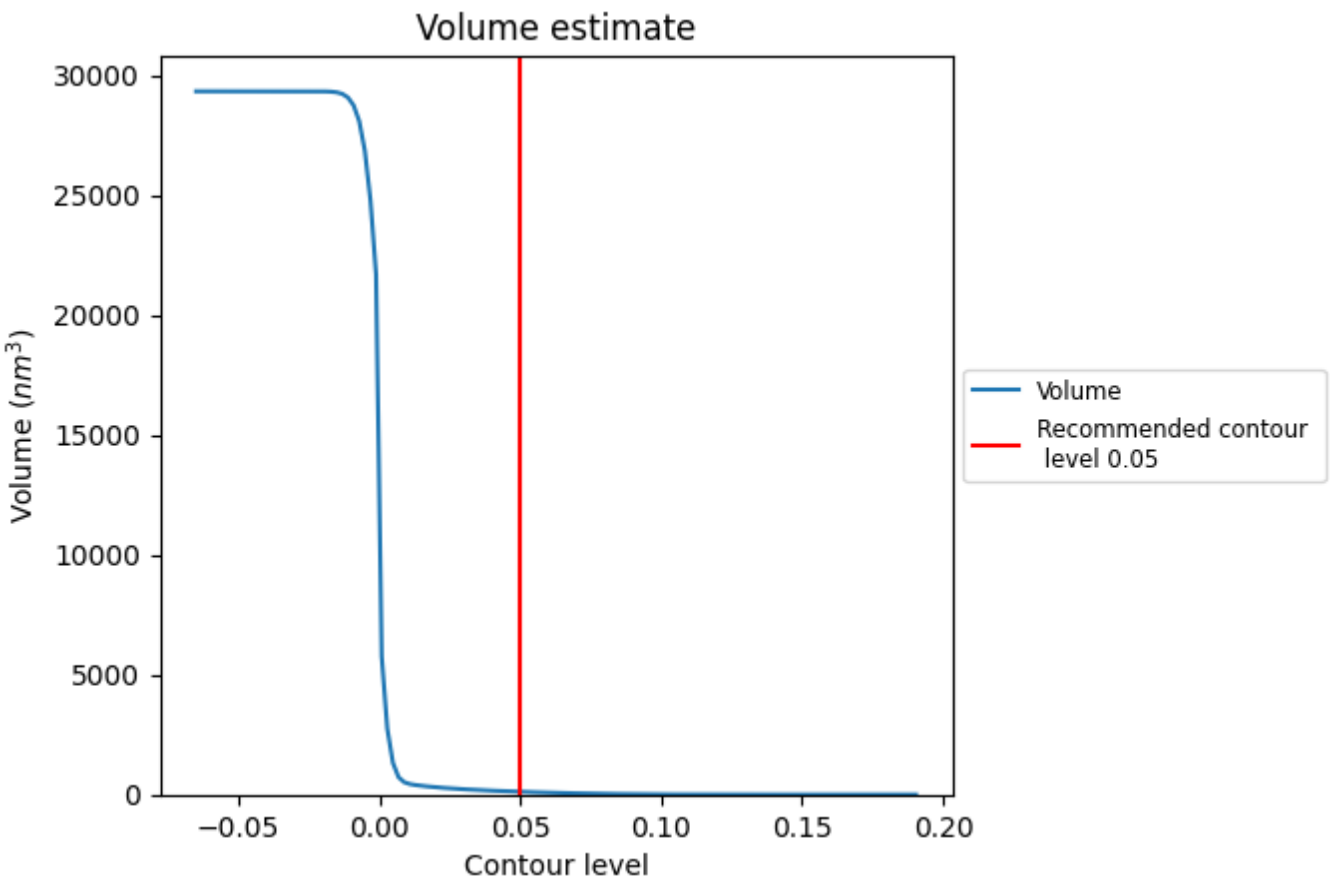
This section contains the results of statistical analysis of the map.

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.

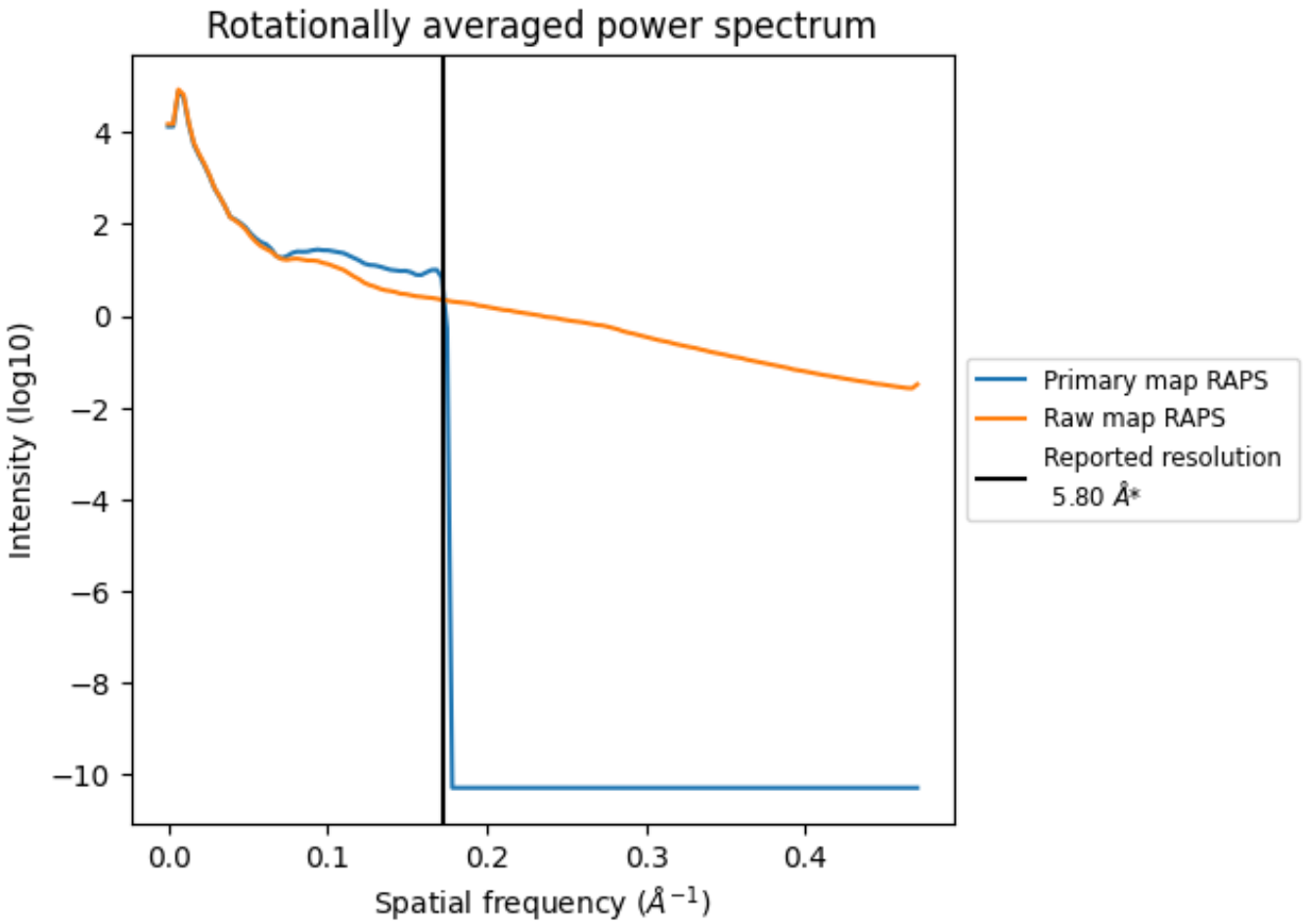
7.2 Volume estimate (i)



The volume at the recommended contour level is 117 nm^3; this corresponds to an approximate mass of 106 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)

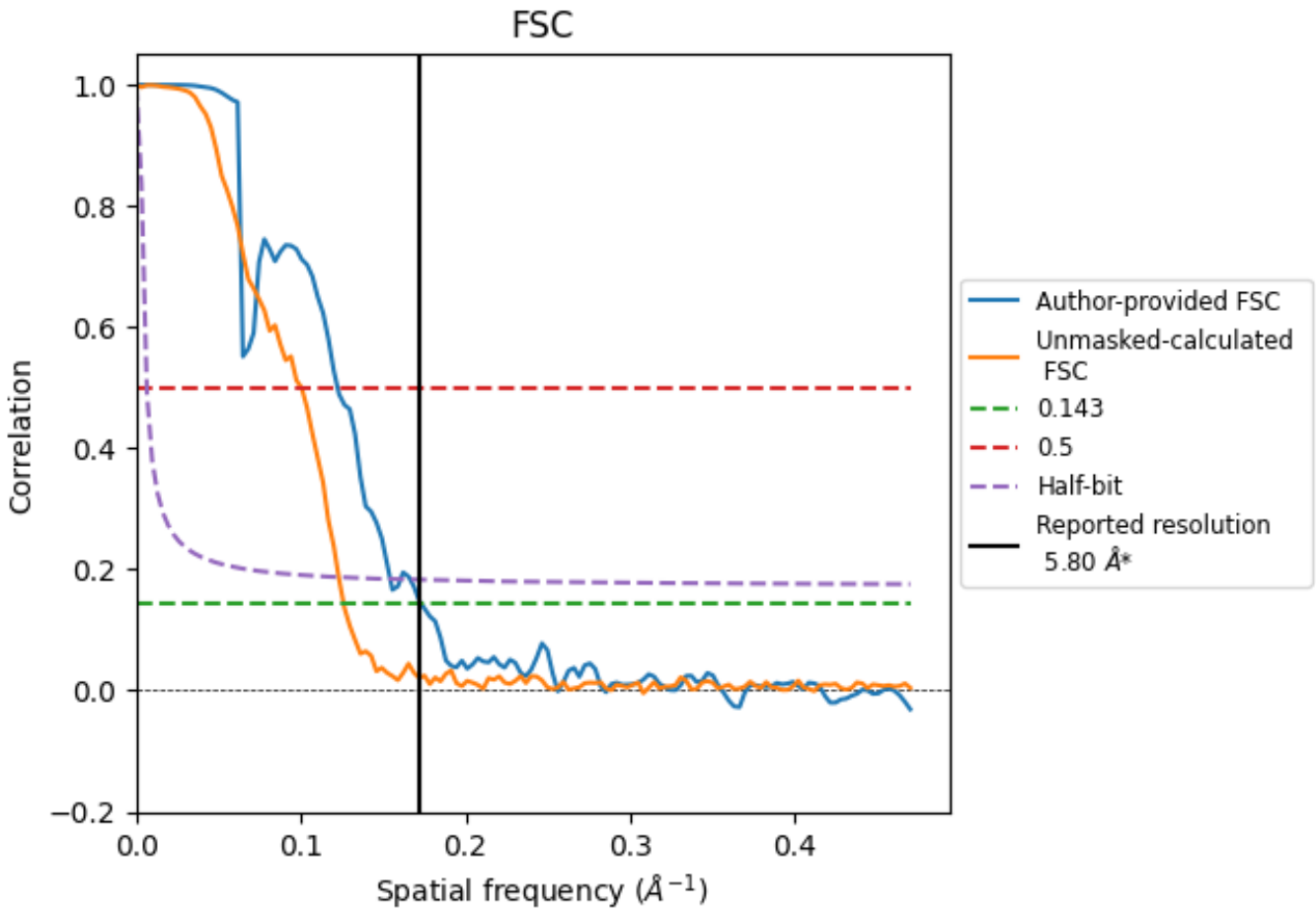


*Reported resolution corresponds to spatial frequency of 0.172 Å^{-1}

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 0.172 Å^{-1}

8.2 Resolution estimates (i)

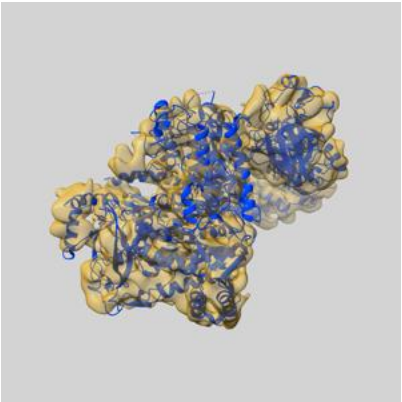
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.80	-	-
Author-provided FSC curve	5.77	8.18	6.48
Unmasked-calculated*	7.94	9.96	8.13

*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 7.94 differs from the reported value 5.8 by more than 10 %

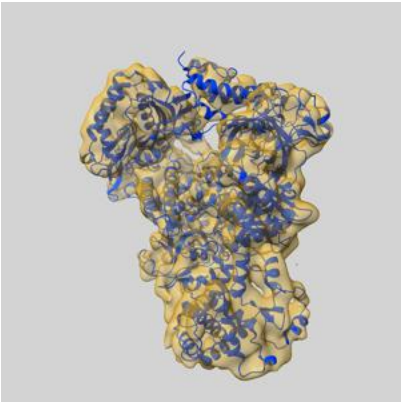
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10089 and PDB model 6S2F. Per-residue inclusion information can be found in section 3 on page 7.

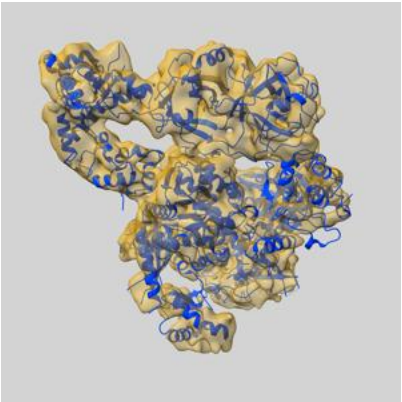
9.1 Map-model overlay (i)



X



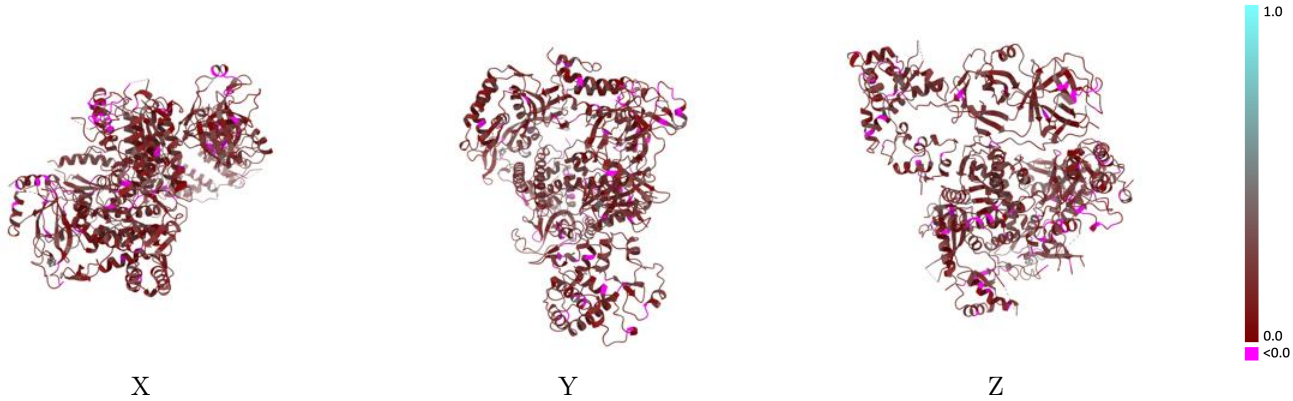
Y



Z

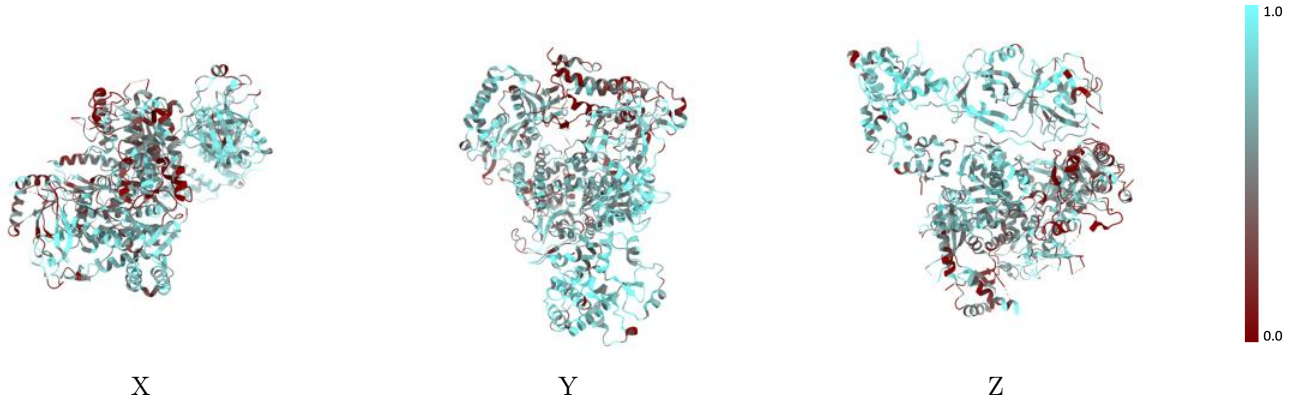
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



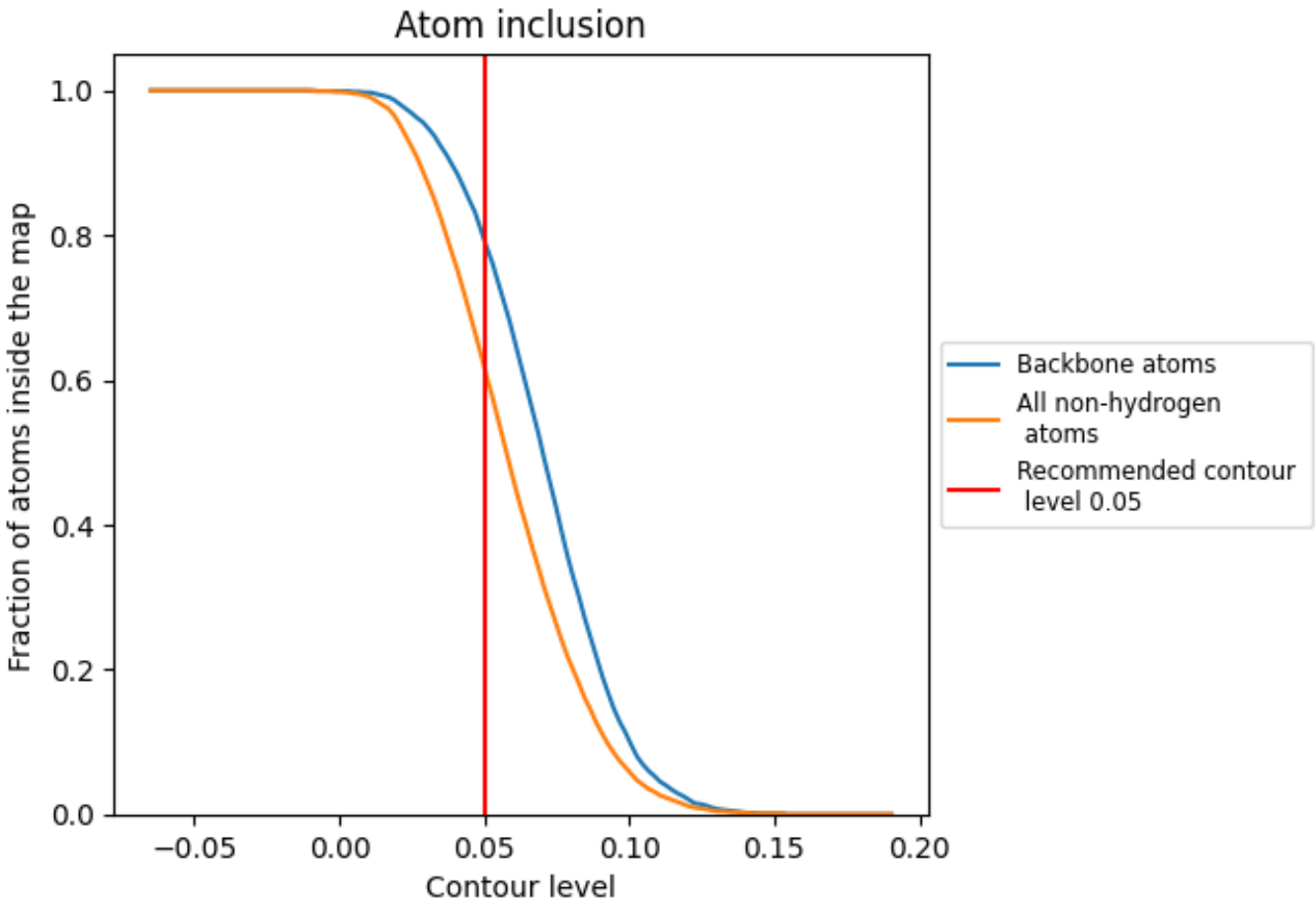
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 62% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6180	0.1730
A	0.5550	0.1670
B	0.7430	0.1850
D	0.7090	0.1800
E	0.7850	0.1970