Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 08:54 am GMT

PDB ID	:	6S2F
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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

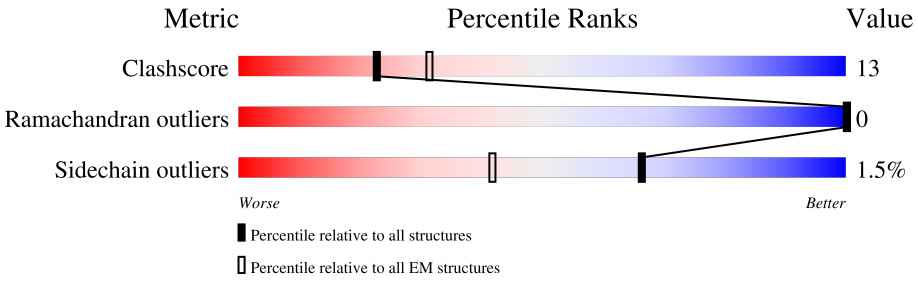
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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)
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	A	1219	24% 57% 24% • 17%
2	D	133	15% 59% 39% •••
3	E	33	9% 45% 33% 21%
4	B	380	8% 67% 30% ••

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

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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
2	D	132	Total	C	N	O	S	0	0
			1031	653	176	195	7		

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

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

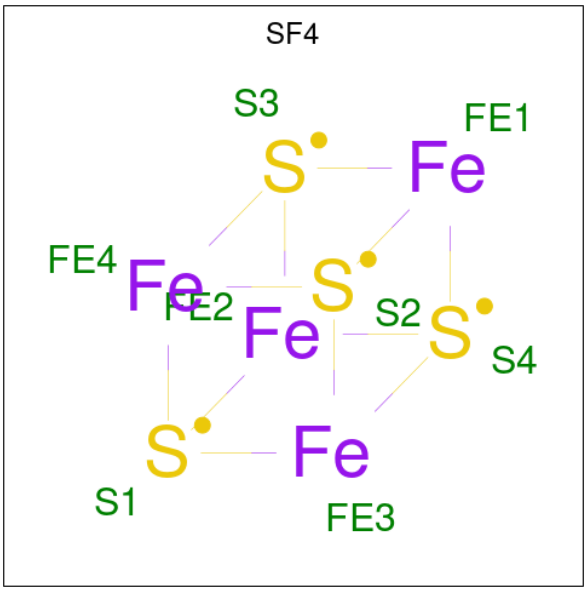
There are 4 discrepancies between the modelled and reference sequences:

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
4	B	375	Total	C	N	O	S	0	0
			3041	1959	505	563	14		

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



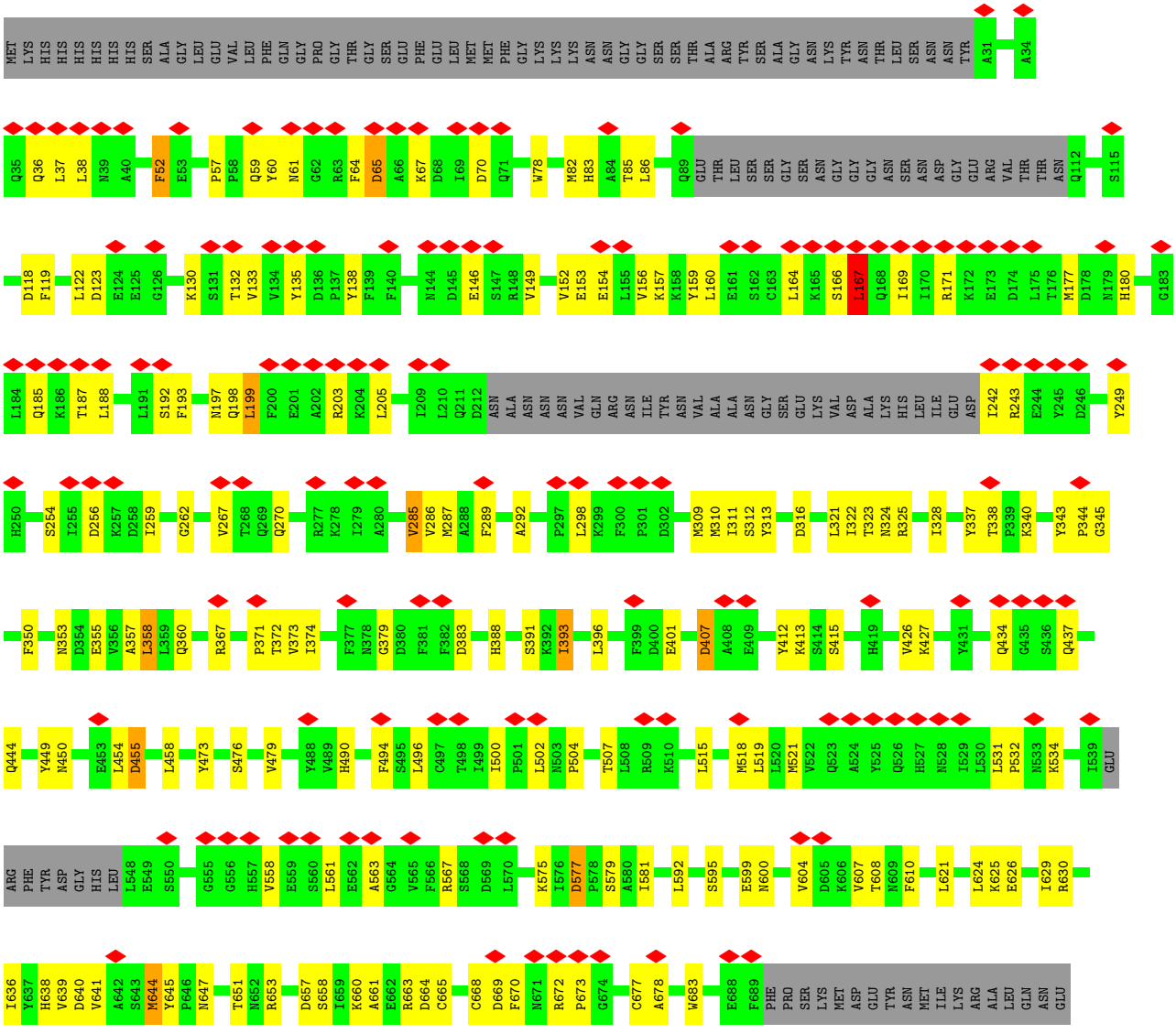
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
5	A	1	8	4	4	0

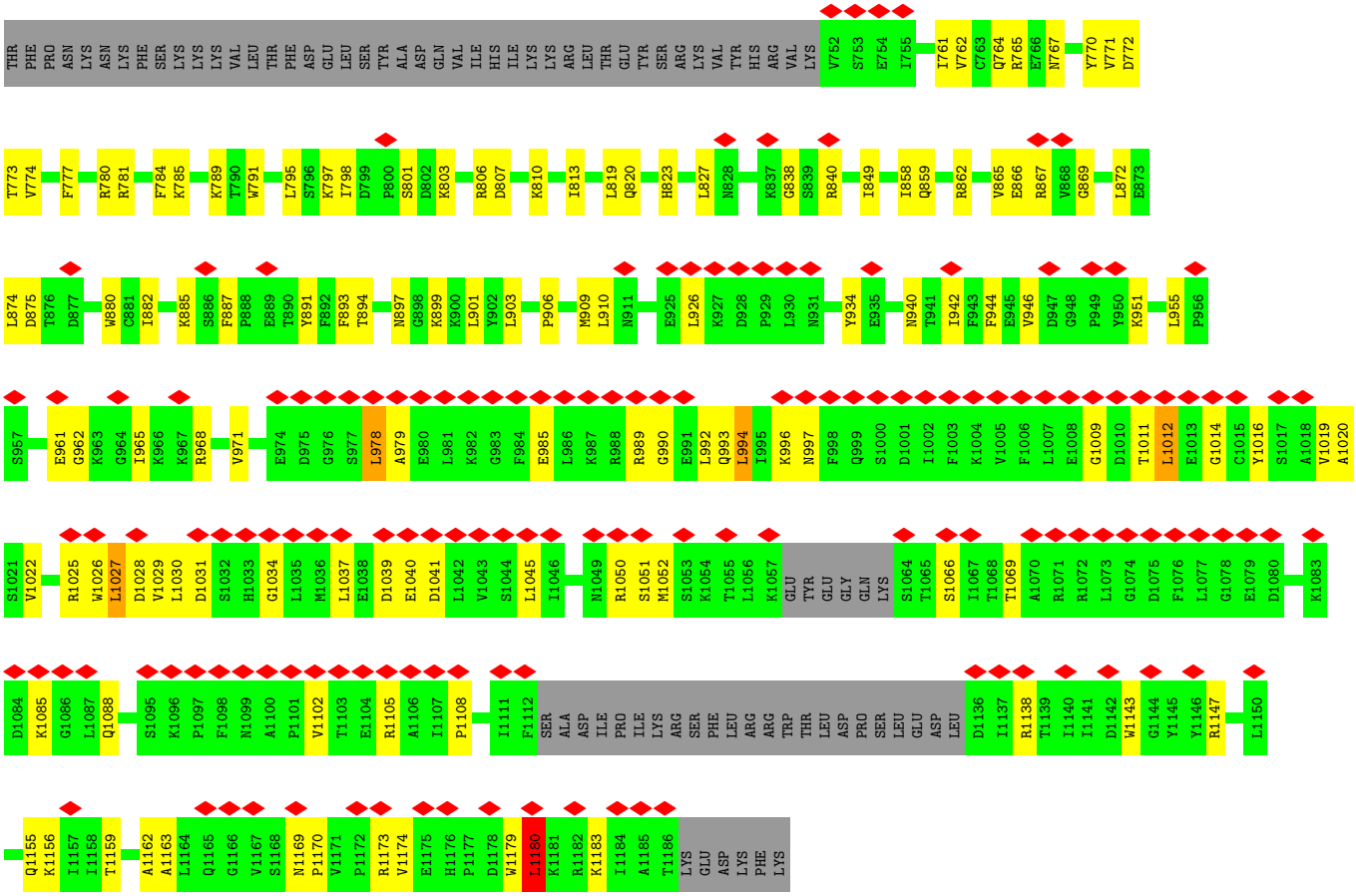
3 Residue-property plots (i)

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

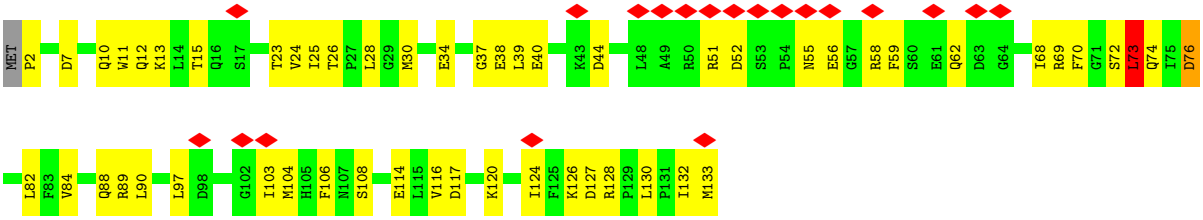
Chain A:





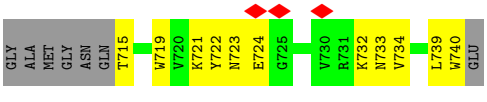
• Molecule 2: Chromosome transmission fidelity protein 8

Chain D:



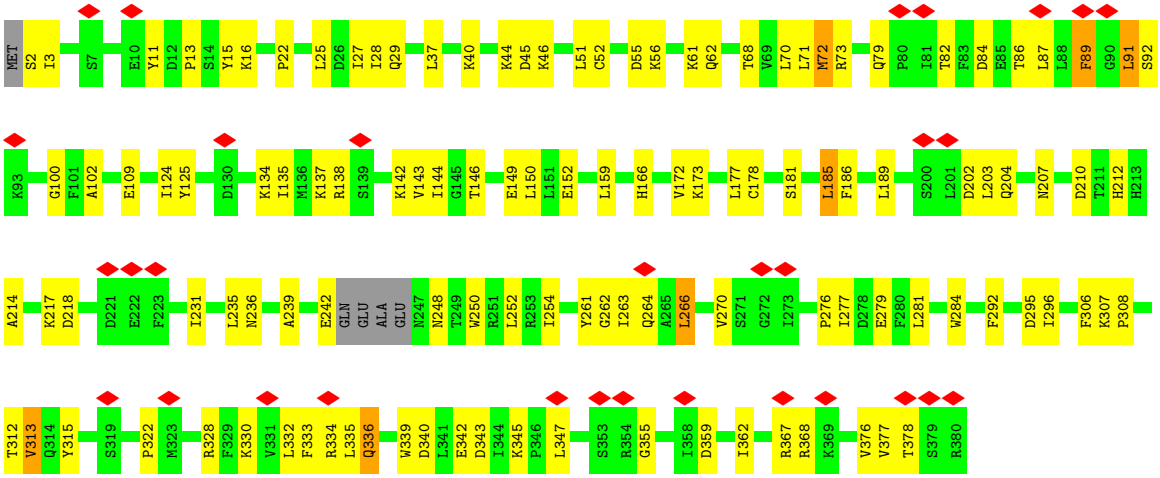
• Molecule 3: Chromosome transmission fidelity protein 18

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 L37 K40 K44 D45 K46 L51 C52 D55 K56 K61 Q62 T68 V69 L70 L71 M72 R73 Q79 P80 I81 T82 F83 D84 E85 T86 L87 L88 F89 G90 L91 S92
K93 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 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

5.1 Standard geometry

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	0.48	1/8338 (0.0%)	0.89	27/11267 (0.2%)
2	D	0.45	0/1047	0.85	2/1407 (0.1%)
3	E	0.57	0/232	0.82	0/316
4	B	0.50	0/3110	0.82	9/4204 (0.2%)
All	All	0.48	1/12727 (0.0%)	0.87	38/17194 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	PHE	CA-CB	-5.86	1.41	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	LEU	CA-CB-CG	8.82	135.59	115.30
1	A	515	LEU	CA-CB-CG	8.76	135.44	115.30
1	A	978	LEU	CA-CB-CG	7.99	133.68	115.30
2	D	73	LEU	CA-CB-CG	7.75	133.11	115.30
4	B	185	LEU	CA-CB-CG	7.74	133.11	115.30
1	A	926	LEU	CA-CB-CG	7.42	132.37	115.30
1	A	358	LEU	CA-CB-CG	7.37	132.26	115.30
1	A	577	ASP	CB-CG-OD1	7.36	124.93	118.30
1	A	994	LEU	CA-CB-CG	6.78	130.89	115.30
1	A	592	LEU	CA-CB-CG	6.57	130.42	115.30
1	A	199	LEU	CA-CB-CG	6.49	130.24	115.30
1	A	455	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	164	LEU	CA-CB-CG	6.11	129.35	115.30
2	D	39	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	518	MET	CA-CB-CG	5.98	123.47	113.30
1	A	122	LEU	CA-CB-CG	5.83	128.71	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	407	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	65	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	454	LEU	CA-CB-CG	5.72	128.45	115.30
1	A	316	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	1027	LEU	CA-CB-CG	5.69	128.40	115.30
1	A	496	LEU	CA-CB-CG	5.64	128.26	115.30
1	A	256	ASP	CB-CG-OD1	5.56	123.31	118.30
4	B	336	GLN	CA-CB-CG	5.55	125.60	113.40
1	A	1180	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	910	LEU	CB-CG-CD2	5.43	120.24	111.00
4	B	266	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	661	ALA	C-N-CA	5.33	135.02	121.70
4	B	332	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	188	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	502	LEU	CA-CB-CG	5.17	127.18	115.30
4	B	335	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	A	205	LEU	CA-CB-CG	5.15	127.14	115.30
4	B	56	LYS	CD-CE-NZ	-5.11	99.95	111.70
4	B	91	LEU	C-N-CA	5.07	134.38	121.70
1	A	123	ASP	CB-CG-OD1	5.04	122.83	118.30
4	B	89	PHE	C-N-CA	-5.03	111.74	122.30
4	B	185	LEU	CB-CG-CD1	5.01	119.52	111.00

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	187	0
2	D	1031	0	1044	49	0
3	E	225	0	220	15	0
4	B	3041	0	3052	90	0
5	A	8	0	0	3	0
All	All	12459	0	12383	311	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 (311) 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:2:SER:N	4:B:92:SER:HG	1.82	0.78
4:B:266:LEU:HB3	4:B:315:TYR:HB2	1.68	0.76
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:561:LEU:HD11	1:A:874:LEU:HD23	1.88	0.55
4:B:261:TYR:OH	4:B:284:TRP:O	2.23	0.55
1:A:657:ASP:N	1:A:657:ASP:OD1	2.39	0.55
2:D:11:TRP:CD1	2:D:117:ASP:HA	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:625:LYS:NZ	1:A:626:GLU:OE2	2.35	0.53
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:289:PHE:HA	1:A:313:TYR:HA	1.89	0.53
4:B:214:ALA:O	4:B:217:LYS:NZ	2.40	0.53
1:A:357:ALA:O	1:A:360:GLN:NE2	2.38	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
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: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
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
4:B:342:GLU:OE1	4:B:345:LYS:NZ	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:772:ASP:N	1:A:772:ASP:OD1	2.44	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:N	4:B:202: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
2:D:126:LYS:O	3:E:722:TYR:OH	2.27	0.49
4:B:13:PRO:O	4:B:16:LYS:NZ	2.37	0.49
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:D:72:SER:HG	4:B:2:SER:HG	1.50	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:575:LYS:HG2	1:A:629:ILE:HD12	1.98	0.45
1:A:521:MET:HE1	1:A:531:LEU:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:11:TRP:O	2:D:15:THR:OG1	2.35	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:125:TYR:HB2	4:B:178:CYS:SG	2.58	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
1:A:801:SER:OG	1:A:801:SER:O	2.34	0.43
4:B:2:SER:OG	4:B:3:ILE:N	2.52	0.43
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
1:A:789:LYS:HA	1:A:789:LYS:HD2	1.80	0.42
4:B:28:ILE:HD13	4:B:28:ILE:HA	1.83	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
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
1:A:893:PHE:HB2	1:A:901:LEU:HG	2.01	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
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
1:A:1040:GLU:CD	3:E:719:TRP:HE1	2.24	0.41
2:D:24:VAL:HG13	2:D:25:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	889 (98%)	14 (2%)	62	79
2	D	114/120 (95%)	112 (98%)	2 (2%)	59	77
3	E	24/28 (86%)	24 (100%)	0	100	100
4	B	343/352 (97%)	338 (98%)	5 (2%)	65	80
All	All	1384/1590 (87%)	1363 (98%)	21 (2%)	66	80

All (21) 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	393	ILE
1	A	630	ARG
1	A	644	MET
1	A	872	LEU
1	A	885	LYS
1	A	978	LEU
1	A	1012	LEU

Continued on next page...

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Mol	Chain	Res	Type
1	A	1180	LEU
2	D	73	LEU
2	D	76	ASP
4	B	52	CYS
4	B	68	THR
4	B	72	MET
4	B	185	LEU
4	B	313	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	197	ASN
1	A	794	ASN
1	A	931	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	336	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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.

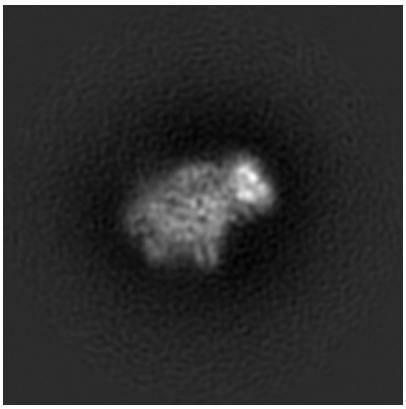
6 Map visualisation

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.

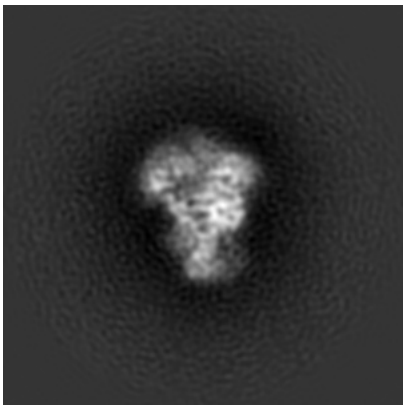
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

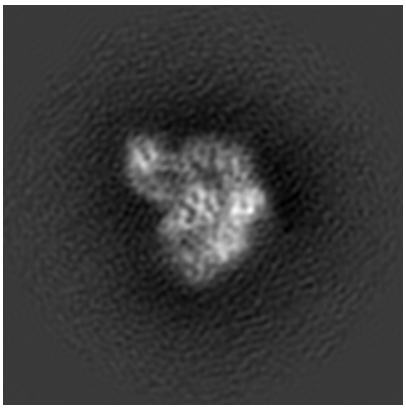
6.1.1 Primary map



X

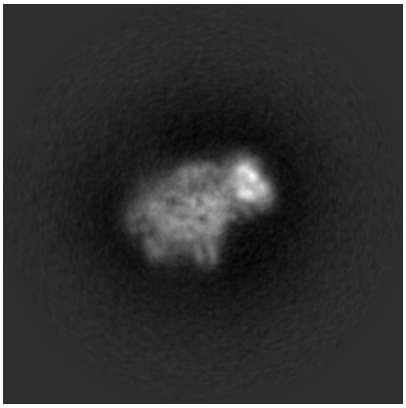


Y

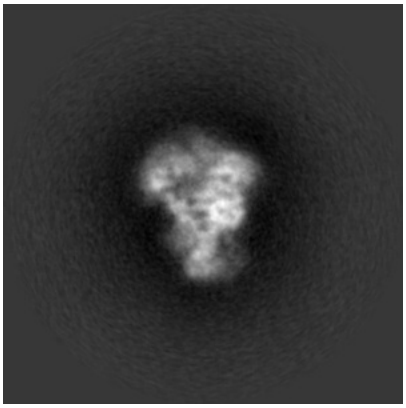


Z

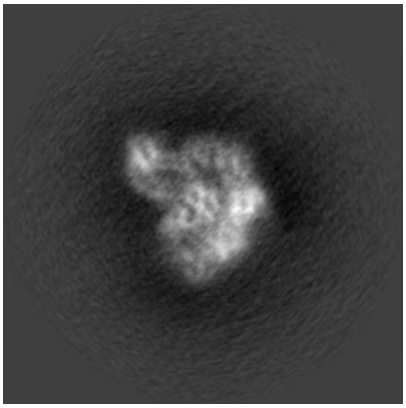
6.1.2 Raw map



X



Y

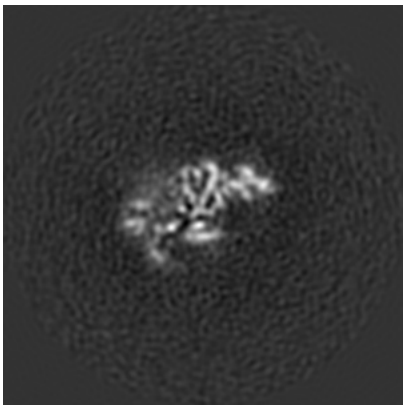


Z

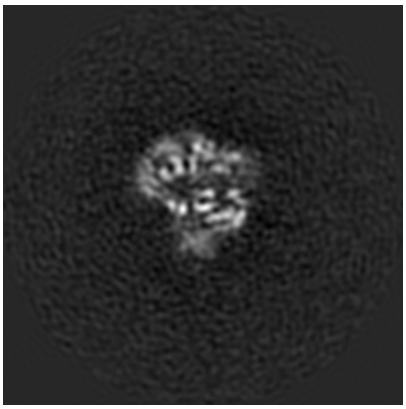
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

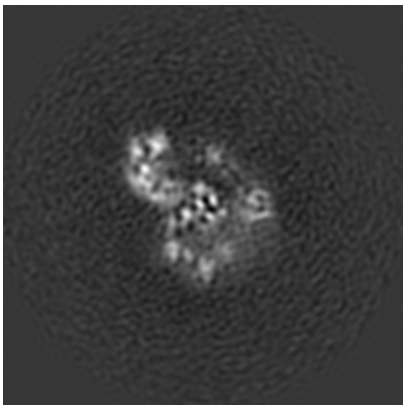
6.2.1 Primary map



X Index: 145

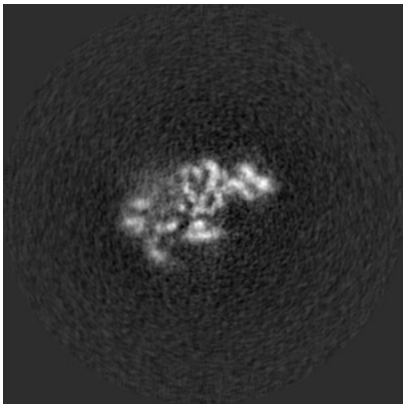


Y Index: 145

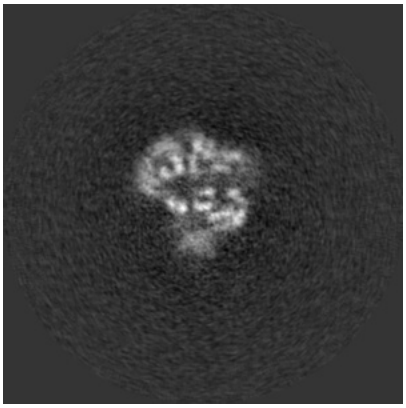


Z Index: 145

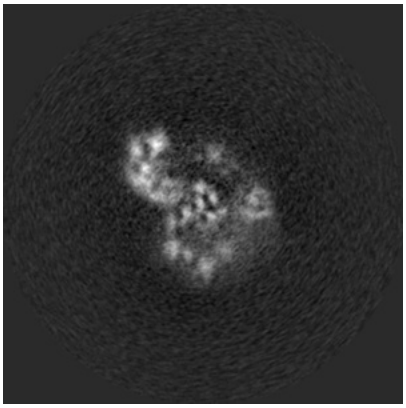
6.2.2 Raw map



X Index: 145



Y Index: 145

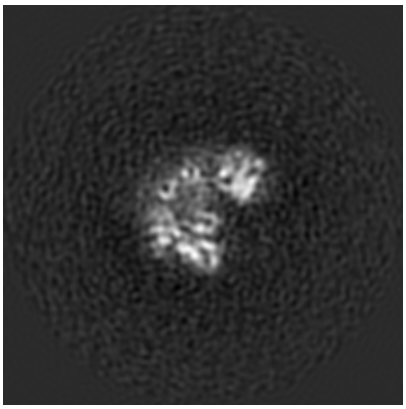


Z Index: 145

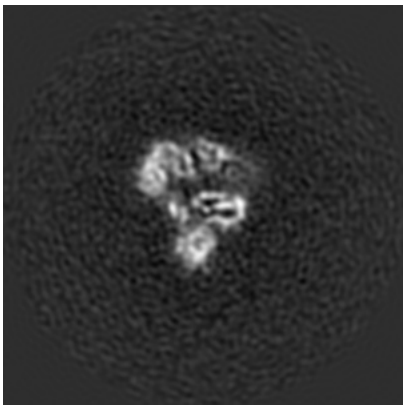
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

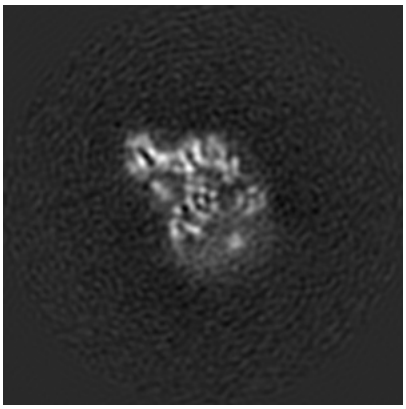
6.3.1 Primary map



X Index: 168

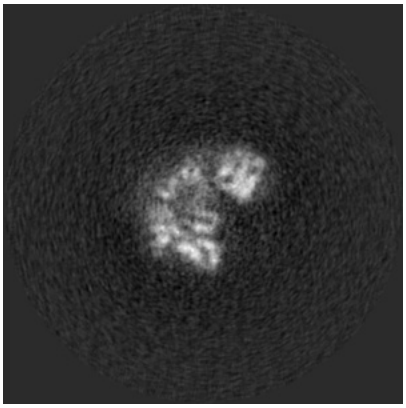


Y Index: 151

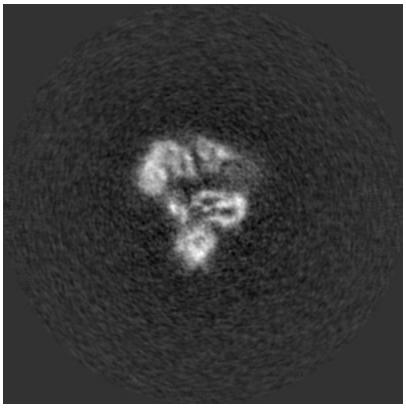


Z Index: 152

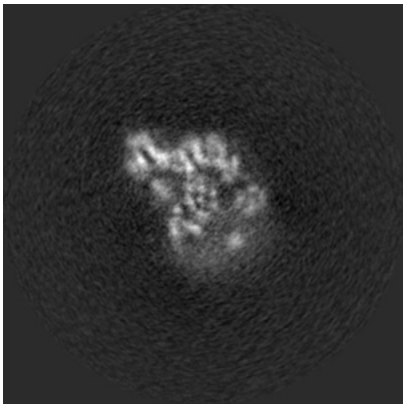
6.3.2 Raw map



X Index: 168



Y Index: 151

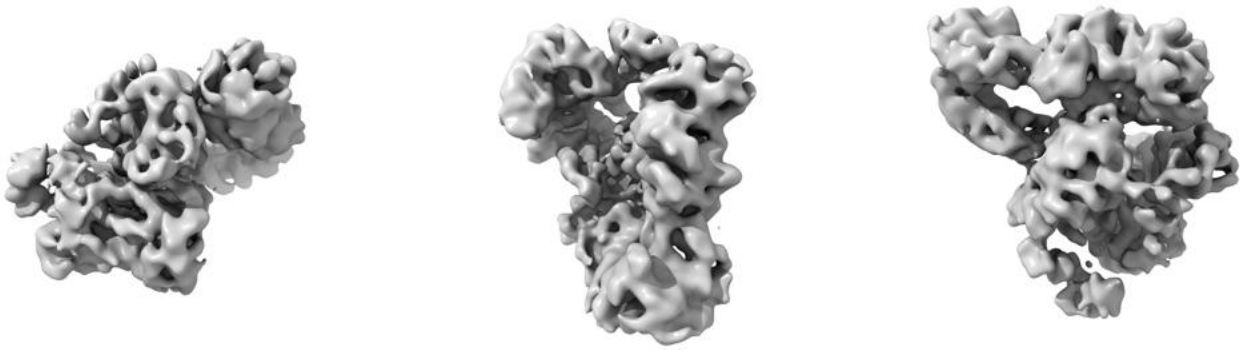


Z Index: 152

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

6.4 Orthogonal surface views (i)

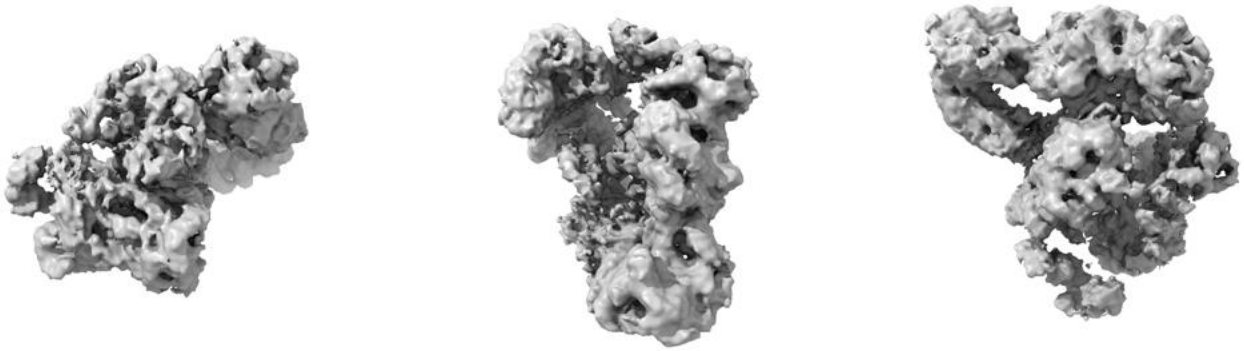
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

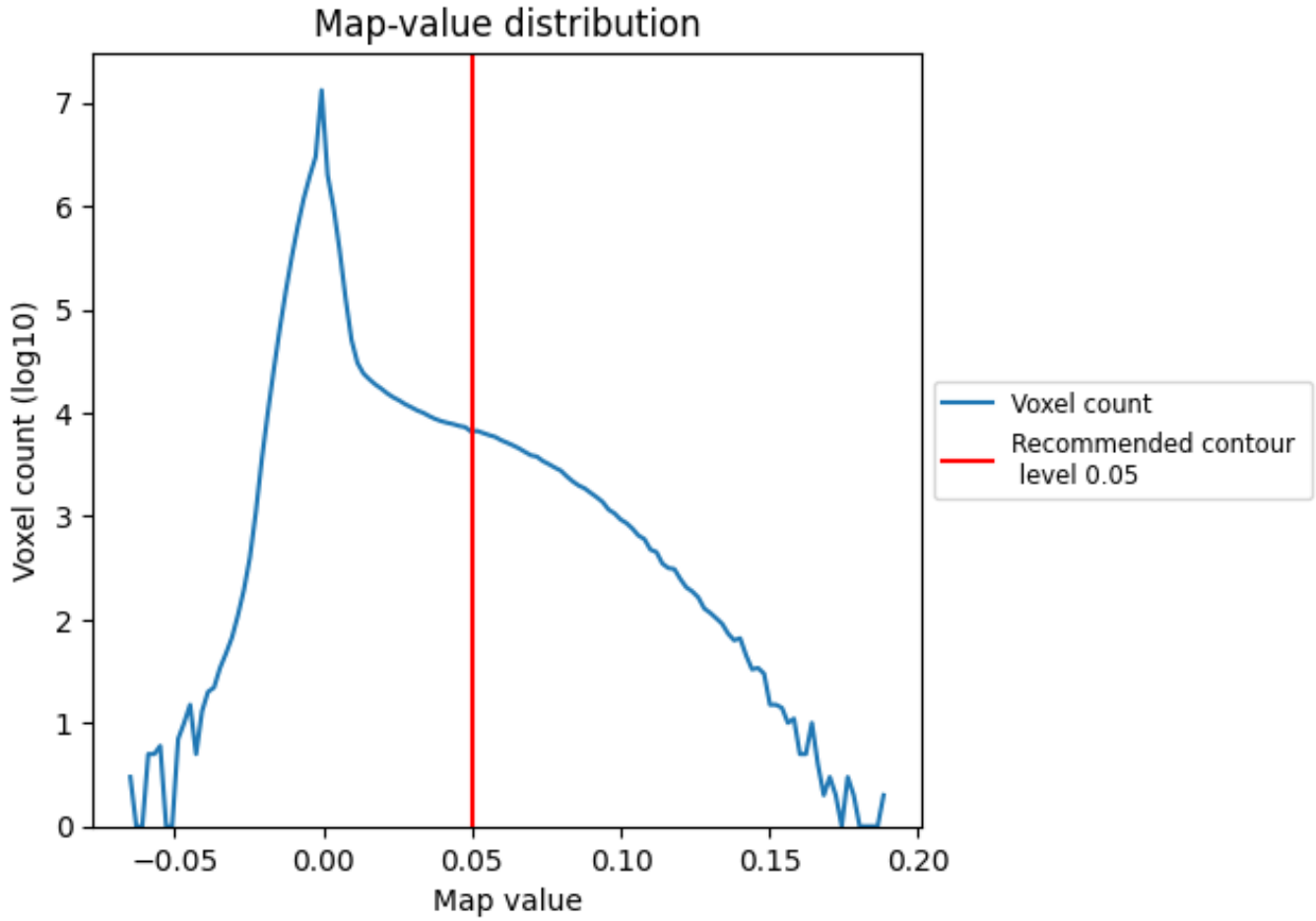
6.5 Mask visualisation (i)

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

7 Map analysis

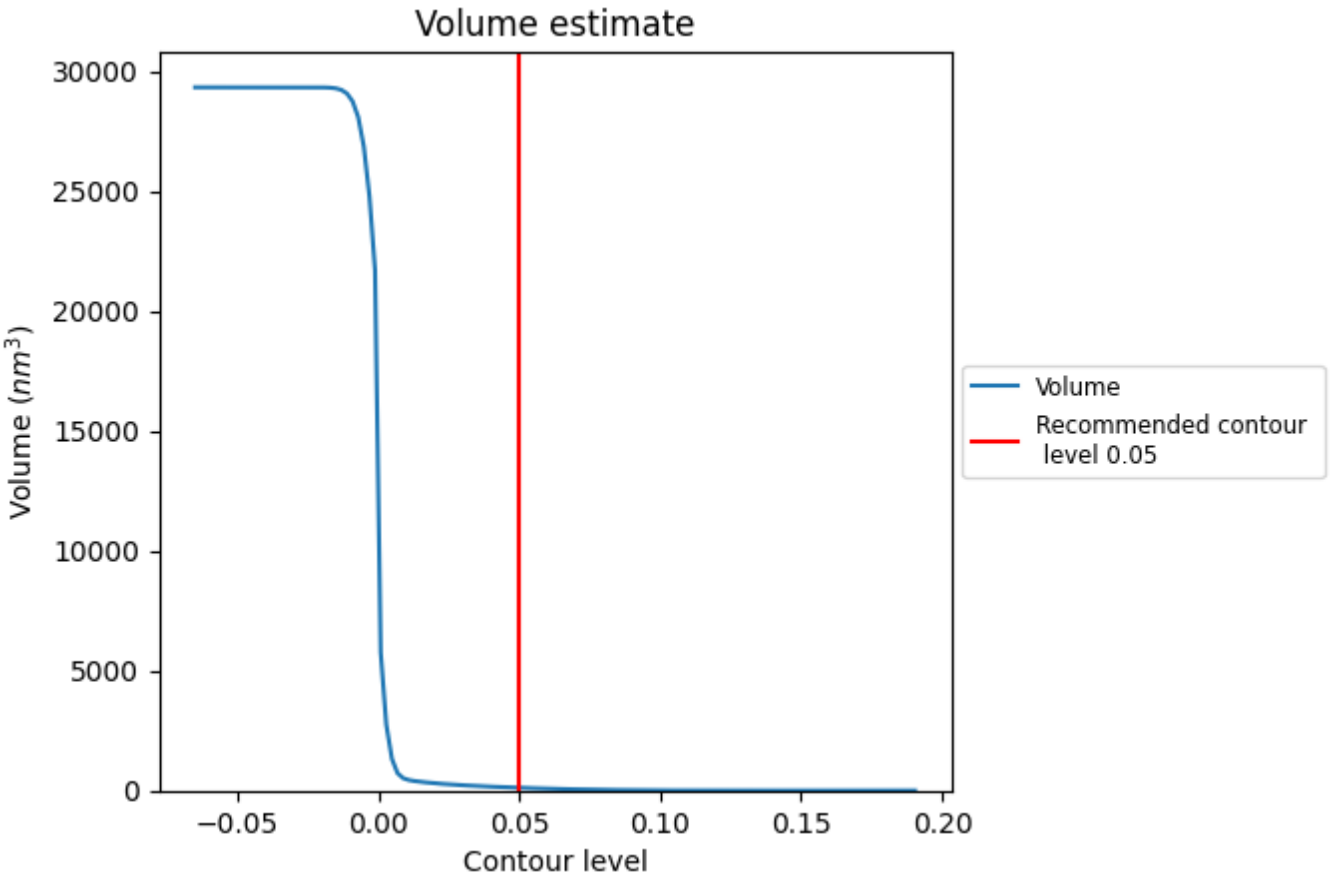
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

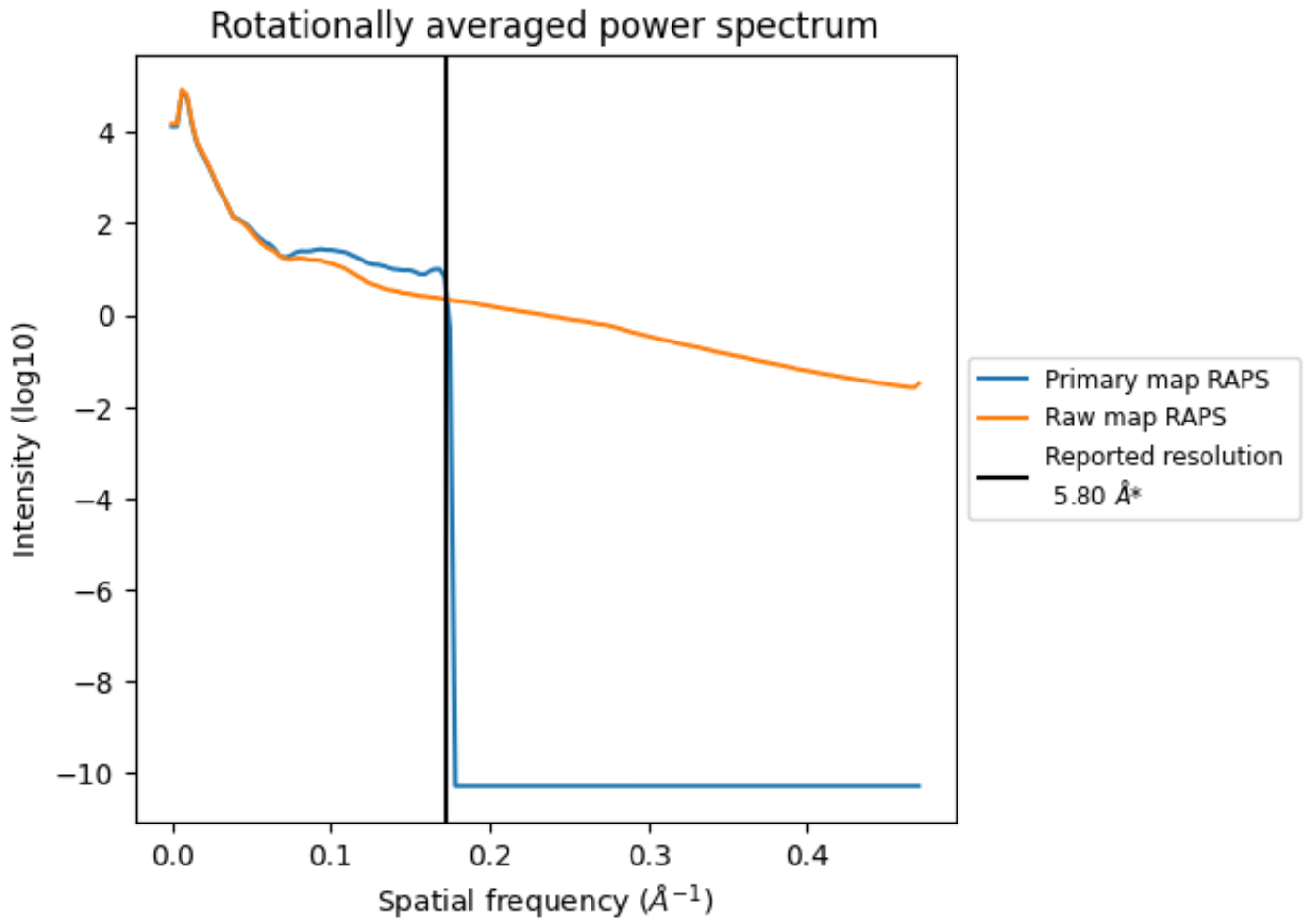
7.2 Volume estimate (i)



The volume at the recommended contour level is 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)

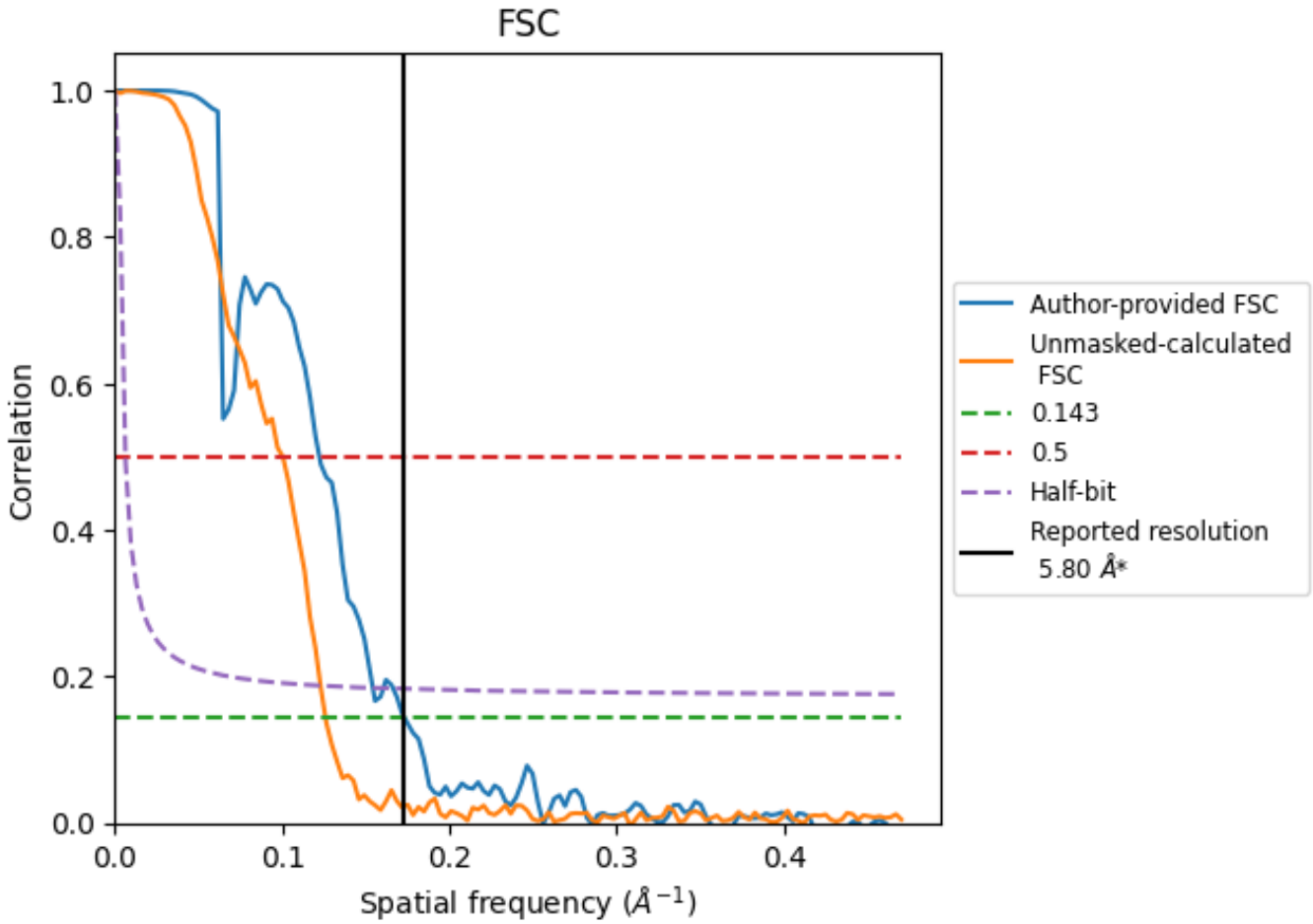


*Reported resolution corresponds to spatial frequency of 0.172 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



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

8.2 Resolution estimates (i)

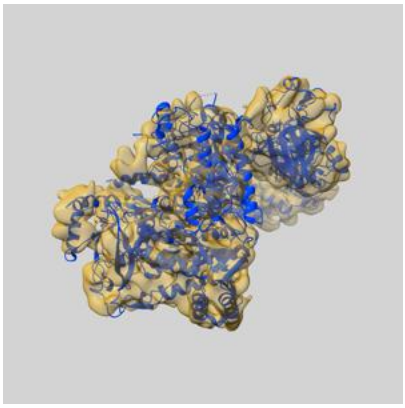
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.80	-	-
Author-provided FSC curve	5.77	8.18	6.48
Unmasked-calculated*	7.94	9.96	8.13

*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 %

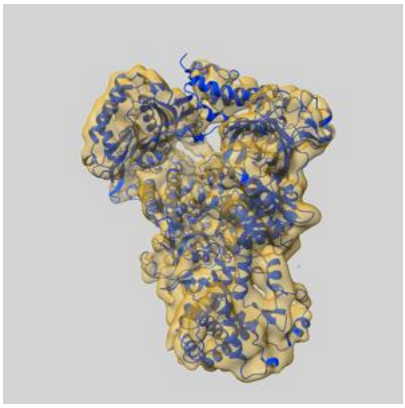
9 Map-model fit

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 6.

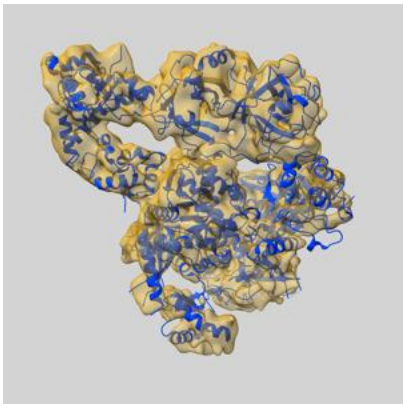
9.1 Map-model overlay



X



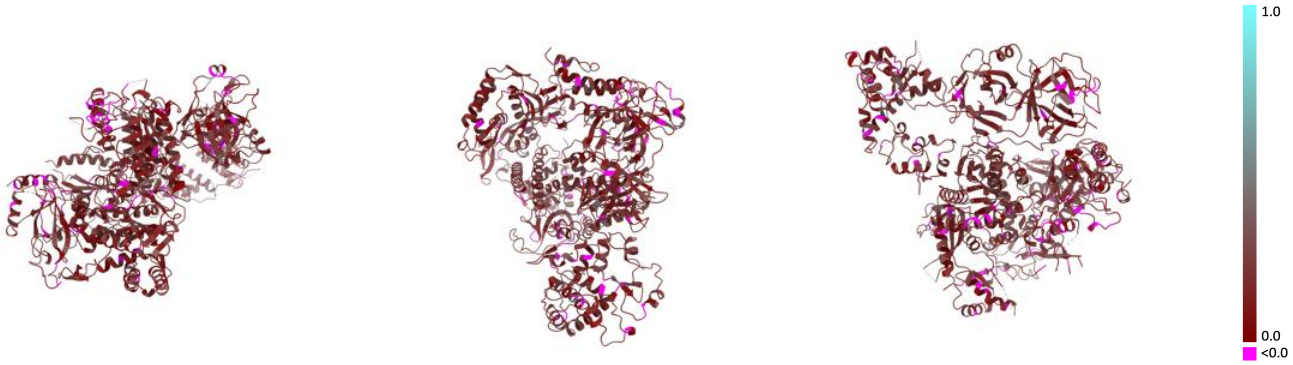
Y



Z

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

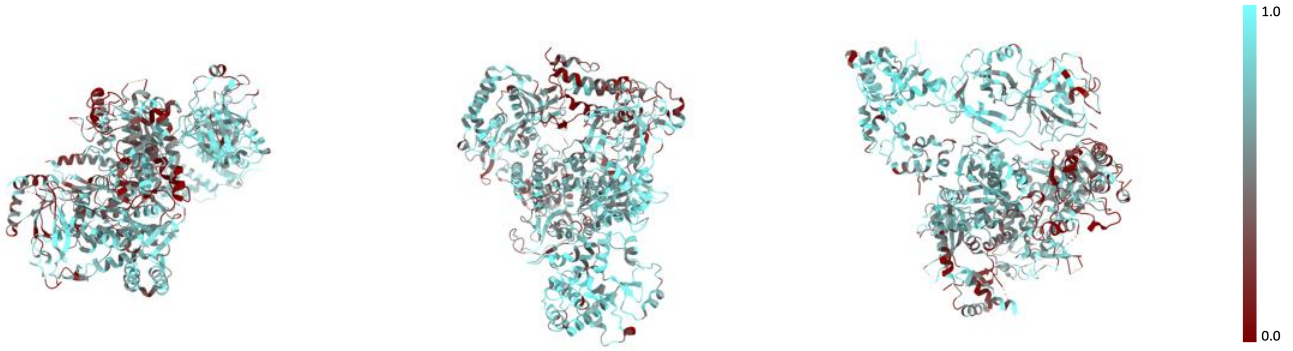
9.2 Q-score mapped to coordinate model (i)



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.

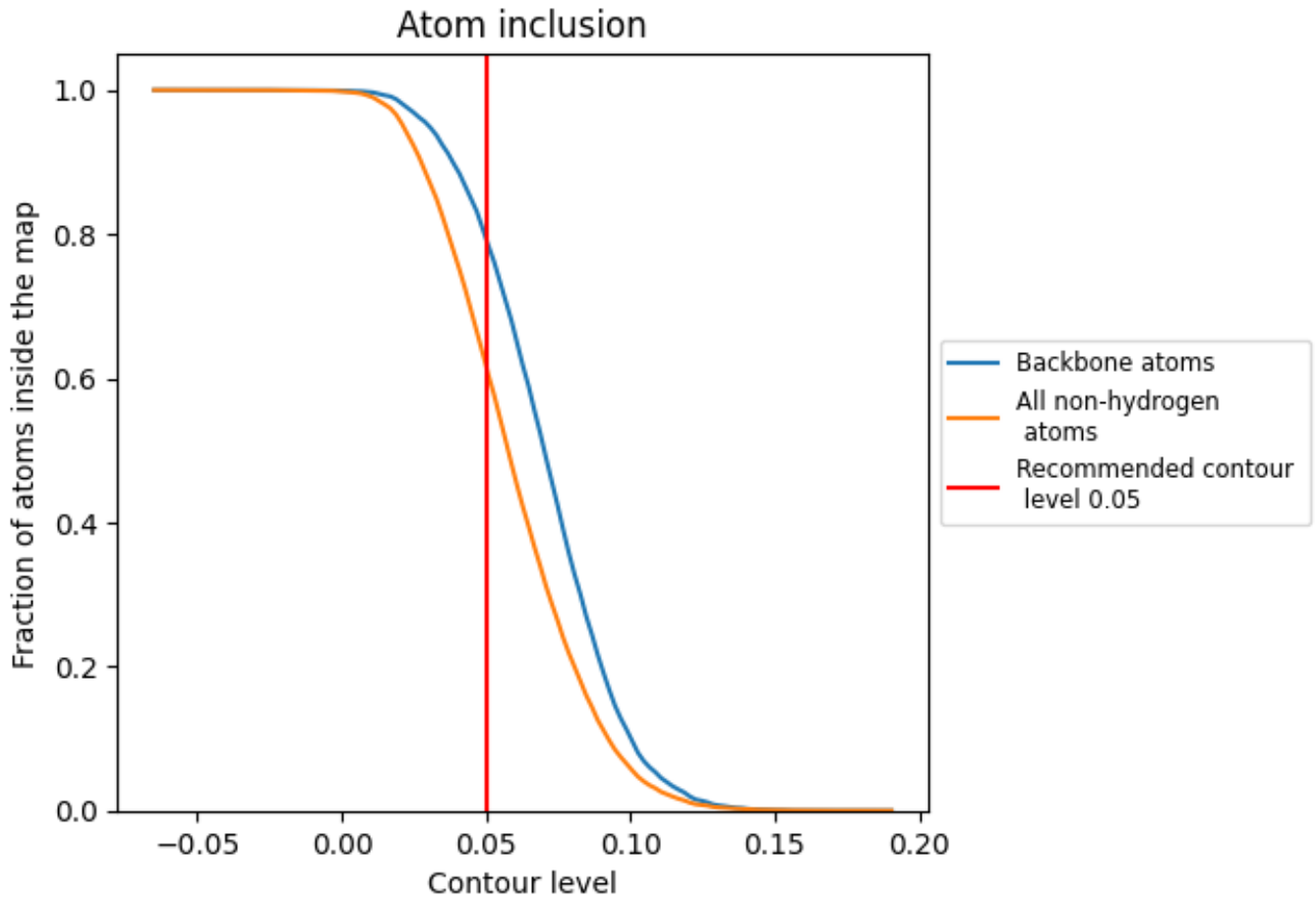
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

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

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	0.6177	0.1730
A	0.5547	0.1670
B	0.7427	0.1850
D	0.7094	0.1800
E	0.7854	0.1970