Full wwPDB EM Validation Report ⓘ

Aug 15, 2026 – 03:27 PM EDT

PDB ID	:	9YB4 / pdb_00009yb4
EMDB ID	:	EMD-72748
Title	:	Localized reconstruction of the asymmetric unit of the low pH treated back neutralized SINV/EEEV.
Authors	:	Bandyopadhyay, A.; Klose, T.; Kuhn, R.J.
Deposited on	:	2025-09-16
Resolution	:	3.10 Å(reported)
Based on initial model	:	6MX4

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:

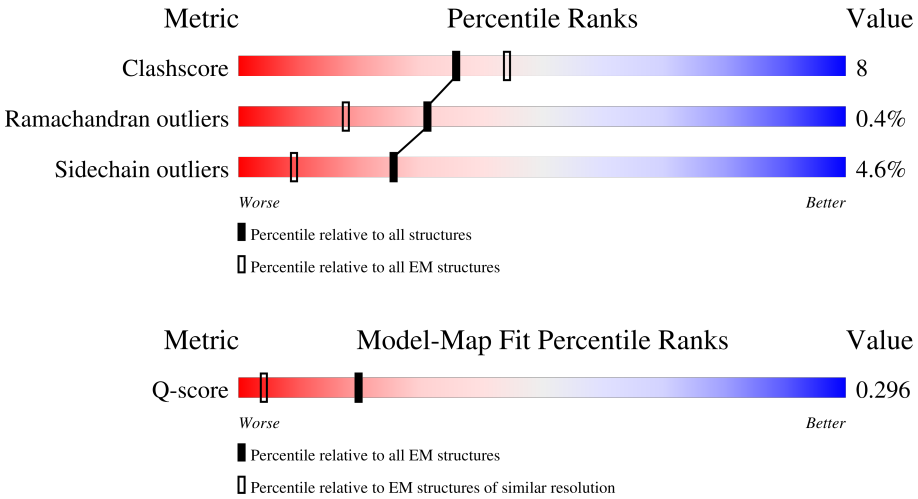
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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.



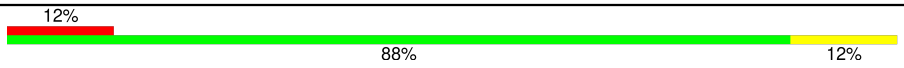
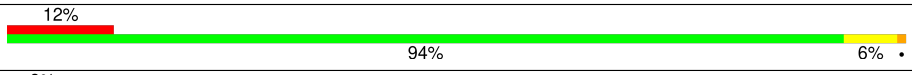
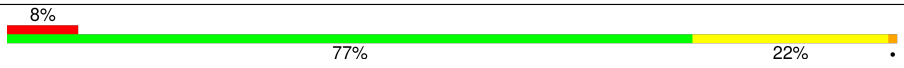
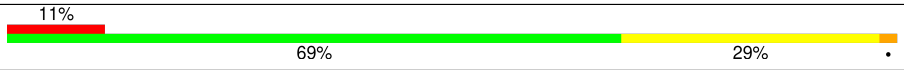
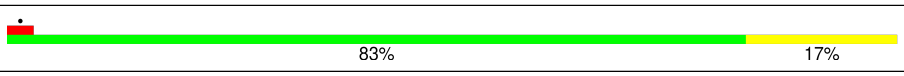
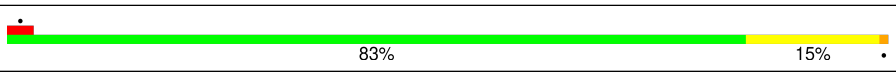
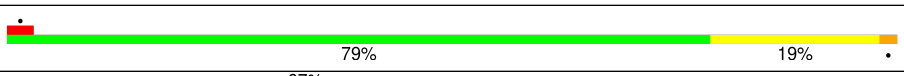
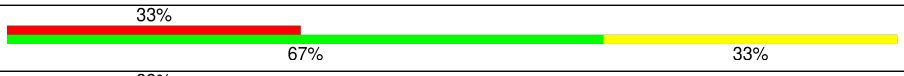
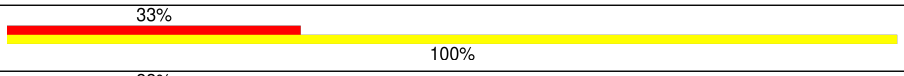
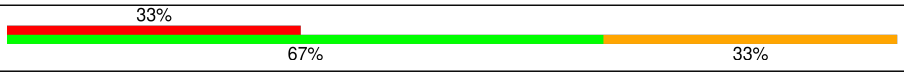
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	441	76% 22%
1	B	441	84% 16%
1	C	441	84% 15%
1	D	441	81% 18%

Continued on next page...

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Mol	Chain	Length	Quality of chain
2	P	160	
2	Q	160	
2	R	160	
2	S	160	
3	a	418	
3	d	418	
4	b	419	
4	c	419	
5	E	3	
5	F	3	
5	G	3	
5	H	3	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 31820 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 E1 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	441	Total	C	N	O	S	0	0
			3371	2148	562	641	20		
1	B	441	Total	C	N	O	S	0	0
			3371	2148	562	641	20		
1	C	441	Total	C	N	O	S	0	0
			3371	2148	562	641	20		
1	D	441	Total	C	N	O	S	0	0
			3371	2148	562	641	20		

- Molecule 2 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	160	Total	C	N	O	S	0	0
			1239	778	221	233	7		
2	Q	160	Total	C	N	O	S	0	0
			1239	778	221	233	7		
2	R	160	Total	C	N	O	S	0	0
			1239	778	221	233	7		
2	S	160	Total	C	N	O	S	0	0
			1239	778	221	233	7		

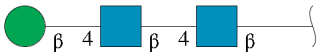
- Molecule 3 is a protein called E2 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	418	Total	C	N	O	S	0	0
			3288	2080	596	588	24		
3	d	418	Total	C	N	O	S	0	0
			3288	2080	596	588	24		

- Molecule 4 is a protein called E2 glycoprotein.

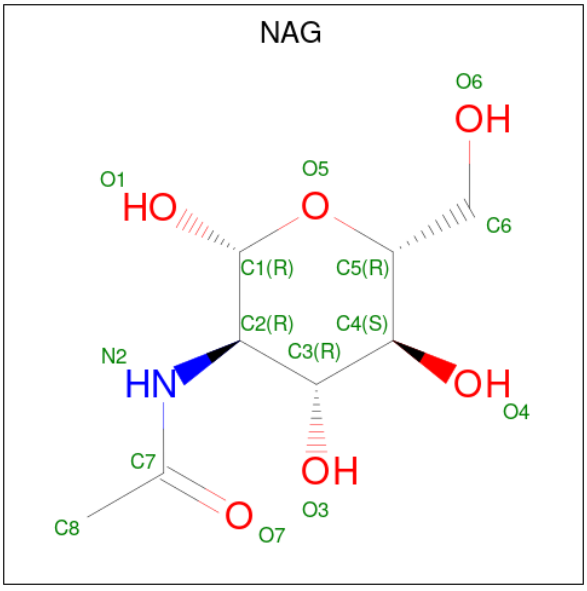
Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	419	Total	C	N	O	S	0	0
			3296	2084	597	591	24		
4	c	419	Total	C	N	O	S	0	0
			3296	2084	597	591	24		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	3	Total	C	N	O	0	0
			39	22	2	15		
5	F	3	Total	C	N	O	0	0
			39	22	2	15		
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	H	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
6	a	1	Total	C	N	O	0
			14	8	1	5	
6	b	1	Total	C	N	O	0
			14	8	1	5	
6	c	1	Total	C	N	O	0
			14	8	1	5	
6	d	1	Total	C	N	O	0
			14	8	1	5	

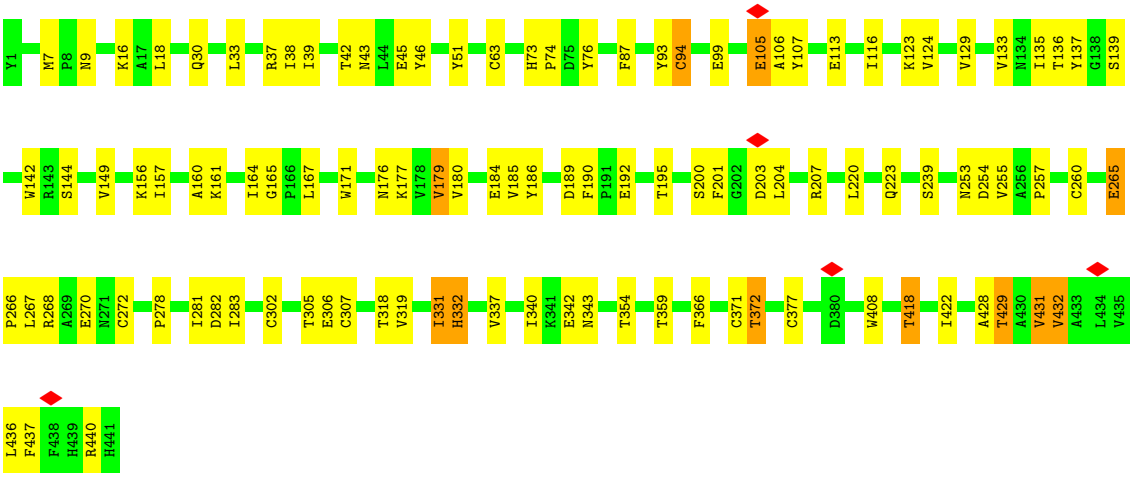
3 Residue-property plots (i)

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: E1 glycoprotein

Chain A:

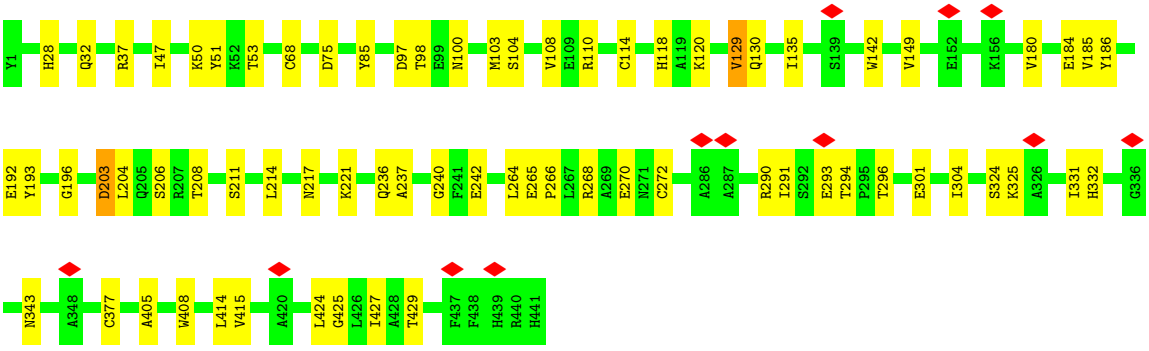




• Molecule 1: E1 glycoprotein

Chain B:

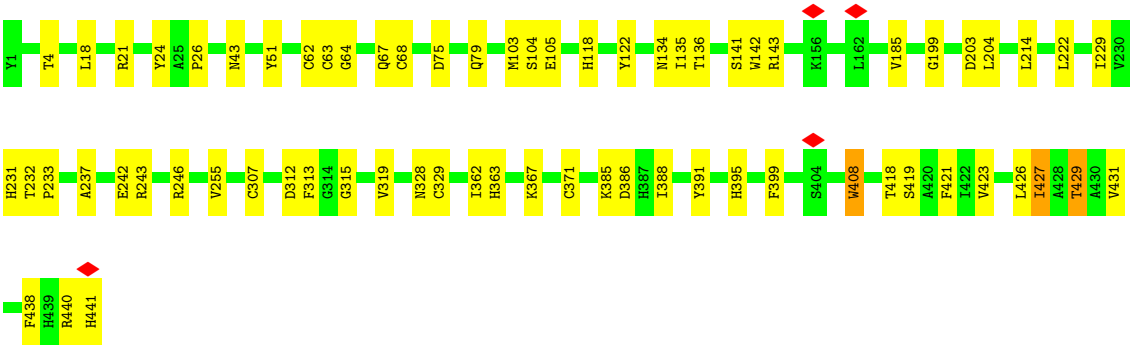




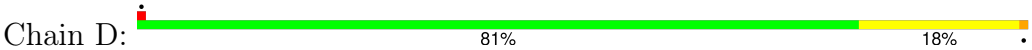
• Molecule 1: E1 glycoprotein

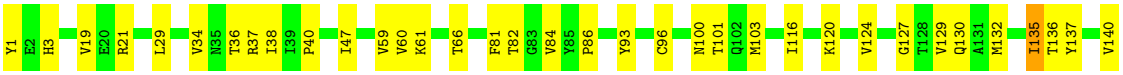
Chain C:



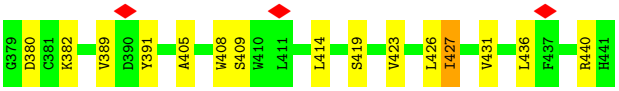


• Molecule 1: E1 glycoprotein

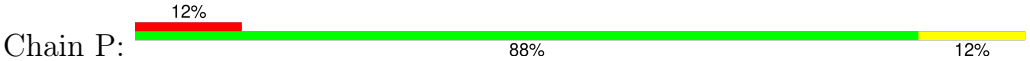


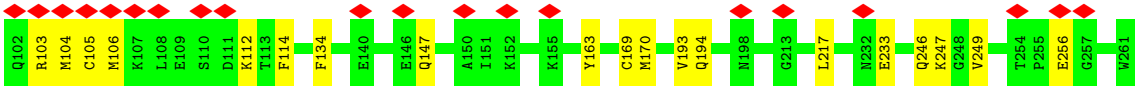




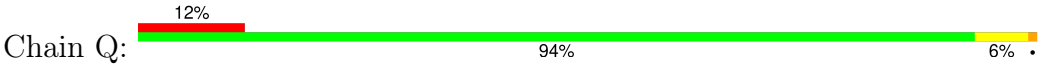


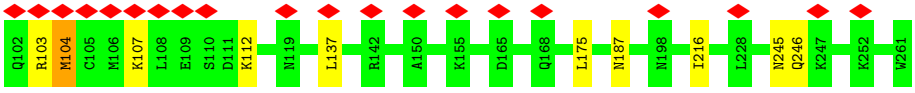
• Molecule 2: Capsid protein



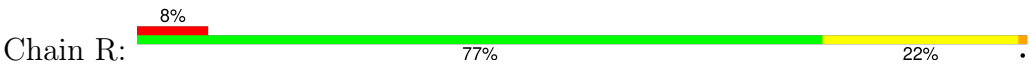


• Molecule 2: Capsid protein

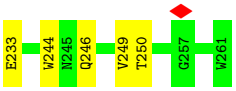




• Molecule 2: Capsid protein



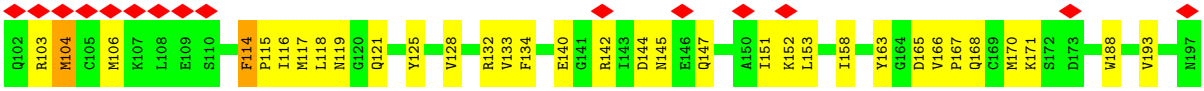


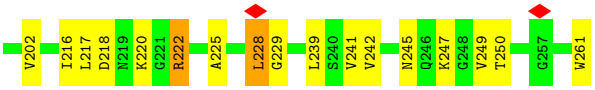


• Molecule 2: Capsid protein

Chain S:



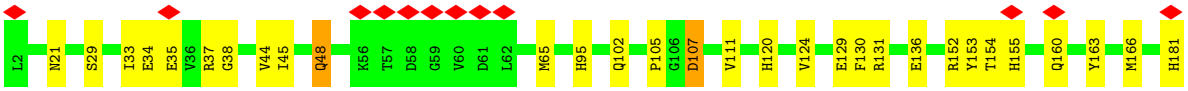


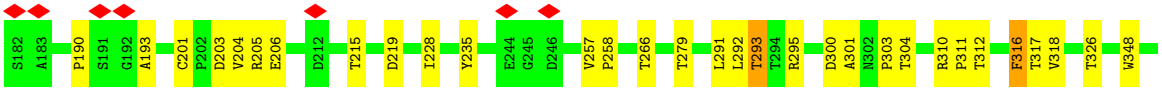


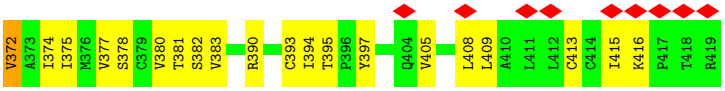
• Molecule 3: E2 glycoprotein

Chain a:





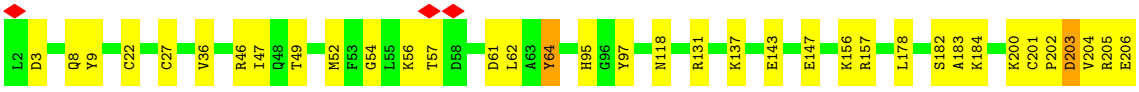




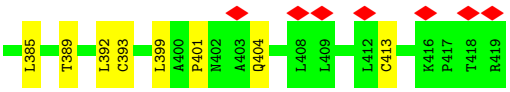
• Molecule 3: E2 glycoprotein

Chain d:





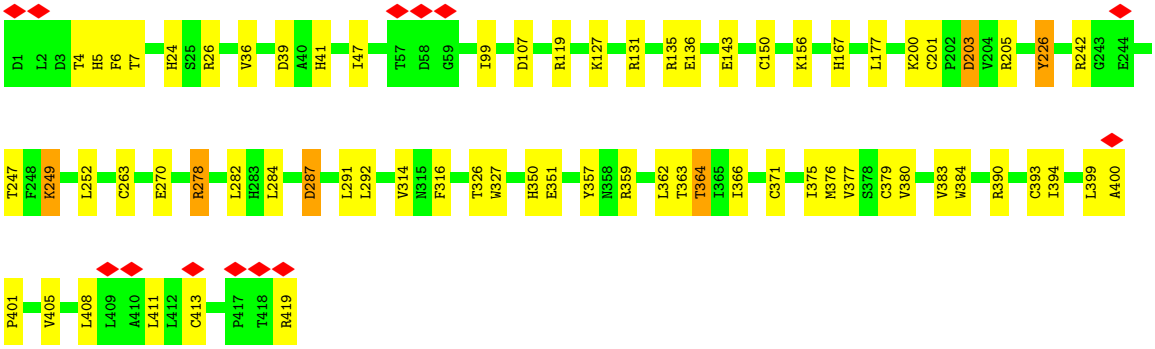




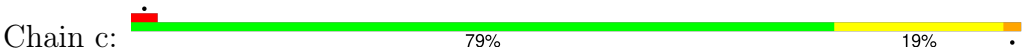
• Molecule 4: E2 glycoprotein

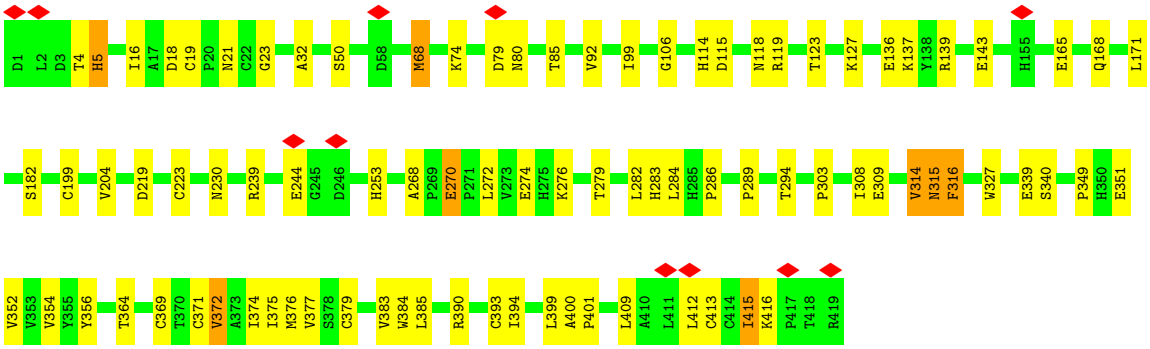
Chain b:





• Molecule 4: E2 glycoprotein





• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



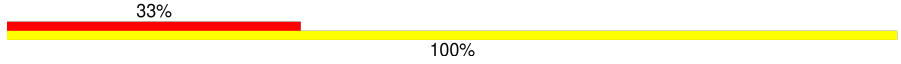


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	958879	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 ($e^-/Å^2$)	36.2	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.716	Depositor
Minimum map value	-0.352	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	279.30002, 279.30002, 279.30002	wwPDB
Map dimensions	210, 210, 210	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.55	0/3464	0.97	0/4728
1	B	0.49	0/3464	0.89	0/4728
1	C	0.49	0/3464	0.90	0/4728
1	D	0.52	0/3464	0.96	0/4728
2	P	0.74	0/1266	1.24	0/1711
2	Q	0.73	0/1266	1.24	0/1711
2	R	0.67	0/1266	1.14	0/1711
2	S	0.68	0/1266	1.14	0/1711
3	a	0.60	0/3383	1.03	0/4613
3	d	0.54	0/3383	0.95	0/4613
4	b	0.62	0/3391	1.07	0/4624
4	c	0.51	0/3391	0.89	0/4624
All	All	0.57	0/32468	1.00	0/44230

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	C	0	3
1	D	0	2
2	Q	0	1
3	d	0	2
4	b	0	3
All	All	0	11

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	122	TYR	Sidechain
1	C	143	ARG	Sidechain
1	C	440	ARG	Sidechain
1	D	186	TYR	Sidechain
1	D	321	TYR	Sidechain
2	Q	103	ARG	Sidechain
4	b	226	TYR	Sidechain
4	b	242	ARG	Sidechain
4	b	278	ARG	Sidechain
3	d	131	ARG	Sidechain
3	d	46	ARG	Sidechain

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	3371	0	3275	75	0
1	B	3371	0	3273	44	0
1	C	3371	0	3275	42	0
1	D	3371	0	3274	54	0
2	P	1239	0	1225	22	0
2	Q	1239	0	1225	8	0
2	R	1239	0	1225	25	0
2	S	1239	0	1225	36	0
3	a	3288	0	3250	57	0
3	d	3288	0	3250	48	0
4	b	3296	0	3257	52	0
4	c	3296	0	3257	66	0
5	E	39	0	34	1	0
5	F	39	0	34	2	0
5	G	39	0	34	6	0
5	H	39	0	34	2	0
6	a	14	0	13	0	0
6	b	14	0	13	0	0
6	c	14	0	13	0	0
6	d	14	0	13	0	0
All	All	31820	0	31199	489	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 (489) 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)
3:a:393:CYS:SG	3:a:413:CYS:HB2	1.71	1.31
4:b:394:ILE:CD1	4:b:413:CYS:SG	2.24	1.24
4:b:394:ILE:HG12	4:b:413:CYS:SG	1.78	1.22
3:a:393:CYS:SG	3:a:413:CYS:CB	2.32	1.17
4:c:393:CYS:SG	4:c:413:CYS:CB	2.34	1.16
4:b:394:ILE:CG1	4:b:413:CYS:SG	2.34	1.14
1:A:440:ARG:NH1	2:P:249:VAL:HG11	1.64	1.11
1:A:440:ARG:HH12	2:P:249:VAL:HG11	1.04	1.09
4:b:394:ILE:HD13	4:b:413:CYS:SG	1.93	1.06
4:c:393:CYS:SG	4:c:409:LEU:CD1	2.45	1.05
4:c:393:CYS:SG	4:c:413:CYS:HB2	1.97	1.05
4:c:393:CYS:SG	4:c:409:LEU:HD11	2.02	0.98
3:d:54:GLY:HA2	3:d:62:LEU:HA	1.47	0.93
1:C:134:ASN:ND2	5:G:1:NAG:C1	2.36	0.89
1:A:440:ARG:HH12	2:P:249:VAL:CG1	1.85	0.88
4:c:393:CYS:HG	4:c:413:CYS:CB	1.86	0.88
2:P:106:MET:HG2	2:P:217:LEU:HD12	1.54	0.87
3:a:393:CYS:HG	3:a:413:CYS:HB2	1.39	0.86
1:D:59:VAL:HG12	1:D:103:MET:HB2	1.57	0.86
4:b:394:ILE:HD13	4:b:413:CYS:HG	1.38	0.85
3:a:44:VAL:HG12	3:a:102:GLN:HG2	1.60	0.84
4:b:393:CYS:SG	4:b:411:LEU:HD12	2.19	0.82
4:b:393:CYS:SG	4:b:411:LEU:CD1	2.68	0.81
1:A:440:ARG:NH1	2:P:249:VAL:HG21	1.96	0.81
4:b:200:LYS:NZ	4:b:201:CYS:O	2.13	0.80
2:R:250:THR:HG21	4:c:399:LEU:HD12	1.65	0.79
1:D:283:ILE:HD12	1:D:284:PRO:HD2	1.65	0.77
4:c:393:CYS:SG	4:c:413:CYS:HB3	2.24	0.77
1:D:37:ARG:HD2	1:D:268:ARG:HD2	1.69	0.74
4:b:394:ILE:HD11	4:b:413:CYS:SG	2.27	0.74
1:D:367:LYS:HD2	1:D:374:ALA:HB1	1.70	0.73
1:B:405:ALA:HA	1:B:408:TRP:HB2	1.70	0.73
1:A:440:ARG:HH11	2:P:249:VAL:HG21	1.54	0.71
3:a:129:GLU:OE2	3:a:131:ARG:NH2	2.24	0.71
1:D:184:GLU:N	1:D:184:GLU:OE1	2.24	0.71
1:C:21:ARG:HB2	1:C:24:TYR:HB2	1.72	0.70
4:c:393:CYS:HG	4:c:413:CYS:HB2	1.47	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:246:GLN:HB3	4:b:419:ARG:HG2	1.74	0.70
3:d:393:CYS:SG	3:d:413:CYS:CB	2.80	0.70
1:A:440:ARG:NH1	2:P:249:VAL:CG1	2.47	0.69
1:A:440:ARG:CZ	2:P:249:VAL:HG11	2.23	0.69
1:C:134:ASN:HD22	5:G:1:NAG:C1	2.04	0.69
1:C:438:PHE:HA	1:C:441:HIS:HB3	1.73	0.69
2:R:117:MET:N	2:R:142:ARG:O	2.26	0.69
3:d:278:ARG:NH1	3:d:339:GLU:OE2	2.25	0.69
4:b:270:GLU:OE1	4:b:270:GLU:N	2.26	0.68
1:D:149:VAL:HG13	1:D:164:ILE:HG22	1.75	0.68
4:b:4:THR:HA	4:b:7:THR:HG22	1.74	0.68
1:B:221:LYS:NZ	4:c:270:GLU:OE2	2.27	0.67
3:d:393:CYS:SG	3:d:413:CYS:HB2	2.34	0.67
2:R:112:LYS:HD2	2:R:175:LEU:HG	1.77	0.67
2:Q:245:ASN:OD1	2:Q:246:GLN:N	2.28	0.67
1:B:184:GLU:OE2	1:B:186:TYR:OH	2.13	0.66
4:c:399:LEU:C	4:c:401:PRO:HD3	2.20	0.65
3:d:270:GLU:OE1	3:d:270:GLU:N	2.26	0.65
1:D:405:ALA:HA	1:D:408:TRP:HB2	1.77	0.65
3:d:147:GLU:OE1	3:d:147:GLU:N	2.29	0.65
2:S:144:ASP:O	2:S:145:ASN:CG	2.40	0.65
4:c:272:LEU:HB2	4:c:283:HIS:HB2	1.79	0.65
2:S:152:LYS:NZ	2:S:153:LEU:O	2.27	0.65
3:a:393:CYS:HG	3:a:413:CYS:CB	2.01	0.64
1:C:243:ARG:HA	1:C:246:ARG:NH2	2.13	0.64
2:R:151:ILE:HD12	2:R:151:ILE:H	1.63	0.64
1:B:97:ASP:OD1	1:B:98:THR:OG1	2.15	0.64
2:S:106:MET:HB2	2:S:217:LEU:HD23	1.78	0.64
1:C:104:SER:HB2	1:C:232:THR:HG23	1.80	0.63
1:D:293:GLU:OE1	1:D:293:GLU:N	2.31	0.63
4:b:24:HIS:HB3	4:c:92:VAL:HG12	1.81	0.63
2:R:250:THR:HG23	4:c:400:ALA:HB2	1.80	0.63
4:b:167:HIS:CD2	4:b:249:LYS:HA	2.33	0.63
3:d:36:VAL:HG23	3:d:47:ILE:HG12	1.79	0.63
1:D:61:LYS:HE3	1:D:66:THR:HG23	1.80	0.63
3:a:393:CYS:SG	3:a:413:CYS:HB3	2.36	0.63
1:A:306:GLU:OE1	1:A:307:CYS:N	2.32	0.62
2:R:246:GLN:OE1	2:R:246:GLN:N	2.26	0.62
1:A:260:CYS:HA	1:A:272:CYS:HB3	1.82	0.62
3:a:206:GLU:OE1	3:a:206:GLU:N	2.32	0.62
1:D:1:TYR:CG	1:D:21:ARG:HD3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:368:LEU:O	3:d:372:VAL:HG23	2.00	0.62
1:A:9:ASN:HD22	1:A:167:LEU:HD21	1.64	0.61
1:D:419:SER:O	1:D:423:VAL:HG12	2.01	0.61
2:R:250:THR:HG21	4:c:399:LEU:CD1	2.30	0.61
2:S:220:LYS:HE2	2:S:220:LYS:HA	1.82	0.61
4:c:393:CYS:HB2	4:c:413:CYS:HG	1.65	0.60
1:D:84:VAL:HG13	1:D:86:PRO:HD3	1.82	0.60
2:S:193:VAL:HG12	2:S:202:VAL:HG12	1.84	0.60
3:d:62:LEU:HD11	3:d:157:ARG:HH22	1.67	0.60
3:a:291:LEU:HD11	3:a:293:THR:HG23	1.84	0.60
2:S:158:ILE:HD13	3:d:392:LEU:HD11	1.83	0.60
1:C:142:TRP:HE1	5:G:1:NAG:H3	1.66	0.60
1:C:67:GLN:OE1	1:C:67:GLN:N	2.35	0.59
1:D:61:LYS:HE3	1:D:66:THR:CG2	2.32	0.59
2:R:121:GLN:OE1	2:R:121:GLN:N	2.35	0.59
1:B:304:ILE:HD11	1:B:377:CYS:HB3	1.82	0.59
1:C:419:SER:O	1:C:423:VAL:HG12	2.02	0.59
1:A:192:GLU:OE1	1:A:192:GLU:N	2.22	0.59
1:A:422:ILE:HD13	3:a:382:SER:HB3	1.85	0.59
3:d:182:SER:OG	3:d:183:ALA:N	2.36	0.59
3:d:54:GLY:HA2	3:d:62:LEU:CA	2.29	0.59
1:A:179:VAL:HG22	1:A:186:TYR:HB2	1.84	0.59
2:S:140:GLU:N	2:S:140:GLU:OE1	2.34	0.59
3:d:385:LEU:O	3:d:389:THR:HG23	2.03	0.58
1:C:134:ASN:HD21	5:G:1:NAG:C1	2.16	0.58
1:A:16:LYS:NZ	1:A:340:ILE:O	2.33	0.58
1:C:18:LEU:HD12	1:C:26:PRO:HB2	1.84	0.58
2:R:116:ILE:HA	2:R:143:ILE:HA	1.85	0.58
2:Q:104:MET:HA	2:Q:107:LYS:HE2	1.84	0.58
4:c:276:LYS:HB3	4:c:279:THR:HB	1.84	0.58
1:B:203:ASP:OD1	1:B:203:ASP:N	2.35	0.58
1:A:440:ARG:HH21	1:A:440:ARG:HG3	1.69	0.57
1:C:362:ILE:HG22	1:C:363:HIS:CD2	2.39	0.57
2:S:103:ARG:O	2:S:106:MET:HG3	2.04	0.57
3:a:397:TYR:HD2	3:a:405:VAL:HG22	1.68	0.57
3:d:203:ASP:OD1	3:d:203:ASP:N	2.29	0.57
3:d:206:GLU:OE1	3:d:206:GLU:N	2.37	0.57
3:a:311:PRO:C	3:a:312:THR:HG23	2.29	0.57
1:C:204:LEU:HD21	1:C:214:LEU:HD23	1.87	0.57
1:D:96:CYS:O	1:D:100:ASN:ND2	2.35	0.57
1:C:229:ILE:HD11	1:C:231:HIS:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:279:THR:HG22	3:a:317:THR:HG22	1.86	0.56
4:b:107:ASP:OD2	4:c:139:ARG:NH2	2.38	0.56
1:B:114:CYS:O	1:B:118:HIS:ND1	2.39	0.56
1:D:1:TYR:N	1:D:283:ILE:O	2.38	0.56
4:b:292:LEU:HD21	4:b:316:PHE:CZ	2.40	0.56
1:A:171:TRP:HZ2	1:A:257:PRO:HG2	1.70	0.56
3:a:35:GLU:OE2	3:a:37:ARG:NH2	2.35	0.55
3:d:52:MET:HE1	3:d:97:TYR:CE1	2.41	0.55
1:A:436:LEU:HA	1:A:440:ARG:HD3	1.88	0.55
1:B:180:VAL:HG22	1:B:185:VAL:HG12	1.87	0.55
4:c:379:CYS:O	4:c:383:VAL:HG12	2.06	0.55
4:c:393:CYS:SG	4:c:409:LEU:HD13	2.43	0.55
1:A:76:TYR:CE1	1:A:105:GLU:HG3	2.42	0.55
1:A:18:LEU:HG	1:A:332:HIS:ND1	2.22	0.55
2:R:244:TRP:HZ3	4:c:400:ALA:HA	1.72	0.55
1:A:51:TYR:HB3	1:A:204:LEU:HD21	1.88	0.55
1:B:203:ASP:OD2	1:B:240:GLY:N	2.28	0.54
4:c:168:GLN:NE2	4:c:230:ASN:OD1	2.40	0.54
4:c:340:SER:O	4:c:340:SER:OG	2.17	0.54
4:c:393:CYS:CB	4:c:413:CYS:HG	2.20	0.54
1:C:51:TYR:OH	1:C:237:ALA:O	2.25	0.54
1:D:389:VAL:HG12	1:D:391:TYR:H	1.73	0.54
2:S:165:ASP:OD1	2:S:166:VAL:N	2.41	0.54
3:a:311:PRO:O	3:a:312:THR:CG2	2.56	0.54
1:C:134:ASN:HD21	1:C:142:TRP:CD1	2.26	0.54
2:Q:112:LYS:HB2	2:Q:175:LEU:CD1	2.38	0.54
2:S:245:ASN:OD1	2:S:247:LYS:N	2.41	0.54
4:b:41:HIS:ND1	4:b:150:CYS:HB2	2.21	0.54
1:A:165:GLY:HA3	1:A:278:PRO:HG2	1.88	0.54
1:A:440:ARG:NH1	2:P:249:VAL:CG2	2.70	0.54
4:c:16:ILE:HD11	4:c:68:MET:HB3	1.89	0.54
3:a:304:THR:HG21	3:a:316:PHE:CZ	2.42	0.54
3:d:292:LEU:HD21	3:d:316:PHE:HZ	1.73	0.54
1:D:38:ILE:HA	1:D:129:VAL:HG12	1.89	0.54
1:A:74:PRO:HD2	1:A:107:TYR:CE1	2.43	0.53
2:S:117:MET:HA	2:S:117:MET:HE2	1.88	0.53
3:a:311:PRO:O	3:a:312:THR:HG23	2.08	0.53
2:S:134:PHE:HD1	2:S:163:TYR:HB2	1.73	0.53
2:S:142:ARG:NH2	2:S:144:ASP:HA	2.23	0.53
4:b:203:ASP:OD1	4:b:203:ASP:N	2.32	0.53
1:A:184:GLU:OE2	1:A:186:TYR:OH	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:107:ASP:OD1	3:a:107:ASP:N	2.37	0.53
3:d:184:LYS:HD3	3:d:216:THR:HA	1.90	0.53
1:A:200:SER:OG	1:A:201:PHE:N	2.40	0.53
3:d:362:LEU:O	3:d:366:ILE:HG22	2.08	0.53
1:A:337:VAL:HG11	1:A:366:PHE:HA	1.91	0.53
3:a:408:LEU:HD23	3:a:409:LEU:H	1.73	0.53
4:b:292:LEU:HD21	4:b:316:PHE:HZ	1.73	0.53
4:b:205:ARG:HA	4:b:205:ARG:NE	2.24	0.53
1:B:293:GLU:OE1	1:B:293:GLU:N	2.41	0.53
1:A:318:THR:HG22	1:A:354:THR:HG22	1.90	0.53
1:D:427:ILE:O	1:D:431:VAL:HG12	2.09	0.53
4:c:21:ASN:OD1	4:c:23:GLY:N	2.34	0.53
1:A:136:THR:HG1	1:A:142:TRP:CD1	2.28	0.52
1:A:203:ASP:N	1:A:203:ASP:OD1	2.41	0.52
1:B:50:LYS:HD2	1:B:242:GLU:OE2	2.10	0.52
3:a:34:GLU:O	3:a:48:GLN:HB2	2.09	0.52
3:a:204:VAL:HG12	3:a:206:GLU:OE1	2.09	0.52
2:P:169:CYS:SG	2:P:170:MET:HE2	2.50	0.52
4:c:371:CYS:HA	4:c:374:ILE:HG22	1.92	0.52
1:C:142:TRP:NE1	5:G:1:NAG:H3	2.24	0.52
1:D:148:TYR:HD2	1:D:153:THR:HG21	1.75	0.52
3:a:377:VAL:O	3:a:381:THR:HG23	2.10	0.52
1:A:46:TYR:HE2	1:A:192:GLU:HA	1.74	0.52
1:C:199:GLY:N	1:C:203:ASP:OD1	2.43	0.52
2:P:103:ARG:HA	2:P:106:MET:HG3	1.92	0.52
1:D:145:ALA:HB3	1:D:157:ILE:HG12	1.91	0.51
1:A:116:ILE:HD11	3:a:258:PRO:HB2	1.91	0.51
1:A:38:ILE:HG22	1:A:129:VAL:HG22	1.92	0.51
1:B:110:ARG:NH1	1:B:211:SER:O	2.43	0.51
4:c:282:LEU:HB2	4:c:314:VAL:HG23	1.91	0.51
2:S:115:PRO:HA	2:S:125:TYR:HA	1.92	0.51
4:b:119:ARG:HA	4:b:119:ARG:NE	2.26	0.51
1:B:196:GLY:O	1:B:217:ASN:ND2	2.42	0.51
4:c:286:PRO:HG3	4:c:308:ILE:HG22	1.93	0.51
3:d:274:GLU:HB3	3:d:281:ILE:HB	1.92	0.51
1:A:30:GLN:NE2	1:A:343:ASN:OD1	2.44	0.51
1:C:427:ILE:O	1:C:431:VAL:HG12	2.11	0.51
2:S:114:PHE:HZ	2:S:128:VAL:HB	1.75	0.51
1:B:293:GLU:O	1:B:325:LYS:NZ	2.25	0.50
1:B:208:THR:HG22	1:B:211:SER:HB3	1.92	0.50
1:D:129:VAL:HG23	1:D:149:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:44:VAL:HG11	3:a:152:ARG:HH11	1.77	0.50
4:b:357:TYR:HA	4:b:364:THR:HG21	1.93	0.50
3:d:393:CYS:HG	3:d:413:CYS:CB	2.25	0.50
3:a:166:MET:HG2	3:a:235:TYR:HA	1.92	0.50
1:B:75:ASP:HB2	1:B:108:VAL:HG12	1.93	0.50
1:B:192:GLU:HG2	1:B:193:TYR:H	1.75	0.50
2:S:228:LEU:HD11	2:S:242:VAL:HG13	1.93	0.50
4:c:394:ILE:HB	4:c:415:ILE:HD11	1.94	0.50
1:B:37:ARG:HH11	1:B:130:GLN:HG3	1.76	0.50
1:A:268:ARG:NE	1:A:270:GLU:OE2	2.32	0.50
1:B:85:TYR:HA	1:B:100:ASN:HD22	1.77	0.50
1:C:231:HIS:CE1	1:C:233:PRO:HG3	2.46	0.50
2:P:134:PHE:CD1	2:P:163:TYR:HB2	2.47	0.50
3:a:203:ASP:O	3:a:205:ARG:NH2	2.37	0.50
1:C:307:CYS:HA	1:C:315:GLY:HA2	1.94	0.50
3:d:3:ASP:OD1	3:d:3:ASP:N	2.42	0.49
2:Q:245:ASN:CG	2:Q:246:GLN:H	2.18	0.49
1:A:113:GLU:OE1	3:a:37:ARG:NH1	2.44	0.49
1:A:265:GLU:HB2	1:A:266:PRO:HD3	1.94	0.49
1:C:68:CYS:HB3	1:C:103:MET:SD	2.52	0.49
1:D:290:ARG:HB2	1:D:293:GLU:OE1	2.12	0.49
1:D:96:CYS:HB3	1:D:100:ASN:OD1	2.12	0.49
2:P:246:GLN:HG2	4:b:419:ARG:HD3	1.94	0.49
1:A:42:THR:HG21	1:A:267:LEU:HD13	1.95	0.49
1:C:328:ASN:OD1	1:C:328:ASN:N	2.43	0.49
2:R:117:MET:HE2	2:R:117:MET:HA	1.94	0.49
4:b:135:ARG:NH1	4:b:326:THR:OG1	2.46	0.49
4:c:32:ALA:N	4:c:50:SER:OG	2.33	0.49
1:A:124:VAL:HG22	1:A:176:ASN:HA	1.93	0.49
4:c:119:ARG:HA	4:c:119:ARG:NE	2.28	0.49
1:D:135:ILE:HD12	1:D:162:LEU:HD22	1.95	0.49
4:b:26:ARG:NH1	4:c:143:GLU:O	2.45	0.49
1:C:229:ILE:HD12	4:c:18:ASP:OD2	2.12	0.48
1:D:130:GLN:HA	1:D:149:VAL:HG23	1.93	0.48
4:c:274:GLU:OE1	4:c:283:HIS:NE2	2.31	0.48
3:d:357:TYR:HA	3:d:364:THR:HG21	1.94	0.48
1:A:180:VAL:HG22	1:A:185:VAL:HG12	1.95	0.48
1:B:104:SER:O	1:B:104:SER:OG	2.29	0.48
1:B:265:GLU:HB3	1:B:266:PRO:HD3	1.95	0.48
1:B:28:HIS:CD2	1:B:343:ASN:HB2	2.48	0.48
4:b:362:LEU:O	4:b:366:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:LEU:HD11	4:b:375:ILE:HG21	1.95	0.48
3:a:372:VAL:HA	3:a:375:ILE:HG22	1.95	0.48
4:b:278:ARG:HH11	4:b:359:ARG:HA	1.78	0.48
4:b:287:ASP:OD1	4:b:287:ASP:N	2.34	0.48
3:d:56:LYS:HB2	3:d:61:ASP:HB2	1.94	0.48
4:b:119:ARG:HA	4:b:119:ARG:HE	1.79	0.48
4:c:356:TYR:O	4:c:364:THR:OG1	2.29	0.48
1:A:331:ILE:HD11	1:A:340:ILE:HG21	1.95	0.48
2:R:244:TRP:CZ3	4:c:400:ALA:HA	2.49	0.48
2:S:153:LEU:HD22	2:S:153:LEU:H	1.79	0.48
3:a:203:ASP:H	3:a:205:ARG:HH22	1.61	0.48
2:S:229:GLY:HA2	2:S:261:TRP:CG	2.49	0.48
1:A:189:ASP:OD1	1:A:190:PHE:N	2.47	0.47
1:D:283:ILE:HD12	1:D:284:PRO:CD	2.38	0.47
1:A:74:PRO:HD2	1:A:107:TYR:HE1	1.78	0.47
1:D:19:VAL:HG13	1:D:29:LEU:HD22	1.97	0.47
1:D:81:PHE:O	1:D:101:THR:HA	2.13	0.47
1:D:162:LEU:HD21	1:D:164:ILE:HD11	1.95	0.47
4:c:18:ASP:OD1	4:c:19:CYS:N	2.47	0.47
1:B:53:THR:HG21	1:B:236:GLN:OE1	2.14	0.47
1:C:103:MET:HE3	1:C:103:MET:HB3	1.76	0.47
4:c:393:CYS:CB	4:c:413:CYS:SG	3.03	0.47
4:c:294:THR:HG21	4:c:316:PHE:CE2	2.50	0.47
1:A:302:CYS:HB3	1:A:319:VAL:HG22	1.97	0.47
1:A:440:ARG:NH2	2:P:249:VAL:HG11	2.30	0.47
4:b:41:HIS:HA	4:b:131:ARG:HB2	1.95	0.47
4:c:412:LEU:HD12	4:c:413:CYS:N	2.30	0.47
3:d:56:LYS:HG2	3:d:57:THR:H	1.77	0.47
1:C:255:VAL:HG13	4:c:303:PRO:HG3	1.96	0.47
2:R:116:ILE:HG22	2:R:143:ILE:HA	1.96	0.47
2:S:218:ASP:OD1	2:S:222:ARG:HG2	2.14	0.47
3:a:95:HIS:C	3:a:95:HIS:CD2	2.93	0.47
3:a:105:PRO:HG3	3:a:130:PHE:H	1.80	0.47
3:a:393:CYS:CB	3:a:413:CYS:SG	3.03	0.47
4:c:118:ASN:OD1	4:c:118:ASN:N	2.48	0.47
3:d:200:LYS:NZ	3:d:202:PRO:O	2.47	0.47
1:B:37:ARG:HG2	1:B:270:GLU:HG3	1.96	0.47
1:B:425:GLY:O	1:B:429:THR:HG22	2.15	0.47
2:P:246:GLN:CB	4:b:419:ARG:HG2	2.43	0.47
2:S:168:GLN:HA	2:S:171:LYS:NZ	2.30	0.47
4:b:393:CYS:SG	4:b:411:LEU:HD11	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:136:GLU:OE2	4:c:268:ALA:HB2	2.15	0.47
1:C:312:ASP:HB3	1:C:391:TYR:CE1	2.51	0.46
1:D:93:TYR:O	3:d:226:TYR:OH	2.25	0.46
3:d:204:VAL:C	3:d:205:ARG:HD2	2.39	0.46
1:C:386:ASP:O	1:C:388:ILE:N	2.47	0.46
2:S:245:ASN:OD1	2:S:245:ASN:C	2.59	0.46
1:A:428:ALA:O	1:A:431:VAL:HG12	2.16	0.46
1:B:268:ARG:NH2	1:B:270:GLU:OE2	2.48	0.46
1:D:436:LEU:HD21	2:S:158:ILE:CD1	2.46	0.46
1:B:204:LEU:HD11	1:B:214:LEU:HD13	1.98	0.46
1:A:139:SER:O	1:A:139:SER:OG	2.26	0.46
2:S:158:ILE:HG21	3:d:392:LEU:HD11	1.97	0.46
4:b:376:MET:HE3	4:b:377:VAL:N	2.30	0.46
4:c:239:ARG:NH2	3:d:143:GLU:OE1	2.44	0.46
3:a:136:GLU:N	3:a:136:GLU:OE1	2.49	0.46
1:D:266:PRO:HG2	1:D:268:ARG:HD3	1.98	0.46
2:Q:104:MET:SD	2:Q:104:MET:N	2.83	0.46
3:a:310:ARG:O	3:a:312:THR:HG23	2.16	0.46
3:a:415:ILE:HG12	3:a:416:LYS:H	1.81	0.46
4:c:284:LEU:HD13	4:c:327:TRP:CZ3	2.51	0.46
1:A:73:HIS:O	1:A:74:PRO:C	2.59	0.45
1:D:47:ILE:HG22	1:D:120:LYS:HG2	1.98	0.45
4:c:376:MET:HE2	4:c:376:MET:HA	1.97	0.45
4:c:351:GLU:O	4:c:354:VAL:HG12	2.15	0.45
1:A:93:TYR:O	1:A:94:CYS:HB3	2.16	0.45
4:c:393:CYS:SG	4:c:409:LEU:HD12	2.50	0.45
3:d:348:TRP:N	3:d:351:GLU:OE2	2.35	0.45
1:A:7:MET:HE1	1:A:33:LEU:HD13	1.99	0.45
1:B:206:SER:OG	1:B:208:THR:O	2.33	0.45
1:B:427:ILE:HD12	1:B:427:ILE:HA	1.88	0.45
4:b:284:LEU:HD12	4:b:327:TRP:CH2	2.52	0.45
4:c:115:ASP:CG	4:c:115:ASP:O	2.59	0.45
1:A:160:ALA:HB1	1:A:281:ILE:HD11	1.99	0.45
1:B:142:TRP:HD1	5:F:1:NAG:H82	1.82	0.45
2:P:247:LYS:HA	2:P:247:LYS:HD3	1.79	0.45
2:S:216:ILE:HD11	2:S:225:ALA:HB3	1.98	0.45
3:d:61:ASP:HB3	3:d:64:TYR:HB2	1.99	0.45
3:a:393:CYS:HB2	3:a:413:CYS:SG	2.57	0.45
1:C:399:PHE:CD1	1:C:399:PHE:C	2.94	0.45
2:S:225:ALA:HB1	2:S:241:VAL:CG2	2.47	0.45
3:a:190:PRO:HG2	3:a:193:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:291:LEU:HD12	4:b:292:LEU:N	2.31	0.45
1:B:37:ARG:NH1	1:B:130:GLN:OE1	2.50	0.44
1:C:136:THR:HB	1:C:142:TRP:HA	1.98	0.44
1:C:242:GLU:OE1	1:C:246:ARG:NH2	2.50	0.44
1:D:268:ARG:NE	1:D:270:GLU:OE2	2.49	0.44
2:R:118:LEU:HD12	2:R:119:ASN:N	2.32	0.44
3:a:154:THR:HG22	3:a:257:VAL:O	2.17	0.44
3:d:137:LYS:HE3	3:d:307:TRP:CH2	2.52	0.44
1:A:45:GLU:OE1	1:A:123:LYS:NZ	2.31	0.44
1:A:176:ASN:N	1:A:176:ASN:OD1	2.49	0.44
4:c:137:LYS:HB2	4:c:289:PRO:HG2	1.99	0.44
1:C:62:CYS:C	1:C:64:GLY:N	2.75	0.44
1:C:395:HIS:C	1:C:395:HIS:CD2	2.95	0.44
1:D:264:LEU:HD12	1:D:264:LEU:HA	1.61	0.44
4:c:384:TRP:HE3	4:c:385:LEU:HD22	1.83	0.44
2:P:112:LYS:HA	2:P:114:PHE:CE2	2.52	0.44
1:D:265:GLU:HB2	1:D:266:PRO:HD3	2.00	0.44
1:C:426:LEU:O	1:C:429:THR:HG22	2.18	0.44
2:Q:112:LYS:H	2:Q:112:LYS:HD2	1.82	0.44
1:B:192:GLU:HG2	1:B:193:TYR:N	2.33	0.44
2:R:103:ARG:HA	2:R:106:MET:HG2	1.99	0.44
4:b:390:ARG:CZ	4:b:413:CYS:HA	2.48	0.44
1:A:177:LYS:HB3	1:A:189:ASP:HA	2.00	0.44
2:P:147:GLN:HE21	2:P:170:MET:HG3	1.83	0.44
4:b:399:LEU:C	4:b:401:PRO:HD3	2.43	0.44
1:A:37:ARG:HB3	1:A:39:ILE:HD11	2.00	0.44
1:A:149:VAL:HG13	1:A:164:ILE:HG22	2.00	0.44
1:A:440:ARG:NH1	2:P:249:VAL:CB	2.81	0.44
3:a:291:LEU:HD12	3:a:292:LEU:N	2.33	0.44
4:b:143:GLU:CD	3:d:239:ARG:HH12	2.25	0.44
1:A:177:LYS:HD3	1:A:190:PHE:CE2	2.53	0.43
1:D:3:HIS:CG	1:D:19:VAL:HG12	2.53	0.43
1:D:186:TYR:CZ	1:D:248:LYS:HD2	2.53	0.43
2:Q:107:LYS:HD3	2:Q:187:ASN:HB2	1.99	0.43
2:Q:112:LYS:HD2	2:Q:112:LYS:N	2.33	0.43
4:b:4:THR:O	4:b:5:HIS:C	2.60	0.43
4:b:384:TRP:CD1	4:b:384:TRP:C	2.95	0.43
4:c:74:LYS:HB2	4:c:74:LYS:HE3	1.71	0.43
1:A:429:THR:O	1:A:432:VAL:HG12	2.18	0.43
1:D:137:TYR:O	1:D:140:VAL:HG12	2.19	0.43
2:R:120:GLY:HA3	2:S:147:GLN:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:GLN:HB2	1:C:222:LEU:HD12	2.01	0.43
3:a:416:LYS:H	3:a:416:LYS:HG3	1.69	0.43
1:C:312:ASP:C	1:C:312:ASP:OD1	2.61	0.43
4:b:36:VAL:HG23	4:b:47:ILE:HG12	2.00	0.43
3:d:95:HIS:CE1	3:d:157:ARG:HD3	2.53	0.43
1:D:142:TRP:CB	5:H:1:NAG:H5	2.48	0.43
1:A:161:LYS:HB2	1:A:282:ASP:HB3	2.00	0.43
1:B:68:CYS:HB3	1:B:103:MET:SD	2.59	0.43
2:S:132:ARG:NH1	3:d:401:PRO:HB3	2.33	0.43
3:a:38:GLY:HA2	3:a:45:ILE:HG22	2.00	0.43
3:a:155:HIS:O	3:a:155:HIS:ND1	2.45	0.43
4:b:379:CYS:O	4:b:383:VAL:HG23	2.19	0.43
1:A:192:GLU:O	1:A:195:THR:HG22	2.18	0.43
1:B:47:ILE:HG22	1:B:120:LYS:HG2	2.00	0.43
1:B:50:LYS:HD3	4:b:39:ASP:OD2	2.19	0.43
2:R:154:LYS:HD2	2:R:163:TYR:OH	2.18	0.43
1:D:367:LYS:CD	1:D:374:ALA:HB1	2.46	0.43
2:S:118:LEU:O	2:S:121:GLN:HG2	2.19	0.43
3:a:300:ASP:OD1	3:a:301:ALA:N	2.52	0.43
1:B:291:ILE:O	1:B:294:THR:HG22	2.19	0.42
2:R:110:SER:HA	2:R:113:THR:HG23	2.01	0.42
4:c:85:THR:HG22	4:c:106:GLY:HA3	2.00	0.42
3:d:118:ASN:OD1	3:d:118:ASN:N	2.52	0.42
1:A:440:ARG:HG3	1:A:440:ARG:NH2	2.34	0.42
1:D:161:LYS:HB3	1:D:161:LYS:HZ2	1.84	0.42
1:A:207:ARG:HD3	1:A:207:ARG:HA	1.74	0.42
2:P:134:PHE:HD1	2:P:163:TYR:HB2	1.84	0.42
2:R:131:GLY:H	2:R:174:THR:HG21	1.84	0.42
2:S:118:LEU:O	2:S:119:ASN:C	2.62	0.42
2:S:188:TRP:CD1	2:S:216:ILE:HG22	2.55	0.42
4:c:349:PRO:HA	4:c:352:VAL:HG12	2.00	0.42
1:A:371:CYS:O	1:A:372:THR:HG22	2.19	0.42
1:D:378:LYS:HE2	1:D:378:LYS:HB3	1.76	0.42
2:R:105:CYS:SG	2:R:106:MET:SD	3.18	0.42
1:A:260:CYS:HA	1:A:272:CYS:CB	2.48	0.42
1:B:290:ARG:HB2	1:B:293:GLU:CD	2.45	0.42
3:a:394:ILE:HG21	3:a:415:ILE:HD12	2.01	0.42
3:d:404:GLN:HA	3:d:404:GLN:OE1	2.19	0.42
1:A:43:ASN:OD1	1:A:43:ASN:C	2.63	0.42
2:R:107:LYS:HD2	2:R:189:HIS:HA	2.02	0.42
3:a:203:ASP:H	3:a:205:ARG:NH2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:311:PRO:C	3:a:312:THR:CG2	2.91	0.42
1:D:147:VAL:HG21	1:D:164:ILE:HD12	2.01	0.42
2:R:244:TRP:CD1	2:R:244:TRP:N	2.87	0.42
4:c:390:ARG:O	4:c:394:ILE:HG23	2.20	0.42
3:d:310:ARG:HG3	3:d:311:PRO:HD2	2.00	0.42
4:b:379:CYS:SG	4:b:380:VAL:N	2.92	0.42
1:A:171:TRP:CZ2	1:A:257:PRO:HG2	2.53	0.42
1:C:408:TRP:HA	1:C:408:TRP:CE3	2.55	0.42
3:a:44:VAL:HG23	3:a:153:TYR:HD2	1.84	0.42
3:d:292:LEU:HD21	3:d:316:PHE:CZ	2.54	0.42
1:A:177:LYS:HD3	1:A:190:PHE:CZ	2.54	0.42
1:C:62:CYS:O	1:C:64:GLY:N	2.52	0.42
1:D:142:TRP:CD1	5:H:1:NAG:H3	2.55	0.42
2:R:136:PRO:HB2	2:R:138:HIS:CE1	2.55	0.42
2:S:151:ILE:HG13	2:S:167:PRO:HD3	2.02	0.42
1:A:137:TYR:CD1	1:A:283:ILE:HD11	2.55	0.41
1:A:167:LEU:HD23	1:A:167:LEU:HA	1.79	0.41
1:C:367:LYS:HE3	1:C:367:LYS:HB2	1.82	0.41
4:c:165:GLU:CD	4:c:165:GLU:H	2.28	0.41
1:A:106:ALA:HB1	1:A:220:LEU:HD21	2.01	0.41
2:P:106:MET:HG2	2:P:217:LEU:CD1	2.39	0.41
2:S:144:ASP:O	2:S:145:ASN:OD1	2.38	0.41
3:a:397:TYR:CE2	3:a:405:VAL:HA	2.56	0.41
4:c:384:TRP:CE3	4:c:385:LEU:HD22	2.55	0.41
3:d:376:MET:HE2	3:d:376:MET:HA	2.02	0.41
1:A:418:THR:OG1	3:a:378:SER:CB	2.68	0.41
2:R:113:THR:O	2:R:113:THR:OG1	2.37	0.41
4:b:4:THR:HA	4:b:7:THR:CG2	2.45	0.41
4:c:4:THR:O	4:c:5:HIS:C	2.64	0.41
3:d:201:CYS:O	3:d:203:ASP:N	2.53	0.41
3:d:392:LEU:HD12	3:d:392:LEU:HA	1.73	0.41
3:d:399:LEU:HD23	3:d:399:LEU:HA	1.86	0.41
1:A:255:VAL:HG22	3:a:303:PRO:HB3	2.01	0.41
1:B:32:GLN:HB3	5:F:1:NAG:H83	2.02	0.41
1:C:243:ARG:HA	1:C:246:ARG:HH22	1.83	0.41
1:D:1:TYR:CD1	1:D:21:ARG:HD3	2.56	0.41
3:a:21:ASN:OD1	3:a:21:ASN:C	2.63	0.41
3:d:368:LEU:HD23	3:d:368:LEU:HA	1.79	0.41
1:D:116:ILE:HD13	1:D:116:ILE:HA	1.81	0.41
4:b:177:LEU:CD2	4:b:177:LEU:H	2.33	0.41
3:d:201:CYS:O	3:d:202:PRO:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASP:OD1	1:A:189:ASP:C	2.64	0.41
1:A:342:GLU:N	1:A:342:GLU:OE1	2.53	0.41
1:B:51:TYR:OH	1:B:237:ALA:O	2.39	0.41
4:b:177:LEU:H	4:b:177:LEU:HD23	1.85	0.41
1:D:40:PRO:HA	1:D:127:GLY:HA3	2.03	0.41
1:D:81:PHE:CE2	1:D:224:ARG:HA	2.56	0.41
4:b:371:CYS:O	4:b:375:ILE:HG23	2.20	0.41
4:b:376:MET:HE3	4:b:376:MET:C	2.46	0.41
1:B:37:ARG:HE	1:B:37:ARG:HB2	1.70	0.41
1:D:34:VAL:CG2	1:D:132:MET:HG2	2.51	0.41
2:S:166:VAL:HG22	2:S:170:MET:SD	2.61	0.41
3:a:377:VAL:HA	3:a:380:VAL:HG22	2.03	0.41
4:b:408:LEU:CD1	4:b:413:CYS:HB3	2.51	0.41
4:c:127:LYS:HZ3	4:c:127:LYS:HG3	1.81	0.41
4:c:372:VAL:HA	4:c:375:ILE:HG22	2.03	0.41
5:E:2:NAG:H4	5:E:3:BMA:H2	1.76	0.41
1:A:254:ASP:O	3:a:295:ARG:HD2	2.21	0.41
1:D:440:ARG:HD2	2:S:249:VAL:CG1	2.51	0.41
4:c:351:GLU:H	4:c:351:GLU:HG2	1.66	0.41
1:C:134:ASN:HD21	1:C:142:TRP:HD1	1.68	0.40
1:D:204:LEU:CD1	1:D:214:LEU:HD21	2.51	0.40
1:D:321:TYR:CD1	1:D:321:TYR:C	2.99	0.40
3:a:105:PRO:HB3	3:a:129:GLU:HA	2.02	0.40
4:b:350:HIS:ND1	4:b:351:GLU:HG3	2.36	0.40
5:G:2:NAG:H4	5:G:3:BMA:H2	1.75	0.40
1:B:129:VAL:HG13	1:B:149:VAL:HB	2.04	0.40
1:D:436:LEU:HD21	2:S:158:ILE:HD12	2.03	0.40
2:R:133:VAL:O	2:R:163:TYR:HA	2.21	0.40
3:a:390:ARG:HE	3:a:394:ILE:HG13	1.87	0.40
4:c:369:CYS:O	4:c:372:VAL:HG12	2.21	0.40
1:B:296:THR:H	1:B:324:SER:HG	1.68	0.40
1:C:43:ASN:N	1:C:43:ASN:OD1	2.54	0.40
2:S:104:MET:SD	2:S:104:MET:N	2.89	0.40
3:a:160:GLN:NE2	3:a:163:TYR:OH	2.53	0.40
4:c:80:ASN:HB3	4:c:114:HIS:CD2	2.57	0.40
4:c:339:GLU:OE1	4:c:339:GLU:HA	2.21	0.40
3:d:272:LEU:HB2	3:d:283:HIS:HB2	2.02	0.40
3:d:310:ARG:HB2	3:d:310:ARG:CZ	2.51	0.40
1:B:110:ARG:HA	1:B:204:LEU:HD21	2.03	0.40
3:a:33:ILE:HD13	3:a:124:VAL:HG13	2.03	0.40
4:c:393:CYS:HB2	4:c:413:CYS:SG	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:416:LYS:O	4:c:416:LYS:HD2	2.21	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	439/441 (100%)	401 (91%)	34 (8%)	4 (1%)	14	44
1	B	439/441 (100%)	418 (95%)	21 (5%)	0	100	100
1	C	439/441 (100%)	417 (95%)	20 (5%)	2 (0%)	24	57
1	D	439/441 (100%)	407 (93%)	31 (7%)	1 (0%)	43	73
2	P	158/160 (99%)	150 (95%)	8 (5%)	0	100	100
2	Q	158/160 (99%)	149 (94%)	9 (6%)	0	100	100
2	R	158/160 (99%)	154 (98%)	4 (2%)	0	100	100
2	S	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
3	a	416/418 (100%)	385 (92%)	28 (7%)	3 (1%)	18	49
3	d	416/418 (100%)	396 (95%)	20 (5%)	0	100	100
4	b	417/419 (100%)	383 (92%)	32 (8%)	2 (0%)	24	57
4	c	417/419 (100%)	380 (91%)	33 (8%)	4 (1%)	12	41
All	All	4054/4078 (99%)	3792 (94%)	246 (6%)	16 (0%)	31	61

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	GLU
4	c	315	ASN
4	c	316	PHE

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Mol	Chain	Res	Type
4	b	400	ALA
1	A	156	LYS
1	C	313	PHE
4	c	182	SER
1	A	94	CYS
1	A	99	GLU
3	a	316	PHE
4	c	244	GLU
1	C	63	CYS
1	D	349	GLU
3	a	120	HIS
4	b	405	VAL
3	a	201	CYS

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	370/370 (100%)	347 (94%)	23 (6%)	16	46
1	B	370/370 (100%)	360 (97%)	10 (3%)	39	67
1	C	370/370 (100%)	354 (96%)	16 (4%)	26	57
1	D	370/370 (100%)	351 (95%)	19 (5%)	21	52
2	P	134/134 (100%)	128 (96%)	6 (4%)	24	56
2	Q	134/134 (100%)	131 (98%)	3 (2%)	45	71
2	R	134/134 (100%)	124 (92%)	10 (8%)	12	39
2	S	134/134 (100%)	126 (94%)	8 (6%)	17	47
3	a	366/366 (100%)	348 (95%)	18 (5%)	22	53
3	d	366/366 (100%)	352 (96%)	14 (4%)	29	60
4	b	367/367 (100%)	351 (96%)	16 (4%)	25	56
4	c	367/367 (100%)	349 (95%)	18 (5%)	22	53
All	All	3482/3482 (100%)	3321 (95%)	161 (5%)	25	55

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	CYS
1	A	87	PHE
1	A	133	VAL
1	A	135	ILE
1	A	144	SER
1	A	157	ILE
1	A	179	VAL
1	A	223	GLN
1	A	239	SER
1	A	253	ASN
1	A	265	GLU
1	A	305	THR
1	A	331	ILE
1	A	332	HIS
1	A	359	THR
1	A	372	THR
1	A	377	CYS
1	A	408	TRP
1	A	418	THR
1	A	429	THR
1	A	431	VAL
1	A	432	VAL
1	A	437	PHE
1	B	129	VAL
1	B	135	ILE
1	B	203	ASP
1	B	264	LEU
1	B	272	CYS
1	B	301	GLU
1	B	331	ILE
1	B	332	HIS
1	B	415	VAL
1	B	424	LEU
1	C	4	THR
1	C	75	ASP
1	C	105	GLU
1	C	118	HIS
1	C	135	ILE
1	C	141	SER
1	C	185	VAL
1	C	319	VAL
1	C	329	CYS

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Mol	Chain	Res	Type
1	C	371	CYS
1	C	385	LYS
1	C	408	TRP
1	C	418	THR
1	C	421	PHE
1	C	427	ILE
1	C	429	THR
1	D	36	THR
1	D	60	VAL
1	D	82	THR
1	D	124	VAL
1	D	135	ILE
1	D	136	THR
1	D	147	VAL
1	D	185	VAL
1	D	280	SER
1	D	281	ILE
1	D	321	TYR
1	D	376	THR
1	D	378	LYS
1	D	380	ASP
1	D	382	LYS
1	D	409	SER
1	D	414	LEU
1	D	426	LEU
1	D	427	ILE
2	P	104	MET
2	P	105	CYS
2	P	193	VAL
2	P	194	GLN
2	P	233	GLU
2	P	256	GLU
2	Q	104	MET
2	Q	137	LEU
2	Q	216	ILE
2	R	104	MET
2	R	105	CYS
2	R	123	ASN
2	R	140	GLU
2	R	187	ASN
2	R	193	VAL
2	R	226	ILE

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Mol	Chain	Res	Type
2	R	231	VAL
2	R	233	GLU
2	R	249	VAL
2	S	104	MET
2	S	114	PHE
2	S	116	ILE
2	S	133	VAL
2	S	222	ARG
2	S	228	LEU
2	S	239	LEU
2	S	250	THR
3	a	29	SER
3	a	48	GLN
3	a	65	MET
3	a	107	ASP
3	a	111	VAL
3	a	181	HIS
3	a	215	THR
3	a	219	ASP
3	a	228	ILE
3	a	266	THR
3	a	293	THR
3	a	318	VAL
3	a	326	THR
3	a	348	TRP
3	a	372	VAL
3	a	374	ILE
3	a	383	VAL
3	a	395	THR
4	b	6	PHE
4	b	99	ILE
4	b	127	LYS
4	b	136	GLU
4	b	156	LYS
4	b	203	ASP
4	b	226	TYR
4	b	247	THR
4	b	249	LYS
4	b	252	LEU
4	b	263	CYS
4	b	282	LEU
4	b	287	ASP

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Mol	Chain	Res	Type
4	b	314	VAL
4	b	363	THR
4	b	364	THR
4	c	5	HIS
4	c	68	MET
4	c	79	ASP
4	c	99	ILE
4	c	123	THR
4	c	171	LEU
4	c	199	CYS
4	c	204	VAL
4	c	219	ASP
4	c	223	CYS
4	c	253	HIS
4	c	270	GLU
4	c	309	GLU
4	c	314	VAL
4	c	315	ASN
4	c	372	VAL
4	c	377	VAL
4	c	415	ILE
3	d	8	GLN
3	d	9	TYR
3	d	22	CYS
3	d	27	CYS
3	d	49	THR
3	d	64	TYR
3	d	156	LYS
3	d	178	LEU
3	d	203	ASP
3	d	257	VAL
3	d	318	VAL
3	d	370	THR
3	d	374	ILE
3	d	378	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	30	GLN
1	A	32	GLN

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Mol	Chain	Res	Type
1	A	102	GLN
1	A	125	HIS
1	A	134	ASN
1	B	32	GLN
1	B	35	ASN
1	B	231	HIS
1	B	387	HIS
1	C	134	ASN
1	C	219	ASN
1	C	439	HIS
1	D	3	HIS
1	D	43	ASN
1	D	394	GLN
1	D	441	HIS
2	P	187	ASN
2	P	219	ASN
2	P	246	GLN
2	Q	198	ASN
2	Q	219	ASN
2	R	187	ASN
2	R	197	ASN
2	S	176	GLN
2	S	190	HIS
3	a	120	HIS
3	a	160	GLN
3	a	167	HIS
3	a	306	GLN
3	a	404	GLN
4	b	8	GLN
4	b	48	GLN
4	b	73	GLN
4	b	114	HIS
4	b	120	HIS
4	b	151	ASN
4	b	155	HIS
4	b	167	HIS
4	b	168	GLN
4	b	285	HIS
4	b	402	ASN
4	c	94	HIS
4	c	288	HIS
4	c	391	ASN

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Mol	Chain	Res	Type
3	d	230	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)

12 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	$\#\|Z\| > 2$
5	NAG	E	1	5	14,14,15	0.38	0	17,19,21	0.44	0
5	NAG	E	2	5	14,14,15	0.38	0	17,19,21	0.81	0
5	BMA	E	3	5	11,11,12	0.37	0	15,15,17	0.49	0
5	NAG	F	1	1,5	14,14,15	0.37	0	17,19,21	0.62	0
5	NAG	F	2	5	14,14,15	0.37	0	17,19,21	0.68	0
5	BMA	F	3	5	11,11,12	0.26	0	15,15,17	0.58	0
5	NAG	G	1	5	14,14,15	0.39	0	17,19,21	0.62	0
5	NAG	G	2	5	14,14,15	0.39	0	17,19,21	0.72	0
5	BMA	G	3	5	11,11,12	0.34	0	15,15,17	0.42	0
5	NAG	H	1	1,5	14,14,15	0.43	0	17,19,21	0.77	1 (5%)
5	NAG	H	2	5	14,14,15	0.38	0	17,19,21	0.51	0
5	BMA	H	3	5	11,11,12	0.24	0	15,15,17	0.55	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
5	NAG	E	1	5	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	5/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	F	2	5	-	3/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	NAG	G	1	5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	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})
5	H	1	NAG	O5-C1-C2	-2.24	107.83	111.29

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C1-C2-N2-C7
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	F	1	NAG	C8-C7-N2-C2
5	F	1	NAG	O7-C7-N2-C2
5	F	2	NAG	C3-C2-N2-C7
5	F	2	NAG	C8-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	G	1	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	E	1	NAG	C8-C7-N2-C2
5	E	2	NAG	O5-C5-C6-O6
5	E	1	NAG	O7-C7-N2-C2
5	G	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C4-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	H	2	NAG	C3-C2-N2-C7
5	F	1	NAG	O5-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2

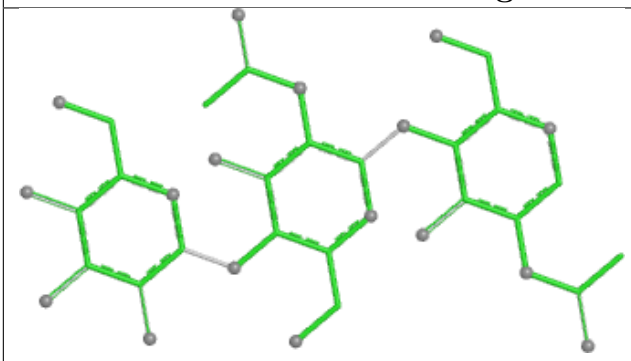
There are no ring outliers.

7 monomers are involved in 11 short contacts:

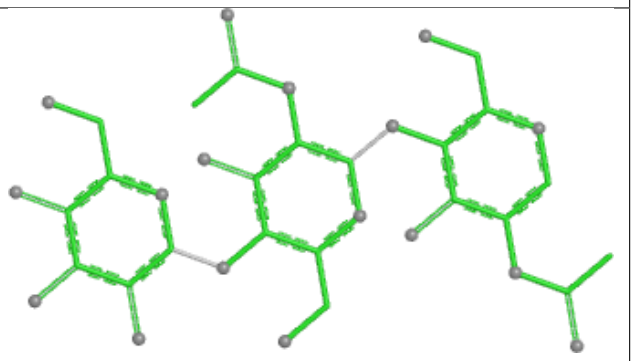
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1	NAG	5	0
5	H	1	NAG	2	0
5	E	3	BMA	1	0
5	F	1	NAG	2	0
5	E	2	NAG	1	0
5	G	2	NAG	1	0
5	G	3	BMA	1	0

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

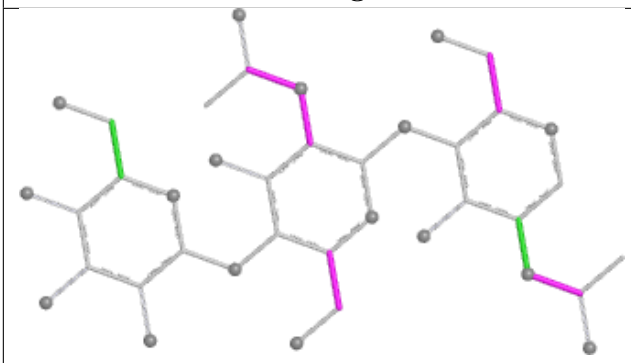
Oligosaccharide Chain E



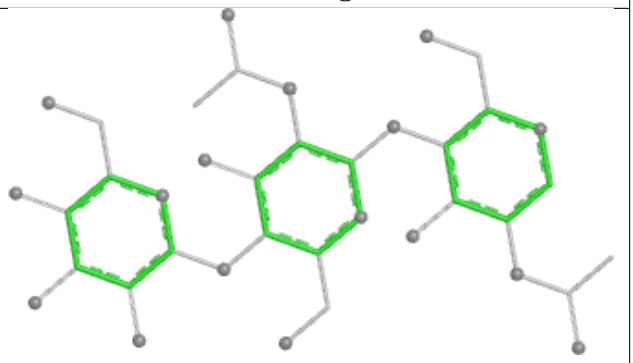
Bond lengths



Bond angles

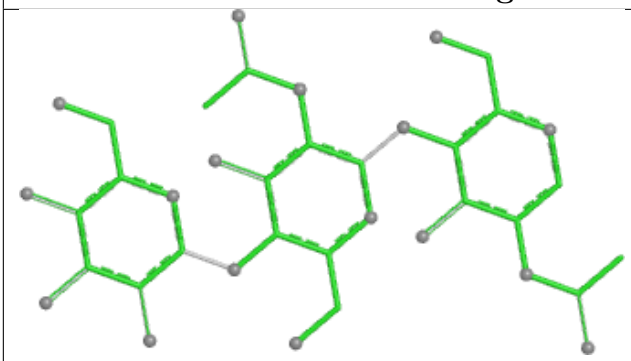


Torsions

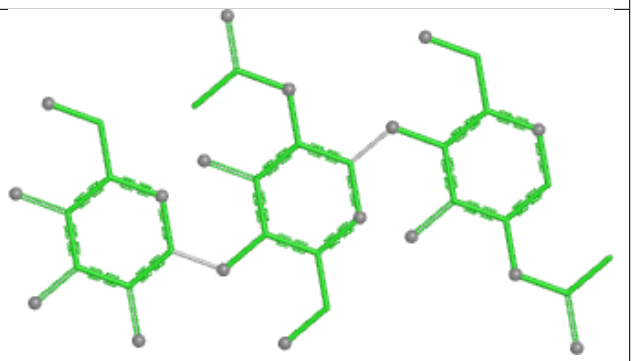


Rings

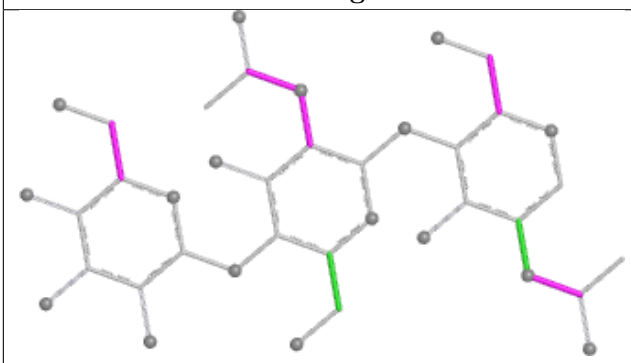
Oligosaccharide Chain F



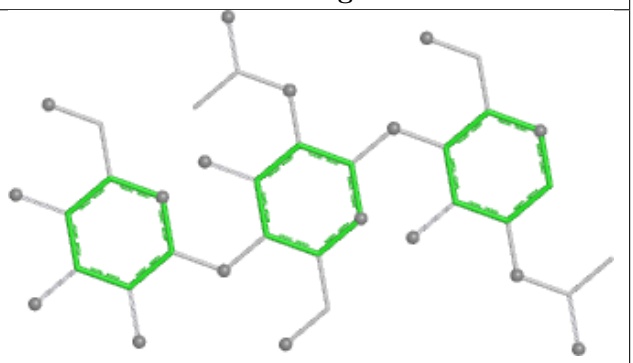
Bond lengths



Bond angles

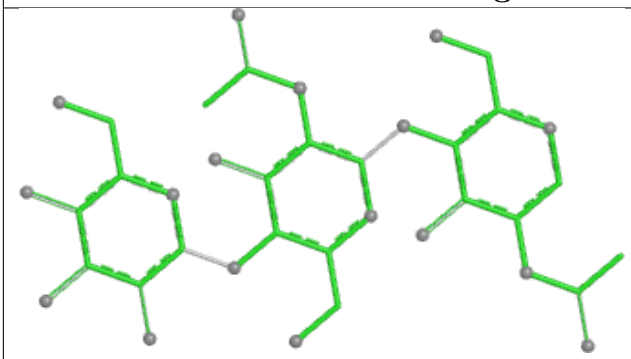


Torsions

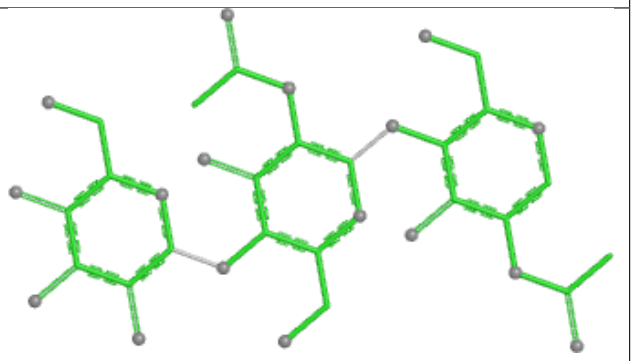


Rings

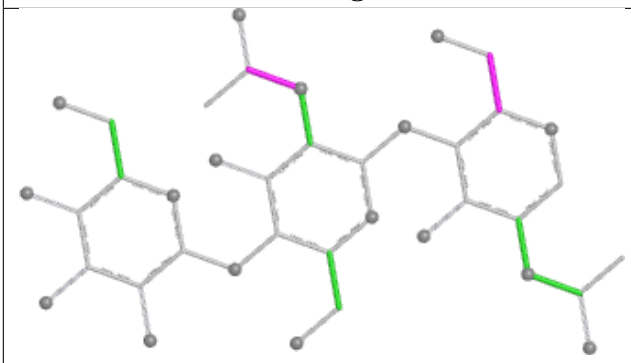
Oligosaccharide Chain G



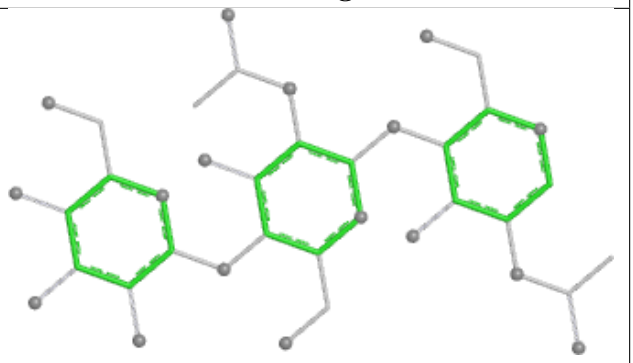
Bond lengths



Bond angles

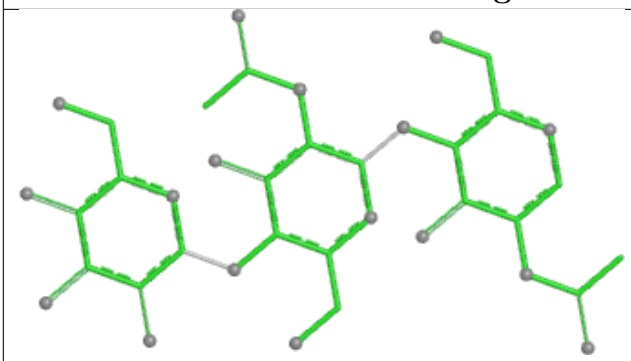


Torsions

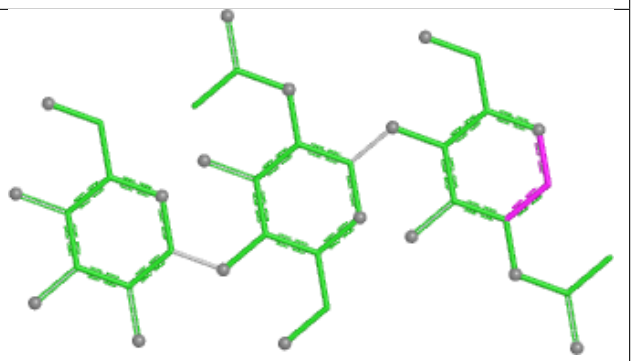


Rings

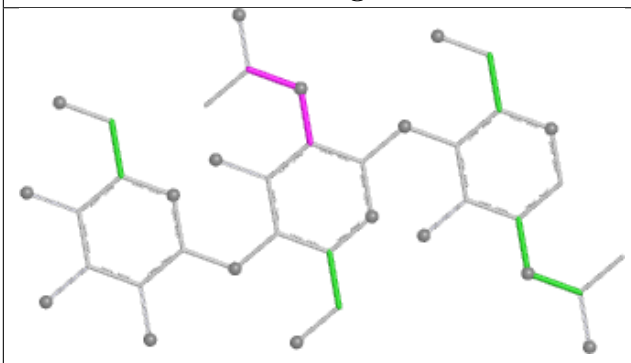
Oligosaccharide Chain H



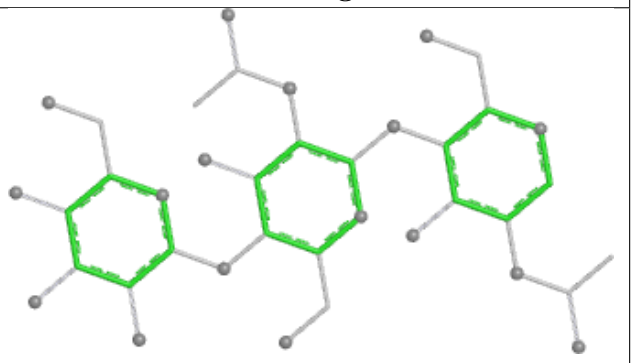
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

4 ligands 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	$\#\|Z\| > 2$
6	NAG	a	501	3	14,14,15	0.39	0	17,19,21	1.02	3 (17%)
6	NAG	b	501	4	14,14,15	0.40	0	17,19,21	1.14	3 (17%)
6	NAG	c	501	4	14,14,15	0.38	0	17,19,21	1.05	3 (17%)
6	NAG	d	501	3	14,14,15	0.38	0	17,19,21	1.07	3 (17%)

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
6	NAG	a	501	3	-	4/6/23/26	0/1/1/1
6	NAG	b	501	4	-	3/6/23/26	0/1/1/1
6	NAG	c	501	4	-	3/6/23/26	0/1/1/1
6	NAG	d	501	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	b	501	NAG	C1-C2-N2	2.84	114.91	110.43
6	d	501	NAG	C2-N2-C7	2.82	126.68	122.90
6	c	501	NAG	C1-C2-N2	2.67	114.64	110.43
6	b	501	NAG	C2-N2-C7	2.66	126.46	122.90
6	a	501	NAG	C1-O5-C5	2.41	115.42	112.19
6	d	501	NAG	C1-C2-N2	2.36	114.15	110.43
6	c	501	NAG	C1-O5-C5	2.35	115.34	112.19
6	a	501	NAG	C1-C2-N2	2.33	114.11	110.43
6	b	501	NAG	C1-O5-C5	2.32	115.29	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	a	501	NAG	C2-N2-C7	2.31	126.00	122.90
6	d	501	NAG	C1-O5-C5	2.10	115.00	112.19
6	c	501	NAG	C2-N2-C7	2.08	125.69	122.90

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	a	501	NAG	C1-C2-N2-C7
6	b	501	NAG	C1-C2-N2-C7
6	b	501	NAG	C8-C7-N2-C2
6	b	501	NAG	O7-C7-N2-C2
6	c	501	NAG	C1-C2-N2-C7
6	c	501	NAG	C8-C7-N2-C2
6	c	501	NAG	O7-C7-N2-C2
6	d	501	NAG	C8-C7-N2-C2
6	d	501	NAG	O7-C7-N2-C2
6	a	501	NAG	C8-C7-N2-C2
6	a	501	NAG	O7-C7-N2-C2
6	a	501	NAG	C3-C2-N2-C7
6	d	501	NAG	C3-C2-N2-C7
6	d	501	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.

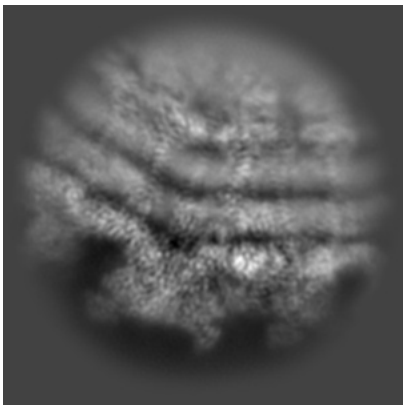
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-72748. These allow visual inspection of the internal detail of the map and identification of artifacts.

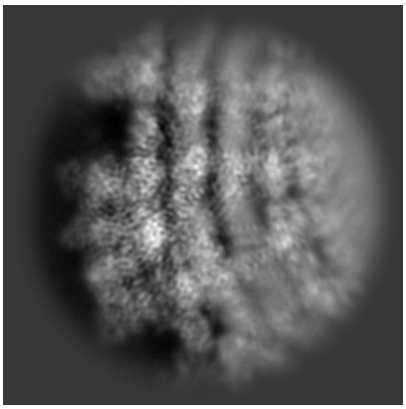
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

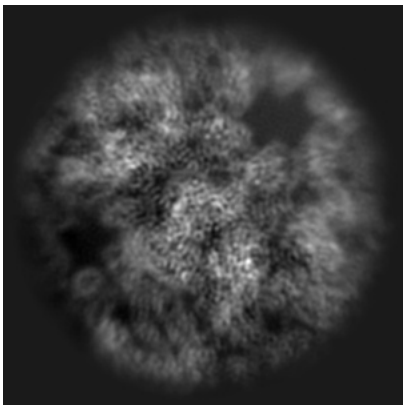
6.1.1 Primary map



X

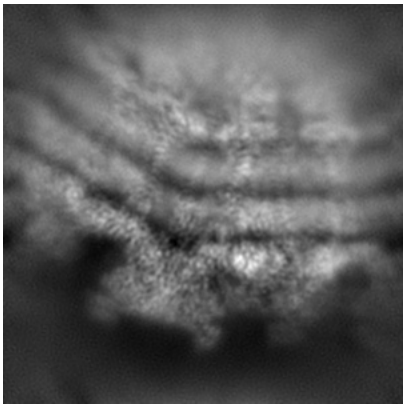


Y

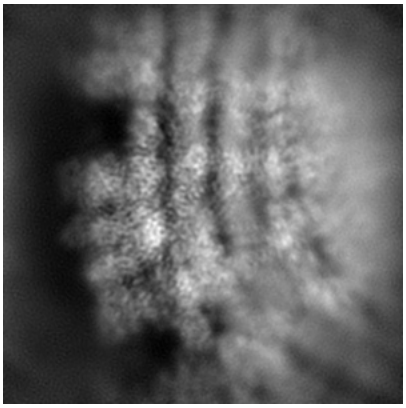


Z

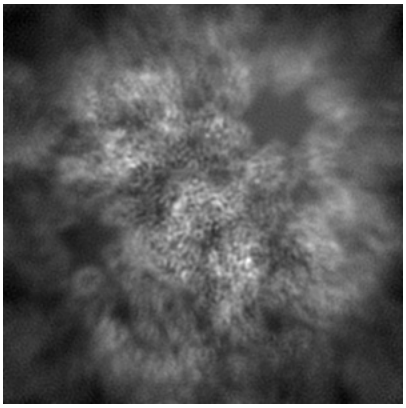
6.1.2 Raw map



X



Y

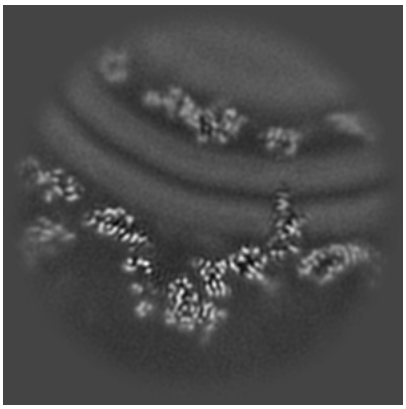


Z

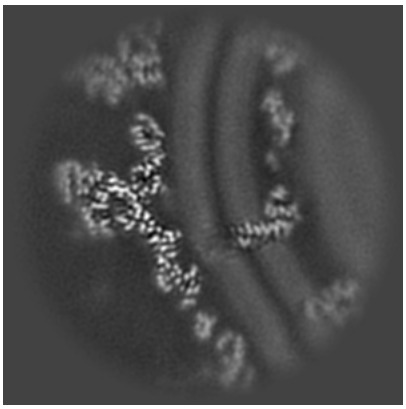
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

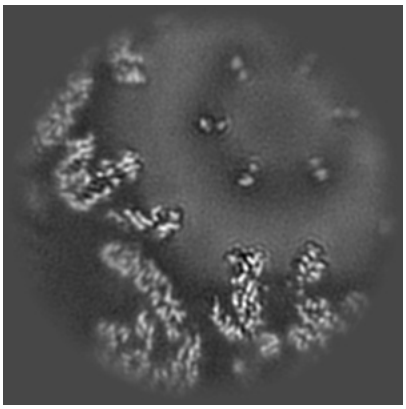
6.2.1 Primary map



X Index: 105

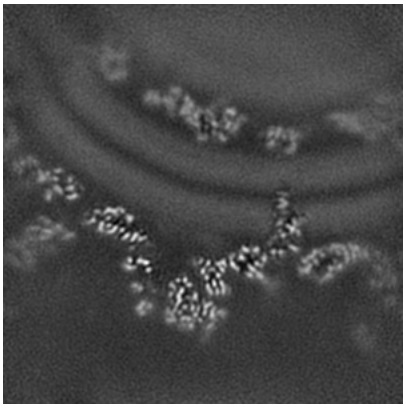


Y Index: 105

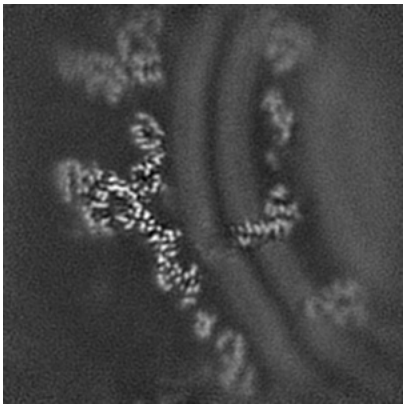


Z Index: 105

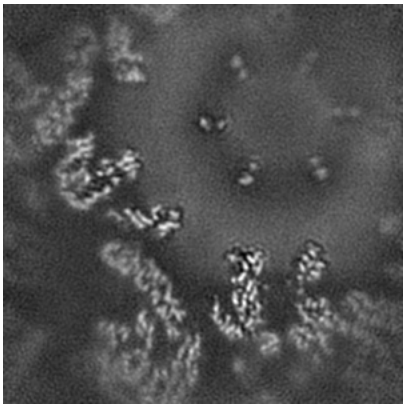
6.2.2 Raw map



X Index: 105



Y Index: 105

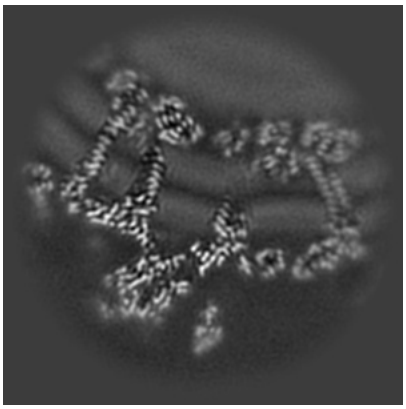


Z Index: 105

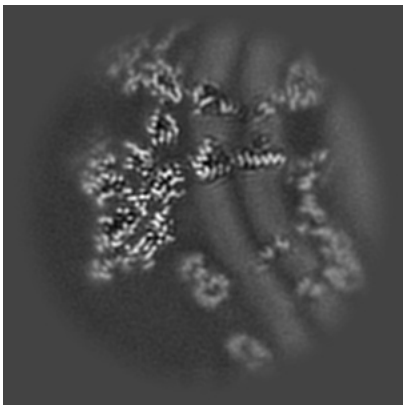
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

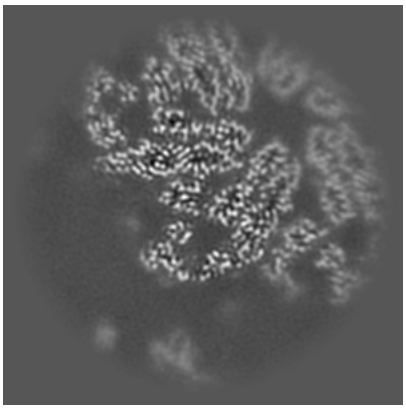
6.3.1 Primary map



X Index: 124

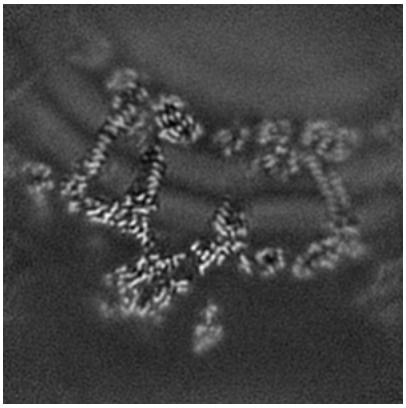


Y Index: 76

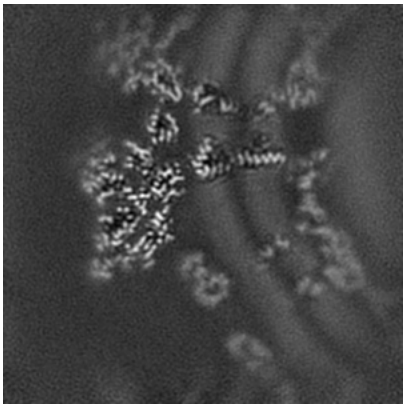


Z Index: 76

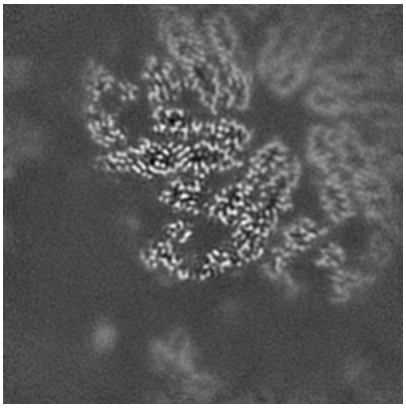
6.3.2 Raw map



X Index: 124



Y Index: 76

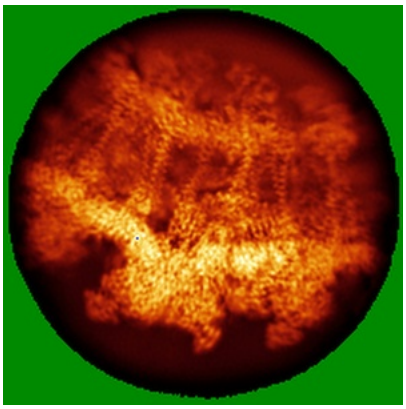


Z Index: 76

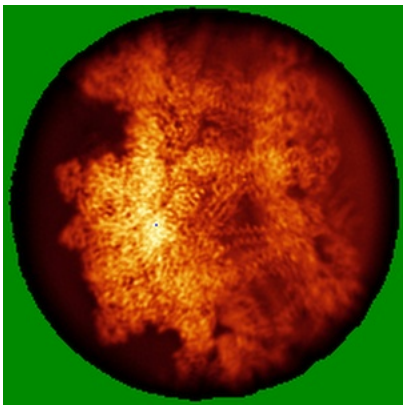
The images above show the largest variance slices of the map in three orthogonal directions.

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

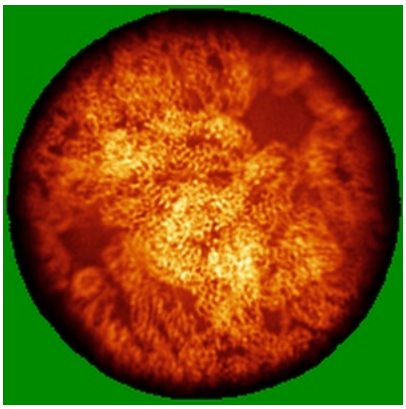
6.4.1 Primary map



X

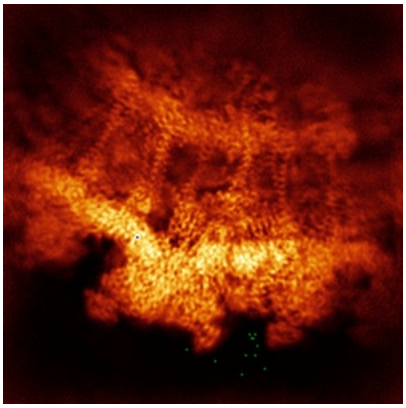


Y

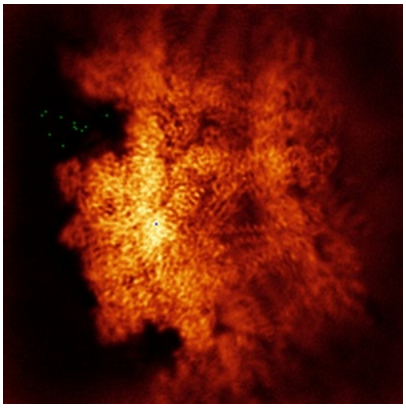


Z

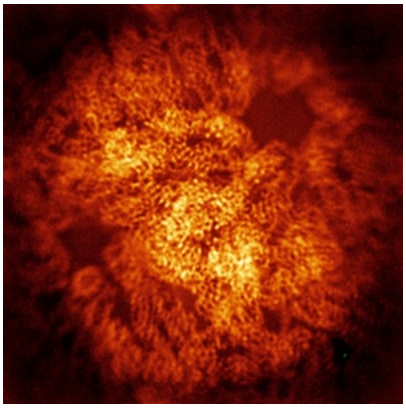
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

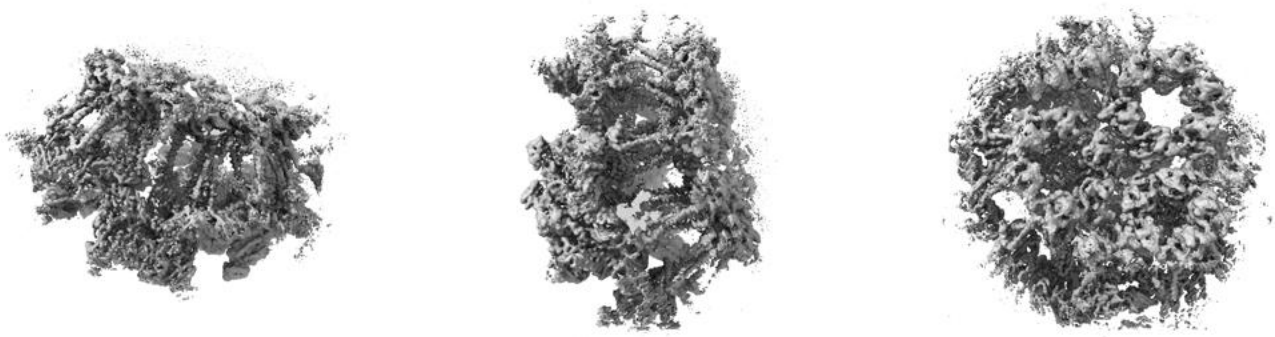
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

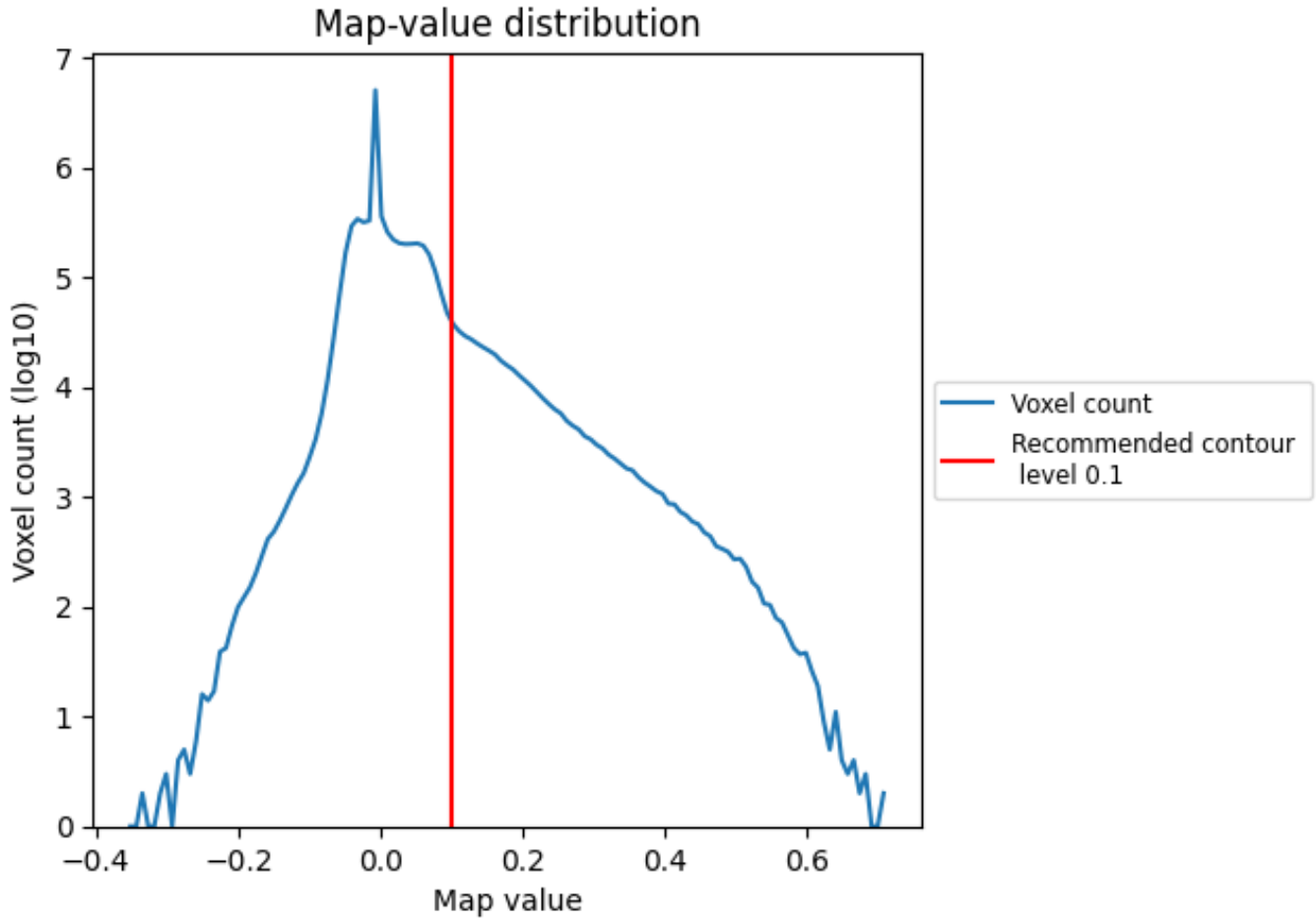
6.6 Mask visualisation (i)

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

7 Map analysis

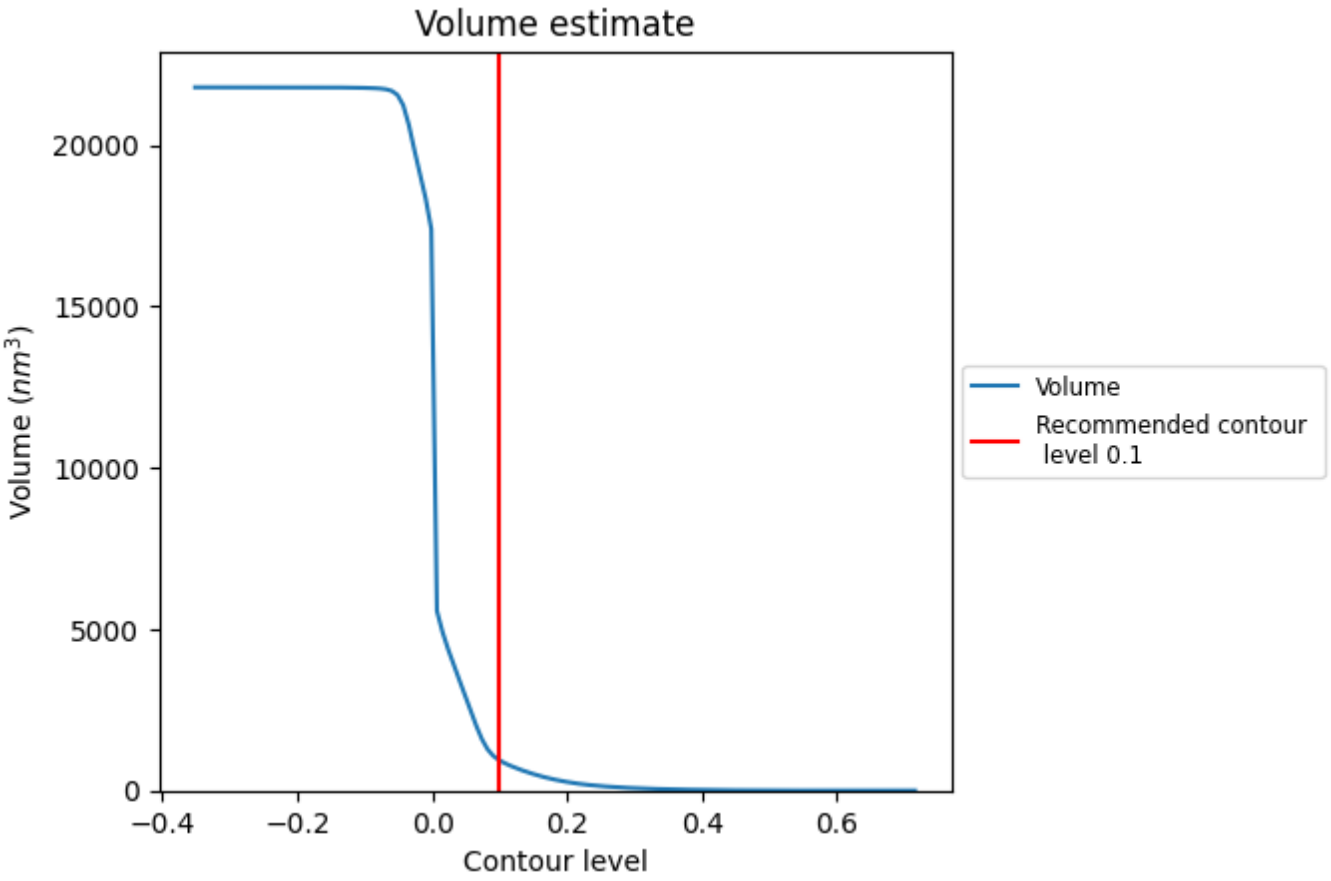
This section contains the results of statistical analysis of the map.

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.

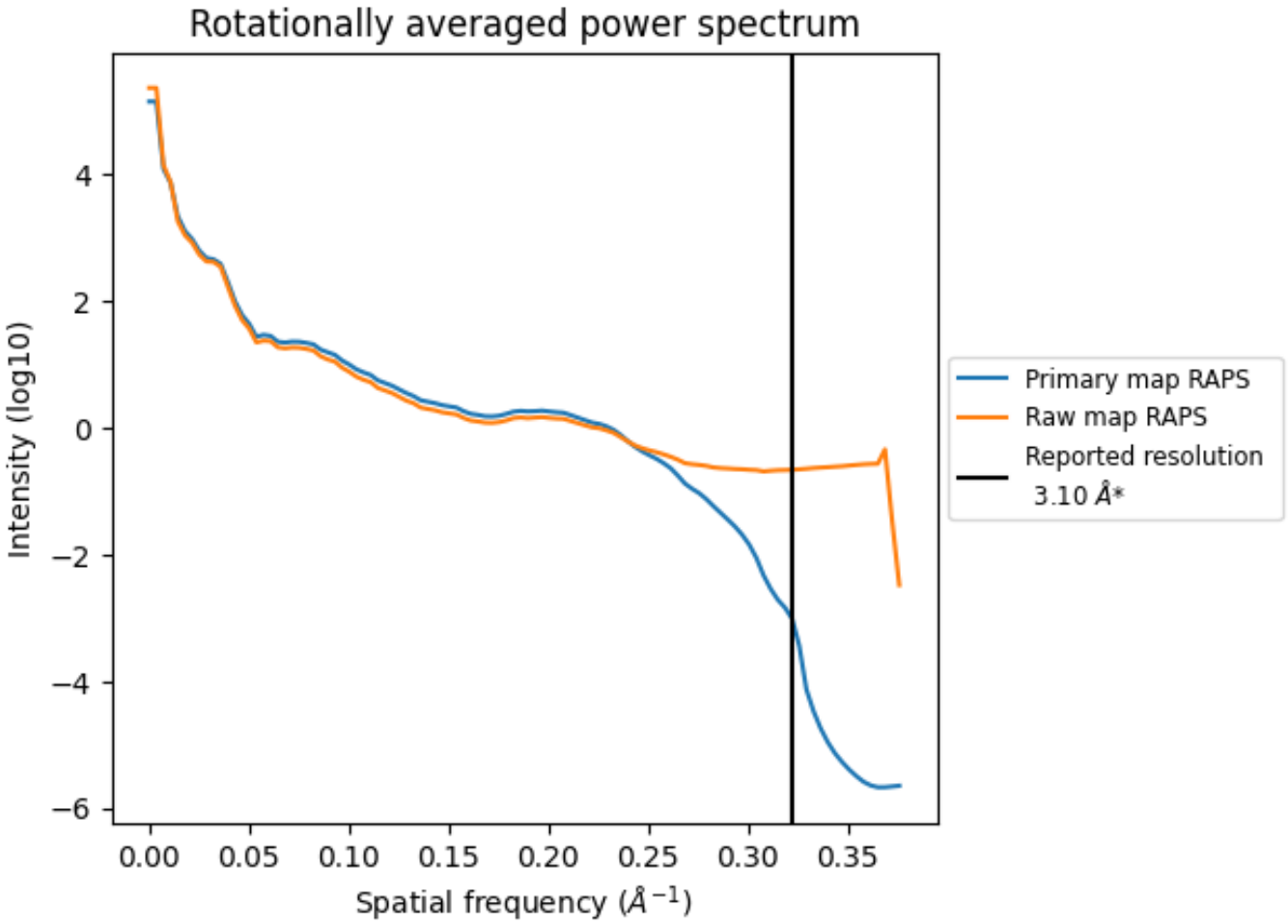
7.2 Volume estimate



The volume at the recommended contour level is 933 nm^3; this corresponds to an approximate mass of 843 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)

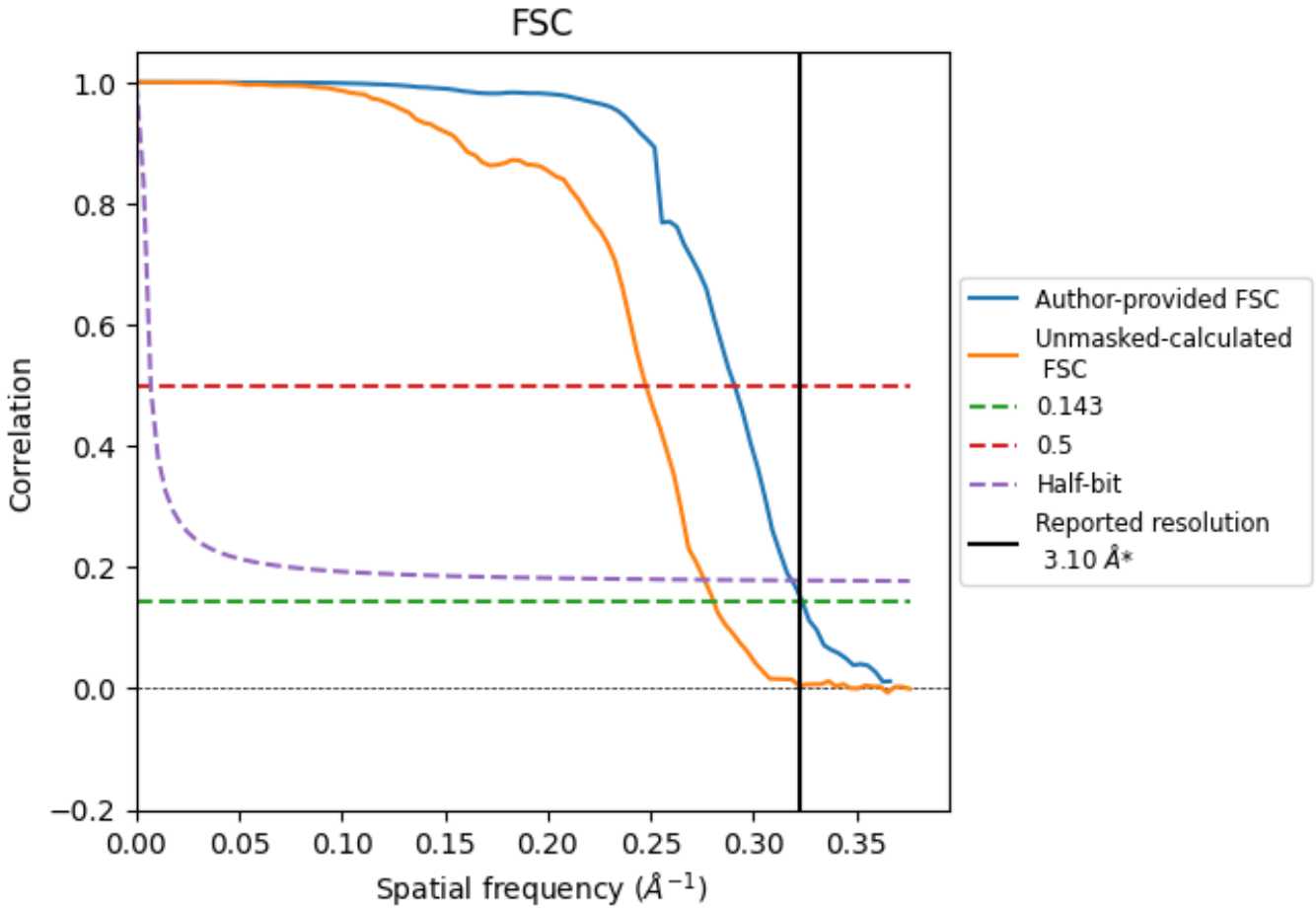


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

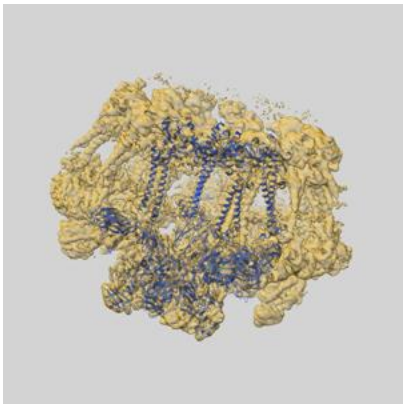
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.09	3.44	3.14
Unmasked-calculated*	3.56	4.04	3.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.56 differs from the reported value 3.1 by more than 10 %

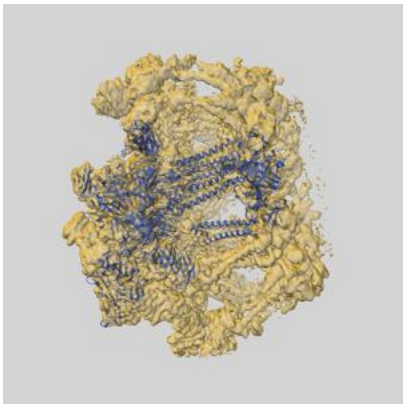
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-72748 and PDB model 9YB4. Per-residue inclusion information can be found in section 3 on page 7.

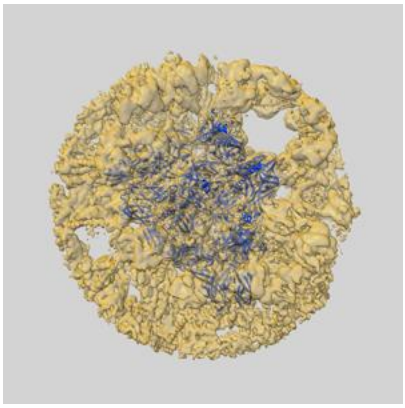
9.1 Map-model overlay



X



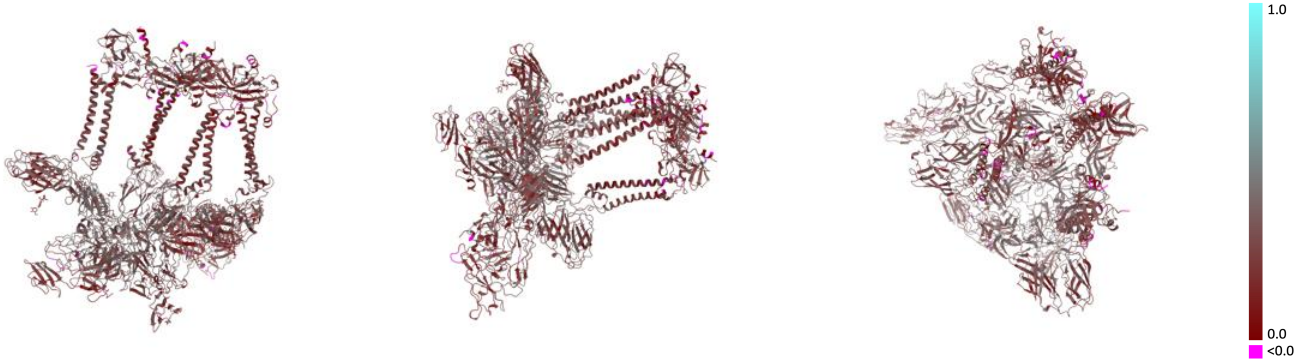
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

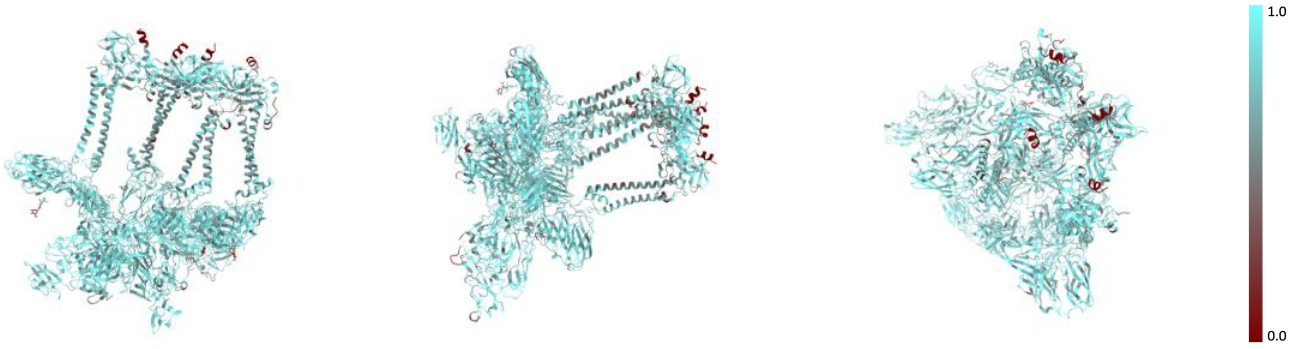
9.2 Q-score mapped to coordinate model (i)



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.

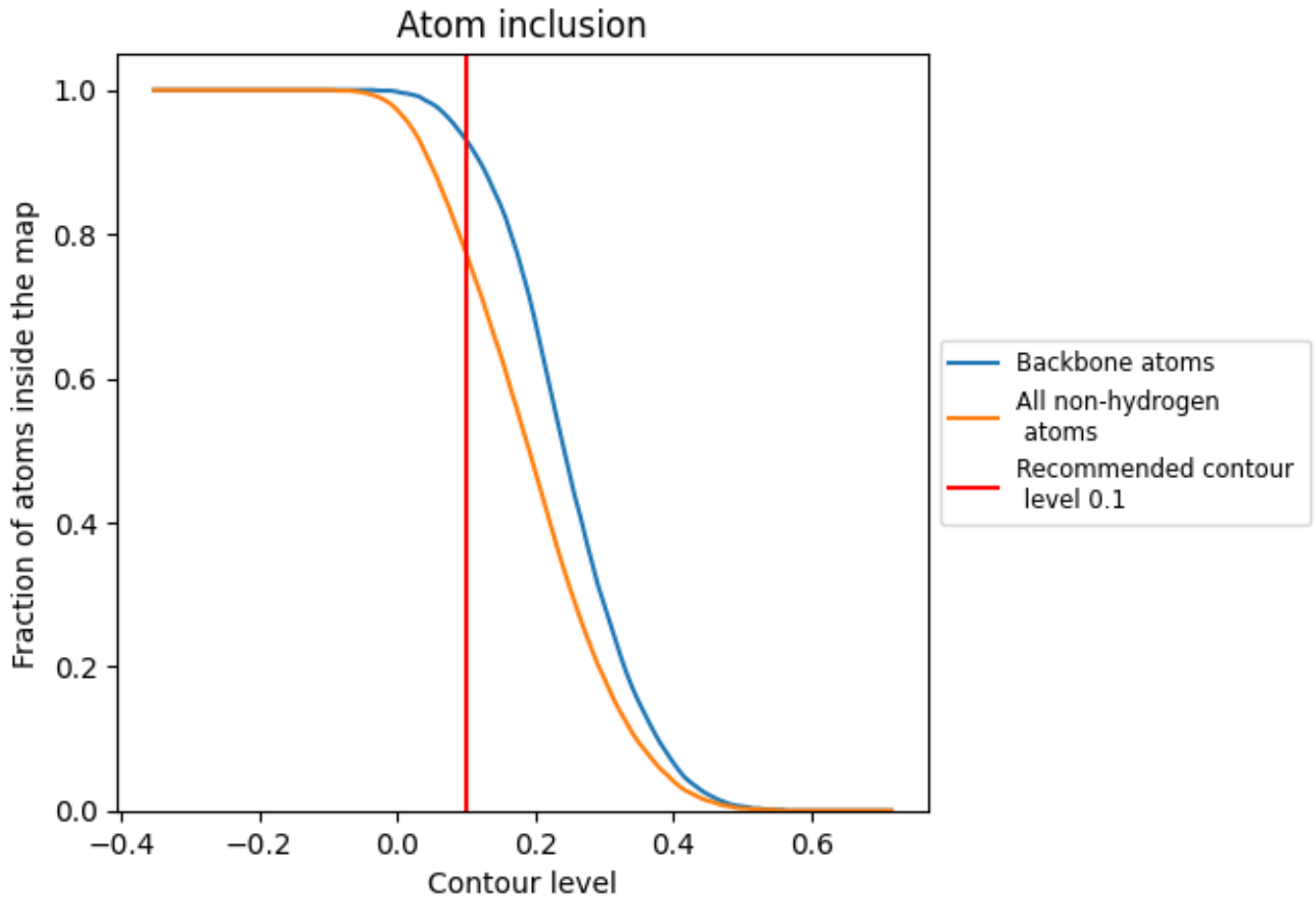
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 77% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7740	0.2960
A	0.7870	0.3070
B	0.7970	0.3140
C	0.8030	0.3120
D	0.8010	0.3130
E	0.3080	0.1240
F	0.5900	0.2560
G	0.4100	0.2020
H	0.5640	0.3350
P	0.6760	0.2390
Q	0.6970	0.2490
R	0.7230	0.2960
S	0.6820	0.2780
a	0.7500	0.2620
b	0.7920	0.2980
c	0.8090	0.3210
d	0.7870	0.2900

