Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 10:36 AM JST

PDB ID	:	5ZYA
EMDB ID	:	EMD-6915
Title	:	SF3b spliceosomal complex bound to E7107
Authors	:	Finci, L.I.; Larsen, N.A.
Deposited on	:	2018-05-23
Resolution	:	3.95 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

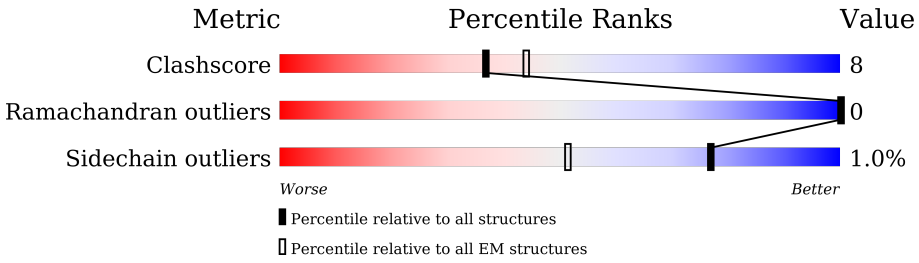
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.95 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	B	86	58% 19% 23%
2	C	1304	7% 47% 15% 38%
3	D	85	91% 9%
4	A	1223	19% 78% 18%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16957 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 Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	66	539	342	93	99	5	0	0

- Molecule 2 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	809	6438	4133	1111	1155	39	0	0

- Molecule 3 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	85	645	396	114	122	13	0	0

- Molecule 4 is a protein called Splicing factor 3B subunit 3.

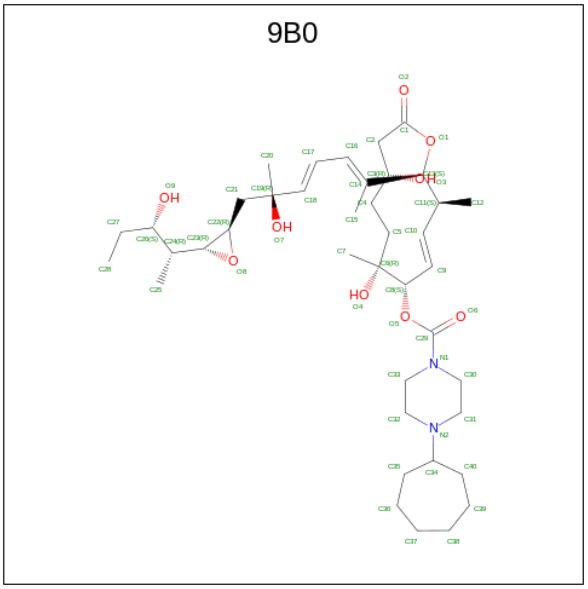
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	1183	9280	5889	1575	1771	45	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ASP	-	expression tag	UNP Q15393
A	1218	ASP	-	expression tag	UNP Q15393
A	1219	TYR	-	expression tag	UNP Q15393
A	1220	LYS	-	expression tag	UNP Q15393
A	1221	ASP	-	expression tag	UNP Q15393
A	1222	ASP	-	expression tag	UNP Q15393

- Molecule 5 is [(2 {S},3 {S},4 {E},6 {S},7 {R},10 {R})-3,7-dimethyl-2-[(2 {E},4 {E},6 {R})-6-methyl-6-oxidanyl-7-[(2 {R},3 {R})-3-[(2 {R},3 {S})-3-oxidanylpentan-2-yl]oxiran-2-yl]he

pta-2,4-dien-2-yl]-7,10-bis(oxidanyl)-12-oxidanylidene-1-oxacyclododec-4-en-6-yl] 4-cyclohep tylpiperazine-1-carboxylate (three-letter code: 9B0) (formula: $C_{40}H_{66}N_2O_9$).



Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			51	40	2	9	

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	D	3	Total	Zn	0
			3	3	

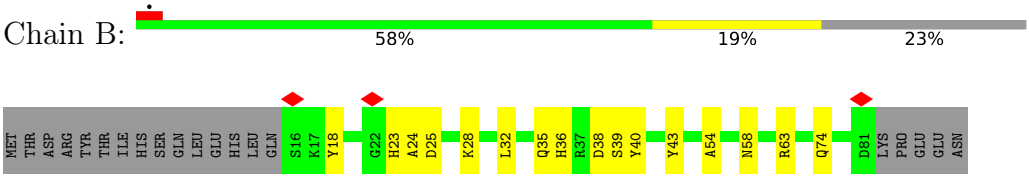
- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	K	0
			1	1	

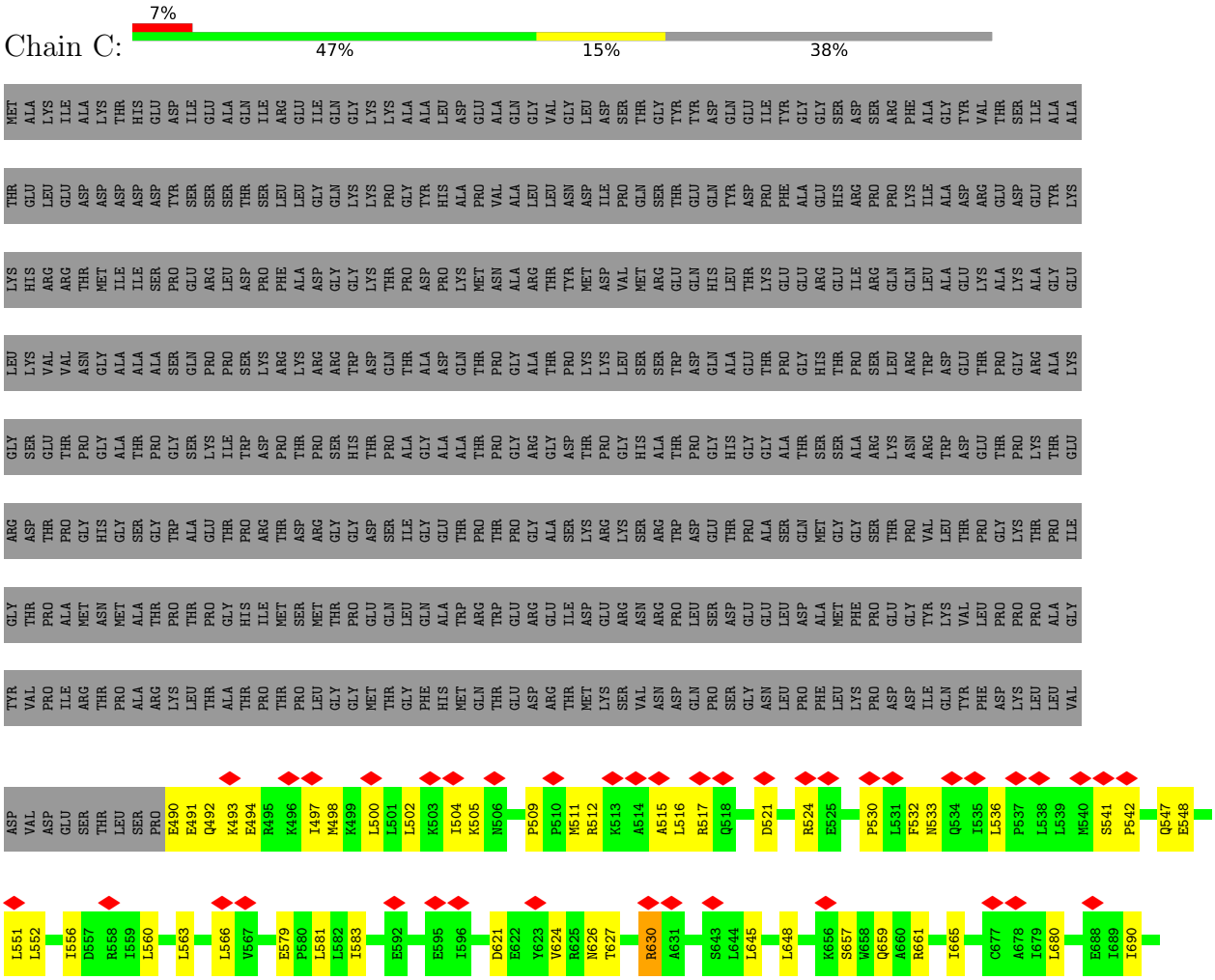
3 Residue-property plots (i)

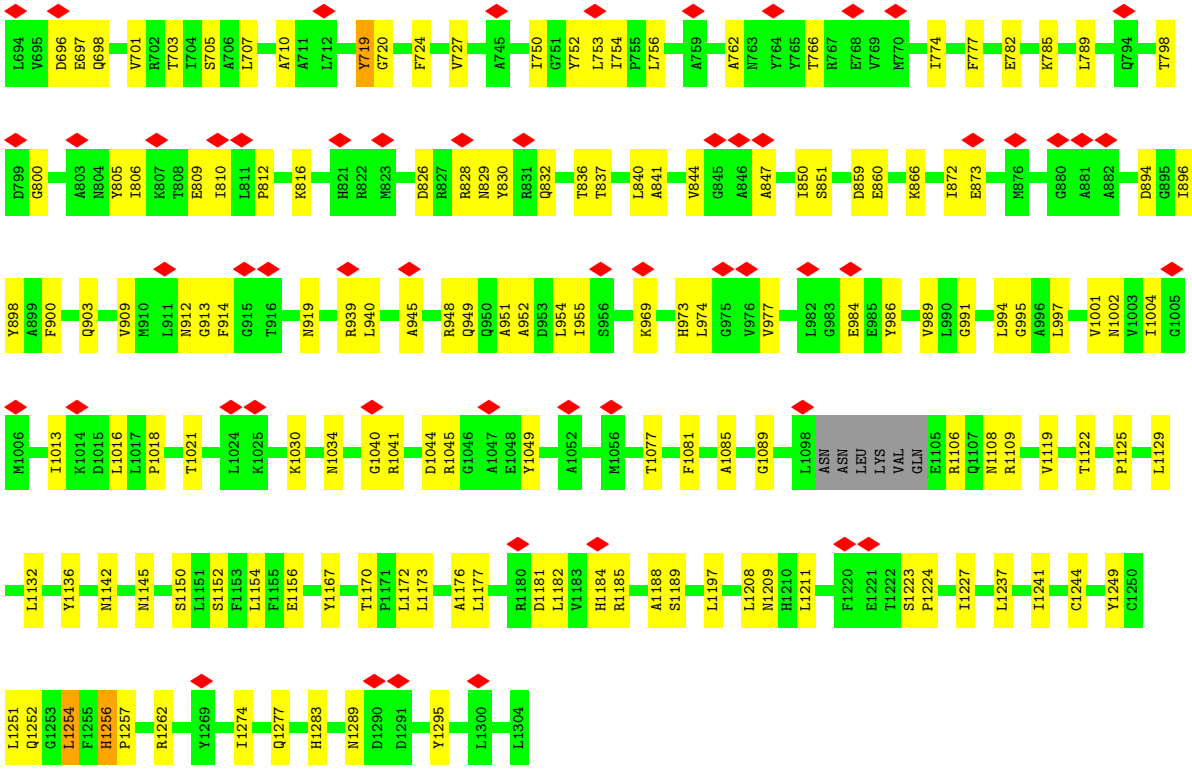
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Splicing factor 3B subunit 5

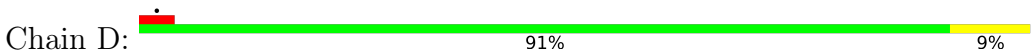


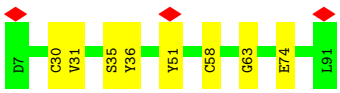
- Molecule 2: Splicing factor 3B subunit 1



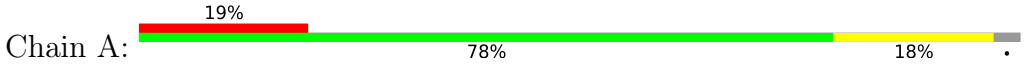


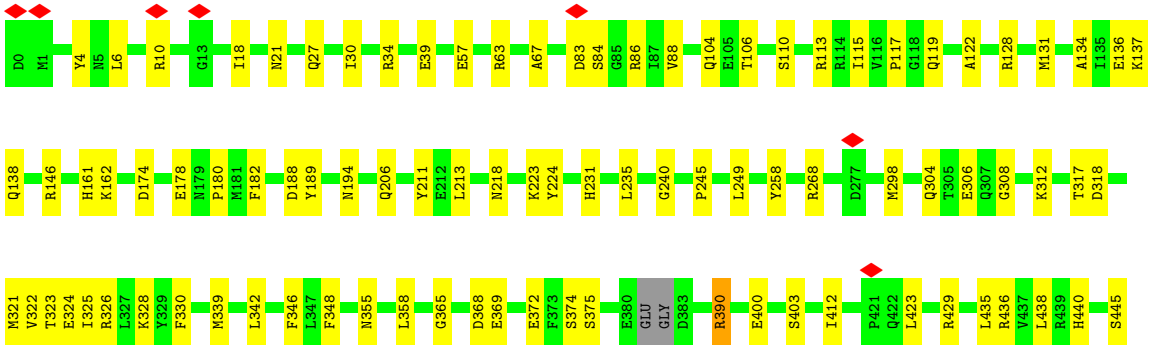
• Molecule 3: PHD finger-like domain-containing protein 5A

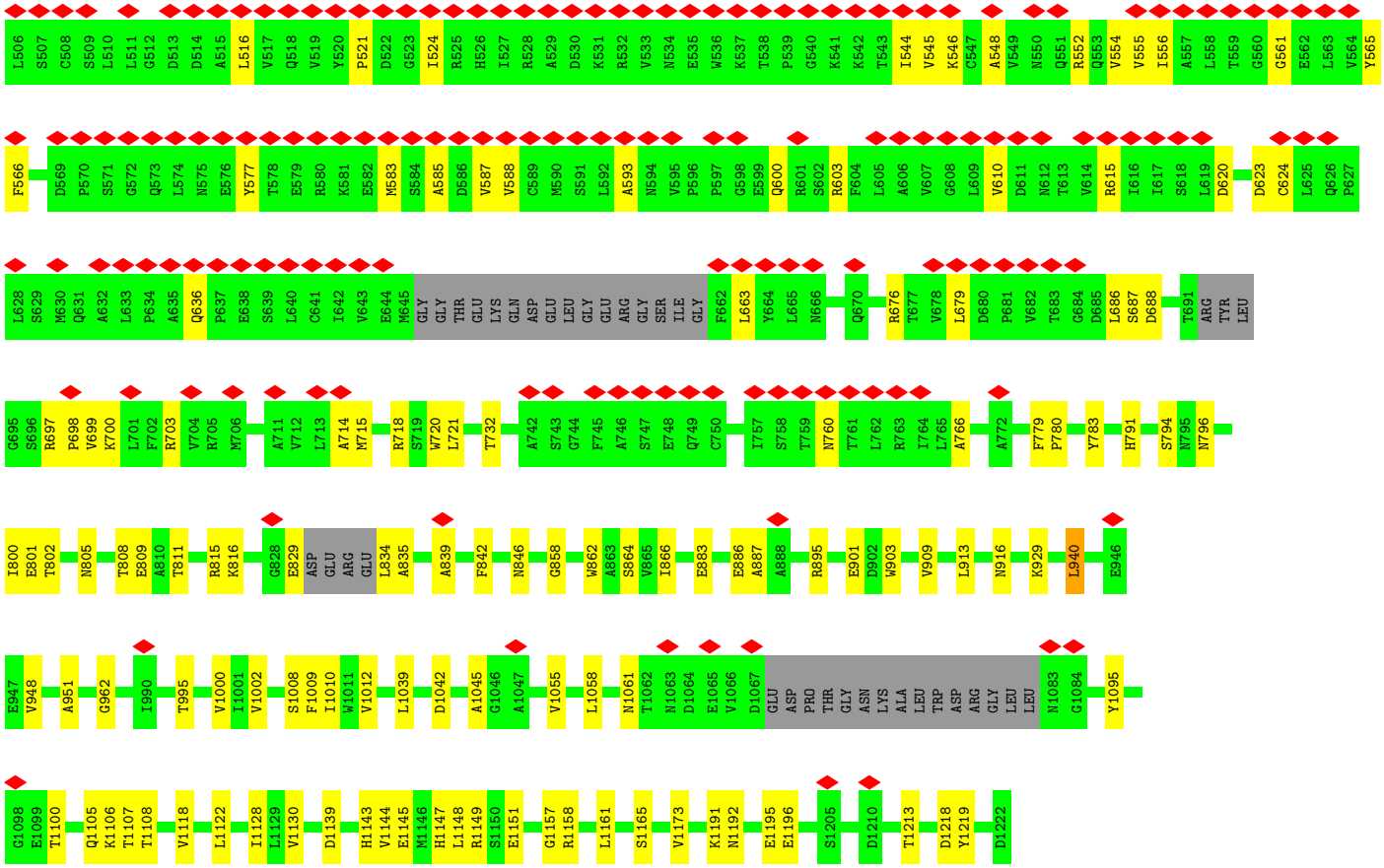




• Molecule 4: Splicing factor 3B subunit 3






L506 S507 C508 S509 L510 L511 G512 D513 D514 A515 L516 V517 Q518 V519 Y520 P521 D522 G523 I524 R525 H526 I527 R528 A529 D530 K531 R532 V533 N534 E535 W536 K537 T538 P539 G540 K541 K542 T543 I544 V545 K546 C547 A548 V549 N550 Q551 R552 Q553 V554 V555 I556 A557 L558 T559 G560 G561 E562 L563 V564 Y565
F566 D569 P570 S571 G572 Q573 L574 N575 E576 Y577 T578 E579 R580 K581 E582 M583 S584 A585 D586 V587 V588 C589 M590 S591 L592 A593 N594 V595 P596 P597 G598 E599 Q600 R601 S602 R603 F604 L605 A606 V607 G608 L609 V610 D611 N612 T613 V614 R615 I616 I617 S618 L619 D620 D623 C624 L625 Q626 P627
L628 S629 M630 Q631 A632 L633 P634 A635 Q636 P637 E638 S639 L640 C641 I642 V643 E644 M645 GLY GLY THR GLU LYS GLN ASP GLU LEU GLY GLU ARG GLY SER ILE GLY F662 L663 Y664 L665 N666 Q670 R676 T677 V678 L679 D680 P681 V682 T683 G684 D685 L686 S687 D688 T691 ARG TYR LEU
G695 S696 R697 P698 V699 K700 L701 F702 R703 V704 R705 M706 A711 V712 L713 A714 M715 R718 S719 W720 L721 T732 A742 S743 G744 F745 A746 S747 E748 Q749 C750 I757 S758 T759 N760 T761 L762 R763 I764 L765 A766 A772 F779 P780 Y783 H791 S794 N795 N796
I800 E801 T802 N805 T808 E809 A810 T811 R815 K816 G828 E829 ASP GLU ARG GLU L834 A835 A839 F842 N846 G858 W862 A863 S864 V865 I866 E883 E886 A887 A888 R895 E901 D902 W903 V909 L913 N916 K929 L940 E946
E947 V948 A951 G962 I990 T995 V1000 I1001 V1002 S1008 F1009 I1010 W1011 V1012 L1039 D1042 A1045 G1046 A1047 V1055 L1058 N1061 T1062 N1063 D1064 E1065 V1066 D1067 GLU ASP PRO THR GLY ASN LYS ALA LEU TRP ASP ARG GLY LEU LEU N1083 G1084 Y1095
G1098 E1099 T1100 Q1105 K1106 T1107 T1108 V1118 L1122 I1128 L1129 V1130 D1139 H1143 V1144 E1145 M1146 H1147 L1148 R1149 S1150 E1151 G1157 R1158 L1161 S1165 V1173 K1191 N1192 E1195 E1196 S1205 D1210 T1213 D1218 Y1219 D1222

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	241288	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 ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.203	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0244	Depositor
Map size (Å)	264.4, 264.4, 264.4	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.322, 1.322, 1.322	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 9B0, K

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	B	0.46	0/555	0.61	0/750
2	C	0.38	0/6559	0.68	6/8877 (0.1%)
3	D	0.40	0/653	0.61	0/877
4	A	0.43	0/9469	0.64	3/12848 (0.0%)
All	All	0.41	0/17236	0.66	9/23352 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	3
All	All	0	4

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	581	LEU	CA-CB-CG	8.43	134.69	115.30
2	C	630	ARG	NE-CZ-NH1	-7.12	116.74	120.30
2	C	500	LEU	CA-CB-CG	6.41	130.05	115.30
4	A	249	LEU	CA-CB-CG	5.72	128.47	115.30
4	A	268	ARG	NE-CZ-NH1	5.51	123.06	120.30
2	C	1172	LEU	CA-CB-CG	5.48	127.91	115.30
2	C	630	ARG	NE-CZ-NH2	5.45	123.03	120.30
4	A	235	LEU	CA-CB-CG	5.26	127.39	115.30
2	C	502	LEU	CA-CB-CG	5.22	127.30	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	74	GLN	Peptide
2	C	1049	TYR	Peptide
2	C	719	TYR	Peptide
2	C	754	ILE	Peptide

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	B	539	0	505	12	0
2	C	6438	0	6646	140	0
3	D	645	0	628	5	0
4	A	9280	0	9192	133	0
5	C	51	0	0	0	0
6	D	3	0	0	0	0
7	A	1	0	0	0	0
All	All	16957	0	16971	280	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 8.

All (280) 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)
2:C:1251:LEU:O	2:C:1254:LEU:CD1	1.67	1.41
2:C:1251:LEU:C	2:C:1254:LEU:HD11	1.45	1.35
2:C:1251:LEU:O	2:C:1254:LEU:HD11	1.03	1.21
2:C:1256:HIS:ND1	2:C:1257:PRO:HD2	1.63	1.12
2:C:1254:LEU:HD12	2:C:1254:LEU:H	1.20	1.07
2:C:1256:HIS:ND1	2:C:1257:PRO:CD	2.31	0.93
4:A:620:ASP:O	4:A:624:CYS:HB2	1.70	0.91
2:C:1173:LEU:O	2:C:1177:LEU:HB2	1.78	0.83
1:B:28:LYS:O	1:B:32:LEU:HB2	1.79	0.82
2:C:1251:LEU:CA	2:C:1254:LEU:HD11	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1251:LEU:C	2:C:1254:LEU:CD1	2.32	0.79
2:C:984:GLU:HG3	2:C:986:TYR:H	1.47	0.78
2:C:873:GLU:HG3	2:C:913:GLY:HA2	1.66	0.77
4:A:1192:ASN:O	4:A:1196:GLU:HB2	1.85	0.76
2:C:894:ASP:O	2:C:898:TYR:HB2	1.86	0.75
4:A:783:TYR:HB2	4:A:801:GLU:HB3	1.69	0.75
2:C:1254:LEU:CD1	2:C:1254:LEU:H	1.97	0.75
2:C:1254:LEU:HD12	2:C:1254:LEU:N	2.01	0.74
2:C:1251:LEU:O	2:C:1254:LEU:HD13	1.86	0.72
2:C:1150:SER:O	2:C:1154:LEU:HB2	1.89	0.72
4:A:791:HIS:HB3	4:A:796:ASN:H	1.55	0.71
2:C:556:ILE:O	2:C:560:LEU:HB2	1.91	0.69
2:C:805:TYR:O	2:C:809:GLU:HB2	1.94	0.68
2:C:847:ALA:O	2:C:851:SER:HB3	1.93	0.68
2:C:1184:HIS:O	2:C:1188:ALA:HB3	1.94	0.68
2:C:665:ILE:HG23	2:C:690:ILE:HD11	1.77	0.66
4:A:122:ALA:HB3	4:A:131:MET:HB3	1.79	0.64
2:C:909:VAL:O	2:C:913:GLY:HA3	1.98	0.63
1:B:24:ALA:O	2:C:1262:ARG:NH1	2.31	0.63
2:C:826:ASP:O	2:C:830:TYR:HB2	1.98	0.63
2:C:626:ASN:OD1	2:C:630:ARG:NH1	2.32	0.63
2:C:697:GLU:OE1	2:C:698:GLN:NE2	2.32	0.63
2:C:494:GLU:O	2:C:498:MET:HB2	1.99	0.62
2:C:812:PRO:O	2:C:816:LYS:HB2	1.99	0.61
2:C:991:GLY:O	2:C:1034:ASN:ND2	2.34	0.61
4:A:464:ARG:HA	4:A:516:LEU:HD11	1.82	0.61
4:A:805:ASN:ND2	4:A:858:GLY:O	2.33	0.61
2:C:1251:LEU:HA	2:C:1254:LEU:HD21	1.82	0.60
2:C:1256:HIS:CE1	2:C:1257:PRO:HD2	2.34	0.60
4:A:1002:VAL:HB	4:A:1010:ILE:HB	1.84	0.60
4:A:330:PHE:O	4:A:390:ARG:NH2	2.33	0.60
2:C:1256:HIS:ND1	2:C:1257:PRO:N	2.49	0.59
3:D:30:CYS:SG	3:D:31:VAL:N	2.75	0.59
4:A:21:ASN:ND2	4:A:27:GLN:O	2.35	0.59
2:C:524:ARG:HH11	2:C:563:LEU:HG	1.66	0.59
4:A:474:ILE:HB	4:A:485:LEU:HB2	1.85	0.59
2:C:948:ARG:O	2:C:952:ALA:HB2	2.03	0.58
2:C:532:PHE:O	2:C:536:LEU:HB2	2.03	0.58
2:C:547:GLN:NE2	3:D:51:TYR:O	2.36	0.58
2:C:511:MET:O	2:C:515:ALA:HB3	2.02	0.58
2:C:1249:TYR:HA	2:C:1252:GLN:HE22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:10:ARG:NH1	4:A:57:GLU:OE2	2.33	0.58
2:C:1002:ASN:OD1	2:C:1041:ARG:NH2	2.37	0.58
4:A:110:SER:HB2	4:A:1158:ARG:HH12	1.69	0.57
2:C:1181:ASP:HB3	2:C:1184:HIS:HD2	1.68	0.57
4:A:588:VAL:HG11	4:A:636:GLN:HE21	1.69	0.57
4:A:583:MET:SD	4:A:615:ARG:NH1	2.78	0.57
4:A:839:ALA:HA	4:A:842:PHE:HB3	1.87	0.57
2:C:645:LEU:HD23	2:C:648:LEU:HD12	1.87	0.57
4:A:30:ILE:HD11	4:A:342:LEU:HD21	1.86	0.57
4:A:524:ILE:HD11	4:A:556:ILE:HG21	1.87	0.57
2:C:1274:ILE:O	4:A:113:ARG:NH2	2.36	0.57
4:A:137:LYS:HB2	4:A:162:LYS:H	1.70	0.56
4:A:864:SER:HB2	4:A:887:ALA:HA	1.86	0.56
2:C:719:TYR:OH	4:A:146:ARG:NH2	2.38	0.56
2:C:945:ALA:HB1	2:C:989:VAL:HG11	1.88	0.56
2:C:949:GLN:HB3	2:C:989:VAL:HG13	1.87	0.56
4:A:476:VAL:HB	4:A:483:LEU:HB3	1.86	0.56
4:A:714:ALA:O	4:A:720:TRP:N	2.36	0.56
4:A:895:ARG:NH2	4:A:901:GLU:OE1	2.38	0.56
4:A:1191:LYS:O	4:A:1195:GLU:HB2	2.05	0.56
4:A:355:ASN:ND2	4:A:400:GLU:OE2	2.39	0.55
4:A:403:SER:O	4:A:436:ARG:NH1	2.39	0.55
2:C:866:LYS:HG3	2:C:909:VAL:HG11	1.88	0.55
4:A:1008:SER:OG	4:A:1009:PHE:N	2.39	0.55
4:A:63:ARG:NH2	4:A:119:GLN:OE1	2.38	0.55
2:C:657:SER:OG	2:C:659:GLN:OE1	2.25	0.55
4:A:554:VAL:HB	4:A:566:PHE:HB2	1.87	0.55
2:C:1085:ALA:O	2:C:1089:GLY:HA2	2.07	0.55
4:A:84:SER:HA	4:A:110:SER:HA	1.88	0.55
2:C:1077:THR:O	2:C:1081:PHE:HB2	2.07	0.54
2:C:1152:SER:O	2:C:1156:GLU:HB2	2.07	0.54
2:C:1184:HIS:O	2:C:1188:ALA:CB	2.55	0.54
4:A:304:GLN:HE21	4:A:308:GLY:HA2	1.72	0.54
4:A:1107:THR:OG1	4:A:1108:THR:N	2.41	0.54
4:A:951:ALA:HB3	4:A:962:GLY:H	1.73	0.54
2:C:661:ARG:NH1	2:C:696:ASP:OD2	2.40	0.54
4:A:811:THR:O	4:A:815:ARG:HB2	2.08	0.53
4:A:585:ALA:HB1	4:A:610:VAL:HB	1.89	0.53
4:A:1039:LEU:HD22	4:A:1106:LYS:HD3	1.89	0.53
2:C:837:THR:HA	2:C:840:LEU:HD12	1.90	0.53
2:C:900:PHE:O	2:C:939:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:NH1	4:A:306:GLU:OE2	2.36	0.53
2:C:896:ILE:O	2:C:900:PHE:HB2	2.08	0.53
2:C:762:ALA:O	2:C:766:THR:OG1	2.23	0.53
2:C:490:GLU:HB3	2:C:493:LYS:HG3	1.90	0.52
2:C:524:ARG:HH12	2:C:566:LEU:HD13	1.74	0.52
4:A:521:PRO:HA	4:A:544:ILE:HG22	1.90	0.52
4:A:883:GLU:HB3	4:A:886:GLU:HB2	1.90	0.52
2:C:1001:VAL:HA	2:C:1004:ILE:HG22	1.92	0.52
2:C:1251:LEU:HD23	2:C:1254:LEU:HD21	1.90	0.52
4:A:791:HIS:CE1	4:A:794:SER:H	2.28	0.52
4:A:1161:LEU:O	4:A:1165:SER:HB2	2.08	0.52
2:C:724:PHE:HD1	2:C:727:VAL:HG21	1.74	0.52
4:A:802:THR:HG23	4:A:887:ALA:HB1	1.92	0.52
2:C:762:ALA:O	2:C:766:THR:CB	2.58	0.51
2:C:847:ALA:O	2:C:851:SER:CB	2.57	0.51
2:C:621:ASP:HB3	2:C:624:VAL:HG22	1.91	0.51
4:A:1042:ASP:HA	4:A:1058:LEU:HD12	1.93	0.51
2:C:948:ARG:O	2:C:952:ALA:CB	2.59	0.51
4:A:34:ARG:NH1	4:A:39:GLU:OE1	2.44	0.51
1:B:54:ALA:O	4:A:429:ARG:NH1	2.43	0.51
2:C:698:GLN:HB2	2:C:701:VAL:HG12	1.93	0.51
4:A:86:ARG:HG2	4:A:106:THR:HA	1.92	0.51
4:A:445:SER:HB2	4:A:766:ALA:HB3	1.92	0.51
4:A:454:GLY:O	4:A:760:ASN:ND2	2.44	0.51
2:C:1040:GLY:O	2:C:1044:ASP:HB2	2.10	0.51
2:C:782:GLU:OE1	2:C:829:ASN:ND2	2.44	0.51
4:A:565:TYR:HD2	4:A:577:TYR:HB2	1.75	0.50
4:A:800:ILE:HG22	4:A:866:ILE:HG12	1.92	0.50
1:B:18:TYR:OH	4:A:113:ARG:NH1	2.45	0.50
4:A:117:PRO:HA	4:A:134:ALA:HB2	1.92	0.50
2:C:1224:PRO:HA	2:C:1227:ILE:HG22	1.93	0.50
2:C:1251:LEU:HA	2:C:1254:LEU:HD11	1.93	0.50
4:A:1147:HIS:O	4:A:1151:GLU:HB2	2.11	0.50
4:A:86:ARG:NH2	4:A:1157:GLY:O	2.44	0.50
4:A:663:LEU:HB3	4:A:679:LEU:HB3	1.94	0.50
4:A:317:THR:OG1	4:A:321:MET:O	2.28	0.50
4:A:829:GLU:HB3	4:A:835:ALA:HB2	1.94	0.50
2:C:512:ARG:O	2:C:516:LEU:HB2	2.11	0.50
4:A:342:LEU:HB2	4:A:346:PHE:HB2	1.94	0.50
4:A:811:THR:O	4:A:815:ARG:CB	2.59	0.50
2:C:798:THR:HG22	2:C:800:GLY:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:TYR:HA	1:B:43:TYR:HD2	1.76	0.49
2:C:1173:LEU:HA	2:C:1176:ALA:HB3	1.94	0.49
4:A:561:GLY:HA2	4:A:587:VAL:HG23	1.94	0.49
2:C:945:ALA:HA	2:C:948:ARG:HB2	1.95	0.49
2:C:1013:ILE:HA	2:C:1016:LEU:HB3	1.94	0.49
2:C:969:LYS:O	2:C:973:HIS:ND1	2.45	0.49
2:C:785:LYS:O	2:C:789:LEU:HB2	2.13	0.49
2:C:894:ASP:O	2:C:898:TYR:CB	2.60	0.49
2:C:1145:ASN:OD1	2:C:1145:ASN:N	2.45	0.49
4:A:423:LEU:HB2	4:A:438:LEU:HB2	1.93	0.49
4:A:721:LEU:N	4:A:732:THR:O	2.46	0.49
4:A:1095:TYR:HB2	4:A:1173:VAL:HG21	1.94	0.49
2:C:517:ARG:O	2:C:521:ASP:HB2	2.13	0.49
2:C:1167:TYR:O	2:C:1170:THR:OG1	2.25	0.49
4:A:808:THR:OG1	4:A:809:GLU:N	2.44	0.49
2:C:859:ASP:OD1	2:C:860:GLU:N	2.46	0.49
2:C:1001:VAL:O	2:C:1045:ARG:NH2	2.46	0.49
4:A:1118:VAL:HG22	4:A:1128:ILE:HG22	1.95	0.48
2:C:1197:LEU:HD13	3:D:74:GLU:HG3	1.95	0.48
4:A:312:LYS:NZ	4:A:365:GLY:O	2.46	0.48
2:C:532:PHE:O	2:C:536:LEU:CB	2.61	0.48
2:C:1185:ARG:O	2:C:1189:SER:OG	2.26	0.48
2:C:1132:LEU:O	2:C:1136:TYR:N	2.47	0.48
2:C:1077:THR:O	2:C:1081:PHE:CB	2.62	0.48
4:A:115:ILE:HG22	4:A:136:GLU:HG2	1.96	0.48
2:C:1119:VAL:HA	2:C:1122:THR:HG22	1.96	0.48
3:D:58:CYS:HB3	3:D:63:GLY:H	1.78	0.48
2:C:491:GLU:HB3	2:C:530:PRO:HG2	1.96	0.47
4:A:829:GLU:O	4:A:834:LEU:N	2.47	0.47
4:A:1144:VAL:O	4:A:1148:LEU:HB2	2.15	0.47
2:C:1208:LEU:HD23	2:C:1211:LEU:HD22	1.96	0.47
3:D:35:SER:OG	3:D:36:TYR:N	2.48	0.47
4:A:115:ILE:HA	4:A:136:GLU:HB3	1.97	0.47
2:C:701:VAL:O	2:C:705:SER:CB	2.63	0.47
2:C:710:ALA:HB1	2:C:752:TYR:HD2	1.80	0.47
2:C:1030:LYS:O	2:C:1034:ASN:HB2	2.14	0.47
4:A:180:PRO:HD2	4:A:213:LEU:HB3	1.97	0.47
4:A:1000:VAL:HB	4:A:1012:VAL:HB	1.96	0.47
2:C:701:VAL:O	2:C:705:SER:HB3	2.15	0.47
2:C:994:LEU:HD13	2:C:997:LEU:HD12	1.97	0.47
4:A:18:ILE:HD12	4:A:67:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:O	1:B:36:HIS:ND1	2.39	0.47
4:A:663:LEU:HD23	4:A:679:LEU:HD23	1.97	0.47
4:A:88:VAL:HG12	4:A:104:GLN:HG2	1.96	0.46
4:A:929:LYS:HD3	4:A:940:LEU:HG	1.97	0.46
2:C:940:LEU:HD12	2:C:948:ARG:HG2	1.98	0.46
4:A:317:THR:HG1	4:A:322:VAL:HA	1.79	0.46
4:A:440:HIS:CE1	4:A:1219:TYR:HH	2.26	0.46
4:A:603:ARG:NH2	4:A:623:ASP:OD2	2.49	0.46
2:C:551:LEU:HD12	2:C:552:LEU:HD22	1.98	0.46
4:A:206:GLN:HE22	4:A:231:HIS:HD2	1.63	0.46
4:A:328:LYS:HD2	4:A:372:GLU:HG3	1.98	0.46
4:A:412:ILE:O	4:A:1105:GLN:NE2	2.48	0.46
2:C:504:ILE:HG22	2:C:551:LEU:HD11	1.96	0.46
2:C:850:ILE:HD13	2:C:872:ILE:HG23	1.98	0.46
2:C:1150:SER:O	2:C:1154:LEU:CB	2.60	0.46
1:B:23:HIS:HE1	1:B:25:ASP:HB2	1.81	0.46
2:C:511:MET:O	2:C:515:ALA:CB	2.64	0.46
4:A:324:GLU:OE1	4:A:326:ARG:NH1	2.47	0.46
1:B:35:GLN:O	1:B:39:SER:OG	2.24	0.45
2:C:812:PRO:O	2:C:816:LYS:CB	2.65	0.45
2:C:1181:ASP:OD1	2:C:1182:LEU:N	2.48	0.45
4:A:138:GLN:HG2	4:A:161:HIS:CE1	2.51	0.45
4:A:258:TYR:HB2	4:A:325:ILE:HD11	1.97	0.45
4:A:435:LEU:O	4:A:779:PHE:N	2.43	0.45
4:A:688:ASP:OD1	4:A:688:ASP:N	2.42	0.45
2:C:1018:PRO:O	2:C:1021:THR:OG1	2.32	0.45
2:C:806:ILE:HA	2:C:810:ILE:HD12	1.99	0.45
4:A:545:VAL:HG12	4:A:546:LYS:HG2	1.99	0.45
4:A:548:ALA:HB3	4:A:555:VAL:HB	1.98	0.45
4:A:561:GLY:HA3	4:A:583:MET:HB2	1.98	0.45
4:A:700:LYS:HB2	4:A:715:MET:HB2	1.98	0.45
2:C:703:THR:O	2:C:707:LEU:HB2	2.17	0.45
2:C:1223:SER:HA	2:C:1224:PRO:HD3	1.85	0.45
1:B:58:ASN:HA	4:A:429:ARG:HH12	1.81	0.44
2:C:505:LYS:HE2	2:C:548:GLU:HB3	1.98	0.44
2:C:720:GLY:H	2:C:756:LEU:HB2	1.82	0.44
4:A:128:ARG:NH2	4:A:178:GLU:O	2.50	0.44
4:A:136:GLU:HG3	4:A:137:LYS:H	1.83	0.44
4:A:829:GLU:O	4:A:835:ALA:N	2.46	0.44
4:A:895:ARG:HG3	4:A:903:TRP:CD2	2.52	0.44
2:C:914:PHE:HD2	2:C:954:LEU:HD11	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:174:ASP:OD2	4:A:240:GLY:N	2.44	0.44
4:A:862:TRP:HZ2	4:A:913:LEU:HB2	1.83	0.44
2:C:828:ARG:O	2:C:832:GLN:HB2	2.18	0.44
4:A:317:THR:OG1	4:A:318:ASP:N	2.50	0.44
4:A:552:ARG:NH1	4:A:600:GLN:O	2.44	0.44
1:B:23:HIS:CE1	1:B:25:ASP:HB2	2.53	0.44
2:C:579:GLU:HG2	2:C:627:THR:HG21	2.00	0.44
4:A:676:ARG:HB2	4:A:686:LEU:HA	1.99	0.44
4:A:1145:GLU:OE2	4:A:1149:ARG:NH2	2.48	0.44
2:C:512:ARG:O	2:C:516:LEU:CB	2.66	0.44
2:C:826:ASP:O	2:C:830:TYR:CB	2.65	0.44
4:A:182:PHE:HB2	4:A:211:TYR:HB2	1.98	0.43
2:C:583:ILE:HG22	2:C:630:ARG:HD2	2.00	0.43
4:A:995:THR:HG22	4:A:1000:VAL:HA	2.00	0.43
2:C:490:GLU:HG3	2:C:492:GLN:H	1.84	0.43
2:C:1125:PRO:HB2	2:C:1129:LEU:HG	2.00	0.43
2:C:762:ALA:O	2:C:766:THR:HB	2.19	0.43
4:A:245:PRO:HD3	4:A:317:THR:HG21	2.01	0.43
2:C:1237:LEU:O	2:C:1241:ILE:HB	2.18	0.43
4:A:317:THR:HA	4:A:323:THR:H	1.84	0.43
4:A:4:TYR:HB3	4:A:1130:VAL:HB	2.00	0.43
4:A:464:ARG:NH1	4:A:473:TYR:OH	2.51	0.43
2:C:841:ALA:HA	2:C:844:VAL:HG12	2.00	0.43
4:A:86:ARG:NH1	4:A:104:GLN:OE1	2.52	0.43
2:C:494:GLU:HA	2:C:497:ILE:HG22	2.01	0.43
4:A:1139:ASP:O	4:A:1143:HIS:ND1	2.38	0.43
4:A:1192:ASN:O	4:A:1196:GLU:CB	2.61	0.43
2:C:832:GLN:O	2:C:836:THR:OG1	2.32	0.42
4:A:816:LYS:NZ	4:A:846:ASN:OD1	2.50	0.42
2:C:974:LEU:HA	2:C:977:VAL:HB	2.01	0.42
2:C:1256:HIS:HA	2:C:1257:PRO:HD3	1.87	0.42
4:A:593:ALA:HA	4:A:703:ARG:HH22	1.85	0.42
2:C:750:ILE:HD13	2:C:753:LEU:HD12	2.02	0.42
4:A:676:ARG:HE	4:A:687:SER:H	1.67	0.42
4:A:714:ALA:N	4:A:720:TRP:O	2.53	0.42
4:A:1100:THR:O	4:A:1122:LEU:N	2.53	0.42
4:A:188:ASP:OD1	4:A:189:TYR:N	2.53	0.42
2:C:774:ILE:HD13	2:C:777:PHE:CE2	2.55	0.41
4:A:368:ASP:OD1	4:A:369:GLU:N	2.53	0.41
4:A:886:GLU:HB3	4:A:909:VAL:HG11	2.02	0.41
4:A:206:GLN:NE2	4:A:231:HIS:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:900:PHE:HA	2:C:903:GLN:NE2	2.36	0.41
2:C:995:GLY:N	2:C:1034:ASN:HD21	2.18	0.41
2:C:828:ARG:O	2:C:832:GLN:CB	2.69	0.41
4:A:1213:THR:HA	4:A:1218:ASP:HB3	2.03	0.41
2:C:509:PRO:HG3	2:C:512:ARG:HH21	1.85	0.41
2:C:530:PRO:HA	2:C:533:ASN:HB3	2.02	0.41
4:A:348:PHE:HD1	4:A:358:LEU:HD13	1.86	0.41
4:A:697:ARG:HA	4:A:698:PRO:HD3	1.90	0.41
2:C:680:LEU:HD13	2:C:680:LEU:HA	1.84	0.41
2:C:785:LYS:O	2:C:789:LEU:CB	2.69	0.41
2:C:951:ALA:O	2:C:955:ILE:HD12	2.21	0.41
2:C:1244:CYS:HB2	2:C:1283:HIS:CE1	2.55	0.41
2:C:1289:ASN:HA	2:C:1295:TYR:CD2	2.55	0.41
4:A:83:ASP:N	4:A:83:ASP:OD1	2.54	0.41
4:A:779:PHE:HA	4:A:780:PRO:HD3	1.92	0.41
4:A:1045:ALA:HA	4:A:1055:VAL:HG22	2.02	0.41
2:C:541:SER:HA	2:C:542:PRO:HD3	1.96	0.41
4:A:699:VAL:HG13	4:A:714:ALA:HB1	2.03	0.41
1:B:38:ASP:OD2	2:C:1277:GLN:NE2	2.54	0.40
2:C:696:ASP:OD1	2:C:697:GLU:N	2.53	0.40
4:A:374:SER:OG	4:A:375:SER:N	2.55	0.40
4:A:223:LYS:HG2	4:A:224:TYR:CD2	2.57	0.40
4:A:6:LEU:HD22	4:A:1128:ILE:HD11	2.02	0.40
4:A:718:ARG:HB2	4:A:720:TRP:NE1	2.36	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	B	64/86 (74%)	59 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	805/1304 (62%)	742 (92%)	63 (8%)	0	100	100
3	D	83/85 (98%)	72 (87%)	11 (13%)	0	100	100
4	A	1171/1223 (96%)	1046 (89%)	125 (11%)	0	100	100
All	All	2123/2698 (79%)	1919 (90%)	204 (10%)	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	B	57/77 (74%)	57 (100%)	0	100	100
2	C	695/1104 (63%)	686 (99%)	9 (1%)	69	81
3	D	73/73 (100%)	73 (100%)	0	100	100
4	A	1026/1057 (97%)	1017 (99%)	9 (1%)	78	87
All	All	1851/2311 (80%)	1833 (99%)	18 (1%)	77	85

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	912	ASN
2	C	919	ASN
2	C	1106	ARG
2	C	1108	ASN
2	C	1109	ARG
2	C	1142	ASN
2	C	1209	ASN
2	C	1254	LEU
2	C	1256	HIS
4	A	194	ASN
4	A	218	ASN
4	A	298	MET
4	A	339	MET

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Mol	Chain	Res	Type
4	A	390	ARG
4	A	916	ASN
4	A	940	LEU
4	A	948	VAL
4	A	1061	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	698	GLN
2	C	878	ASN
2	C	903	GLN
2	C	912	ASN
2	C	919	ASN
2	C	950	GLN
2	C	1142	ASN
2	C	1184	HIS
2	C	1209	ASN
2	C	1283	HIS
4	A	161	HIS
4	A	194	ASN
4	A	206	GLN
4	A	218	ASN
4	A	231	HIS
4	A	304	GLN
4	A	355	ASN
4	A	636	GLN
4	A	749	GLN
4	A	760	ASN
4	A	916	ASN
4	A	1061	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	9B0	C	1401	-	52,54,54	3.47	16 (30%)	61,77,77	3.62	32 (52%)

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	9B0	C	1401	-	-	21/67/91/91	0/3/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1401	9B0	C16-C14	20.31	1.52	1.33
5	C	1401	9B0	C17-C18	6.78	1.52	1.32
5	C	1401	9B0	C2-C1	-5.26	1.40	1.50
5	C	1401	9B0	C40-C34	4.65	1.65	1.53
5	C	1401	9B0	C36-C35	4.09	1.64	1.52
5	C	1401	9B0	C11-C10	-3.69	1.41	1.51
5	C	1401	9B0	C10-C9	3.44	1.42	1.32
5	C	1401	9B0	C23-C22	2.93	1.50	1.46
5	C	1401	9B0	C17-C16	2.51	1.51	1.43
5	C	1401	9B0	C31-N2	2.42	1.51	1.47
5	C	1401	9B0	C39-C40	2.39	1.59	1.52
5	C	1401	9B0	O4-C6	-2.34	1.40	1.44
5	C	1401	9B0	C15-C14	2.21	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1401	9B0	C38-C37	2.18	1.60	1.51
5	C	1401	9B0	C2-C3	2.17	1.58	1.52
5	C	1401	9B0	C34-N2	2.01	1.54	1.48

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1401	9B0	O5-C29-N1	12.94	122.88	111.27
5	C	1401	9B0	C11-C13-C14	-8.52	96.89	113.89
5	C	1401	9B0	C39-C40-C34	7.77	141.00	115.87
5	C	1401	9B0	C13-C14-C16	-7.35	112.14	119.13
5	C	1401	9B0	C39-C38-C37	-6.95	87.02	116.34
5	C	1401	9B0	C38-C37-C36	6.40	143.34	116.34
5	C	1401	9B0	C15-C14-C13	5.88	125.84	115.68
5	C	1401	9B0	C12-C11-C10	-5.38	97.00	109.99
5	C	1401	9B0	C36-C35-C34	-5.13	99.29	115.87
5	C	1401	9B0	C7-C6-C5	-4.96	101.79	110.63
5	C	1401	9B0	C17-C16-C14	-4.89	120.14	127.32
5	C	1401	9B0	O5-C8-C9	4.59	118.35	107.65
5	C	1401	9B0	C37-C36-C35	4.49	129.84	115.84
5	C	1401	9B0	O6-C29-N1	-4.20	117.29	124.32
5	C	1401	9B0	C7-C6-C8	3.91	116.89	110.11
5	C	1401	9B0	C31-N2-C32	-3.46	102.76	109.08
5	C	1401	9B0	C16-C17-C18	-3.07	108.88	127.37
5	C	1401	9B0	C11-C10-C9	-3.06	116.19	125.67
5	C	1401	9B0	C23-O8-C22	2.98	62.50	60.59
5	C	1401	9B0	O5-C29-O6	-2.87	118.82	124.86
5	C	1401	9B0	O1-C1-C2	2.81	116.62	111.46
5	C	1401	9B0	O1-C13-C11	2.76	109.91	106.31
5	C	1401	9B0	C13-O1-C1	-2.62	111.78	116.61
5	C	1401	9B0	C15-C14-C16	-2.49	120.96	124.03
5	C	1401	9B0	C4-C3-C2	-2.43	104.03	112.78
5	C	1401	9B0	O2-C1-C2	-2.35	119.53	124.73
5	C	1401	9B0	C5-C4-C3	2.26	117.99	112.76
5	C	1401	9B0	C30-C31-N2	2.11	114.63	110.59
5	C	1401	9B0	C28-C27-C26	-2.09	109.70	113.61
5	C	1401	9B0	C25-C24-C23	-2.06	107.72	111.40
5	C	1401	9B0	O1-C1-O2	-2.01	118.84	123.70
5	C	1401	9B0	O7-C19-C21	2.01	111.70	107.60

There are no chirality outliers.

All (21) torsion outliers are listed below:

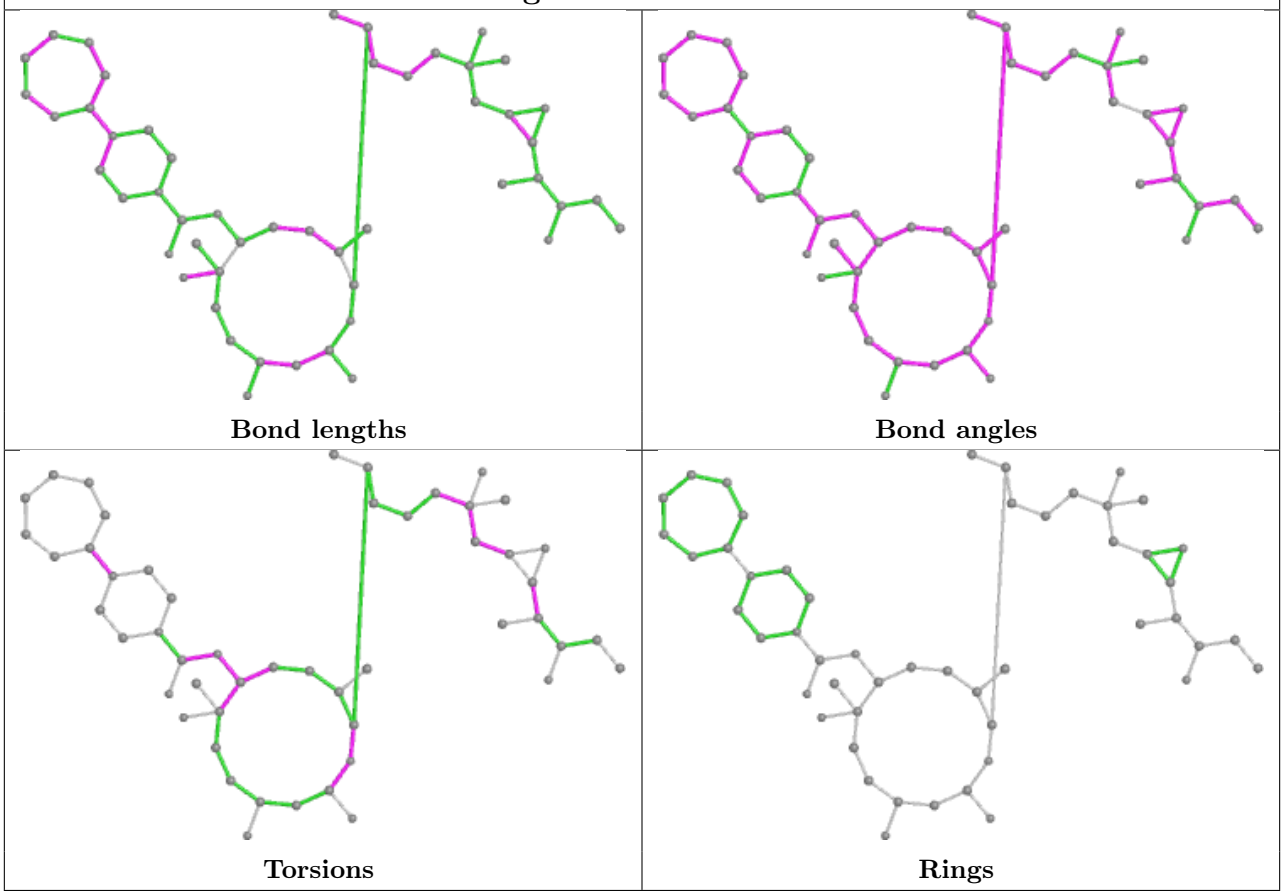
Mol	Chain	Res	Type	Atoms
5	C	1401	9B0	N1-C29-O5-C8
5	C	1401	9B0	O6-C29-O5-C8
5	C	1401	9B0	O5-C8-C9-C10
5	C	1401	9B0	C7-C6-C8-C9
5	C	1401	9B0	O4-C6-C8-C9
5	C	1401	9B0	C14-C13-O1-C1
5	C	1401	9B0	C17-C18-C19-C20
5	C	1401	9B0	C17-C18-C19-O7
5	C	1401	9B0	C17-C18-C19-C21
5	C	1401	9B0	C18-C19-C21-C22
5	C	1401	9B0	C19-C21-C22-C23
5	C	1401	9B0	O8-C23-C24-C25
5	C	1401	9B0	O8-C23-C24-C26
5	C	1401	9B0	C5-C6-C8-C9
5	C	1401	9B0	C11-C13-O1-C1
5	C	1401	9B0	C9-C8-O5-C29
5	C	1401	9B0	C35-C34-N2-C31
5	C	1401	9B0	C22-C23-C24-C26
5	C	1401	9B0	O2-C1-O1-C13
5	C	1401	9B0	C19-C21-C22-O8
5	C	1401	9B0	C22-C23-C24-C25

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 9B0 C 1401



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.

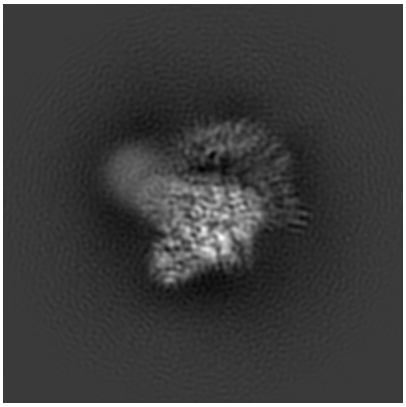
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6915. These allow visual inspection of the internal detail of the map and identification of artifacts.

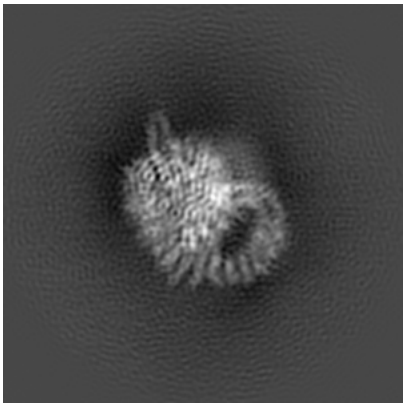
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

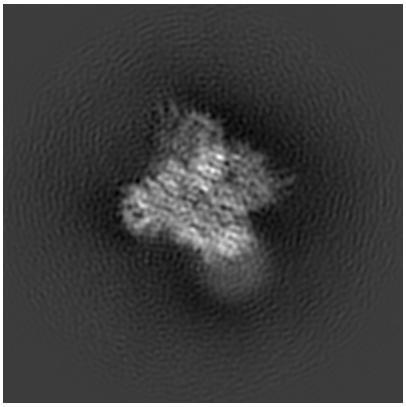
6.1.1 Primary map



X



Y

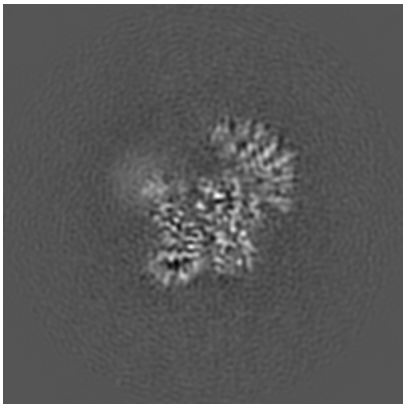


Z

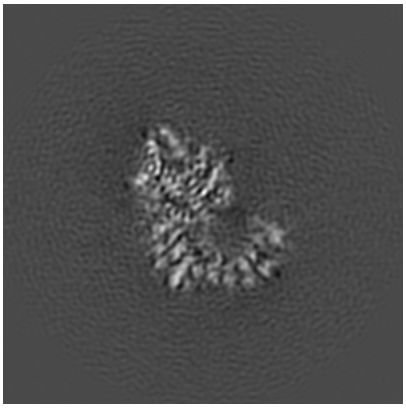
The images above show the map projected in three orthogonal directions.

6.2 Central slices

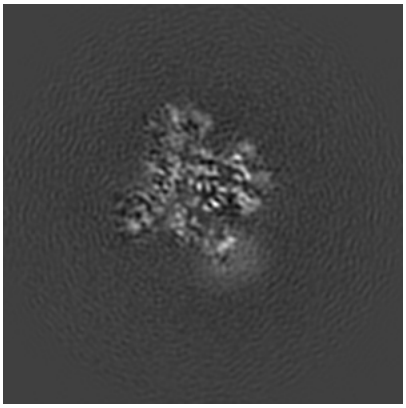
6.2.1 Primary map



X Index: 100



Y Index: 100

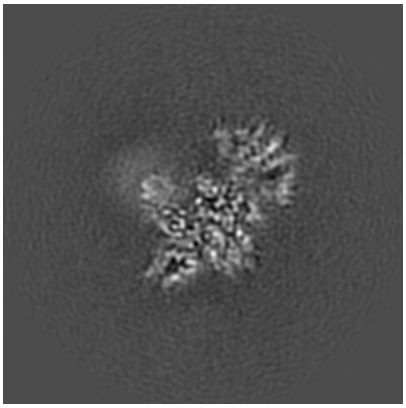


Z Index: 100

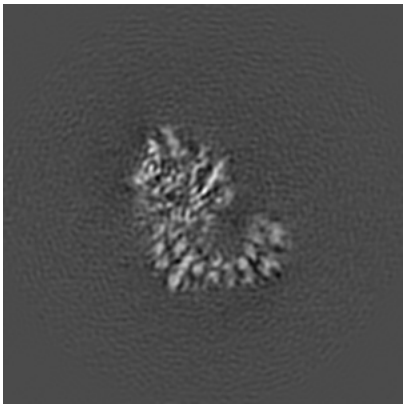
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

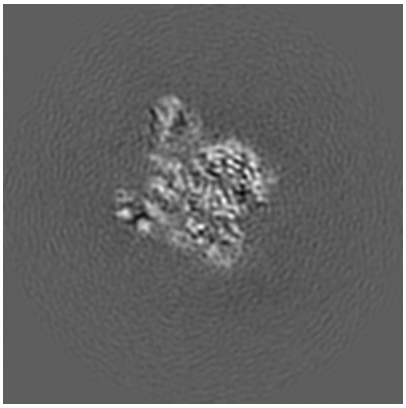
6.3.1 Primary map



X Index: 102



Y Index: 99

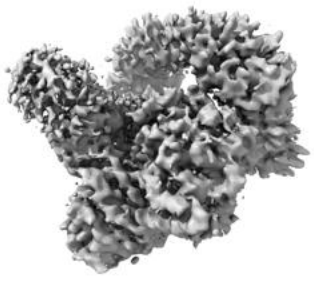


Z Index: 94

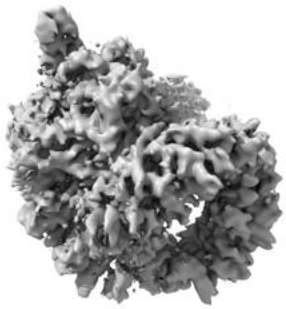
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

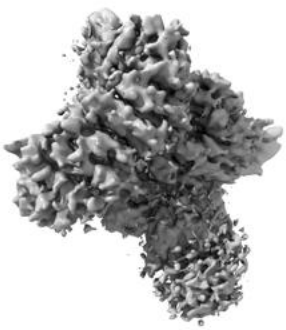
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0244. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

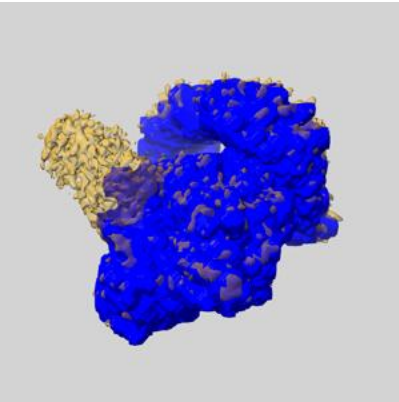
6.5 Mask visualisation (i)

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

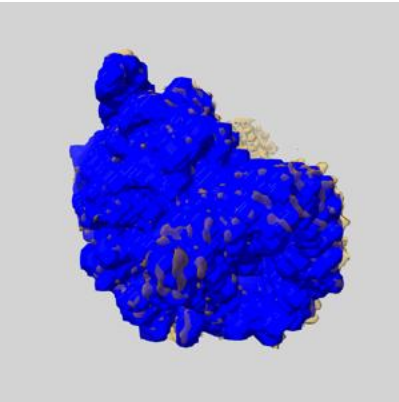
A mask typically either:

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

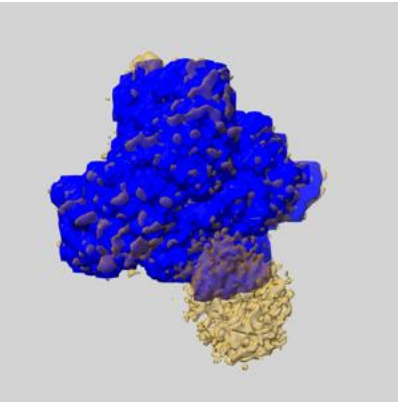
6.5.1 emd_6915_msk_1.map (i)



X



Y

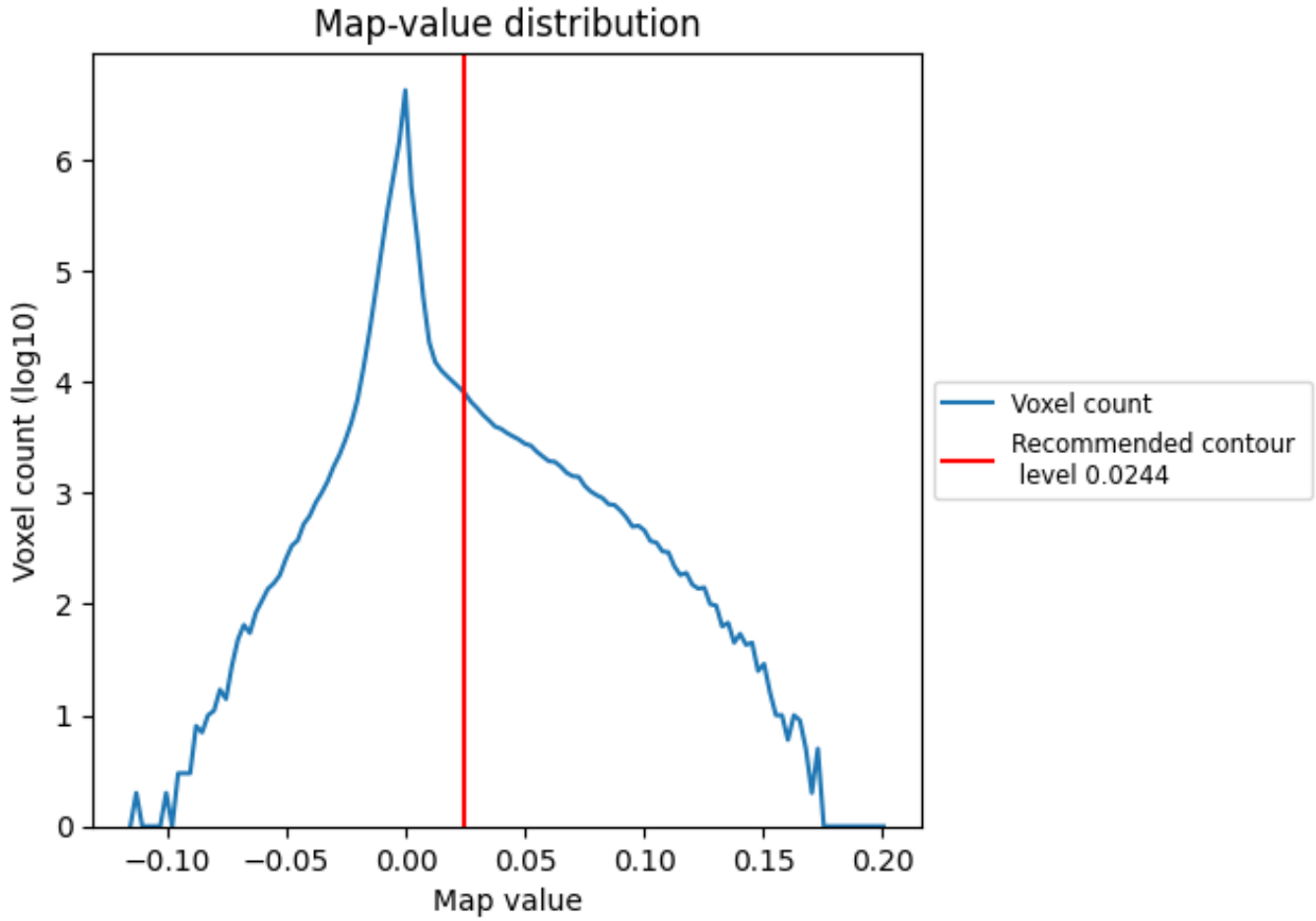


Z

7 Map analysis

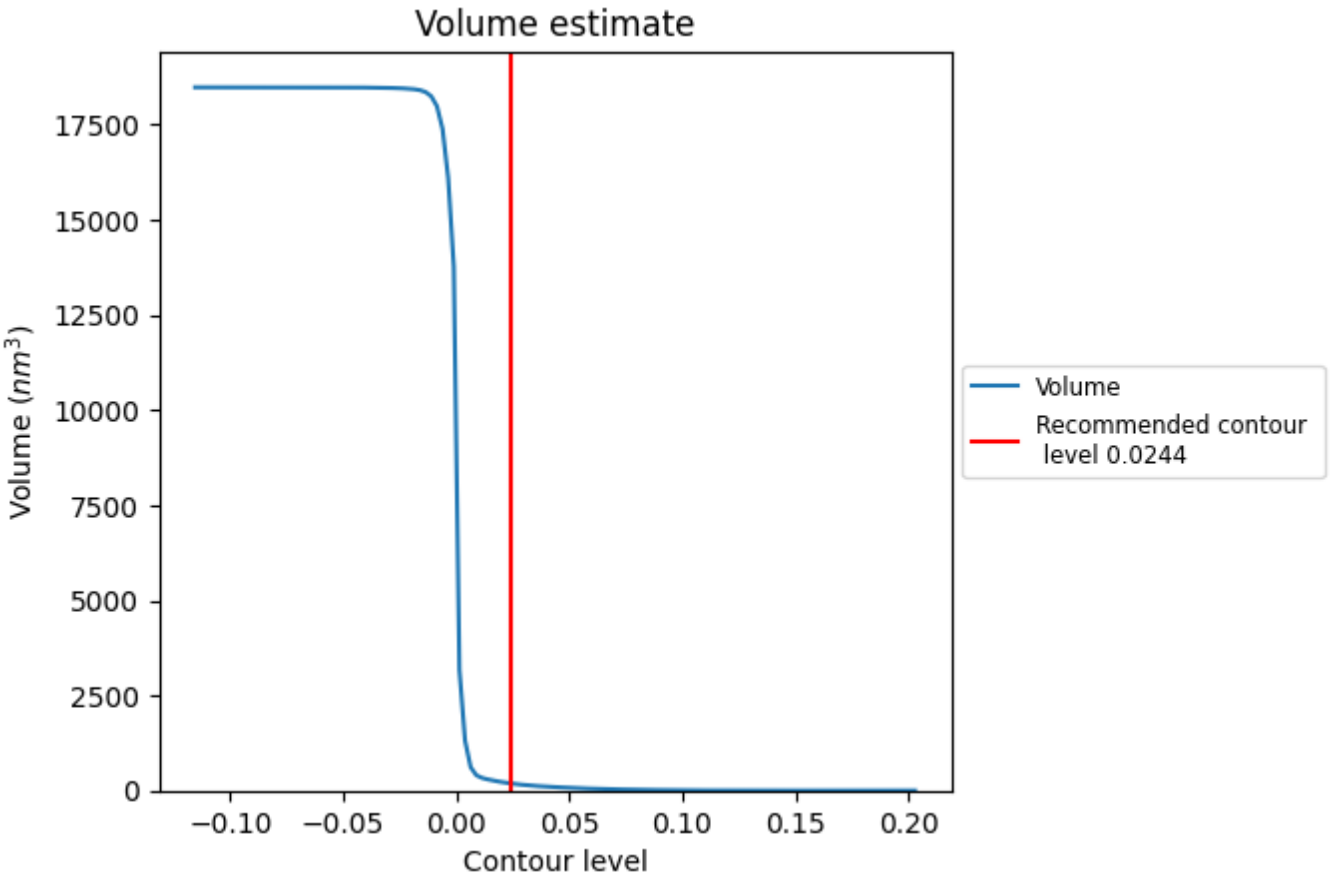
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

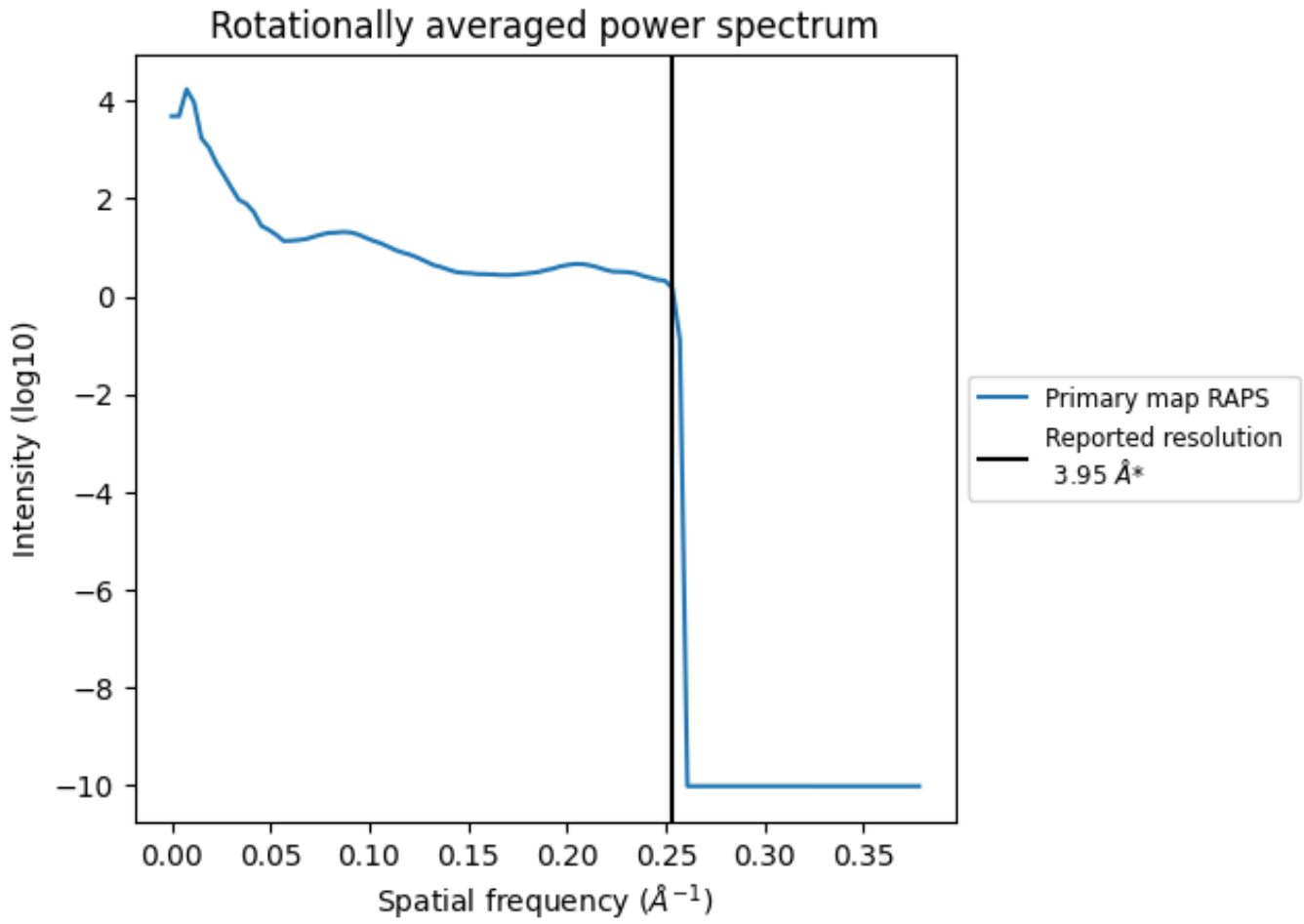
7.2 Volume estimate



The volume at the recommended contour level is 186 nm^3; this corresponds to an approximate mass of 168 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 0.253 Å^{-1}

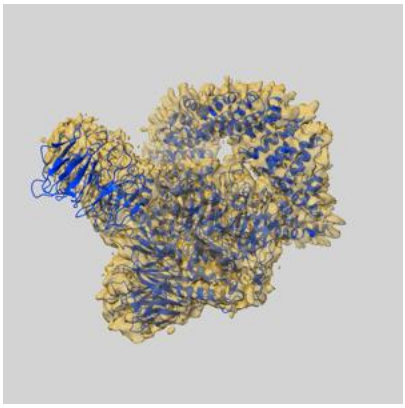
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

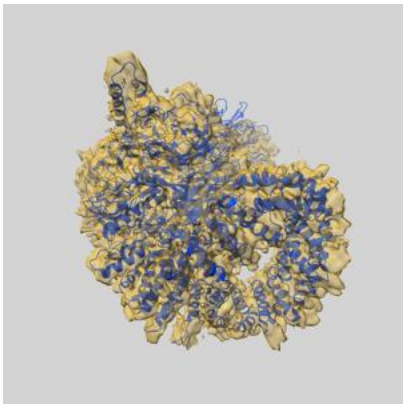
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6915 and PDB model 5ZYA. Per-residue inclusion information can be found in section 3 on page 5.

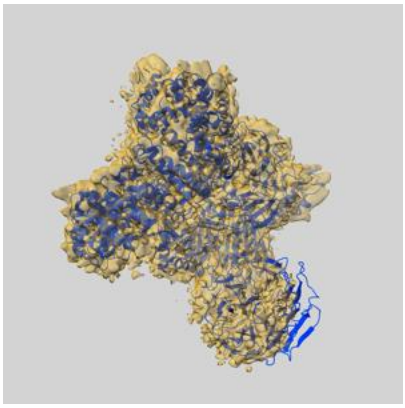
9.1 Map-model overlay



X



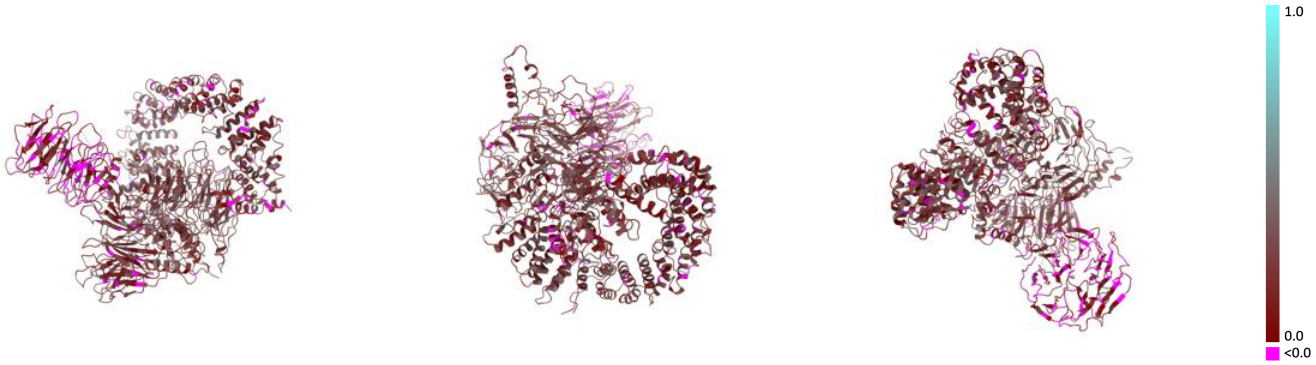
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0244 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.

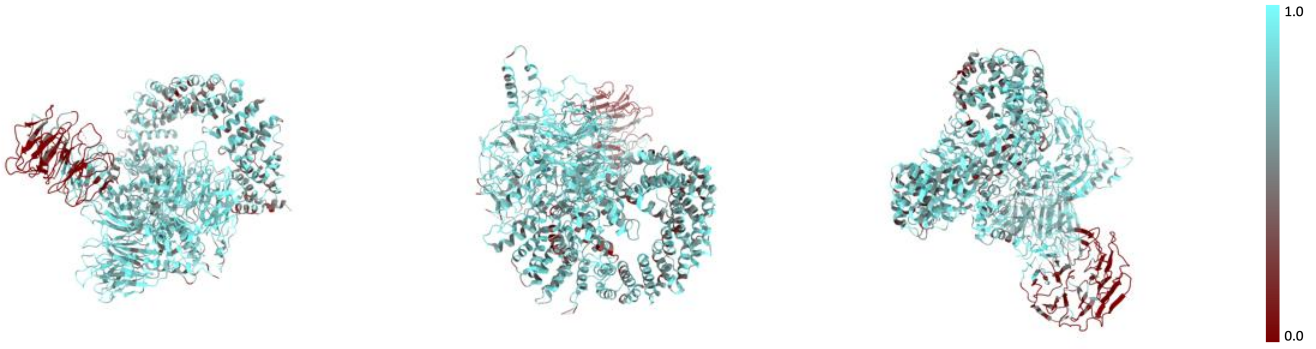
9.2 Q-score mapped to coordinate model (i)



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.

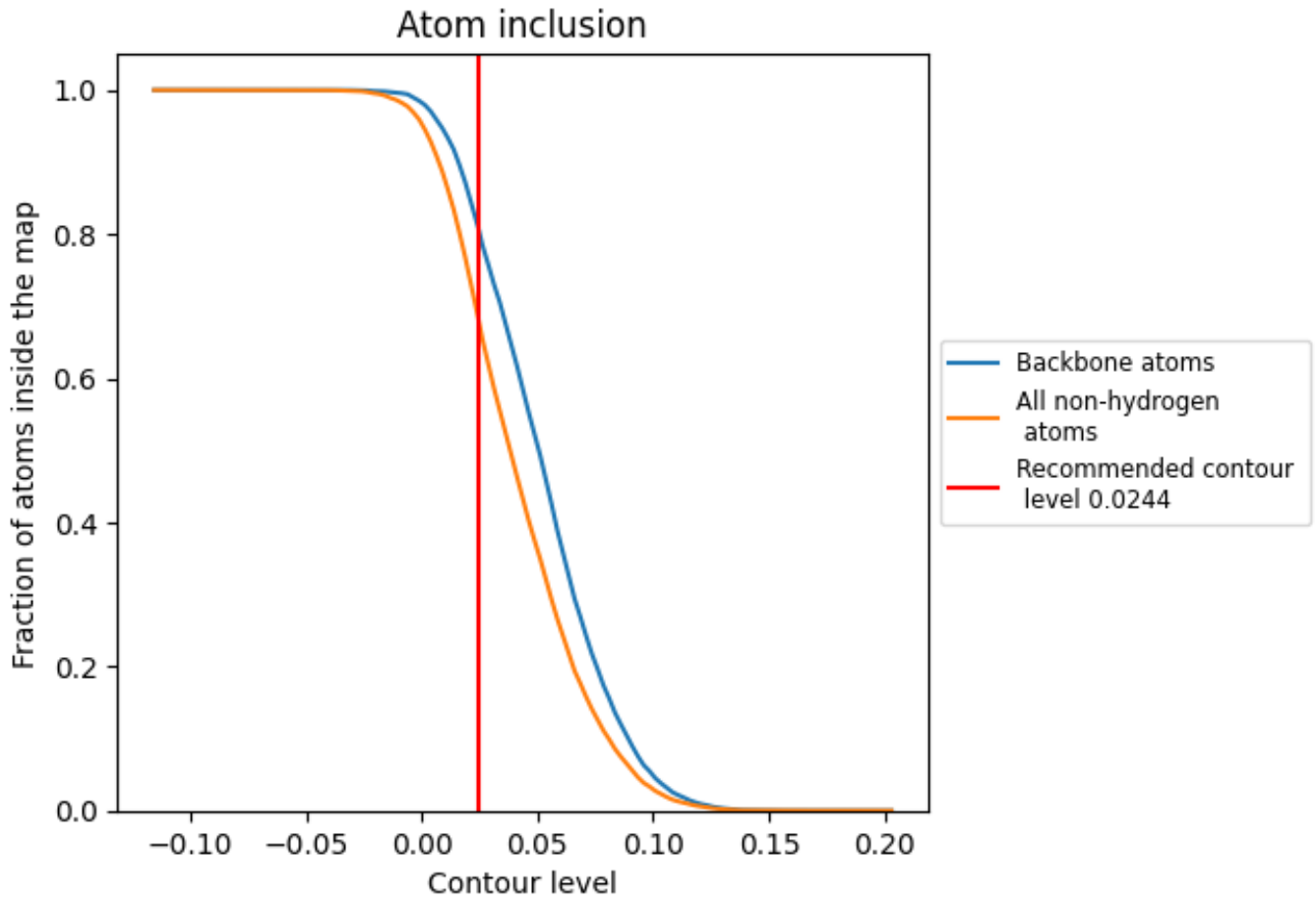
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0244).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 68% 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 (0.0244) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6835	0.2050
A	0.6634	0.1940
B	0.7742	0.2370
C	0.6925	0.2110
D	0.8067	0.2650