



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:48 PM UTC

PDB ID : 6OEV / pdb_00006oev
EMDB ID : EMD-7796
Title : Structure of human Patched1 in complex with native Sonic Hedgehog
Authors : Qi, X.; Li, X.
Deposited on : 2019-03-27
Resolution : 3.80 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

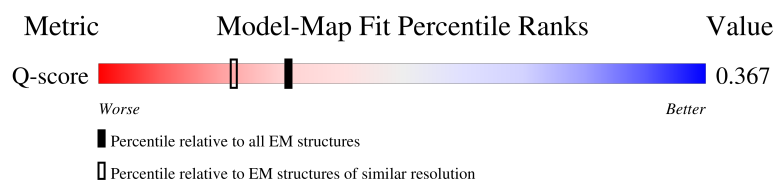
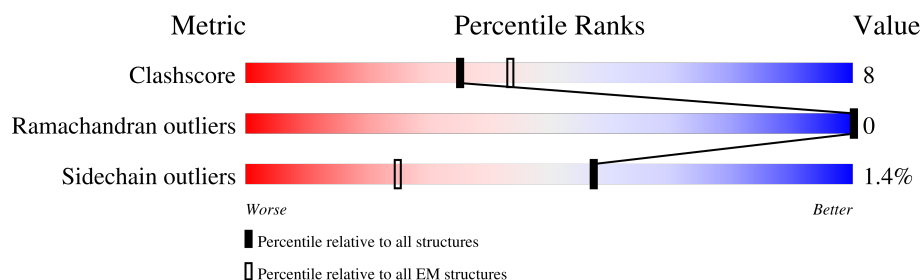
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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 $\leq 5\%$. 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	1447	19% 57% 9% 33%
2	C	175	85% 82% 11% 5%
3	B	2	100% 50% 50%
3	D	2	50% 50%

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
3	NAG	B	1	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8605 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 Protein patched homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	964	Total	C	N	O	S	0	0
			7181	4658	1207	1283	33		

- Molecule 2 is a protein called Sonic hedgehog protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	166	Total	C	N	O	S	0	0
			1339	841	243	249	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	23	PLM	ALA	engineered mutation	UNP Q15465

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

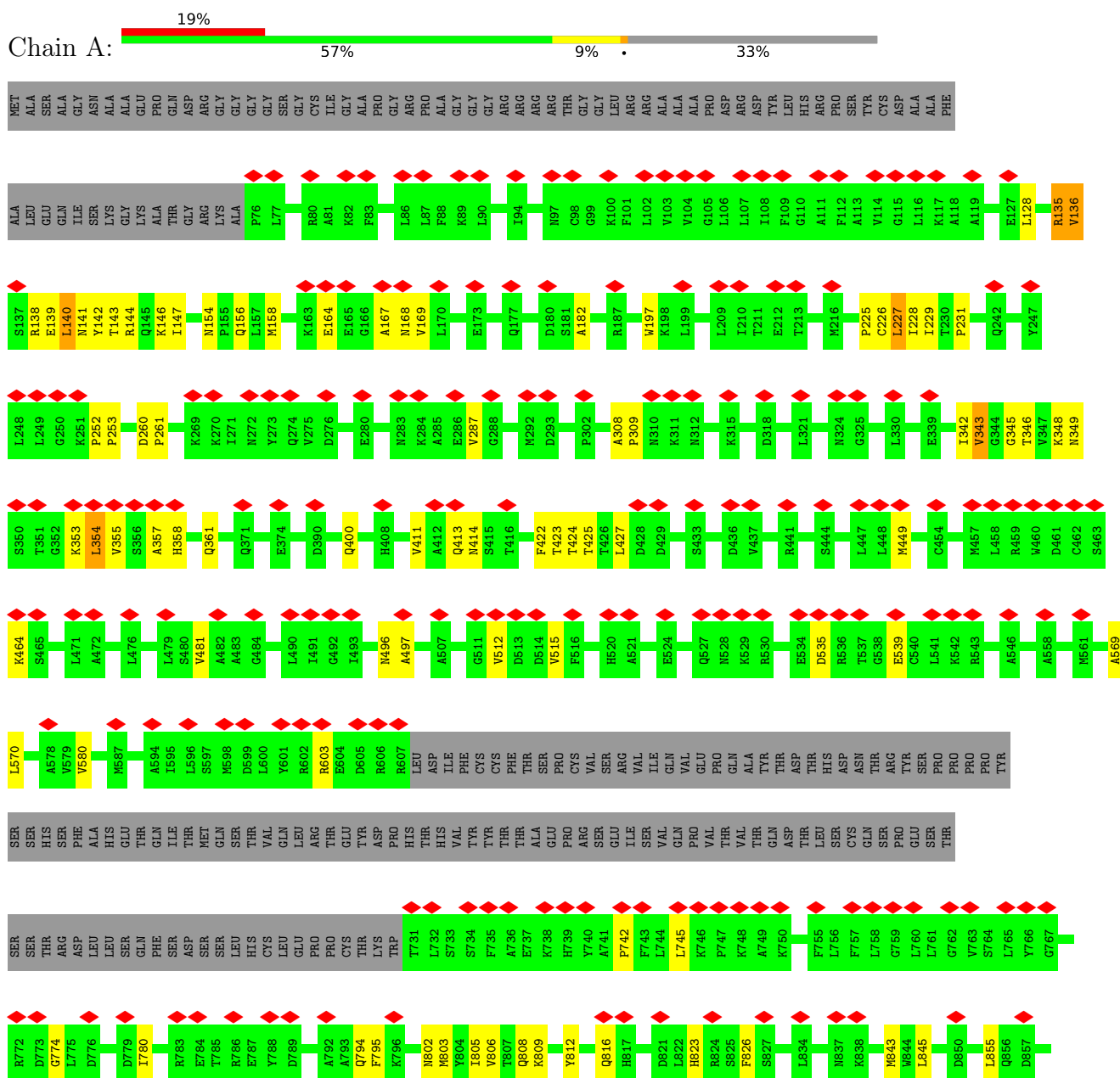
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

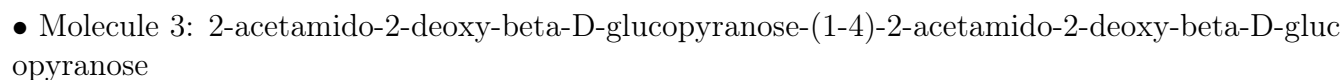
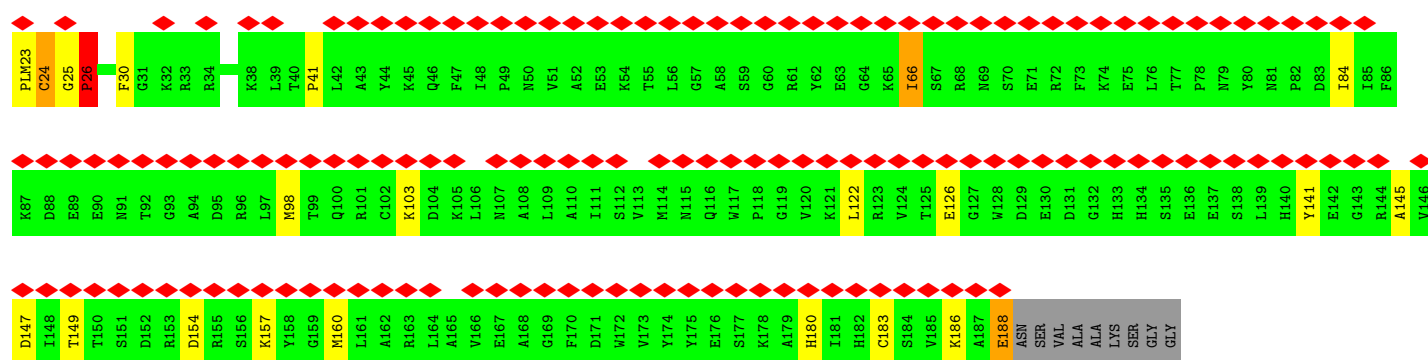
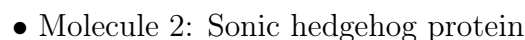
Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Zn	0
			1	1	

3 Residue-property plots

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: Protein patched homolog 1





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	194633	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 ($e^-/\text{\AA}^2$)	1.6	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	2.277	Depositor
Minimum map value	-1.325	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.55	Depositor
Map size ($\text{\AA}$)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.07	2/7336 (0.0%)	1.59	31/9998 (0.3%)
2	C	1.05	0/1352	1.45	3/1819 (0.2%)
All	All	1.07	2/8688 (0.0%)	1.57	34/11817 (0.3%)

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	A	0	2
2	C	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	VAL	N-CA	6.01	1.53	1.46
1	A	876	GLY	N-CA	5.49	1.49	1.44

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ILE	N-CA-C	-14.79	78.59	109.34
1	A	227	LEU	N-CA-C	-13.62	91.04	110.24
1	A	227	LEU	CB-CA-C	12.65	130.06	109.70
1	A	229	ILE	N-CA-C	-9.50	94.12	107.99
1	A	135	ARG	CA-C-O	-9.23	111.39	120.90
1	A	228	ILE	CB-CA-C	8.74	125.63	111.29
1	A	252	PRO	N-CA-CB	7.55	110.40	103.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	PRO	N-CA-CB	7.19	110.14	103.46
1	A	253	PRO	N-CA-CB	7.18	110.79	103.25
2	C	26	PRO	CA-C-N	6.76	133.51	122.21
2	C	26	PRO	C-N-CA	6.76	133.51	122.21
1	A	354	LEU	CB-CA-C	6.54	126.17	111.78
1	A	422	PHE	N-CA-C	-6.49	99.71	108.86
1	A	261	PRO	N-CA-CB	6.46	110.14	103.23
1	A	135	ARG	CA-C-N	6.46	129.23	120.77
1	A	135	ARG	C-N-CA	6.46	129.23	120.77
1	A	870	PRO	N-CA-CB	6.26	110.22	103.33
1	A	957	PRO	N-CA-CB	6.08	109.64	103.25
1	A	990	ALA	CA-C-O	-6.06	114.64	121.00
1	A	228	ILE	N-CA-CB	6.01	121.15	111.23
1	A	869	MET	CA-C-N	5.97	125.68	119.05
1	A	869	MET	C-N-CA	5.97	125.68	119.05
1	A	354	LEU	N-CA-C	-5.96	101.12	110.36
1	A	225	PRO	N-CA-CB	5.95	109.88	103.33
1	A	423	THR	N-CA-C	-5.84	100.53	108.24
1	A	422	PHE	CB-CA-C	5.83	125.65	111.65
1	A	135	ARG	O-C-N	5.75	128.25	122.03
1	A	956	MET	O-C-N	5.75	124.17	121.53
1	A	956	MET	CA-C-N	5.56	126.79	119.84
1	A	956	MET	C-N-CA	5.56	126.79	119.84
1	A	260	ASP	CA-C-N	5.24	124.42	118.97
1	A	260	ASP	C-N-CA	5.24	124.42	118.97
1	A	1012	GLY	CA-C-O	-5.18	118.13	122.33
2	C	26	PRO	O-C-N	-5.16	115.68	122.64

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	TRP	Peptide
1	A	984	THR	Peptide
2	C	26	PRO	Mainchain

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	7181	0	6923	122	0
2	C	1339	0	1320	35	0
3	B	28	0	25	10	0
3	D	28	0	25	4	0
4	A	28	0	25	5	0
5	C	1	0	0	0	0
All	All	8605	0	8318	133	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 (133) 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:A:780:ILE:CD1	2:C:23:PLM:CA	1.92	1.45
1:A:780:ILE:HD11	2:C:23:PLM:CA	1.45	1.38
1:A:1000:ASN:HD21	3:D:1:NAG:C1	1.37	1.37
1:A:780:ILE:CD1	2:C:23:PLM:HA1	1.53	1.33
1:A:414:ASN:ND2	3:B:1:NAG:C1	1.97	1.26
1:A:780:ILE:CD1	2:C:23:PLM:HA2	1.61	1.26
1:A:1000:ASN:ND2	3:D:1:NAG:C1	1.98	1.26
1:A:990:ALA:O	1:A:994:VAL:HG12	1.37	1.23
1:A:141:ASN:ND2	4:A:1501:NAG:C1	2.11	1.14
1:A:780:ILE:HD13	2:C:23:PLM:HA2	1.22	1.10
1:A:414:ASN:HD21	3:B:1:NAG:C1	1.68	1.02
1:A:999:SER:O	1:A:1002:THR:OG1	1.78	0.99
1:A:141:ASN:HD22	4:A:1501:NAG:C1	1.76	0.96
1:A:780:ILE:HD11	2:C:23:PLM:HA1	0.97	0.95
1:A:414:ASN:HD21	3:B:1:NAG:C5	1.82	0.93
1:A:128:LEU:HD21	2:C:23:PLM:CE	2.02	0.89
4:A:1501:NAG:H4	4:A:1506:NAG:O7	1.73	0.87
1:A:780:ILE:HD12	2:C:23:PLM:HA1	1.57	0.84
4:A:1501:NAG:H4	4:A:1506:NAG:C7	2.08	0.83
1:A:128:LEU:HD21	2:C:23:PLM:HE1	1.60	0.83
1:A:414:ASN:HD22	3:B:1:NAG:C1	1.92	0.82
1:A:135:ARG:HA	1:A:138:ARG:NH2	1.95	0.82
1:A:990:ALA:C	1:A:994:VAL:HG12	2.05	0.80
1:A:1000:ASN:HD21	3:D:1:NAG:C2	1.95	0.79
1:A:780:ILE:HD12	2:C:23:PLM:CA	2.11	0.77
1:A:136:VAL:O	1:A:140:LEU:N	2.18	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ASN:HD22	1:A:569:ALA:HA	1.51	0.75
1:A:135:ARG:O	1:A:139:GLU:HG2	1.87	0.74
1:A:780:ILE:HD11	2:C:23:PLM:CB	2.21	0.71
1:A:1018:TRP:CH2	2:C:23:PLM:C4	2.76	0.69
1:A:143:THR:O	1:A:147:ILE:N	2.23	0.68
1:A:812:TYR:O	1:A:816:GLN:NE2	2.28	0.67
1:A:414:ASN:HD21	3:B:1:NAG:C4	2.07	0.67
1:A:1018:TRP:CH2	2:C:23:PLM:H41	2.31	0.66
1:A:141:ASN:HD21	4:A:1501:NAG:C1	2.09	0.65
1:A:1018:TRP:CH2	2:C:23:PLM:H42	2.32	0.65
1:A:1017:PHE:CG	2:C:23:PLM:H31	2.31	0.64
1:A:411:VAL:O	1:A:411:VAL:HG13	1.97	0.64
1:A:135:ARG:HA	1:A:138:ARG:HH21	1.61	0.64
1:A:353:LYS:HG2	1:A:354:LEU:O	1.98	0.64
1:A:497:ALA:HB3	2:C:23:PLM:HF2	1.80	0.63
1:A:1149:VAL:O	1:A:1153:PHE:HB3	2.00	0.62
1:A:156:GLN:HE21	1:A:400:GLN:HE22	1.46	0.61
1:A:226:CYS:O	1:A:227:LEU:C	2.44	0.60
1:A:414:ASN:HD21	3:B:1:NAG:H5	1.64	0.58
1:A:802:ASN:OD1	2:C:26:PRO:O	2.22	0.57
1:A:940:ASN:ND2	2:C:30:PHE:O	2.38	0.57
1:A:140:LEU:HD12	1:A:144:ARG:HH21	1.70	0.56
1:A:154:ASN:HB2	1:A:424:THR:HG21	1.88	0.56
1:A:449:MET:HE2	1:A:512:VAL:HG21	1.88	0.55
1:A:142:TYR:CE1	1:A:146:LYS:HE2	2.41	0.54
1:A:128:LEU:CD2	2:C:23:PLM:CE	2.84	0.52
1:A:158:MET:HE1	1:A:182:ALA:HA	1.90	0.52
1:A:140:LEU:HG	1:A:1016:LEU:HD21	1.91	0.52
1:A:991:ILE:HA	1:A:994:VAL:HG13	1.92	0.52
1:A:512:VAL:HA	1:A:515:VAL:HG12	1.92	0.51
1:A:414:ASN:ND2	3:B:1:NAG:C2	2.72	0.51
1:A:414:ASN:ND2	3:B:1:NAG:O4	2.43	0.51
2:C:186:LYS:HG3	2:C:188:GLU:H	1.76	0.51
1:A:843:MET:SD	1:A:845:LEU:HB3	2.51	0.50
1:A:427:LEU:HD13	2:C:24:CYS:HB3	1.93	0.50
1:A:128:LEU:HD21	2:C:23:PLM:HE2	1.89	0.50
1:A:128:LEU:CD2	2:C:23:PLM:HD2	2.41	0.50
1:A:991:ILE:HA	1:A:994:VAL:CG1	2.42	0.49
1:A:135:ARG:C	1:A:139:GLU:HG2	2.36	0.49
1:A:570:LEU:HD21	1:A:1081:VAL:HG22	1.93	0.49
1:A:991:ILE:O	1:A:995:ARG:HB2	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLU:HG3	1:A:995:ARG:HH22	1.78	0.48
2:C:84:ILE:HG12	2:C:122:LEU:HD21	1.95	0.48
1:A:140:LEU:CG	1:A:1016:LEU:HD21	2.44	0.48
1:A:823:HIS:HB2	1:A:843:MET:HE3	1.95	0.48
1:A:969:ILE:HD11	1:A:972:ALA:HB2	1.94	0.48
1:A:135:ARG:HG2	1:A:138:ARG:NH2	2.28	0.48
1:A:142:TYR:CE2	1:A:808:GLN:NE2	2.82	0.48
1:A:1150:ARG:O	1:A:1154:ALA:HB3	2.13	0.48
1:A:164:GLU:HB2	1:A:167:ALA:HB2	1.96	0.47
1:A:142:TYR:HE1	1:A:146:LYS:HE2	1.79	0.47
1:A:413:GLN:HE21	3:B:1:NAG:C1	2.28	0.47
1:A:348:LYS:HG2	1:A:353:LYS:HA	1.95	0.47
1:A:795:PHE:O	1:A:982:ARG:NH2	2.48	0.47
1:A:1017:PHE:CB	2:C:23:PLM:H31	2.44	0.47
1:A:464:LYS:O	1:A:603:ARG:NH2	2.47	0.47
1:A:794:GLN:HE22	2:C:25:GLY:C	2.23	0.47
1:A:998:CYS:SG	1:A:1008:SER:C	2.98	0.47
1:A:998:CYS:SG	1:A:1009:TYR:HA	2.55	0.46
1:A:346:THR:OG1	1:A:353:LYS:NZ	2.48	0.46
1:A:128:LEU:HD22	2:C:23:PLM:HD2	1.97	0.46
1:A:1013:TYR:N	1:A:1014:PRO:HD2	2.30	0.46
1:A:927:VAL:HG11	1:A:945:ARG:HB2	1.97	0.46
1:A:1043:CYS:O	1:A:1047:LEU:HB2	2.15	0.46
2:C:41:PRO:HB3	2:C:160:MET:HE2	1.96	0.46
1:A:1002:THR:HG22	1:A:1007:SER:HA	1.98	0.46
1:A:411:VAL:O	1:A:411:VAL:CG1	2.63	0.46
1:A:1032:ILE:HA	1:A:1035:VAL:HG12	1.97	0.46
1:A:1081:VAL:HB	1:A:1082:PRO:HD3	1.97	0.45
1:A:1031:PHE:HA	1:A:1034:VAL:HG12	1.98	0.45
1:A:1124:ALA:O	1:A:1128:ASP:HB2	2.17	0.45
1:A:342:ILE:O	1:A:361:GLN:N	2.48	0.45
1:A:1039:THR:HA	1:A:1042:VAL:HG12	1.98	0.45
1:A:742:PRO:HA	1:A:745:LEU:HG	1.98	0.45
2:C:149:THR:HG22	2:C:180:HIS:HA	1.99	0.45
1:A:140:LEU:CD1	1:A:1016:LEU:HD21	2.47	0.45
1:A:1063:MET:HE1	1:A:1163:GLY:N	2.32	0.44
1:A:1036:LEU:HA	1:A:1039:THR:HG22	1.99	0.44
1:A:924:THR:HG23	1:A:945:ARG:HB3	2.00	0.44
2:C:154:ASP:HB3	2:C:157:LYS:HE2	2.00	0.44
1:A:140:LEU:HD11	1:A:1016:LEU:HD21	2.00	0.44
1:A:128:LEU:CD2	2:C:23:PLM:HE1	2.40	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:MET:HE2	1:A:805:ILE:HG13	1.99	0.43
1:A:348:LYS:HA	1:A:354:LEU:H	1.84	0.43
1:A:345:GLY:O	1:A:358:HIS:ND1	2.51	0.43
1:A:414:ASN:ND2	3:B:1:NAG:C4	2.81	0.43
2:C:66:ILE:H	2:C:141:TYR:HB3	1.84	0.43
1:A:806:VAL:HG21	1:A:971:TYR:CE1	2.55	0.42
2:C:98:MET:O	2:C:103:LYS:NZ	2.48	0.42
1:A:168:ASN:HA	1:A:357:ALA:O	2.20	0.42
1:A:535:ASP:O	1:A:539:GLU:N	2.50	0.42
1:A:1028:LEU:HD12	1:A:1083:VAL:HG22	2.02	0.42
1:A:349:ASN:HB3	1:A:354:LEU:HD12	2.01	0.41
1:A:1000:ASN:ND2	3:D:1:NAG:C2	2.69	0.41
1:A:1124:ALA:O	1:A:1128:ASP:CB	2.68	0.41
2:C:126:GLU:HB2	2:C:147:ASP:HB2	2.02	0.41
1:A:855:LEU:HD12	1:A:855:LEU:HA	1.95	0.41
1:A:308:ALA:HB3	1:A:309:PRO:HD3	2.02	0.41
1:A:809:LYS:HG2	1:A:970:GLU:HA	2.02	0.41
2:C:145:ALA:HA	2:C:183:CYS:O	2.21	0.41
1:A:156:GLN:HE21	1:A:400:GLN:NE2	2.15	0.41
1:A:136:VAL:O	1:A:140:LEU:HB2	2.20	0.41
1:A:918:ALA:HA	1:A:921:ILE:HD13	2.01	0.41
1:A:774:GLY:HA3	1:A:984:THR:HG21	2.03	0.41
1:A:805:ILE:HD11	1:A:826:PHE:CZ	2.57	0.40
1:A:481:VAL:HA	1:A:580:VAL:HG23	2.03	0.40
1:A:342:ILE:HG13	1:A:343:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	958/1447 (66%)	862 (90%)	96 (10%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	163/175 (93%)	145 (89%)	18 (11%)	0	100	100
All	All	1121/1622 (69%)	1007 (90%)	114 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	700/1230 (57%)	691 (99%)	9 (1%)	61	71
2	C	139/144 (96%)	136 (98%)	3 (2%)	45	63
All	All	839/1374 (61%)	827 (99%)	12 (1%)	57	70

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LEU
1	A	169	VAL
1	A	287	VAL
1	A	343	VAL
1	A	355	VAL
1	A	425	THR
1	A	984	THR
1	A	994	VAL
1	A	1000	ASN
2	C	24	CYS
2	C	66	ILE
2	C	188	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	141	ASN
1	A	184	GLN
1	A	283	ASN
1	A	400	GLN
1	A	413	GLN
1	A	414	ASN
1	A	501	GLN
1	A	817	HIS
1	A	973	GLN
1	A	979	ASN
1	A	1000	ASN
1	A	1112	ASN
1	A	1166	ASN
2	C	50	ASN
2	C	182	HIS

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 ⓘ

4 monosaccharides are 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	$\# Z > 2$
3	NAG	B	1	3	14,14,15	0.70	0	17,19,21	1.63	2 (11%)
3	NAG	B	2	3	14,14,15	0.65	0	17,19,21	1.79	3 (17%)
3	NAG	D	1	3	14,14,15	0.88	0	17,19,21	2.11	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	2	3	14,14,15	0.76	0	17,19,21	1.68	2 (11%)

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	B	1	3	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	NAG	C1-O5-C5	5.18	119.13	112.19
3	D	1	NAG	C4-C3-C2	5.16	118.58	111.02
3	D	2	NAG	C2-N2-C7	4.53	128.97	122.90
3	D	1	NAG	C2-N2-C7	4.34	128.72	122.90
3	B	1	NAG	C4-C3-C2	3.57	116.25	111.02
3	B	1	NAG	C1-O5-C5	3.37	116.70	112.19
3	B	2	NAG	C4-C3-C2	3.22	115.74	111.02
3	D	2	NAG	C4-C3-C2	3.06	115.50	111.02
3	D	1	NAG	C3-C4-C5	2.58	114.91	110.23
3	D	1	NAG	O5-C5-C6	-2.28	103.23	107.66
3	B	2	NAG	O5-C5-C6	-2.13	103.53	107.66
3	D	1	NAG	C8-C7-N2	2.09	119.58	116.12
3	D	1	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	B	1	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

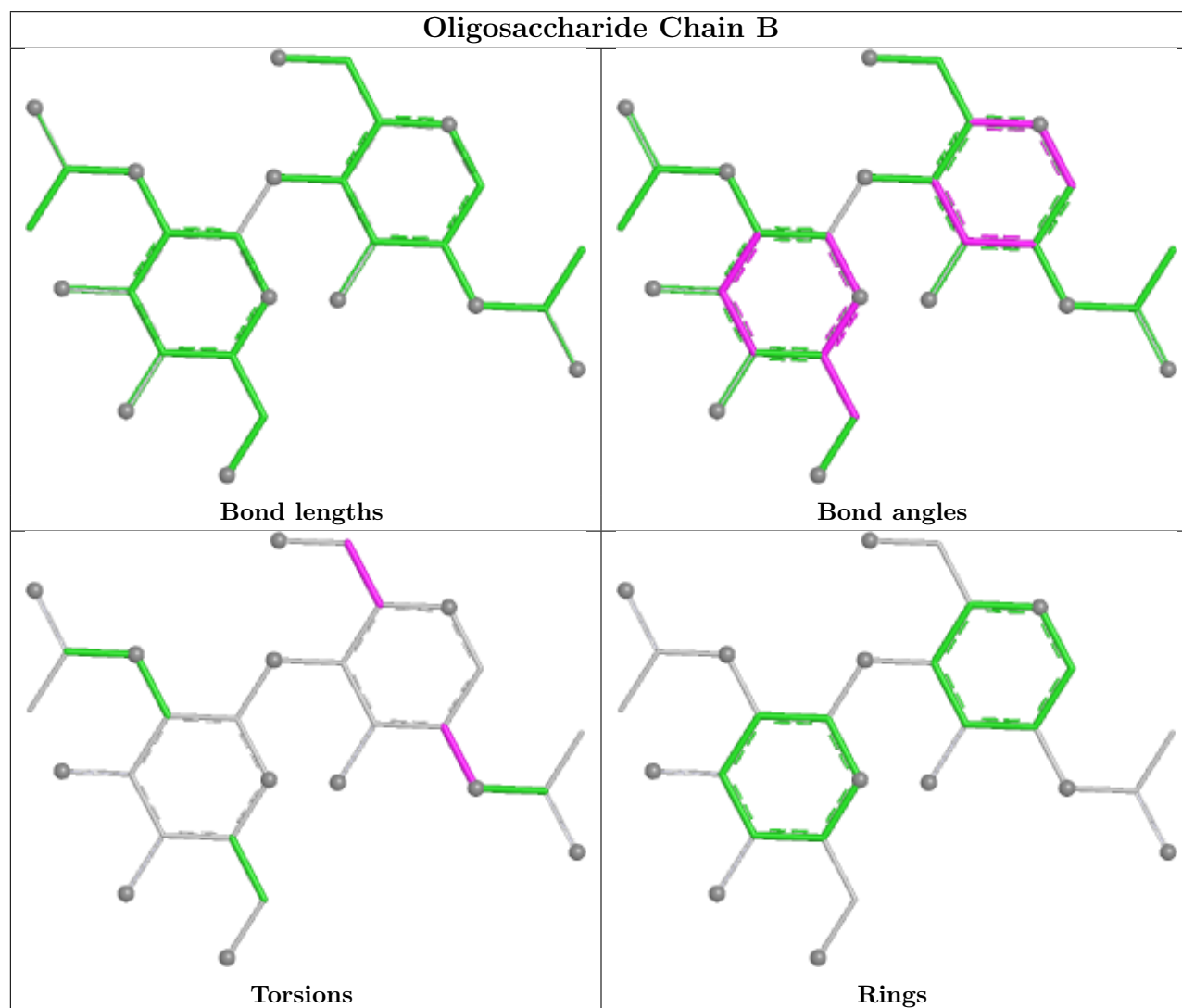
Mol	Chain	Res	Type	Atoms
3	B	1	NAG	C4-C5-C6-O6

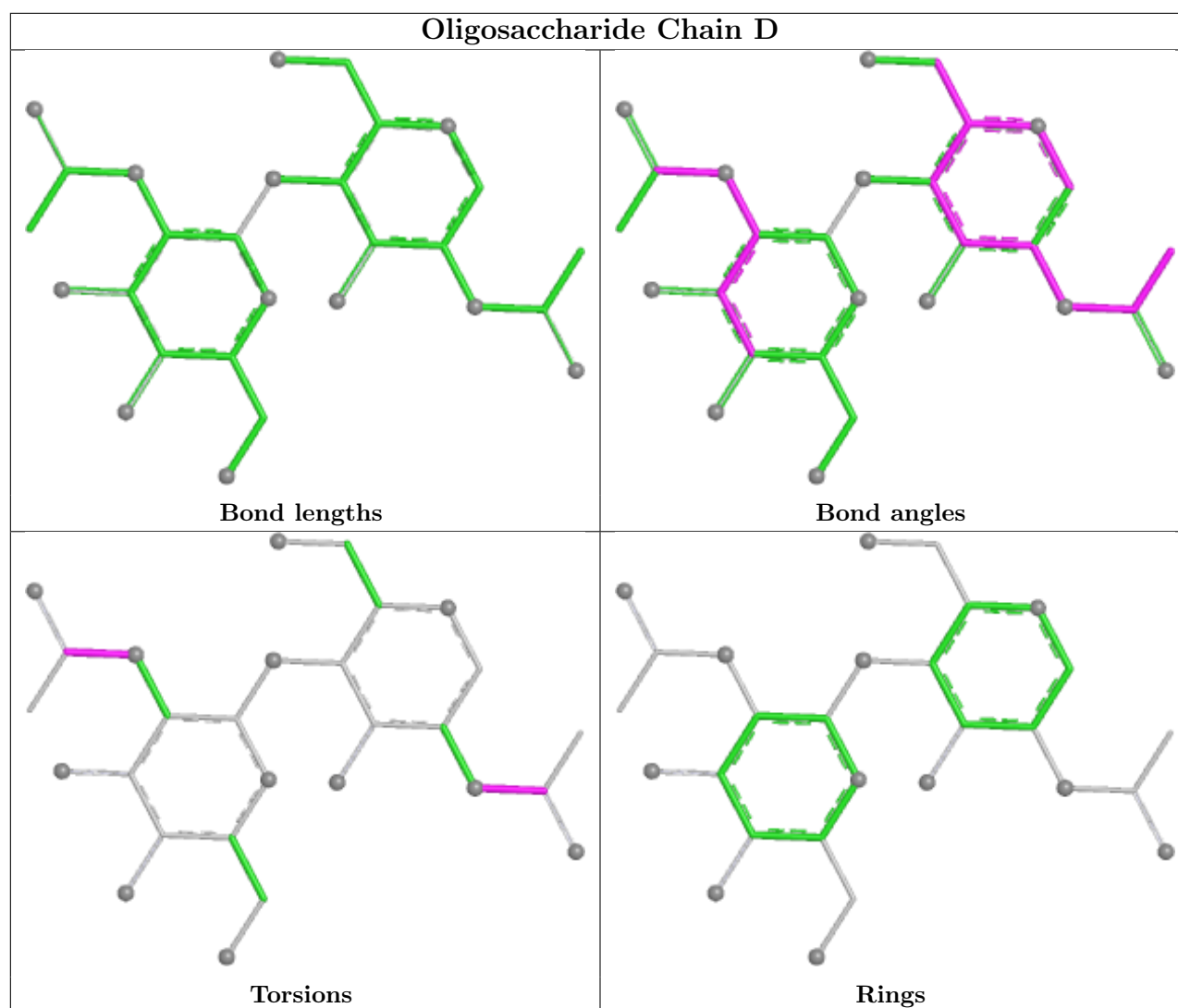
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	4	0
3	B	1	NAG	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
4	NAG	A	1506	-	14,14,15	0.73	0	17,19,21	1.32	3 (17%)
4	NAG	A	1501	-	14,14,15	0.73	0	17,19,21	1.31	2 (11%)

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
4	NAG	A	1506	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1501	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1506	NAG	C4-C3-C2	2.64	114.89	111.02
4	A	1501	NAG	C4-C3-C2	2.63	114.87	111.02
4	A	1506	NAG	C1-O5-C5	2.52	115.56	112.19
4	A	1501	NAG	C1-O5-C5	2.47	115.50	112.19
4	A	1506	NAG	C2-N2-C7	2.03	125.62	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1506	NAG	2	0
4	A	1501	NAG	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

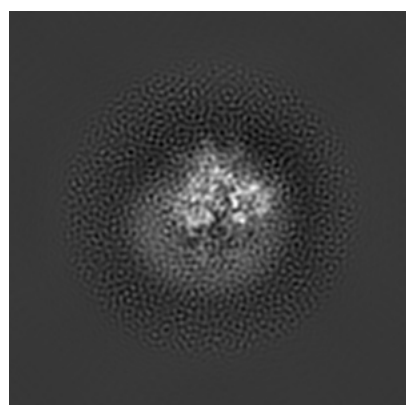
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7796. These allow visual inspection of the internal detail of the map and identification of artifacts.

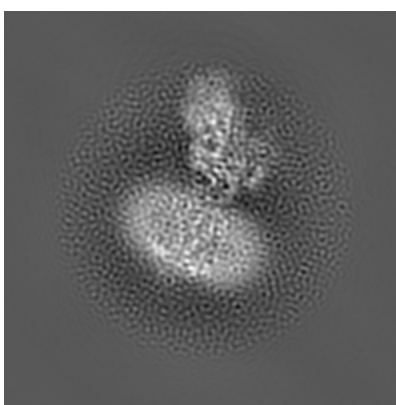
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

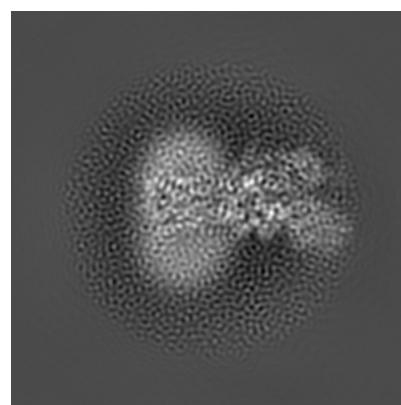
6.1.1 Primary map



X



Y

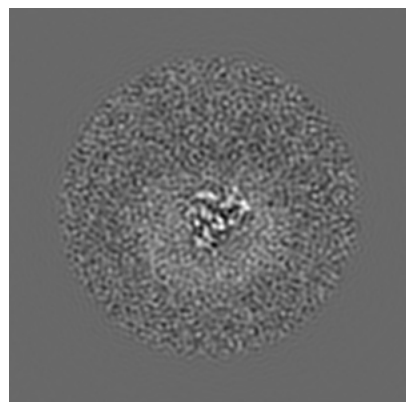


Z

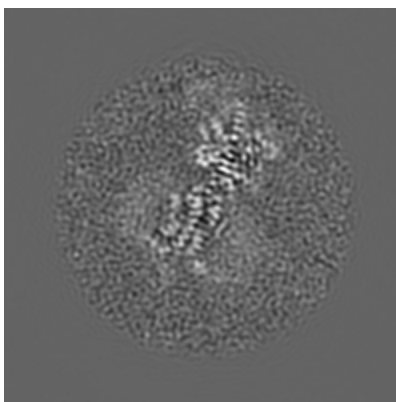
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

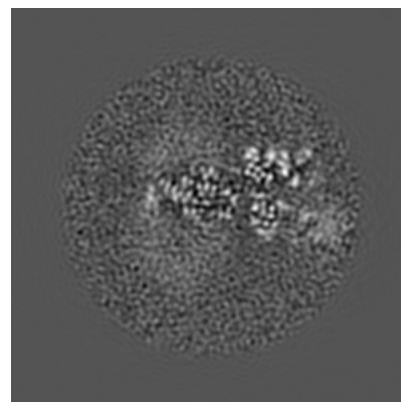
6.2.1 Primary map



X Index: 128



Y Index: 128

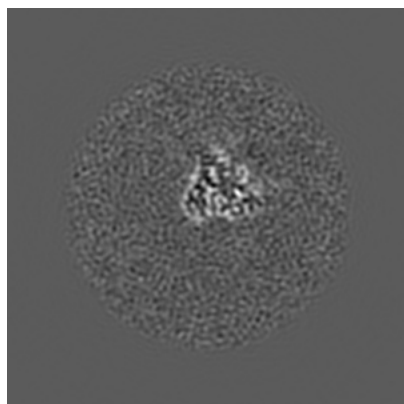


Z Index: 128

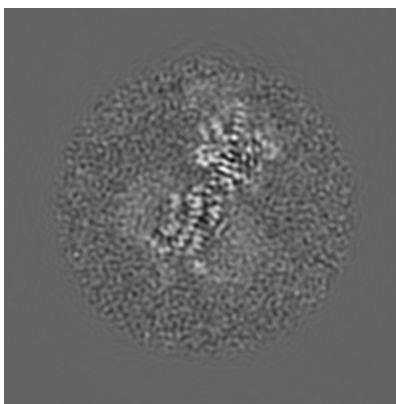
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

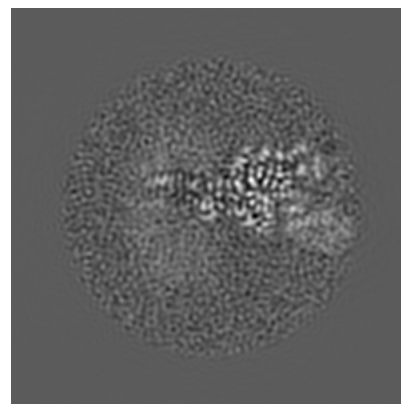
6.3.1 Primary map



X Index: 158



Y Index: 128

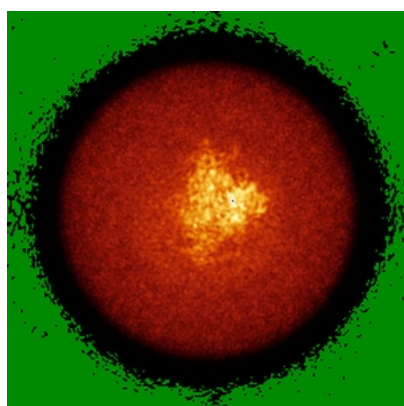


Z Index: 135

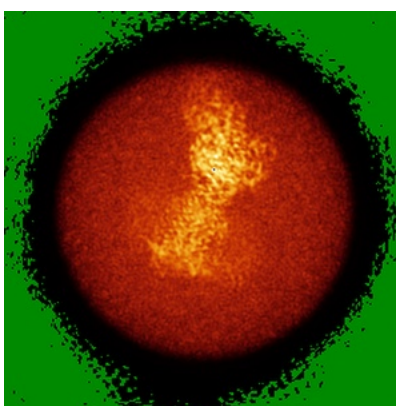
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

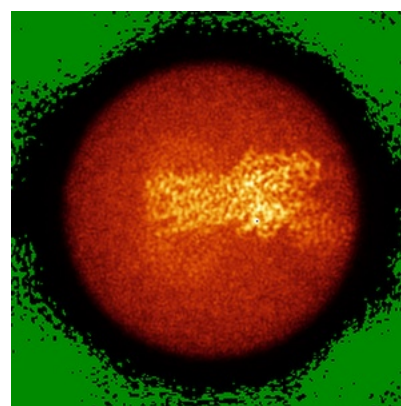
6.4.1 Primary map



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

This section was not generated.

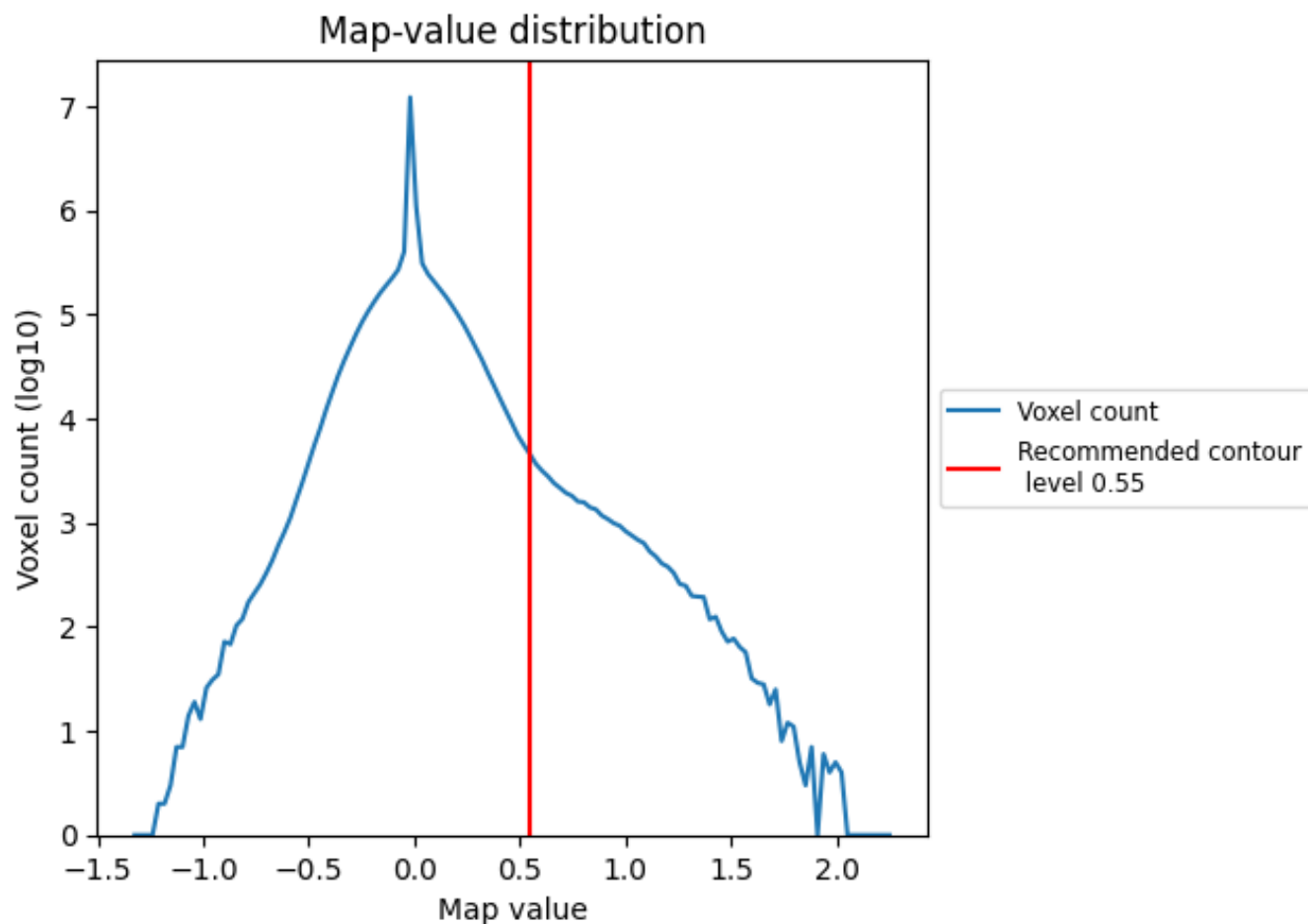
6.6 Mask visualisation

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

7 Map analysis [i](#)

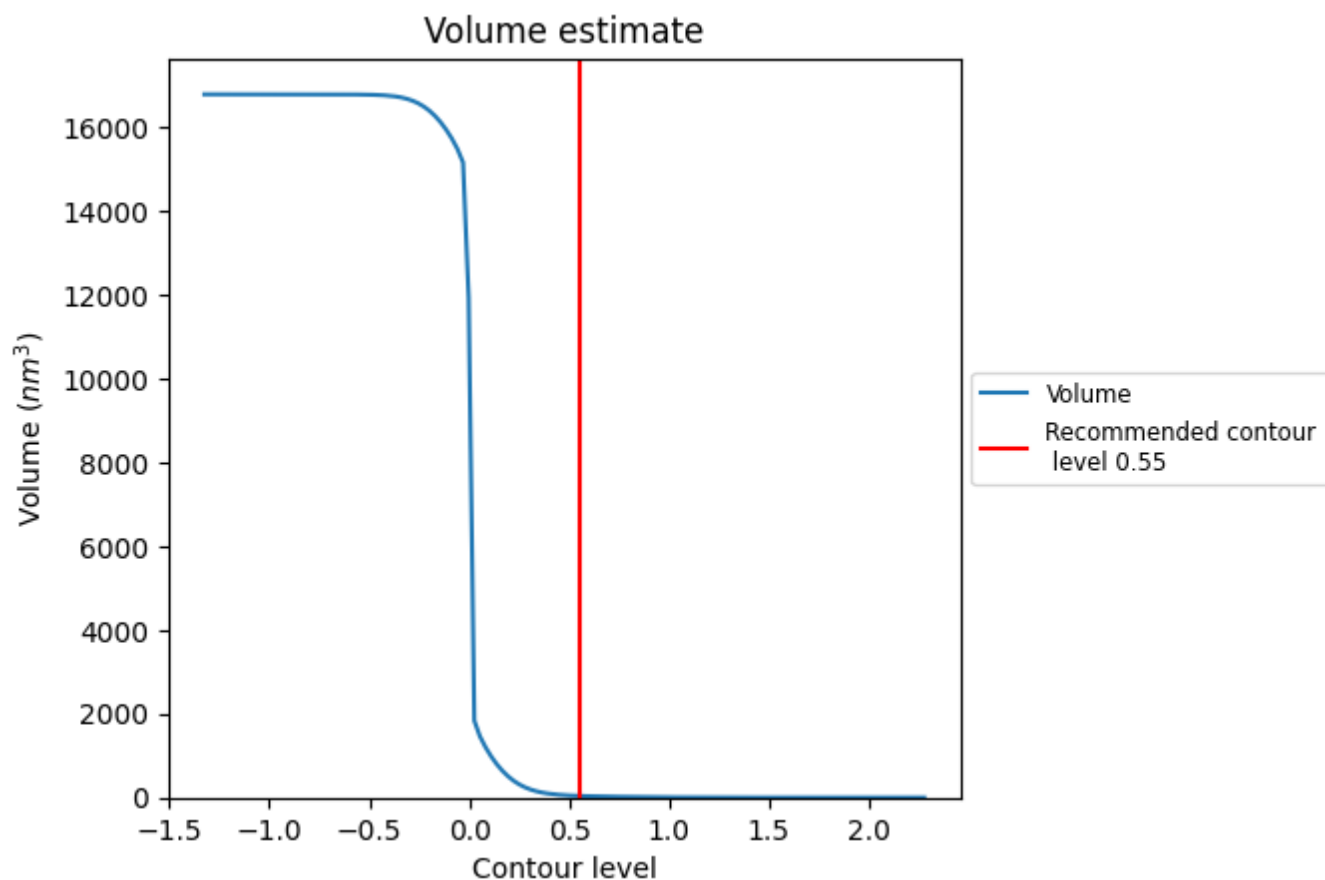
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

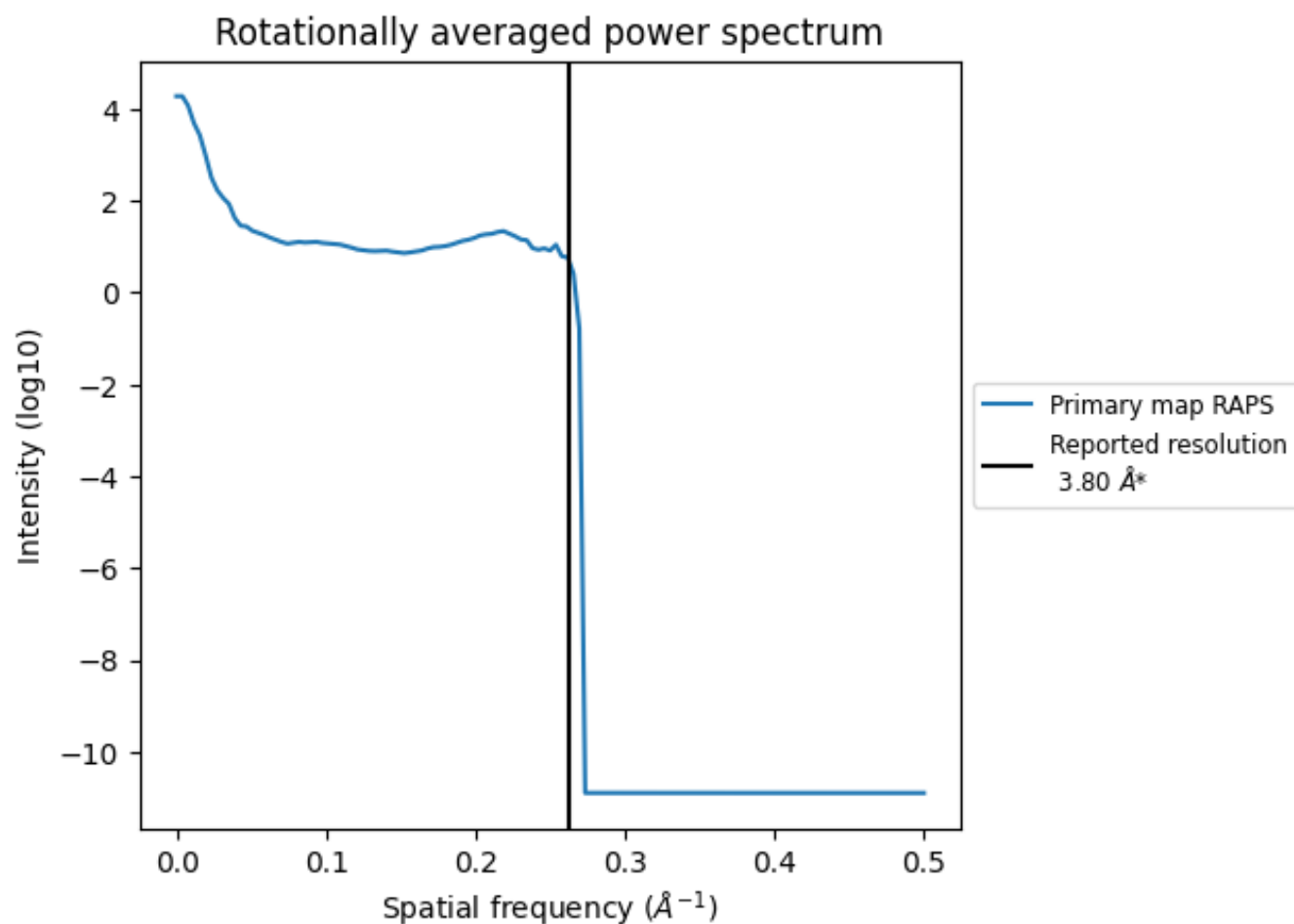
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm³; this corresponds to an approximate mass of 35 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

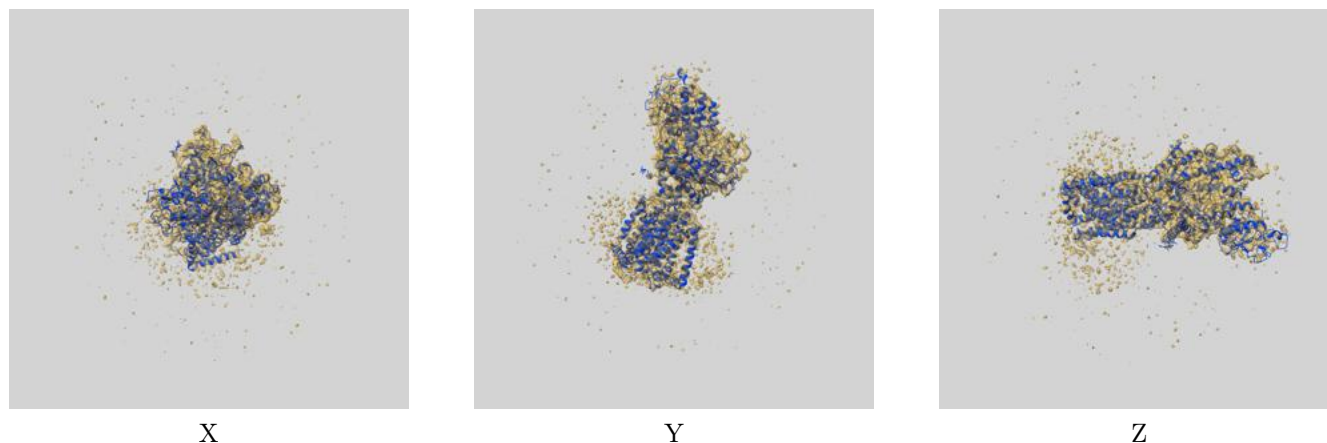
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

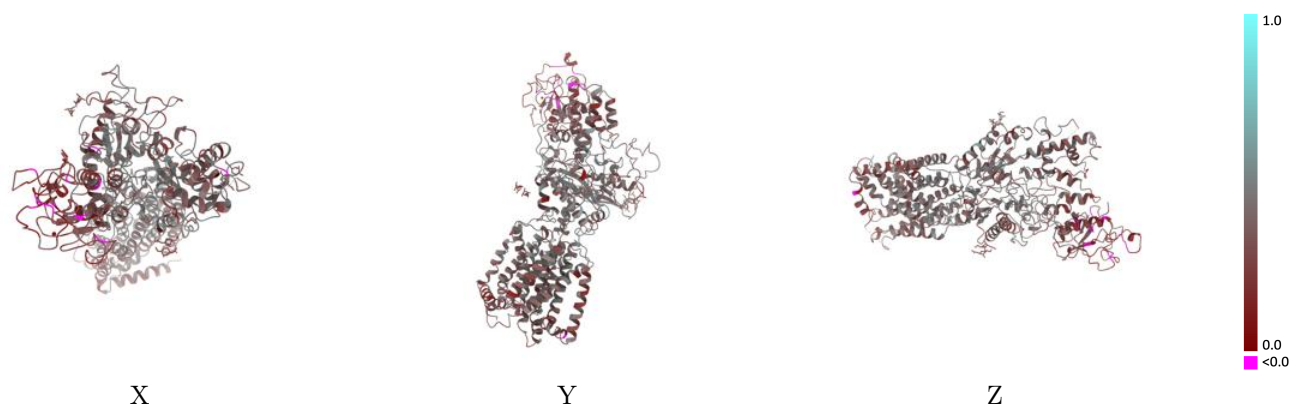
This section contains information regarding the fit between EMDB map EMD-7796 and PDB model 6OEV. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



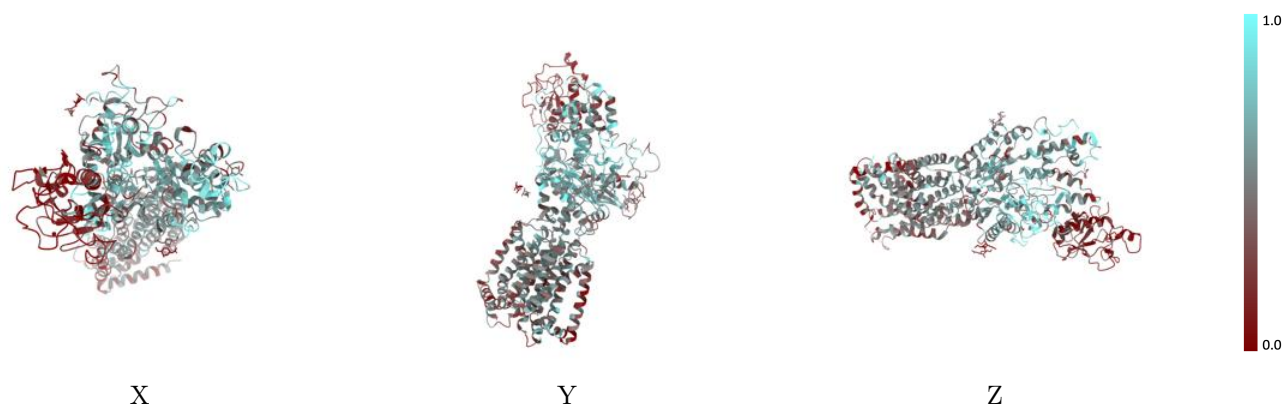
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



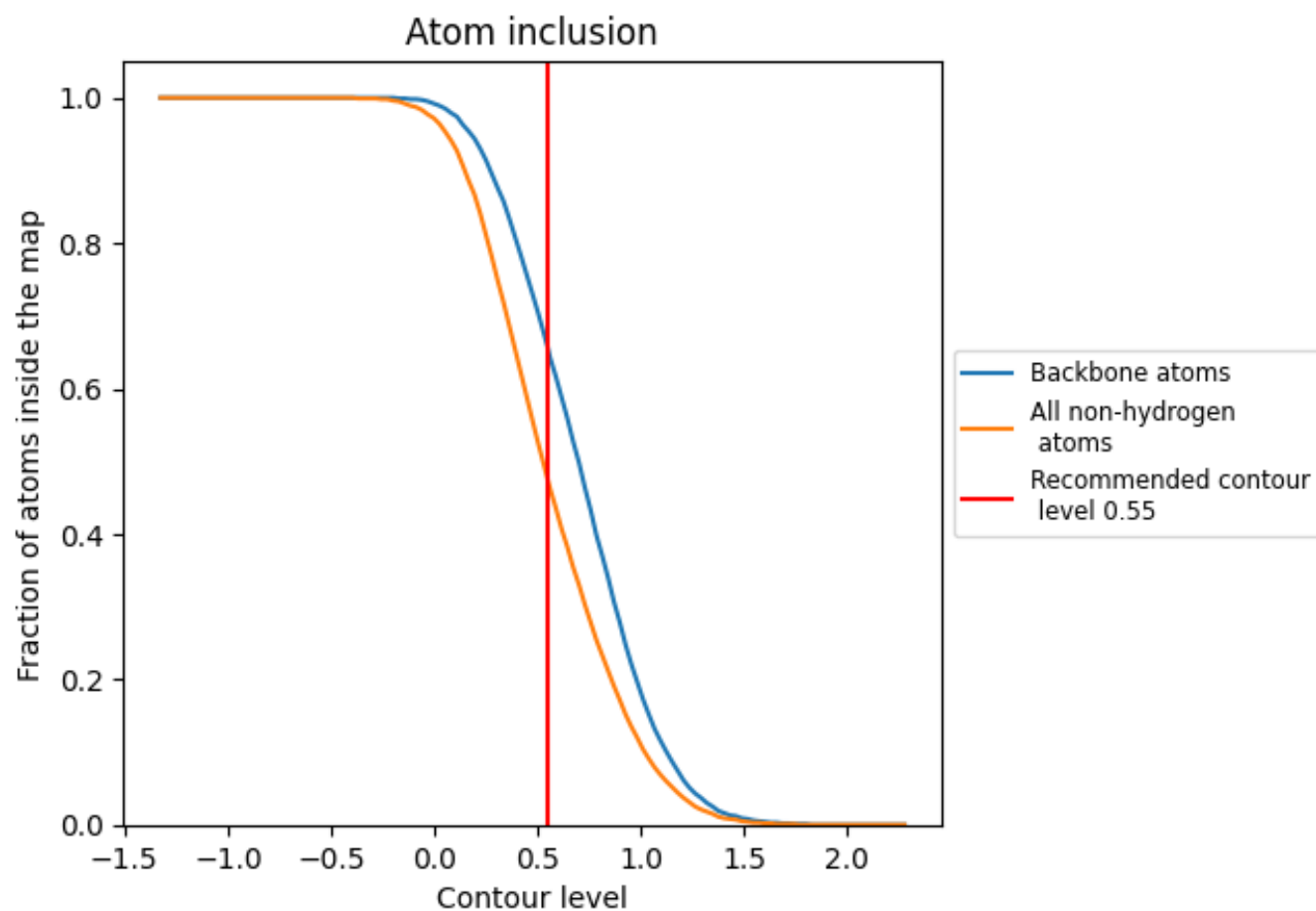
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 48% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4750	0.3670
A	0.5300	0.3880
B	0.1070	0.3000
C	0.1820	0.2520
D	0.3930	0.3420

