Full wwPDB EM Validation Report ⓘ

Jun 11, 2025 – 04:23 PM EDT

PDB ID	:	9NB5 / pdb_00009nb5
EMDB ID	:	EMD-49213
Title	:	Cryo-EM structure of the autoinhibitory CD163 trimer
Authors	:	Huang, C.-S.; White, J.B.R.; Degtjarik, O.; Mosyak, L.
Deposited on	:	2025-02-13
Resolution	:	3.00 Å(reported)
Based on initial model	:	.

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:

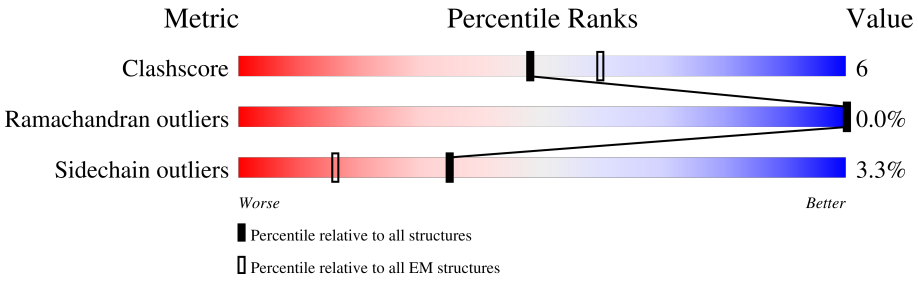
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1012	5% 72% 13% 15%
1	B	1012	5% 72% 13% 14%
1	C	1012	8% 70% 13% • 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19608 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 Scavenger receptor cysteine-rich type 1 protein M130.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	858	Total	C	N	O	S	0	0
			6492	3979	1179	1261	73		
1	B	867	Total	C	N	O	S	0	0
			6549	4012	1189	1275	73		
1	C	848	Total	C	N	O	S	0	0
			6421	3938	1168	1244	71		

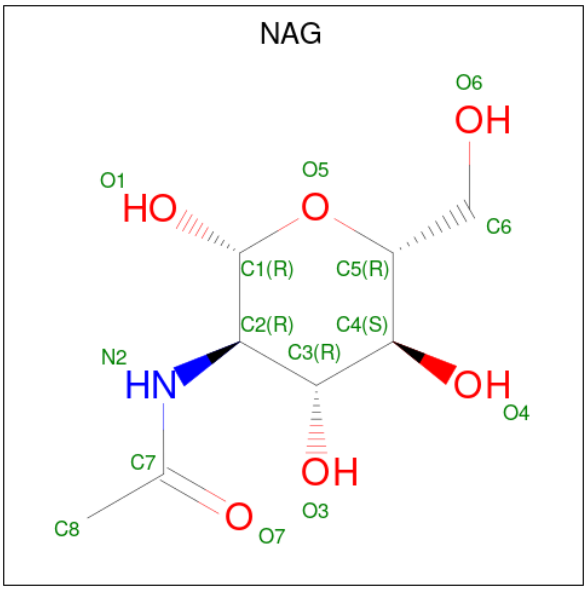
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1046	HIS	-	expression tag	UNP Q86VB7
A	1047	HIS	-	expression tag	UNP Q86VB7
A	1048	HIS	-	expression tag	UNP Q86VB7
A	1049	HIS	-	expression tag	UNP Q86VB7
A	1050	HIS	-	expression tag	UNP Q86VB7
A	1051	HIS	-	expression tag	UNP Q86VB7
A	1052	HIS	-	expression tag	UNP Q86VB7
A	1053	HIS	-	expression tag	UNP Q86VB7
B	1046	HIS	-	expression tag	UNP Q86VB7
B	1047	HIS	-	expression tag	UNP Q86VB7
B	1048	HIS	-	expression tag	UNP Q86VB7
B	1049	HIS	-	expression tag	UNP Q86VB7
B	1050	HIS	-	expression tag	UNP Q86VB7
B	1051	HIS	-	expression tag	UNP Q86VB7
B	1052	HIS	-	expression tag	UNP Q86VB7
B	1053	HIS	-	expression tag	UNP Q86VB7
C	1046	HIS	-	expression tag	UNP Q86VB7
C	1047	HIS	-	expression tag	UNP Q86VB7
C	1048	HIS	-	expression tag	UNP Q86VB7
C	1049	HIS	-	expression tag	UNP Q86VB7
C	1050	HIS	-	expression tag	UNP Q86VB7
C	1051	HIS	-	expression tag	UNP Q86VB7
C	1052	HIS	-	expression tag	UNP Q86VB7
C	1053	HIS	-	expression tag	UNP Q86VB7

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A	7	Total Ca 7 7	0
2	B	7	Total Ca 7 7	0
2	C	6	Total Ca 6 6	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0

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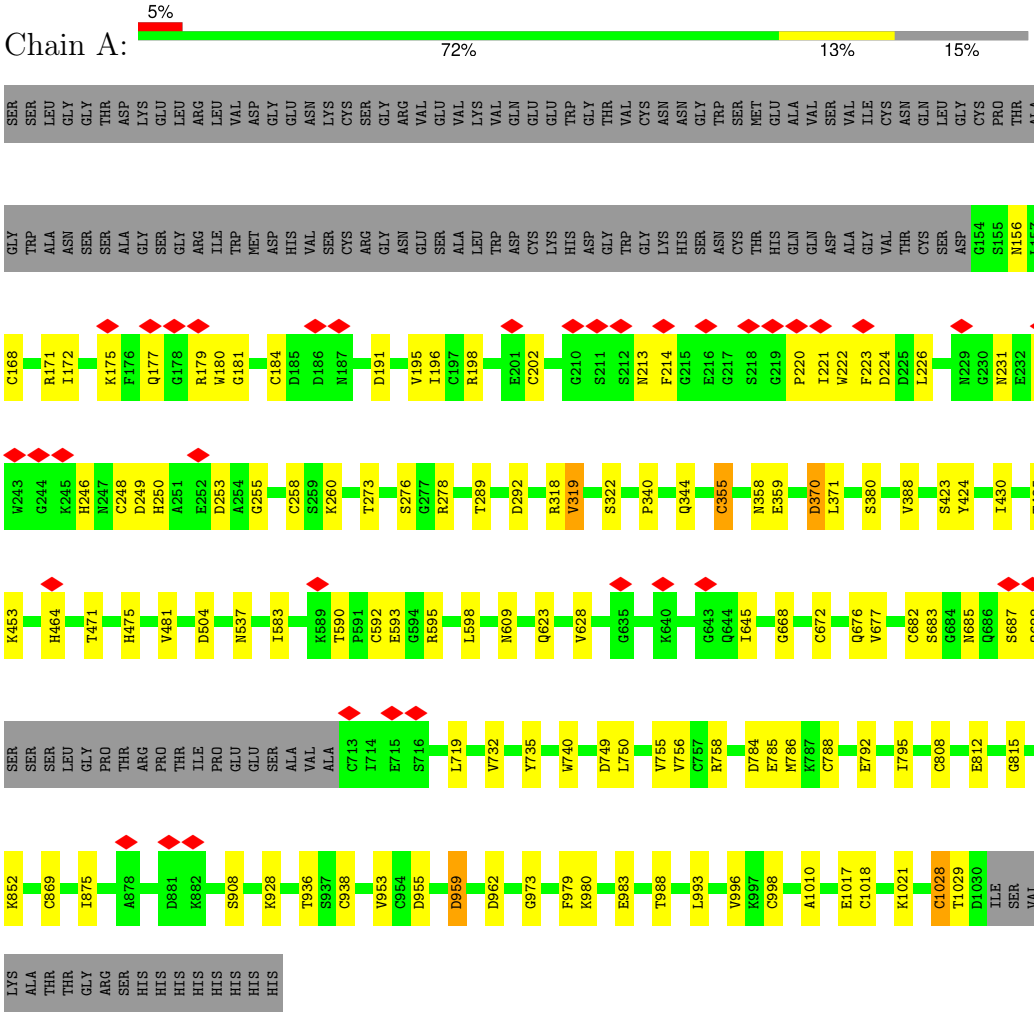
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

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.

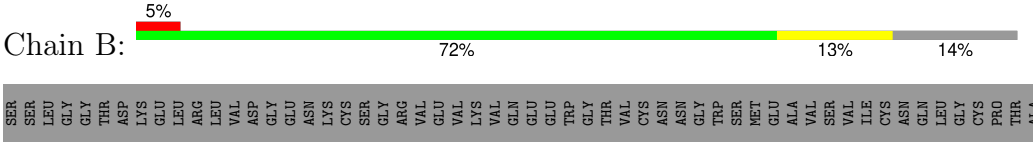
• Molecule 1: Scavenger receptor cysteine-rich type 1 protein M130

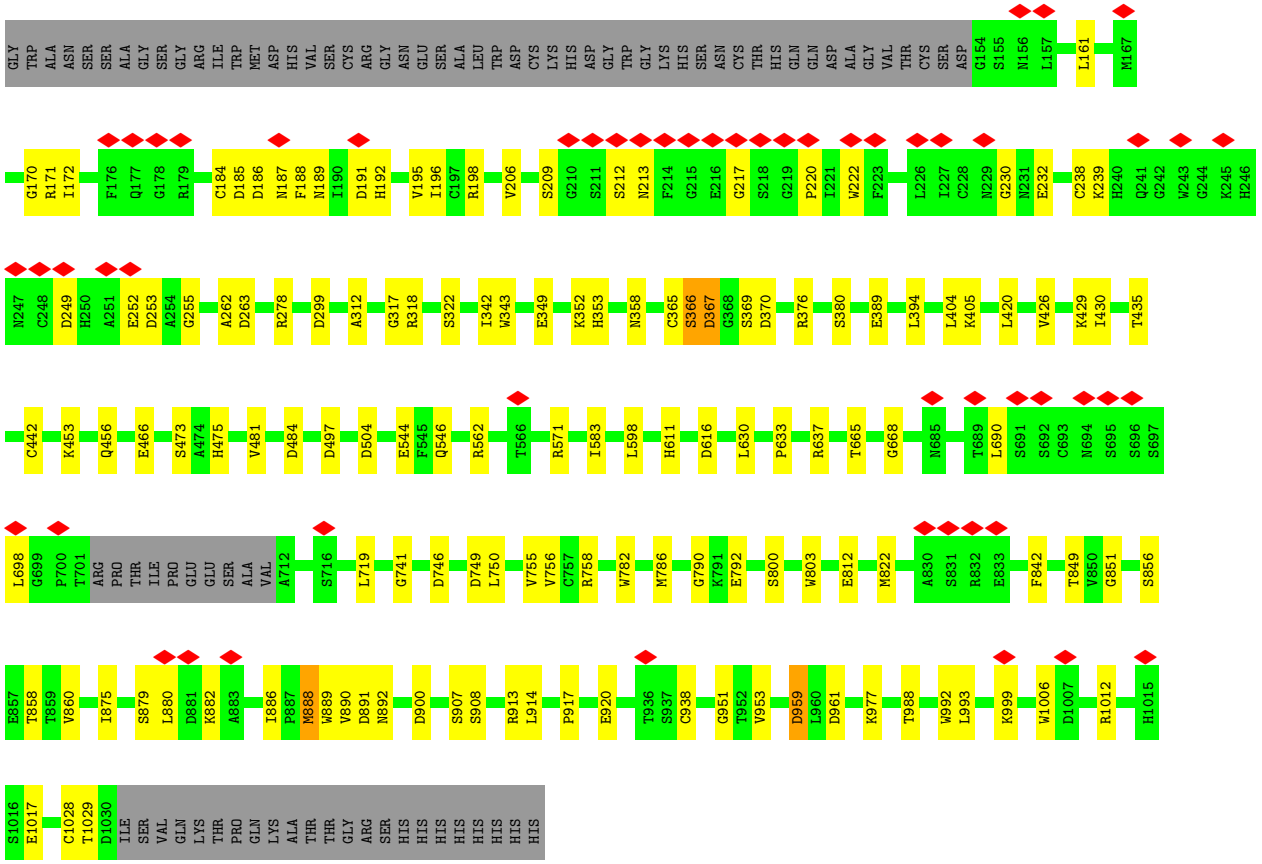
Chain A:



• Molecule 1: Scavenger receptor cysteine-rich type 1 protein M130

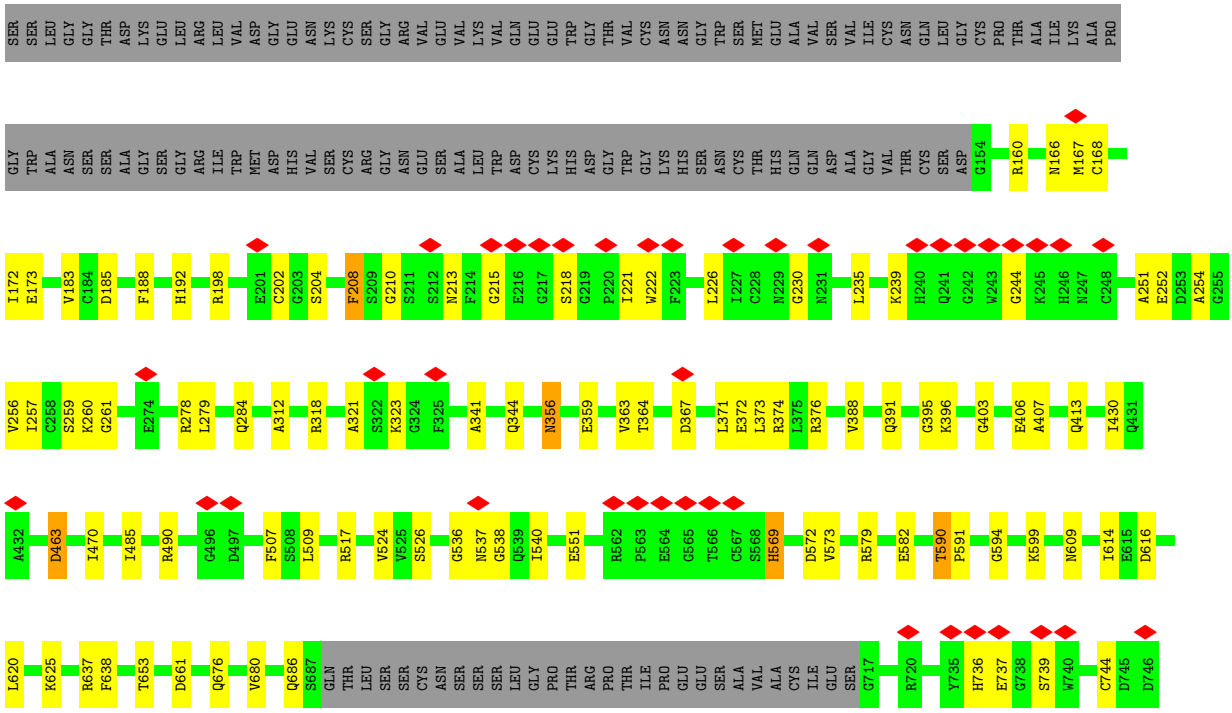
Chain B:

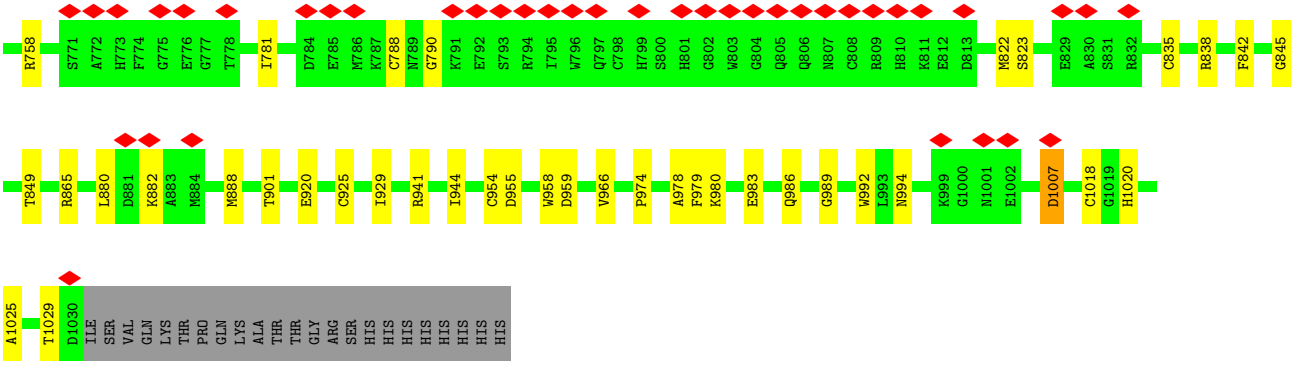




• Molecule 1: Scavenger receptor cysteine-rich type 1 protein M130

Chain C:




R758
S771 A772 H773 F774 G775 E776 G777 T778
I781
D784 E785 M786 K787 C788 N789 G790
K791 E792 S793 R794 I795 W796 Q797 C798 H799 S800 H801 G802 W803 G804 Q805 Q806 N807 C808 R809 H810 K811 E812 D813
M822 S823
E829 A830 S831 R832
C835
R838
F842
G845
T849
R865
L880 D881 K882 A883 M884
M888
T901
E920
C925
I929
R941
I944
C954 D955
W958 D959
V966
P974
A978 F979 K980
E983
Q986
G989
W992 L993 N994
K999 G1000 N1001 E1002
D1007
C1018 G1019 H1020
A1025
T1029
D1030
ILE SER VAL GLN LYS THR PRO GLN LYS ALA THR THR GLY ARG SER HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	391535	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.67	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	7.564	Depositor
Minimum map value	0.000	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.85	Depositor
Map size (Å)	444.0, 444.0, 444.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG

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	0.14	0/6641	0.29	0/8991
1	B	0.19	0/6699	0.37	3/9071 (0.0%)
1	C	0.13	0/6570	0.28	0/8895
All	All	0.16	0/19910	0.31	3/26957 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	369	SER	N-CA-C	8.32	120.34	111.28
1	B	366	SER	N-CA-C	6.68	120.05	109.50
1	B	370	ASP	N-CA-C	5.05	119.42	113.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6492	0	6028	73	0
1	B	6549	0	6082	68	0
1	C	6421	0	5962	77	0
2	A	7	0	0	0	0
2	B	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	6	0	0	0	0
3	A	42	0	39	0	0
3	B	42	0	39	0	0
3	C	42	0	39	0	0
All	All	19608	0	18189	216	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 6.

All (216) 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)
1:C:185:ASP:HB3	1:C:251:ALA:HB1	1.63	0.81
1:B:213:ASN:HA	1:B:349:GLU:HG3	1.68	0.76
1:B:352:LYS:O	1:B:353:HIS:ND1	2.21	0.74
1:A:936:THR:HG22	1:A:938:CYS:H	1.54	0.72
1:C:994:ASN:ND2	1:C:1018:CYS:SG	2.65	0.70
1:C:758:ARG:NH2	1:C:790:GLY:O	2.24	0.70
1:B:184:CYS:SG	1:B:185:ASP:N	2.65	0.69
1:C:183:VAL:HA	1:C:221:ILE:HG12	1.73	0.69
1:C:213:ASN:ND2	1:C:252:GLU:O	2.27	0.68
1:A:213:ASN:HD22	1:A:214:PHE:HD2	1.42	0.67
1:A:318:ARG:NH2	1:A:359:GLU:OE1	2.28	0.66
1:C:318:ARG:HD2	1:C:321:ALA:HB3	1.77	0.66
1:A:1017:GLU:N	1:A:1017:GLU:OE2	2.30	0.64
1:C:979:PHE:HD2	1:C:983:GLU:HG3	1.62	0.64
1:B:186:ASP:O	1:B:187:ASN:ND2	2.31	0.64
1:C:407:ALA:HB1	1:C:470:ILE:HD13	1.80	0.64
1:B:453:LYS:HE3	1:B:453:LYS:HA	1.80	0.63
1:B:1017:GLU:OE2	1:C:356:ASN:ND2	2.28	0.63
1:A:852:LYS:HG2	1:A:875:ILE:HD11	1.80	0.63
1:A:198:ARG:HD2	1:A:233:SER:HA	1.80	0.63
1:C:517:ARG:NH1	1:C:551:GLU:O	2.31	0.62
1:C:372:GLU:OE1	1:C:374:ARG:NH2	2.28	0.62
1:C:625:LYS:O	1:C:686:GLN:NE2	2.33	0.61
1:C:955:ASP:HB2	1:C:980:LYS:HG2	1.83	0.60
1:B:206:VAL:HG11	1:B:262:ALA:HB2	1.82	0.60
1:A:276:SER:HB3	1:A:319:VAL:HG21	1.85	0.59
1:A:758:ARG:NH2	1:A:792:GLU:O	2.34	0.59
1:B:238:CYS:SG	1:B:239:LYS:N	2.75	0.59
1:C:312:ALA:HB3	1:C:367:ASP:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:TRP:O	1:A:246:HIS:NE2	2.37	0.58
1:B:938:CYS:HB3	1:B:1028:CYS:HB2	1.86	0.58
1:A:184:CYS:H	1:A:221:ILE:HG23	1.70	0.57
1:B:907:SER:OG	1:B:908:SER:N	2.38	0.57
1:B:544:GLU:OE1	1:B:562:ARG:NH1	2.38	0.56
1:C:215:GLY:O	1:C:218:SER:OG	2.23	0.56
1:C:185:ASP:O	1:C:188:PHE:HB2	2.06	0.56
1:B:405:LYS:NZ	1:B:442:CYS:O	2.35	0.56
1:C:210:GLY:O	1:C:213:ASN:ND2	2.37	0.56
1:C:279:LEU:HD11	1:C:363:VAL:HG22	1.86	0.56
1:A:171:ARG:NH2	1:A:253:ASP:OD2	2.39	0.56
1:B:249:ASP:HB2	1:B:252:GLU:HB2	1.87	0.55
1:B:914:LEU:H	1:B:914:LEU:HD23	1.71	0.55
1:B:758:ARG:NH1	1:B:792:GLU:O	2.39	0.55
1:C:278:ARG:NH1	1:C:323:LYS:O	2.39	0.55
1:C:341:ALA:HB3	1:C:344:GLN:HG3	1.88	0.54
1:A:583:ILE:HG12	1:A:598:LEU:HD12	1.90	0.54
1:B:278:ARG:NH1	1:B:322:SER:O	2.40	0.54
1:A:732:VAL:HG23	1:A:815:GLY:HA2	1.90	0.54
1:C:929:ILE:HD11	1:C:966:VAL:HG13	1.88	0.54
1:A:166:ASN:O	1:A:167:MET:HG3	2.08	0.54
1:A:380:SER:OG	1:A:475:HIS:ND1	2.37	0.53
1:B:171:ARG:HH12	1:B:212:SER:HB2	1.73	0.53
1:B:583:ILE:HG12	1:B:598:LEU:HD12	1.89	0.53
1:C:989:GLY:O	1:C:1020:HIS:NE2	2.38	0.53
1:B:749:ASP:OD1	1:B:749:ASP:N	2.40	0.53
1:C:609:ASN:HB2	1:C:676:GLN:HB3	1.91	0.53
1:A:719:LEU:HD13	1:A:756:VAL:HG13	1.89	0.53
1:C:538:GLY:O	1:C:569:HIS:NE2	2.41	0.52
1:C:198:ARG:NH2	1:C:230:GLY:O	2.43	0.52
1:C:537:ASN:OD1	1:C:537:ASN:N	2.43	0.52
1:C:222:TRP:HE3	1:C:244:GLY:HA2	1.75	0.51
1:A:179:ARG:NH1	1:A:180:TRP:H	2.09	0.51
1:A:156:ASN:OD1	1:A:156:ASN:N	2.43	0.51
1:A:439:LEU:HD11	1:A:449:LEU:HD11	1.92	0.51
1:A:595:ARG:HD2	1:A:677:VAL:HG11	1.93	0.51
1:C:202:CYS:SG	1:C:260:LYS:HB3	2.50	0.51
1:B:192:HIS:HA	1:B:195:VAL:HG23	1.93	0.51
1:A:292:ASP:HB3	1:A:358:ASN:HB3	1.93	0.50
1:B:822:MET:HA	1:B:842:PHE:O	2.12	0.49
1:C:226:LEU:HD23	1:C:235:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:GLU:OE1	1:C:599:LYS:NZ	2.45	0.49
1:B:171:ARG:NH2	1:B:253:ASP:HB2	2.27	0.49
1:C:185:ASP:N	1:C:251:ALA:O	2.40	0.49
1:A:749:ASP:OD1	1:A:750:LEU:N	2.44	0.49
1:B:161:LEU:HA	1:B:171:ARG:O	2.12	0.49
1:B:367:ASP:OD1	1:B:367:ASP:N	2.45	0.49
1:B:171:ARG:HH21	1:B:217:GLY:HA2	1.77	0.49
1:B:312:ALA:HB3	1:B:366:SER:O	2.12	0.49
1:C:403:GLY:N	1:C:406:GLU:OE1	2.44	0.48
1:C:941:ARG:NH1	1:C:986:GLN:O	2.47	0.48
1:C:463:ASP:N	1:C:463:ASP:OD1	2.47	0.48
1:C:958:TRP:CD1	1:C:978:ALA:HB1	2.49	0.48
1:A:202:CYS:O	1:A:260:LYS:HG2	2.13	0.48
1:C:168:CYS:HB2	1:C:261:GLY:HA3	1.95	0.48
1:C:979:PHE:HB2	1:C:1025:ALA:HB3	1.95	0.48
1:C:1007:ASP:N	1:C:1007:ASP:OD1	2.45	0.48
1:B:900:ASP:OD1	1:B:900:ASP:N	2.47	0.48
1:A:537:ASN:N	1:A:537:ASN:OD1	2.47	0.48
1:A:687:SER:OG	1:A:688:GLN:N	2.47	0.48
1:A:953:VAL:HG13	1:A:993:LEU:HB2	1.95	0.47
1:B:185:ASP:O	1:B:188:PHE:HB2	2.14	0.47
1:B:891:ASP:OD1	1:B:892:ASN:N	2.48	0.47
1:B:209:SER:HB2	1:B:255:GLY:C	2.39	0.47
1:A:592:CYS:HB3	1:A:682:CYS:HB2	1.97	0.47
1:B:389:GLU:HG3	1:B:394:LEU:HD12	1.97	0.47
1:B:1006:TRP:O	1:B:1012:ARG:NH1	2.48	0.47
1:C:166:ASN:OD1	1:C:167:MET:N	2.47	0.47
1:A:504:ASP:HB3	1:A:988:THR:HB	1.97	0.47
1:A:962:ASP:OD1	1:A:998:CYS:HB2	2.14	0.47
1:A:423:SER:O	1:A:471:THR:OG1	2.26	0.47
1:A:278:ARG:NH1	1:A:322:SER:O	2.47	0.46
1:C:835:CYS:SG	1:C:925:CYS:HB2	2.55	0.46
1:A:938:CYS:HB3	1:A:1028:CYS:HB2	1.97	0.46
1:C:823:SER:HB3	1:C:842:PHE:HB3	1.97	0.46
1:A:869:CYS:O	1:A:928:LYS:HG2	2.15	0.46
1:B:504:ASP:OD1	1:B:571:ARG:HB3	2.14	0.46
1:C:536:GLY:O	1:C:569:HIS:ND1	2.48	0.46
1:A:609:ASN:HB2	1:A:676:GLN:HB3	1.98	0.46
1:B:786:MET:HE3	1:B:786:MET:HB3	1.83	0.46
1:C:959:ASP:N	1:C:959:ASP:OD1	2.49	0.46
1:B:376:ARG:HB2	1:B:430:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:PRO:HB3	1:B:637:ARG:HG3	1.98	0.46
1:A:158:GLU:H	1:A:175:LYS:HB3	1.81	0.46
1:C:172:ILE:HD11	1:C:256:VAL:HG13	1.98	0.46
1:C:388:VAL:O	1:C:395:GLY:N	2.49	0.45
1:B:220:PRO:HG2	1:B:222:TRP:CH2	2.51	0.45
1:C:637:ARG:HE	1:C:637:ARG:HB3	1.56	0.45
1:B:172:ILE:HD13	1:B:196:ILE:HD13	1.97	0.45
1:B:882:LYS:HD3	1:B:917:PRO:HG3	1.98	0.45
1:C:842:PHE:CZ	1:C:845:GLY:HA2	2.52	0.45
1:A:628:VAL:HG13	1:A:688:GLN:HG3	1.98	0.45
1:C:822:MET:HA	1:C:842:PHE:O	2.17	0.45
1:B:977:LYS:HE3	1:B:977:LYS:HB2	1.84	0.45
1:C:490:ARG:HD2	1:C:572:ASP:OD2	2.16	0.45
1:A:590:THR:HG22	1:A:592:CYS:H	1.81	0.45
1:B:318:ARG:NH2	1:B:358:ASN:O	2.49	0.45
1:C:838:ARG:NH1	1:C:920:GLU:OE1	2.43	0.45
1:A:979:PHE:CD2	1:A:983:GLU:HG2	2.52	0.45
1:A:370:ASP:OD1	1:A:370:ASP:N	2.48	0.44
1:A:784:ASP:OD1	1:A:785:GLU:N	2.50	0.44
1:B:420:LEU:HD21	1:B:473:SER:HB3	1.98	0.44
1:C:954:CYS:SG	1:C:955:ASP:N	2.90	0.44
1:B:758:ARG:NH2	1:B:790:GLY:O	2.35	0.44
1:C:192:HIS:NE2	1:C:226:LEU:HB3	2.32	0.44
1:B:189:ASN:HB2	1:B:191:ASP:OD1	2.18	0.44
1:A:191:ASP:O	1:A:195:VAL:HG23	2.17	0.44
1:A:226:LEU:HB2	1:A:240:HIS:HB3	2.00	0.44
1:A:453:LYS:HA	1:A:453:LYS:HD3	1.73	0.44
1:A:235:LEU:HD12	1:A:236:TRP:N	2.33	0.44
1:A:340:PRO:HG2	1:A:344:GLN:HG3	2.00	0.44
1:A:645:ILE:HG21	1:A:672:CYS:HB3	2.00	0.44
1:B:999:LYS:HD2	1:B:999:LYS:HA	1.66	0.44
1:A:955:ASP:HB2	1:A:980:LYS:HB2	1.99	0.44
1:A:423:SER:OG	1:A:424:TYR:N	2.51	0.44
1:B:317:GLY:HA3	1:B:456:GLN:HG3	2.00	0.44
1:B:888:MET:N	1:B:913:ARG:O	2.46	0.43
1:A:239:LYS:HE3	1:A:239:LYS:HB2	1.88	0.43
1:B:191:ASP:HB2	1:B:230:GLY:HA3	2.00	0.43
1:B:959:ASP:HB2	1:B:961:ASP:OD1	2.17	0.43
1:C:185:ASP:HA	1:C:254:ALA:HB2	2.00	0.43
1:A:959:ASP:OD1	1:A:959:ASP:N	2.50	0.43
1:C:736:HIS:ND1	1:C:737:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:744:CYS:SG	1:C:781:ILE:HG21	2.59	0.43
1:B:951:GLY:HA3	1:B:992:TRP:CD1	2.53	0.43
1:C:944:ILE:HD11	1:C:992:TRP:HB2	2.00	0.43
1:B:690:LEU:H	1:B:690:LEU:HD23	1.83	0.43
1:A:221:ILE:HG21	1:A:248:CYS:SG	2.59	0.43
1:A:996:VAL:HA	1:A:1010:ALA:HB2	2.01	0.43
1:C:226:LEU:HD12	1:C:226:LEU:HA	1.85	0.43
1:A:171:ARG:HA	1:A:255:GLY:HA2	2.00	0.43
1:C:614:ILE:HD12	1:C:614:ILE:HA	1.90	0.43
1:A:179:ARG:HD2	1:A:179:ARG:HA	1.85	0.42
1:C:849:THR:HG21	1:C:920:GLU:HG2	2.00	0.42
1:A:1021:LYS:NZ	1:B:746:ASP:OD2	2.52	0.42
1:B:879:SER:OG	1:B:880:LEU:N	2.52	0.42
1:A:668:GLY:HA2	1:A:908:SER:O	2.20	0.42
1:A:683:SER:OG	1:A:685:ASN:OD1	2.23	0.42
1:A:735:TYR:HB2	1:A:740:TRP:CZ3	2.54	0.42
1:B:719:LEU:HD21	1:B:756:VAL:HG13	2.00	0.42
1:A:719:LEU:HD23	1:A:719:LEU:HA	1.87	0.42
1:C:376:ARG:C	1:C:430:ILE:HD11	2.44	0.42
1:C:239:LYS:HD2	1:C:239:LYS:HA	1.81	0.42
1:C:204:SER:O	1:C:259:SER:N	2.42	0.42
1:B:698:LEU:HB2	1:B:803:TRP:NE1	2.33	0.42
1:A:792:GLU:N	1:A:792:GLU:OE1	2.53	0.42
1:B:263:ASP:OD1	1:B:263:ASP:N	2.47	0.42
1:C:364:THR:O	1:C:364:THR:OG1	2.34	0.42
1:B:161:LEU:HB3	1:B:170:GLY:HA3	2.01	0.42
1:B:668:GLY:HA2	1:B:908:SER:O	2.19	0.42
1:A:590:THR:HB	1:A:593:GLU:HG2	2.02	0.41
1:A:172:ILE:HG12	1:A:196:ILE:HD13	2.01	0.41
1:A:181:GLY:HA3	1:A:220:PRO:HG2	2.01	0.41
1:B:380:SER:OG	1:B:475:HIS:ND1	2.44	0.41
1:C:160:ARG:NE	1:C:173:GLU:OE1	2.42	0.41
1:C:373:LEU:HB3	1:C:413:GLN:HE22	1.85	0.41
1:A:755:VAL:HG21	1:A:788:CYS:SG	2.60	0.41
1:B:953:VAL:HG13	1:B:993:LEU:HB2	2.03	0.41
1:B:856:SER:O	1:B:860:VAL:HG23	2.20	0.41
1:C:620:LEU:HD23	1:C:680:VAL:HG11	2.01	0.41
1:C:974:PRO:O	1:C:1029:THR:HG22	2.21	0.41
1:B:917:PRO:HA	1:B:920:GLU:HG2	2.02	0.41
1:C:208:PHE:O	1:C:208:PHE:CG	2.74	0.41
1:C:540:ILE:HD11	1:C:569:HIS:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASN:C	1:A:168:CYS:H	2.27	0.41
1:A:231:ASN:OD1	1:A:231:ASN:N	2.54	0.41
1:C:888:MET:HE3	1:C:888:MET:HB2	1.87	0.41
1:B:429:LYS:HA	1:B:429:LYS:HD3	1.83	0.41
1:A:250:HIS:ND1	1:A:250:HIS:O	2.54	0.41
1:C:880:LEU:HG	1:C:882:LYS:H	1.86	0.41
1:A:249:ASP:OD1	1:A:249:ASP:N	2.54	0.41
1:B:851:GLY:HA3	1:B:891:ASP:OD2	2.21	0.41
1:C:590:THR:HG22	1:C:591:PRO:HD2	2.03	0.40
1:A:355:CYS:SG	1:A:358:ASN:HB2	2.61	0.40
1:A:795:ILE:HD12	1:A:795:ILE:HA	1.86	0.40
1:C:594:GLY:HA2	1:C:638:PHE:CD2	2.56	0.40
1:A:786:MET:HE3	1:A:786:MET:HB3	1.98	0.40
1:B:198:ARG:NH2	1:B:232:GLU:O	2.37	0.40
1:C:257:ILE:HD13	1:C:284:GLN:NE2	2.36	0.40
1:C:485:ILE:HD13	1:C:485:ILE:HA	1.89	0.40
1:A:177:GLN:OE1	1:A:177:GLN:N	2.55	0.40
1:A:973:GLY:HA3	1:A:1029:THR:OG1	2.21	0.40
1:B:318:ARG:O	1:B:318:ARG:HG3	2.22	0.40
1:B:849:THR:HG23	1:B:886:ILE:HG13	2.04	0.40
1:C:579:ARG:NH2	1:C:661:ASP:OD2	2.55	0.40
1:B:741:GLY:HA3	1:B:782:TRP:CD1	2.56	0.40
1:C:526:SER:HB3	1:C:865:ARG:HH12	1.86	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	854/1012 (84%)	825 (97%)	28 (3%)	1 (0%)	48 81
1	B	863/1012 (85%)	839 (97%)	24 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	844/1012 (83%)	823 (98%)	21 (2%)	0	100	100
All	All	2561/3036 (84%)	2487 (97%)	73 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	VAL

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	698/826 (84%)	678 (97%)	20 (3%)	37	70
1	B	705/826 (85%)	676 (96%)	29 (4%)	26	60
1	C	688/826 (83%)	669 (97%)	19 (3%)	38	70
All	All	2091/2478 (84%)	2023 (97%)	68 (3%)	35	67

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	PHE
1	A	224	ASP
1	A	238	CYS
1	A	258	CYS
1	A	273	THR
1	A	289	THR
1	A	355	CYS
1	A	370	ASP
1	A	371	LEU
1	A	388	VAL
1	A	430	ILE
1	A	435	THR
1	A	464	HIS
1	A	481	VAL

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Mol	Chain	Res	Type
1	A	623	GLN
1	A	808	CYS
1	A	812	GLU
1	A	959	ASP
1	A	1018	CYS
1	A	1028	CYS
1	B	299	ASP
1	B	342	ILE
1	B	343	TRP
1	B	365	CYS
1	B	367	ASP
1	B	404	LEU
1	B	426	VAL
1	B	435	THR
1	B	466	GLU
1	B	481	VAL
1	B	484	ASP
1	B	497	ASP
1	B	546	GLN
1	B	611	HIS
1	B	616	ASP
1	B	630	LEU
1	B	665	THR
1	B	750	LEU
1	B	755	VAL
1	B	800	SER
1	B	812	GLU
1	B	858	THR
1	B	875	ILE
1	B	888	MET
1	B	889	TRP
1	B	890	VAL
1	B	959	ASP
1	B	988	THR
1	B	1029	THR
1	C	208	PHE
1	C	356	ASN
1	C	359	GLU
1	C	371	LEU
1	C	391	GLN
1	C	396	LYS
1	C	463	ASP

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Mol	Chain	Res	Type
1	C	507	PHE
1	C	509	LEU
1	C	524	VAL
1	C	569	HIS
1	C	573	VAL
1	C	590	THR
1	C	616	ASP
1	C	653	THR
1	C	739	SER
1	C	788	CYS
1	C	901	THR
1	C	1007	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	434	ASN
1	A	723	ASN
1	A	806	GLN
1	A	946	HIS
1	B	241	GLN
1	B	464	HIS
1	B	623	GLN
1	B	686	GLN
1	B	736	HIS
1	B	968	GLN
1	C	425	GLN
1	C	553	HIS
1	C	622	GLN
1	C	651	HIS
1	C	657	GLN
1	C	805	GLN

5.3.3 RNA

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)

Of 29 ligands modelled in this entry, 20 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
3	NAG	A	1208	1	14,14,15	0.69	0	17,19,21	0.76	0
3	NAG	B	1208	1	14,14,15	0.77	0	17,19,21	0.89	0
3	NAG	A	1209	1	14,14,15	0.73	0	17,19,21	0.82	0
3	NAG	A	1210	1	14,14,15	0.75	0	17,19,21	0.90	0
3	NAG	C	1207	1	14,14,15	0.72	0	17,19,21	0.81	0
3	NAG	B	1210	1	14,14,15	0.73	0	17,19,21	0.78	0
3	NAG	B	1209	1	14,14,15	0.72	0	17,19,21	0.78	0
3	NAG	C	1208	1	14,14,15	0.76	0	17,19,21	1.00	1 (5%)
3	NAG	C	1209	1	14,14,15	0.71	0	17,19,21	0.84	0

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
3	NAG	A	1208	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1208	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1209	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1210	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1207	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1210	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1209	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1208	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1209	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1208	NAG	C1-O5-C5	2.56	115.62	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1208	NAG	C8-C7-N2-C2
3	B	1208	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

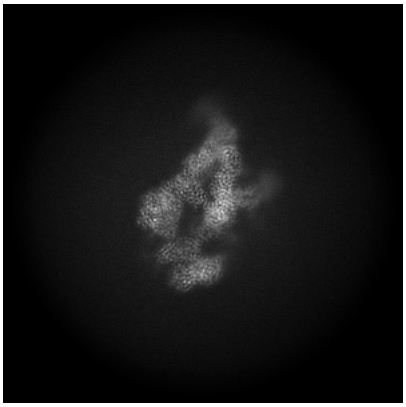
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-49213. These allow visual inspection of the internal detail of the map and identification of artifacts.

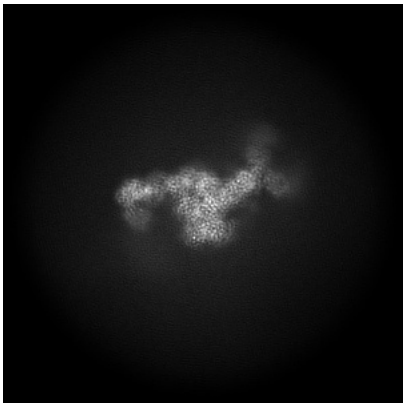
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

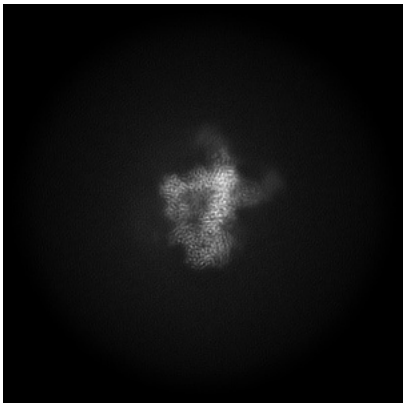
6.1.1 Primary map



X



Y



Z

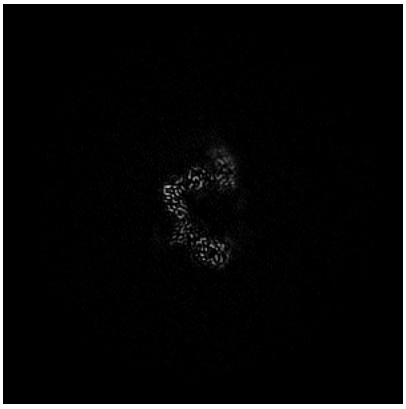
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 200

Y Index: 200

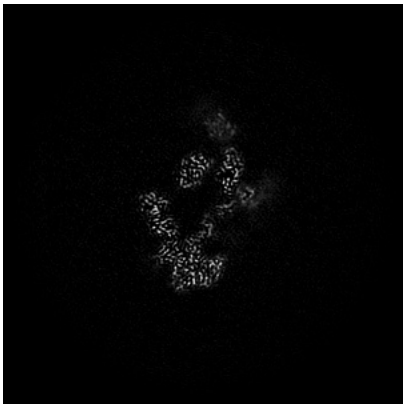


Z Index: 200

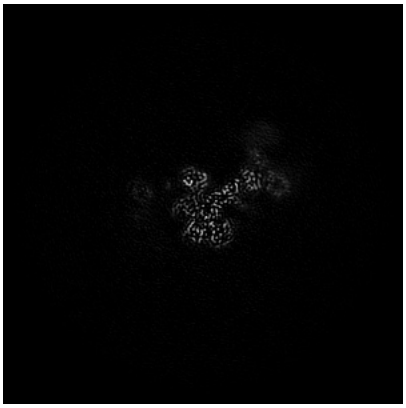
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

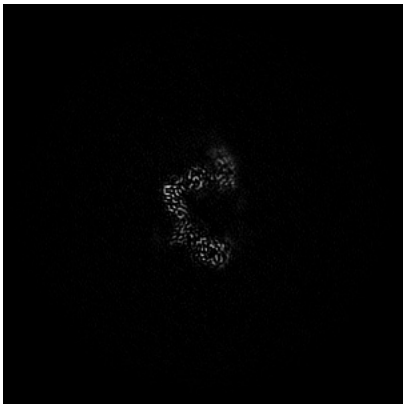
6.3.1 Primary map



X Index: 212



Y Index: 220

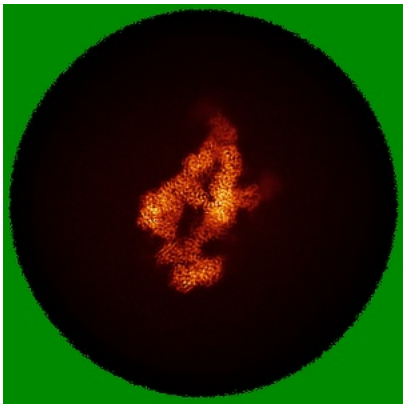


Z Index: 200

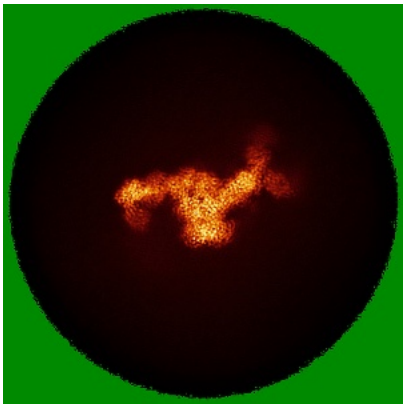
The images above show the largest variance slices of the map in three orthogonal directions.

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

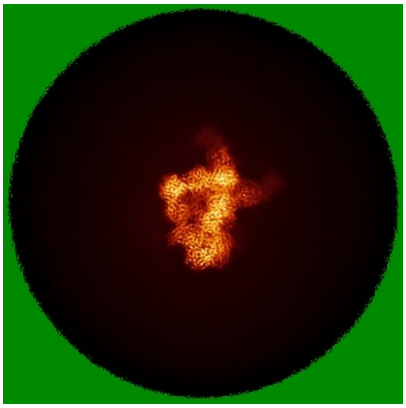
6.4.1 Primary map



X



Y



Z

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

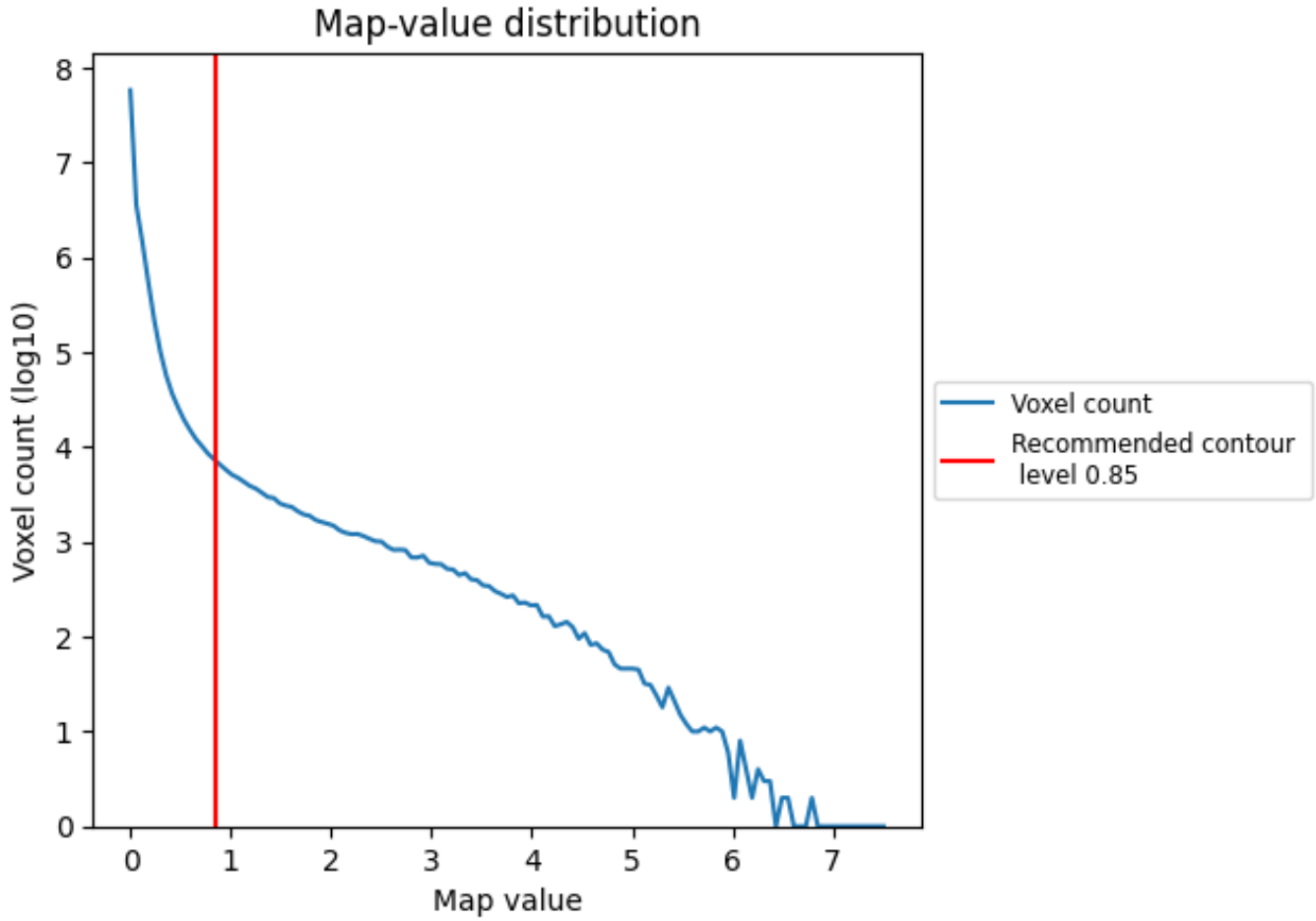
6.6 Mask visualisation (i)

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

7 Map analysis

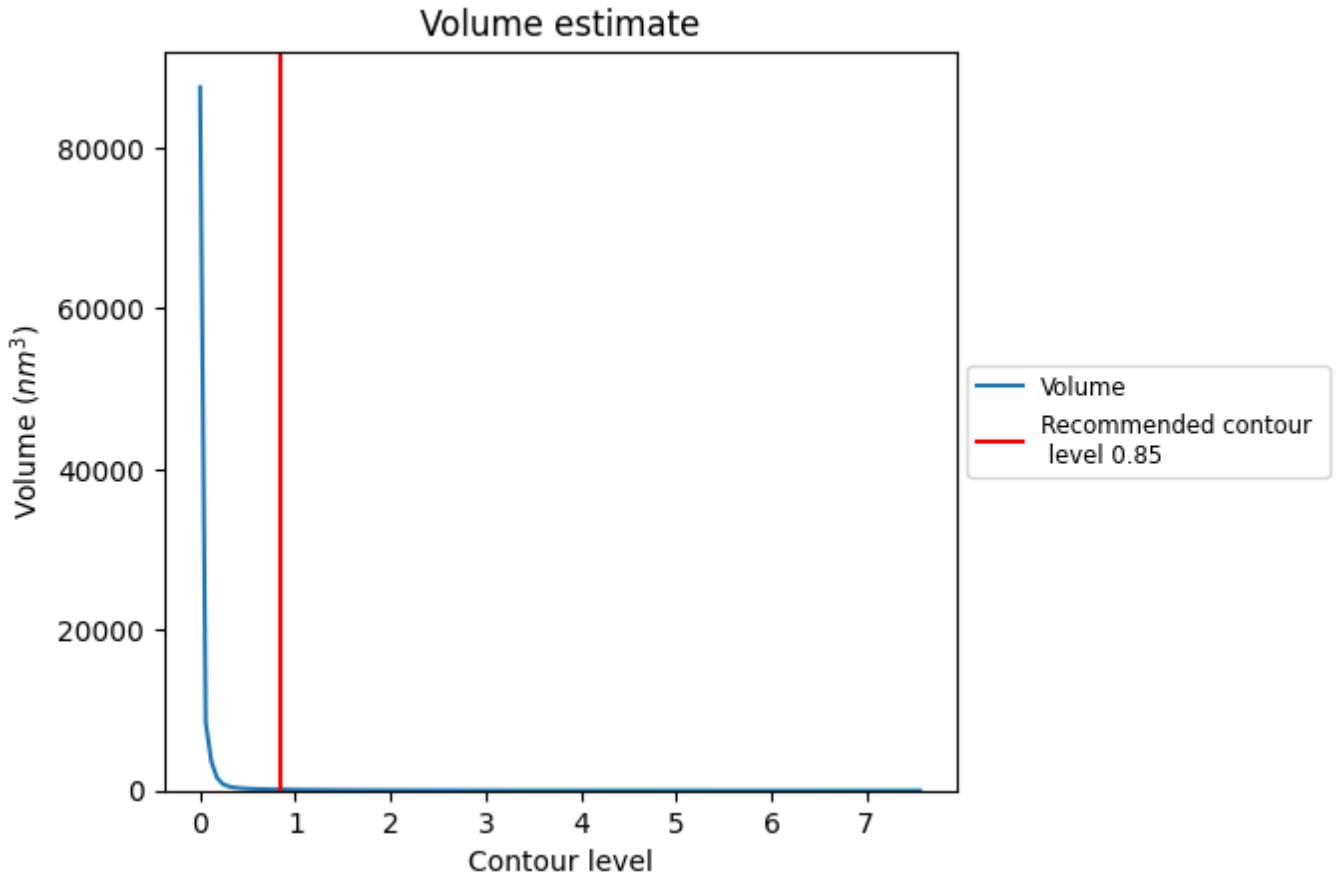
This section contains the results of statistical analysis of the map.

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.

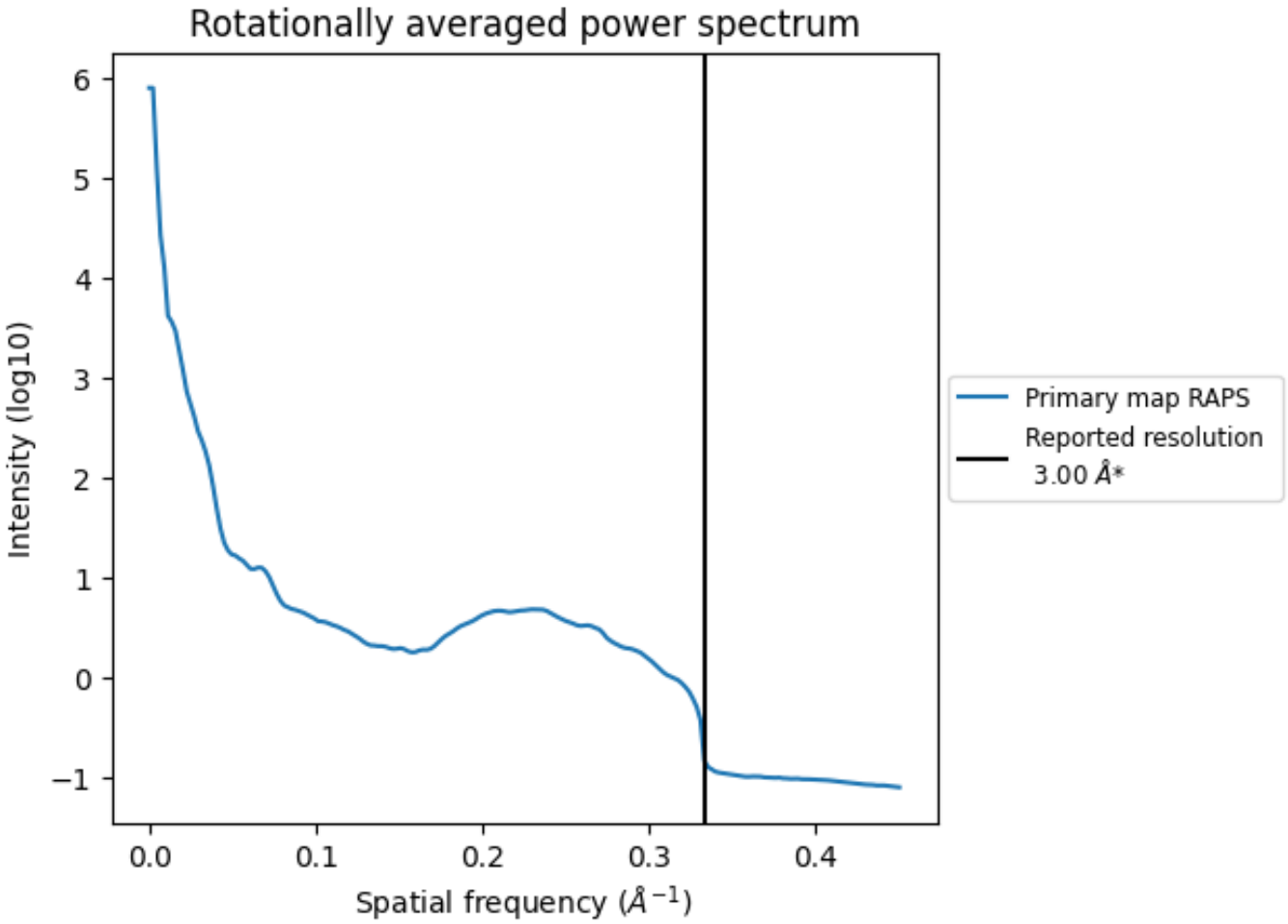
7.2 Volume estimate



The volume at the recommended contour level is 126 nm^3; this corresponds to an approximate mass of 113 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 0.333 $Å^{-1}$

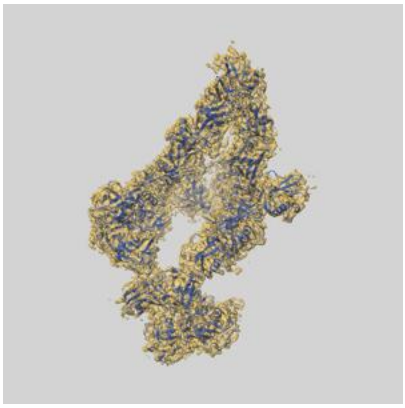
8 Fourier-Shell correlation (i)

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

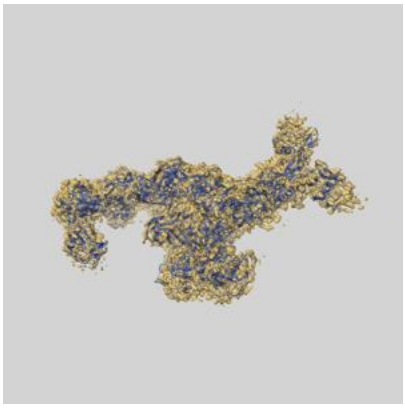
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-49213 and PDB model 9NB5. Per-residue inclusion information can be found in section 3 on page 6.

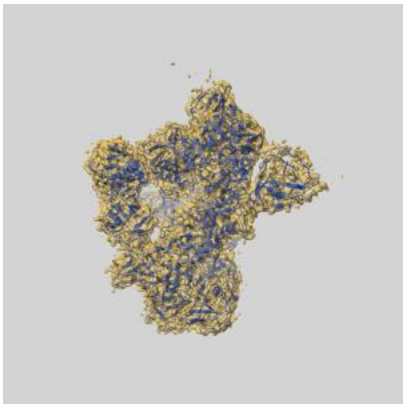
9.1 Map-model overlay



X



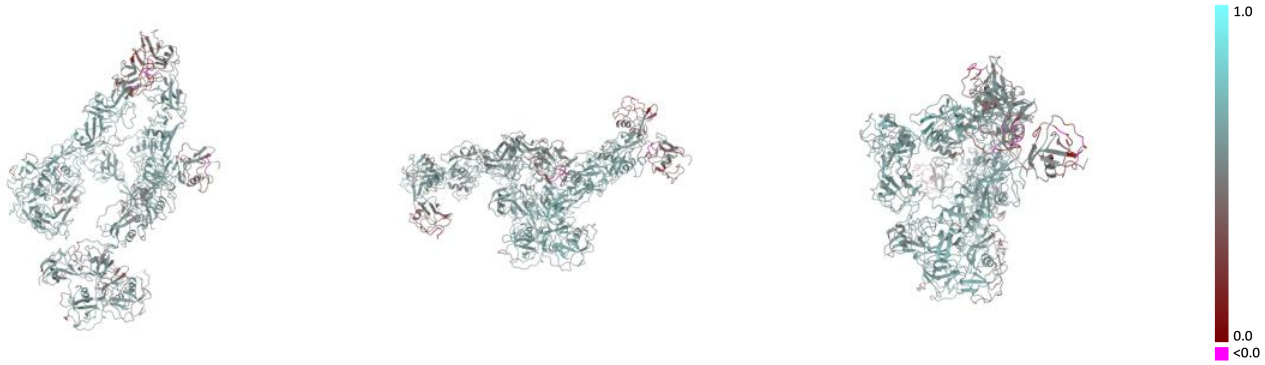
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.85 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.

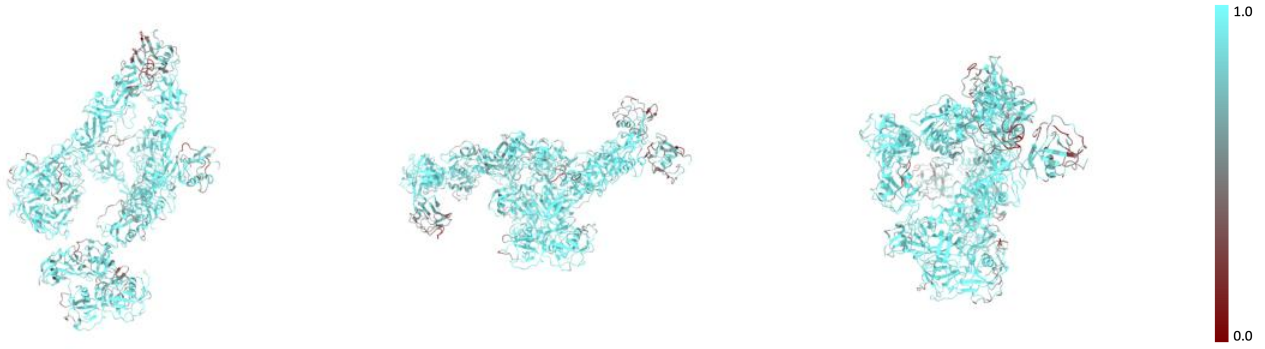
9.2 Q-score mapped to coordinate model (i)



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.

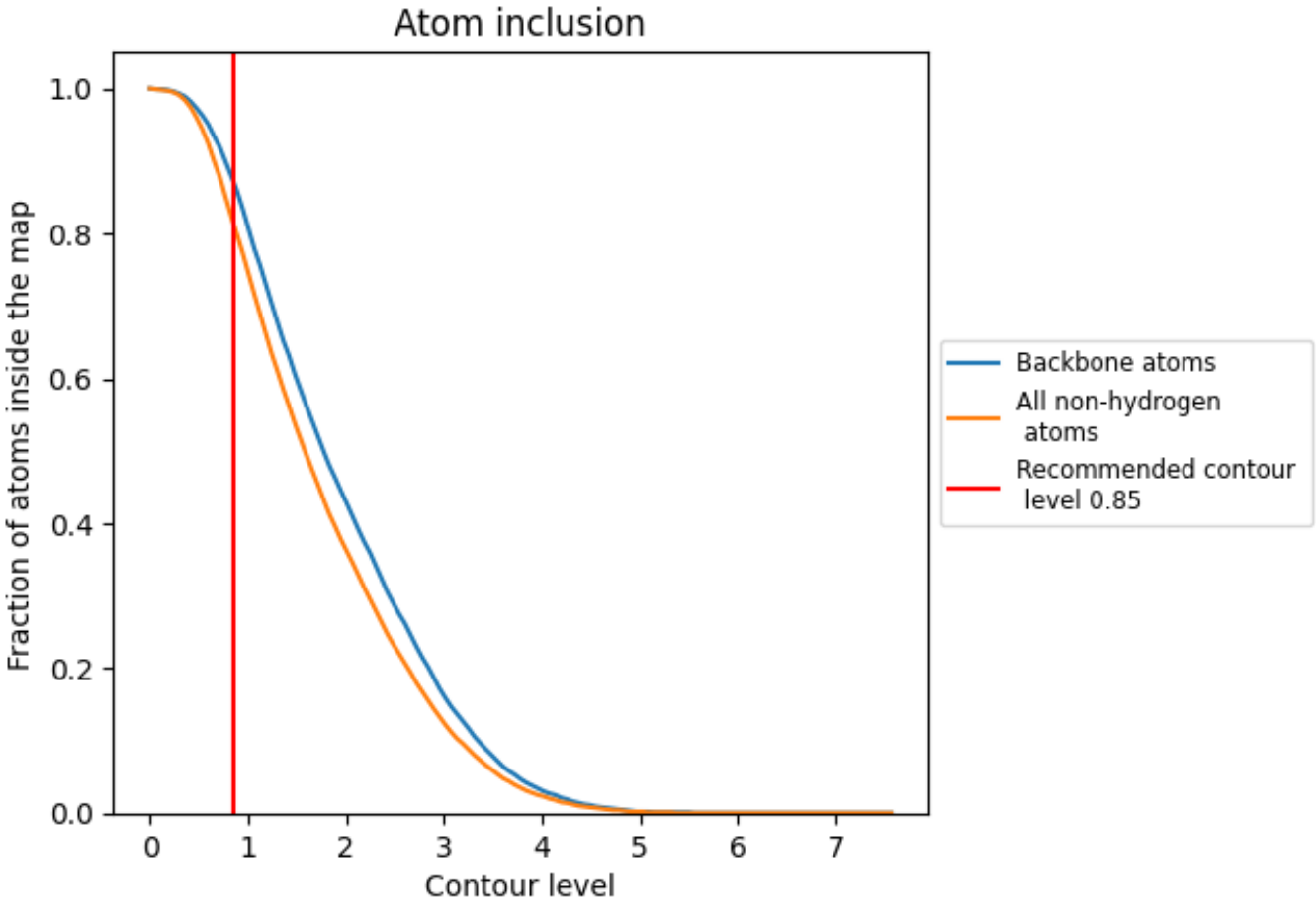
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.85).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 81% 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 (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8140	0.5330
A	0.8460	0.5470
B	0.8360	0.5530
C	0.7600	0.4990