Full wwPDB EM Validation Report (i)

Aug 15, 2026 – 01:18 PM EDT

PDB ID	:	9YB2 / pdb_00009yb2
EMDB ID	:	EMD-72746
Title	:	Localized reconstruction of the asymmetric unit of SINV/EEEV at 40C sample.
Authors	:	Bandyopadhyay, A.; Klose, T.; Kuhn, R.J.
Deposited on	:	2025-09-16
Resolution	:	4.10 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 (i) 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 (1)) were used in the production of this report:

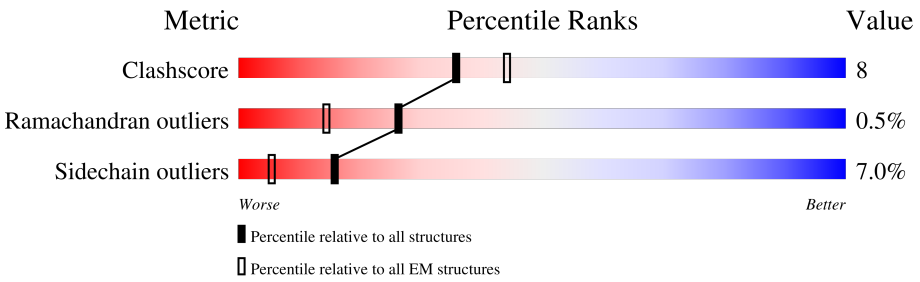
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13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

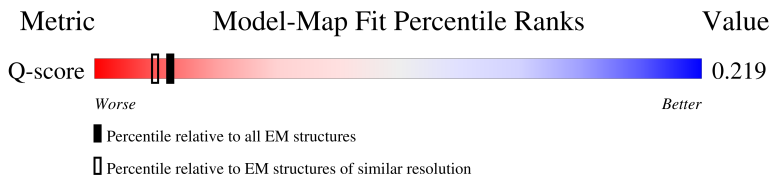
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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	437	75% 22%
1	B	437	70% 26%
1	C	437	81% 18%
1	D	437	74% 22%

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Mol	Chain	Length	Quality of chain
2	P	160	6% 89% 9%
2	Q	160	5% 92% 8%
2	R	160	88% 11%
2	S	160	7% 88% 12%
3	a	420	6% 76% 22%
3	b	420	8% 73% 24%
3	c	420	5% 78% 21%
3	d	420	7% 73% 24%
4	E	3	33% 33% 67%
4	F	3	33% 33% 67%
4	G	3	33% 67% 33%
4	H	3	67% 67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	d	501	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31679 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
			Total	C	N	O	S		
1	C	437	3329	2121	551	637	20	0	0
1	D	437	3329	2121	551	637	20	0	0
1	B	437	3329	2121	551	637	20	0	0
1	A	437	3329	2121	551	637	20	0	0

- Molecule 2 is a protein called Capsid protein.

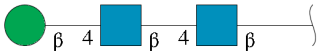
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	R	159	1230	773	219	231	7	0	0
2	S	160	1239	778	221	233	7	0	0
2	Q	160	1239	778	221	233	7	0	0
2	P	160	1239	778	221	233	7	0	0

- Molecule 3 is a protein called E2 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	420	3301	2087	598	592	24	0	0
3	d	420	3301	2087	598	592	24	0	0
3	b	420	3301	2087	598	592	24	0	0
3	a	420	3301	2087	598	592	24	0	0

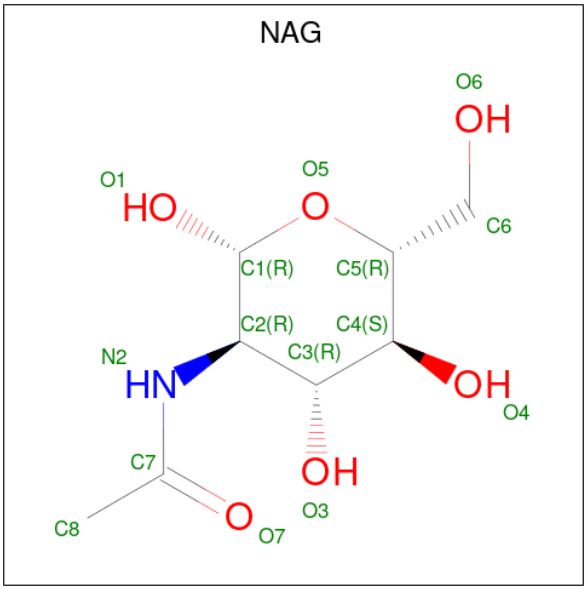
- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



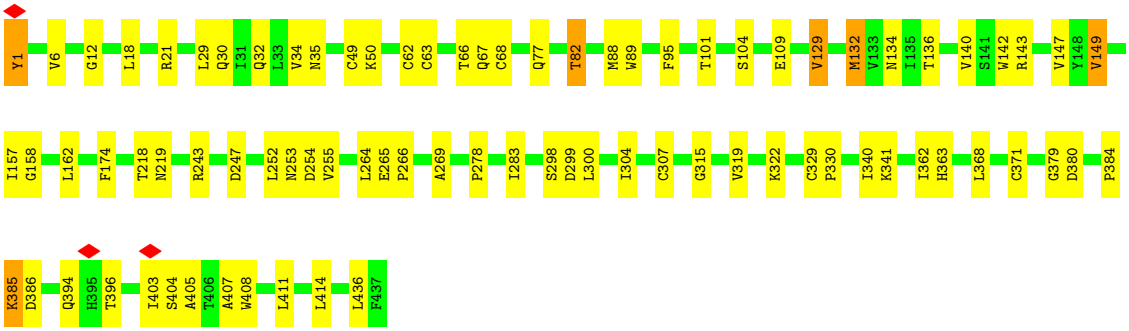
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	c	1	14	8	1	5	0
5	d	1	14	8	1	5	0
5	b	1	14	8	1	5	0
5	a	1	14	8	1	5	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

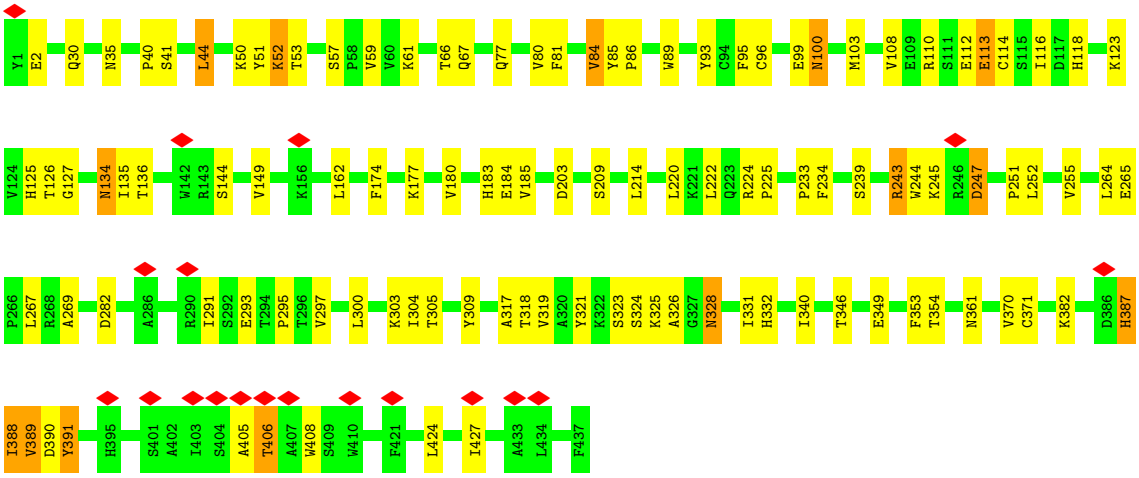
• Molecule 1: E1 glycoprotein

Chain C:



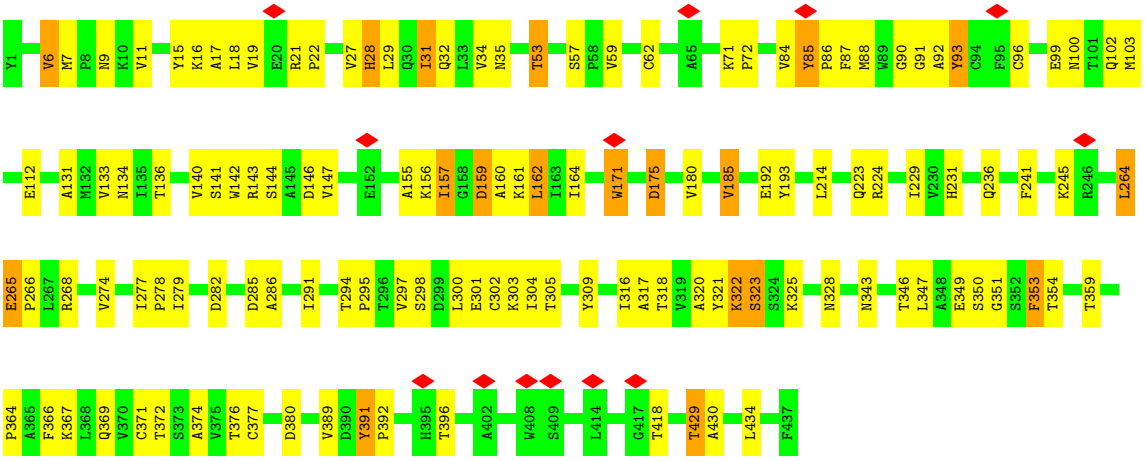
• Molecule 1: E1 glycoprotein

Chain D:



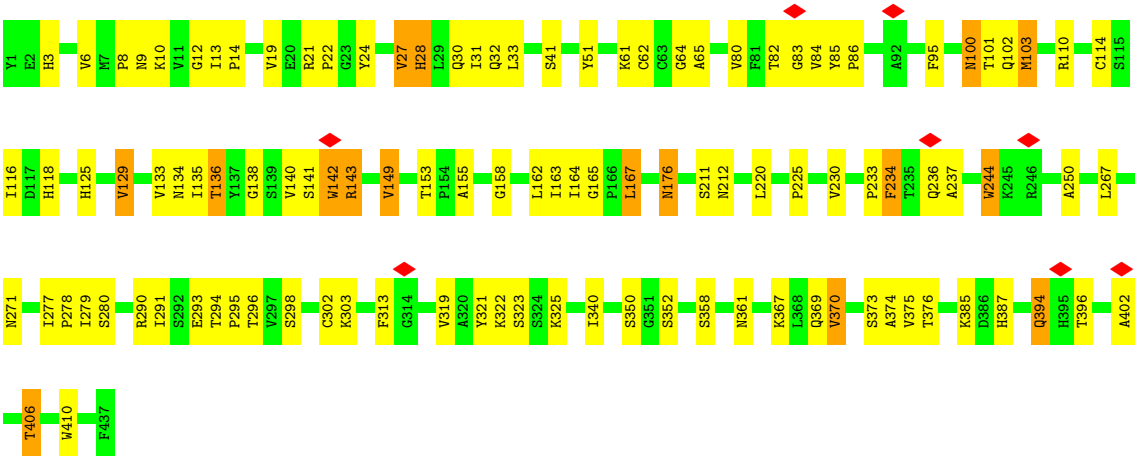
• Molecule 1: E1 glycoprotein

Chain B:



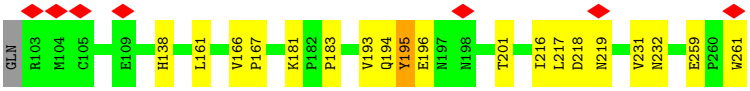
- Molecule 1: E1 glycoprotein

Chain A:



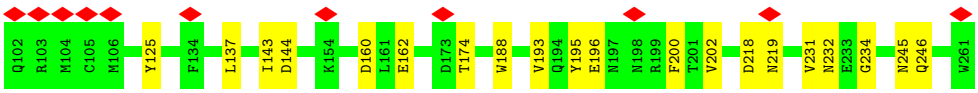
- Molecule 2: Capsid protein

Chain R:



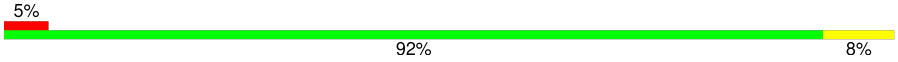
- Molecule 2: Capsid protein

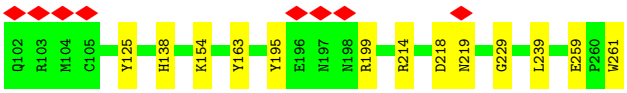
Chain S:



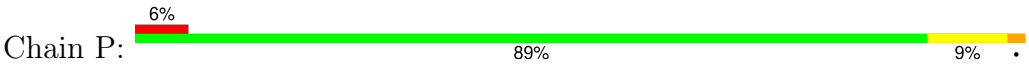
- Molecule 2: Capsid protein

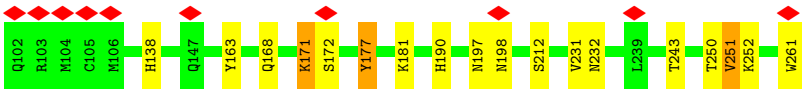
Chain Q:



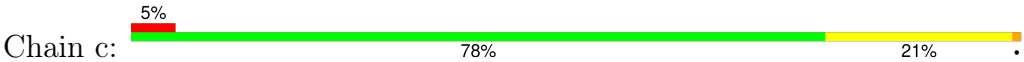


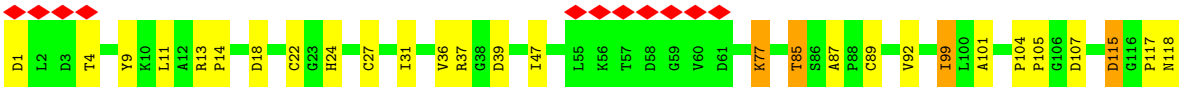
• Molecule 2: Capsid protein

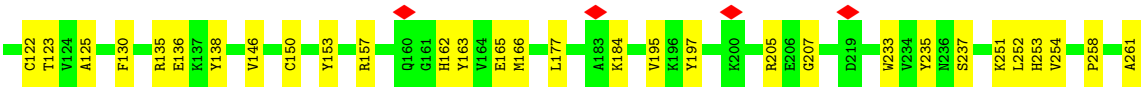


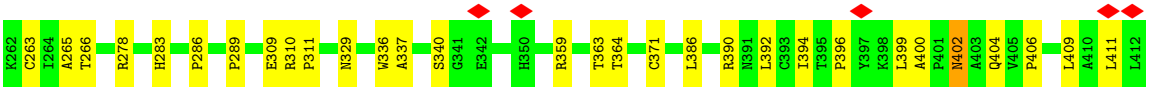


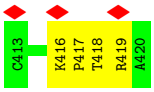
• Molecule 3: E2 glycoprotein



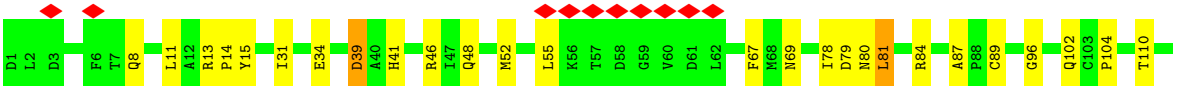


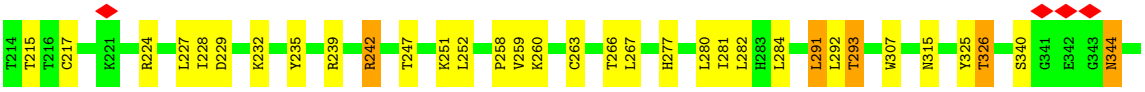


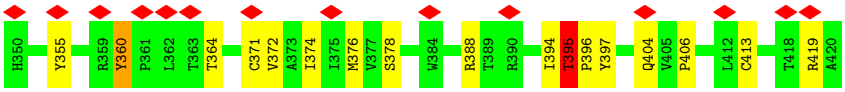




• Molecule 3: E2 glycoprotein

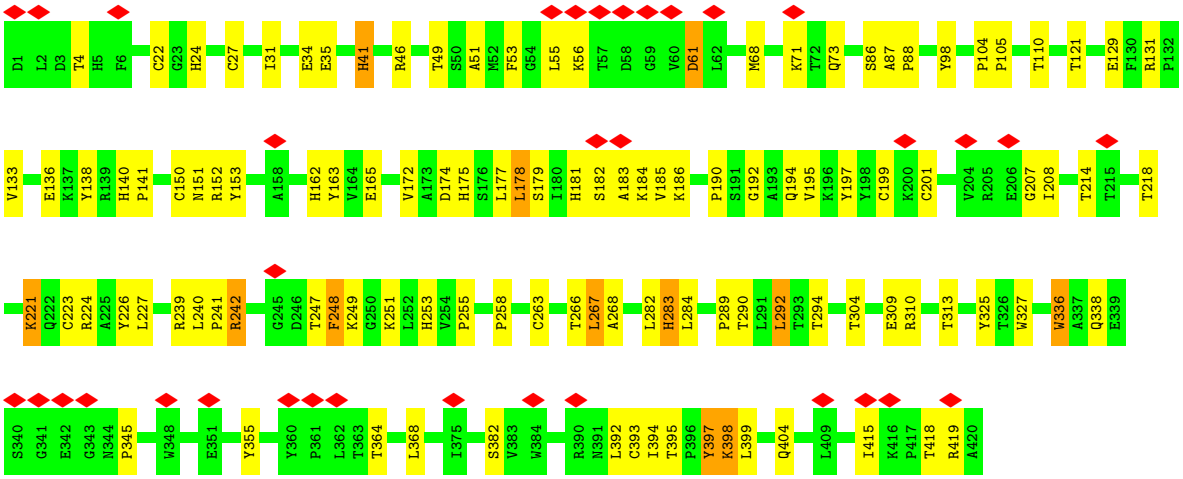






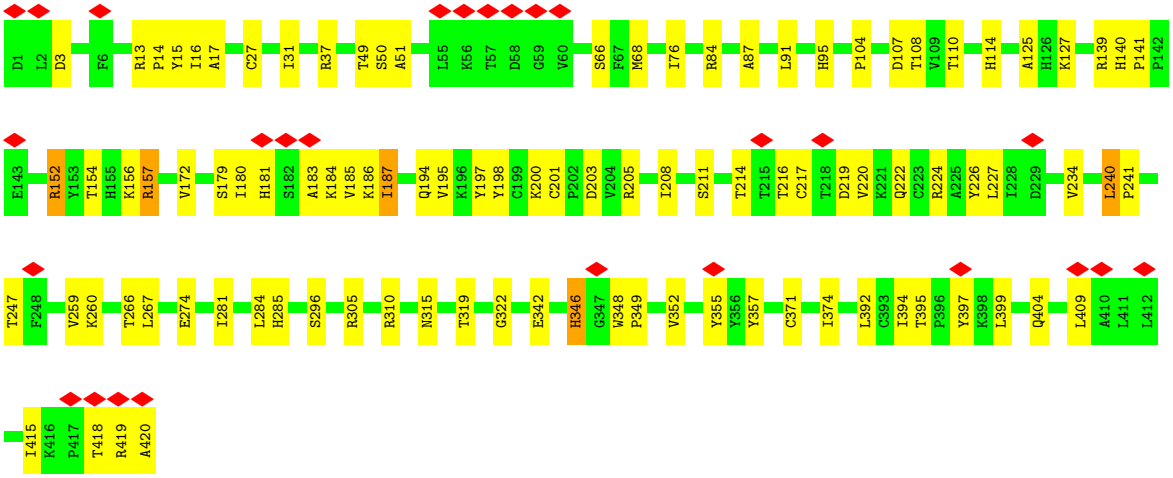
• Molecule 3: E2 glycoprotein

Chain b:



• Molecule 3: E2 glycoprotein

Chain a:



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

Chain E:

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

Chain F:

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

Chain G:

• Molecule 4: 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	428120	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	1.763	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	292.6, 292.6, 292.6	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.30	0/3419	0.47	1/4668 (0.0%)
1	B	0.27	0/3419	0.50	0/4668
1	C	0.37	1/3419 (0.0%)	0.68	0/4668
1	D	0.30	0/3419	0.57	1/4668 (0.0%)
2	P	0.59	0/1266	1.14	2/1711 (0.1%)
2	Q	0.32	0/1266	0.76	0/1711
2	R	0.39	0/1257	0.76	0/1699
2	S	0.39	0/1266	0.87	0/1711
3	a	0.34	0/3396	0.61	0/4631
3	b	0.35	0/3396	0.60	0/4631
3	c	0.38	0/3396	0.65	4/4631 (0.1%)
3	d	0.29	0/3396	0.56	1/4631 (0.0%)
All	All	0.35	1/32315 (0.0%)	0.64	9/44028 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
2	P	0	2
2	Q	0	1
2	R	0	1
3	a	0	2
3	b	0	1
3	c	0	2
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	386	ASP	N-CA	-5.04	1.39	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	c	418	THR	CA-CB-CG2	5.75	120.27	110.50
3	c	418	THR	CA-C-N	5.64	132.31	121.54
3	c	418	THR	C-N-CA	5.64	132.31	121.54
3	c	404	GLN	OE1-CD-NE2	-5.48	117.12	122.60
2	P	171	LYS	CA-CB-CG	5.48	125.06	114.10
1	D	309	TYR	CA-CB-CG	5.30	123.44	113.90
2	P	190	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	A	385	LYS	CD-CE-NZ	-5.11	95.56	111.90
3	d	395	THR	N-CA-C	5.06	121.00	109.81

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ARG	Sidechain
1	B	268	ARG	Peptide
1	D	391	TYR	Peptide
2	P	163	TYR	Sidechain
2	P	177	TYR	Sidechain
2	Q	259	GLU	Peptide
2	R	259	GLU	Peptide
3	a	152	ARG	Sidechain
3	a	310	ARG	Sidechain
3	b	55	LEU	Peptide
3	c	205	ARG	Peptide
3	c	419	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	3329	0	3239	63	0
1	B	3329	0	3239	81	0
1	C	3329	0	3238	39	0
1	D	3329	0	3239	69	0
2	P	1239	0	1225	8	0
2	Q	1239	0	1225	6	0
2	R	1230	0	1217	8	0
2	S	1239	0	1225	11	0
3	a	3301	0	3262	47	0
3	b	3301	0	3262	62	0
3	c	3301	0	3262	43	0
3	d	3301	0	3263	78	0
4	E	39	0	34	1	0
4	F	39	0	34	1	0
4	G	39	0	34	0	0
4	H	39	0	34	0	0
5	a	14	0	13	0	0
5	b	14	0	13	0	0
5	c	14	0	13	0	0
5	d	14	0	13	7	0
All	All	31679	0	31084	492	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 (492) 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:d:281:ILE:HG23	5:d:501:NAG:H81	1.47	0.97
1:C:385:LYS:HA	3:c:340:SER:HB2	1.54	0.88
3:d:281:ILE:HG23	5:d:501:NAG:C8	2.04	0.87
2:R:183:PRO:HB3	2:R:196:GLU:HA	1.58	0.83
3:a:201:CYS:HB2	3:a:216:THR:HB	1.61	0.80
1:B:391:TYR:CD2	1:B:392:PRO:HD2	2.17	0.79
3:d:281:ILE:CG2	5:d:501:NAG:H81	2.14	0.77
1:A:41:SER:HB2	1:A:125:HIS:HB2	1.67	0.76
3:b:395:THR:HB	3:b:398:LYS:HB2	1.67	0.75
2:S:193:VAL:HG21	2:S:200:PHE:HB3	1.69	0.74
3:c:162:HIS:O	3:c:253:HIS:ND1	2.22	0.73
3:c:336:TRP:CD1	3:c:337:ALA:H	2.07	0.72
3:b:283:HIS:HB3	3:b:313:THR:HG22	1.71	0.72
1:B:7:MET:HE3	1:B:15:TYR:CD1	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:VAL:O	1:A:100:ASN:ND2	2.24	0.71
3:d:197:TYR:H	3:d:205:ARG:HH11	1.39	0.71
3:b:152:ARG:NH1	3:b:263:CYS:SG	2.64	0.71
1:C:49:CYS:SG	1:C:50:LYS:N	2.64	0.70
1:B:140:VAL:O	1:B:142:TRP:CD1	2.45	0.70
1:B:32:GLN:O	1:B:134:ASN:N	2.23	0.69
1:D:183:HIS:HA	1:D:264:LEU:HD21	1.74	0.69
1:C:143:ARG:NH2	1:C:157:ILE:O	2.26	0.69
1:B:297:VAL:HG12	1:B:323:SER:HB3	1.74	0.69
1:B:62:CYS:SG	3:b:226:TYR:OH	2.50	0.68
1:D:41:SER:HB3	1:D:125:HIS:HB3	1.74	0.68
3:d:8:GLN:HG3	3:d:252:LEU:HD13	1.76	0.68
1:D:252:LEU:HA	1:D:255:VAL:HG22	1.75	0.68
2:R:195:TYR:HD2	2:R:201:THR:HG22	1.60	0.67
2:P:168:GLN:HA	2:P:171:LYS:HG3	1.77	0.67
3:d:31:ILE:HG13	3:d:113:PHE:HE1	1.60	0.67
1:C:82:THR:HA	1:C:101:THR:HA	1.76	0.67
1:C:12:GLY:O	1:C:32:GLN:NE2	2.29	0.66
1:B:418:THR:HG23	3:b:382:SER:HB3	1.78	0.66
1:C:140:VAL:O	1:C:142:TRP:CD1	2.49	0.66
1:A:62:CYS:SG	3:a:226:TYR:OH	2.54	0.65
3:d:80:ASN:ND2	3:d:114:HIS:O	2.20	0.65
1:B:57:SER:OG	3:b:240:LEU:O	2.15	0.65
1:B:143:ARG:NH2	1:B:157:ILE:O	2.31	0.64
3:d:360:TYR:CD2	3:d:364:THR:HG23	2.32	0.64
1:D:323:SER:N	1:D:349:GLU:OE1	2.29	0.64
3:a:179:SER:O	3:a:186:LYS:N	2.20	0.64
1:B:71:LYS:HG3	1:B:72:PRO:HD2	1.78	0.64
3:b:181:HIS:HB3	3:b:184:LYS:H	1.62	0.64
1:B:6:VAL:HA	1:B:278:PRO:HA	1.79	0.63
1:A:116:ILE:HD12	3:a:260:LYS:HB2	1.80	0.63
1:C:363:HIS:CD2	1:C:405:ALA:HB2	2.33	0.63
3:a:201:CYS:HB2	3:a:217:CYS:H	1.64	0.63
1:C:304:ILE:HG21	1:C:379:GLY:HA3	1.78	0.63
1:B:34:VAL:HG22	1:B:35:ASN:HD22	1.65	0.62
3:c:87:ALA:HB3	3:c:104:PRO:HG3	1.82	0.62
3:d:87:ALA:HB3	3:d:104:PRO:HG3	1.81	0.62
3:b:221:LYS:O	3:b:224:ARG:NH1	2.32	0.62
1:A:21:ARG:NH2	1:A:22:PRO:O	2.33	0.62
1:B:301:GLU:O	1:B:320:ALA:N	2.26	0.61
3:a:14:PRO:HG2	3:a:68:MET:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:NH1	1:A:211:SER:O	2.33	0.61
3:a:108:THR:HG22	3:a:125:ALA:HA	1.81	0.61
1:C:34:VAL:HB	1:C:132:MET:HB3	1.83	0.61
3:b:87:ALA:HB3	3:b:104:PRO:HG3	1.83	0.61
3:d:14:PRO:HB3	3:d:52:MET:H	1.65	0.61
1:D:134:ASN:ND2	1:D:144:SER:HB3	2.16	0.60
1:D:57:SER:HB2	3:d:242:ARG:HG2	1.83	0.60
3:b:185:VAL:O	3:b:214:THR:OG1	2.18	0.60
2:S:218:ASP:OD1	2:S:219:ASN:N	2.35	0.60
1:D:110:ARG:NH1	1:D:209:SER:O	2.34	0.60
3:b:41:HIS:ND1	3:b:151:ASN:OD1	2.34	0.60
1:B:323:SER:H	1:B:350:SER:H	1.48	0.60
1:B:159:ASP:OD1	1:B:159:ASP:N	2.35	0.60
1:B:318:THR:HA	1:B:354:THR:HA	1.83	0.59
3:d:187:ILE:H	3:d:213:HIS:CD2	2.19	0.59
1:B:32:GLN:HB3	1:B:134:ASN:HB3	1.84	0.59
1:C:1:TYR:HD1	1:C:1:TYR:H1	1.50	0.59
1:A:313:PHE:HA	1:A:358:SER:HB3	1.84	0.59
3:a:140:HIS:CG	3:a:141:PRO:HD2	2.38	0.59
1:B:136:THR:O	1:B:136:THR:HG23	2.02	0.59
3:a:87:ALA:HB3	3:a:104:PRO:HG2	1.84	0.59
3:c:107:ASP:N	3:c:107:ASP:OD1	2.35	0.58
3:d:284:LEU:HD11	3:d:292:LEU:HD12	1.84	0.58
1:C:253:ASN:ND2	1:C:254:ASP:OD1	2.36	0.58
1:D:134:ASN:HD21	4:F:1:NAG:HN2	1.50	0.58
3:a:181:HIS:HB2	3:a:186:LYS:HD3	1.85	0.58
3:b:68:MET:HA	3:b:73:GLN:HA	1.85	0.58
2:S:193:VAL:HG23	2:S:202:VAL:HG13	1.85	0.58
3:d:129:GLU:HB3	3:d:131:ARG:HH11	1.68	0.58
1:D:247:ASP:OD1	1:D:247:ASP:N	2.36	0.58
1:A:165:GLY:HA2	1:A:278:PRO:HD2	1.85	0.58
2:S:245:ASN:OD1	2:S:246:GLN:N	2.37	0.58
2:P:197:ASN:CG	2:P:198:ASN:H	2.12	0.58
3:d:181:HIS:HB2	3:d:186:LYS:HG3	1.85	0.58
3:d:133:VAL:HB	3:d:148:LEU:HD23	1.86	0.58
3:d:197:TYR:O	3:d:205:ARG:NE	2.37	0.58
1:C:136:THR:HG21	4:E:1:NAG:H62	1.85	0.57
1:B:155:ALA:O	1:B:162:LEU:N	2.35	0.57
1:D:149:VAL:HG12	1:D:149:VAL:O	2.05	0.57
1:D:328:ASN:N	1:D:328:ASN:OD1	2.37	0.57
1:B:102:GLN:NE2	1:B:103:MET:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:LEU:HA	1:C:255:VAL:HG12	1.87	0.57
1:D:44:LEU:HD23	1:D:44:LEU:H	1.69	0.57
3:d:84:ARG:N	3:d:110:THR:O	2.30	0.57
3:d:79:ASP:N	3:d:79:ASP:OD1	2.36	0.57
1:C:21:ARG:HH21	1:C:21:ARG:HG3	1.69	0.56
1:B:59:VAL:HB	1:B:103:MET:HB3	1.87	0.56
1:A:155:ALA:HB3	1:A:162:LEU:HB2	1.87	0.56
3:c:166:MET:HE3	3:c:235:TYR:HB2	1.87	0.56
3:b:172:VAL:O	3:b:227:LEU:N	2.37	0.56
1:D:388:ILE:HG12	1:D:389:VAL:H	1.70	0.56
2:Q:218:ASP:OD1	2:Q:219:ASN:N	2.38	0.56
3:d:52:MET:HG3	3:d:96:GLY:HA2	1.88	0.56
3:a:219:ASP:HB2	3:a:222:GLN:HB2	1.86	0.56
1:B:96:CYS:O	1:B:100:ASN:ND2	2.39	0.56
3:b:165:GLU:HA	3:b:251:LYS:HA	1.88	0.56
1:C:407:ALA:O	1:C:411:LEU:N	2.38	0.56
1:D:95:PHE:HB2	3:d:224:ARG:HD3	1.88	0.56
1:A:163:ILE:HB	1:A:280:SER:HB2	1.86	0.56
1:D:125:HIS:CG	1:D:126:THR:H	2.24	0.55
3:a:84:ARG:HB3	3:a:110:THR:HB	1.88	0.55
1:A:367:LYS:HA	1:A:376:THR:HA	1.88	0.55
3:d:172:VAL:HG23	3:d:227:LEU:HB3	1.89	0.55
1:D:388:ILE:HG23	1:D:389:VAL:N	2.22	0.55
3:d:165:GLU:HA	3:d:251:LYS:HA	1.89	0.55
1:C:147:VAL:HG11	1:C:162:LEU:HD11	1.86	0.55
1:D:80:VAL:HG12	1:D:103:MET:HB3	1.87	0.55
1:B:321:TYR:HE1	1:B:353:PHE:H	1.52	0.55
3:d:277:HIS:HA	3:d:340:SER:HB3	1.88	0.55
1:B:9:ASN:ND2	1:B:274:VAL:H	2.05	0.55
3:d:41:HIS:HB3	3:d:133:VAL:HG13	1.89	0.55
3:d:172:VAL:O	3:d:227:LEU:N	2.39	0.55
1:D:61:LYS:NZ	1:D:66:THR:OG1	2.39	0.55
1:D:96:CYS:O	1:D:100:ASN:ND2	2.40	0.55
1:A:19:VAL:HG23	1:A:27:VAL:HG13	1.89	0.55
1:C:32:GLN:O	1:C:134:ASN:N	2.40	0.54
1:D:77:GLN:NE2	1:D:220:LEU:O	2.38	0.54
1:D:93:TYR:O	3:d:224:ARG:NH1	2.38	0.54
2:S:137:LEU:HD13	2:S:162:GLU:HG2	1.88	0.54
1:B:328:ASN:HB3	1:B:346:THR:HB	1.88	0.54
1:A:302:CYS:HA	1:A:319:VAL:HG12	1.89	0.54
3:c:47:ILE:HG13	3:c:99:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ALA:HA	1:A:101:THR:HG21	1.90	0.54
3:b:150:CYS:SG	3:b:263:CYS:N	2.81	0.54
1:D:225:PRO:HA	1:D:233:PRO:HG2	1.89	0.54
1:A:30:GLN:HG2	1:A:136:THR:HG23	1.88	0.54
1:B:53:THR:HG21	1:B:236:GLN:HE22	1.73	0.54
3:b:31:ILE:HD11	3:b:121:THR:HA	1.90	0.54
1:B:164:ILE:HA	1:B:279:ILE:HA	1.90	0.54
3:d:114:HIS:HA	3:d:119:ARG:HA	1.90	0.54
1:A:21:ARG:HD2	1:A:22:PRO:HD2	1.89	0.54
1:A:28:HIS:CE1	1:A:138:GLY:H	2.26	0.54
1:A:14:PRO:HB3	1:A:32:GLN:HB2	1.90	0.53
3:d:281:ILE:CG1	5:d:501:NAG:H81	2.37	0.53
3:b:49:THR:HG22	3:b:51:ALA:H	1.71	0.53
3:d:13:ARG:NH2	3:d:229:ASP:OD2	2.41	0.53
3:b:283:HIS:HA	3:b:313:THR:HA	1.89	0.53
1:A:250:ALA:HA	3:a:305:ARG:HH11	1.73	0.53
1:D:388:ILE:HG23	1:D:389:VAL:H	1.73	0.53
1:B:21:ARG:HD3	1:B:22:PRO:HD2	1.89	0.53
1:B:140:VAL:O	1:B:142:TRP:HD1	1.90	0.53
1:D:389:VAL:HG12	1:D:390:ASP:CG	2.34	0.53
1:B:28:HIS:O	1:B:28:HIS:ND1	2.41	0.53
3:c:409:LEU:HD12	3:c:416:LYS:HG2	1.91	0.53
3:d:39:ASP:N	3:d:39:ASP:OD1	2.40	0.53
1:C:265:GLU:HB3	1:C:266:PRO:HD3	1.91	0.53
1:A:167:LEU:HB3	1:A:277:ILE:HG22	1.91	0.53
3:d:84:ARG:HD2	3:b:88:PRO:HG2	1.90	0.53
1:D:174:PHE:CZ	1:D:269:ALA:HB2	2.44	0.52
1:D:424:LEU:HA	1:D:427:ILE:HG12	1.92	0.52
1:B:347:LEU:HD12	1:B:351:GLY:HA3	1.91	0.52
1:B:364:PRO:HD2	1:B:380:ASP:HA	1.92	0.52
2:R:195:TYR:CD2	2:R:201:THR:HG22	2.41	0.52
2:P:212:SER:HG	2:P:261:TRP:CD1	2.28	0.52
3:d:197:TYR:O	3:d:205:ARG:HB2	2.10	0.52
1:D:112:GLU:OE1	3:d:46:ARG:NH1	2.42	0.52
3:b:179:SER:HB2	3:b:186:LYS:HG3	1.92	0.52
1:D:295:PRO:HG3	1:D:325:LYS:HB3	1.91	0.52
1:B:367:LYS:HA	1:B:376:THR:HA	1.92	0.52
3:a:201:CYS:N	3:a:217:CYS:SG	2.82	0.52
1:A:370:VAL:O	1:A:373:SER:OG	2.28	0.52
3:c:336:TRP:CD1	3:c:337:ALA:N	2.78	0.52
3:b:248:PHE:HD1	3:b:249:LYS:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:197:TYR:O	3:a:205:ARG:HA	2.10	0.52
1:D:86:PRO:HG2	1:D:93:TYR:HB3	1.92	0.52
1:B:229:ILE:O	1:B:231:HIS:ND1	2.41	0.52
1:A:136:THR:HB	1:A:142:TRP:HA	1.91	0.52
3:d:150:CYS:SG	3:d:263:CYS:N	2.82	0.52
3:b:190:PRO:HG2	3:b:192:GLY:O	2.10	0.52
1:D:325:LYS:HG2	1:D:326:ALA:H	1.75	0.52
3:c:396:PRO:HA	3:c:399:LEU:HG	1.91	0.52
1:D:113:GLU:HA	3:d:258:PRO:HG3	1.91	0.51
1:B:297:VAL:HA	1:B:323:SER:HA	1.92	0.51
1:D:53:THR:HG22	1:D:108:VAL:HG12	1.93	0.51
1:B:369:GLN:HA	1:B:374:ALA:HA	1.93	0.51
1:A:220:LEU:HD22	1:A:236:GLN:HA	1.93	0.51
3:a:91:LEU:H	3:a:91:LEU:HD23	1.76	0.51
3:d:138:TYR:HD1	3:d:140:HIS:H	1.59	0.51
1:D:405:ALA:HA	1:D:408:TRP:CE3	2.45	0.51
1:A:176:ASN:N	1:A:176:ASN:OD1	2.43	0.51
1:C:143:ARG:HH12	1:C:158:GLY:HA3	1.75	0.51
1:D:52:LYS:HE2	1:D:53:THR:H	1.75	0.51
1:B:143:ARG:HH22	1:B:160:ALA:H	1.57	0.51
3:a:154:THR:HG23	3:a:156:LYS:H	1.75	0.51
3:d:315:ASN:HB3	5:d:501:NAG:O7	2.10	0.50
3:d:360:TYR:CG	3:d:364:THR:HG23	2.46	0.50
2:P:250:THR:O	2:P:251:VAL:HG13	2.11	0.50
3:b:129:GLU:OE1	3:b:131:ARG:NH1	2.44	0.50
1:D:265:GLU:O	1:D:267:LEU:N	2.38	0.50
3:c:146:VAL:O	3:c:265:ALA:N	2.42	0.50
3:d:394:ILE:HG12	3:d:394:ILE:O	2.11	0.50
3:b:34:GLU:HG3	3:b:35:GLU:HG3	1.93	0.50
3:b:140:HIS:CG	3:b:141:PRO:HD2	2.46	0.50
3:d:196:LYS:H	3:d:196:LYS:HD2	1.77	0.50
3:b:129:GLU:HB2	3:b:131:ARG:NH2	2.27	0.50
3:b:392:LEU:O	3:b:393:CYS:C	2.54	0.50
1:B:291:ILE:O	1:B:294:THR:OG1	2.21	0.50
1:B:322:LYS:HA	1:B:350:SER:HA	1.94	0.50
3:b:86:SER:OG	3:b:105:PRO:O	2.26	0.50
1:D:180:VAL:HG22	1:D:185:VAL:HG22	1.94	0.49
3:c:13:ARG:HD2	3:c:14:PRO:HD2	1.93	0.49
3:c:115:ASP:C	3:c:117:PRO:HD2	2.37	0.49
3:c:122:CYS:SG	3:c:123:THR:N	2.85	0.49
3:c:136:GLU:N	3:c:136:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:194:GLN:HB3	3:b:208:ILE:HA	1.94	0.49
1:C:299:ASP:HB2	1:C:322:LYS:HE2	1.94	0.49
1:A:82:THR:OG1	1:A:83:GLY:N	2.44	0.49
1:D:183:HIS:O	1:D:183:HIS:ND1	2.45	0.49
3:b:199:CYS:HA	3:b:223:CYS:HA	1.94	0.49
1:C:174:PHE:CE2	1:C:269:ALA:HB2	2.48	0.49
3:c:77:LYS:HD3	3:c:77:LYS:H	1.77	0.49
3:b:292:LEU:HB2	3:b:327:TRP:HE3	1.78	0.49
1:B:429:THR:HG22	1:B:430:ALA:H	1.77	0.49
1:B:264:LEU:HG	1:B:265:GLU:H	1.77	0.49
1:A:244:TRP:CD1	1:A:244:TRP:C	2.91	0.49
1:D:125:HIS:CD2	1:D:126:THR:H	2.30	0.49
1:B:136:THR:OG1	1:B:141:SER:O	2.26	0.48
3:d:114:HIS:ND1	3:d:118:ASN:O	2.46	0.48
1:B:7:MET:HG2	1:B:31:ILE:HD13	1.95	0.48
1:A:323:SER:OG	1:A:325:LYS:O	2.29	0.48
3:c:37:ARG:NH1	3:c:39:ASP:OD2	2.42	0.48
3:d:344:ASN:ND2	3:d:355:TYR:HB2	2.28	0.48
1:A:129:VAL:HG22	1:A:149:VAL:HG11	1.96	0.48
1:A:164:ILE:HG13	1:A:279:ILE:HG12	1.95	0.48
3:a:49:THR:OG1	3:a:50:SER:N	2.47	0.48
3:a:203:ASP:O	3:a:205:ARG:NH1	2.46	0.48
3:c:150:CYS:SG	3:c:263:CYS:N	2.86	0.48
1:D:222:LEU:HA	1:D:234:PHE:HA	1.96	0.48
1:D:387:HIS:CE1	3:d:340:SER:HG	2.32	0.48
3:b:197:TYR:HB2	3:b:207:GLY:N	2.28	0.48
3:a:195:VAL:HG12	3:a:227:LEU:HA	1.94	0.48
1:A:225:PRO:HA	1:A:233:PRO:HG3	1.95	0.48
3:b:163:TYR:HB3	3:b:251:LYS:HB2	1.96	0.48
3:b:336:TRP:CZ2	3:b:338:GLN:HB2	2.49	0.48
1:B:349:GLU:CD	1:B:349:GLU:H	2.22	0.47
1:A:103:MET:SD	1:A:103:MET:N	2.86	0.47
3:a:180:ILE:HA	3:a:185:VAL:HA	1.96	0.47
3:d:84:ARG:HB3	3:d:110:THR:HB	1.95	0.47
1:D:116:ILE:HD11	3:d:260:LYS:HD2	1.96	0.47
1:D:328:ASN:HA	1:D:346:THR:HA	1.97	0.47
3:d:185:VAL:HG22	3:d:215:THR:HG22	1.96	0.47
1:D:40:PRO:HA	1:D:127:GLY:HA3	1.97	0.47
3:a:13:ARG:HB3	3:a:234:VAL:HG12	1.96	0.47
3:a:194:GLN:HB3	3:a:208:ILE:HA	1.96	0.47
1:A:84:VAL:HG21	1:A:102:GLN:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:107:ASP:HA	3:a:127:LYS:HA	1.97	0.47
1:B:31:ILE:HD12	1:B:279:ILE:HD13	1.95	0.47
2:S:137:LEU:CD1	2:S:162:GLU:HG2	2.45	0.47
3:c:153:TYR:HA	3:c:258:PRO:HA	1.97	0.47
3:a:152:ARG:O	3:a:259:VAL:HG12	2.13	0.47
1:D:96:CYS:HB3	1:D:99:GLU:HB2	1.97	0.47
1:B:59:VAL:HG22	3:b:242:ARG:HG3	1.97	0.47
1:C:21:ARG:HH21	1:C:21:ARG:CG	2.28	0.46
3:d:293:THR:HG23	3:d:326:THR:HB	1.97	0.46
2:Q:229:GLY:O	2:Q:239:LEU:HA	2.15	0.46
3:b:195:VAL:HG23	3:b:226:TYR:O	2.16	0.46
3:b:240:LEU:HD23	3:b:241:PRO:HD2	1.97	0.46
1:D:331:ILE:HG22	1:D:370:VAL:HG12	1.98	0.46
1:B:131:ALA:O	1:B:147:VAL:N	2.34	0.46
3:b:289:PRO:HB3	3:b:309:GLU:HG2	1.98	0.46
2:R:138:HIS:HB3	2:R:261:TRP:CE3	2.51	0.46
2:P:231:VAL:HG22	2:P:232:ASN:N	2.30	0.46
3:c:85:THR:OG1	3:c:89:CYS:SG	2.66	0.46
3:d:179:SER:HB3	3:d:186:LYS:HB2	1.96	0.46
1:D:2:GLU:HG2	1:D:282:ASP:HB2	1.98	0.46
1:A:163:ILE:N	1:A:280:SER:O	2.43	0.46
3:c:289:PRO:HG3	3:c:309:GLU:HG3	1.98	0.46
1:C:414:LEU:HD13	3:c:371:CYS:SG	2.55	0.46
1:D:303:LYS:O	1:D:318:THR:N	2.42	0.46
1:A:295:PRO:HB3	1:A:325:LYS:HG2	1.97	0.46
3:c:36:VAL:HG22	3:c:47:ILE:HG22	1.96	0.46
3:c:105:PRO:HG3	3:c:130:PHE:HB2	1.97	0.46
3:d:187:ILE:O	3:d:213:HIS:NE2	2.48	0.46
1:B:86:PRO:HB2	1:B:93:TYR:CZ	2.51	0.46
1:B:396:THR:HG23	1:B:396:THR:O	2.16	0.46
1:A:298:SER:O	1:A:322:LYS:HB3	2.16	0.46
3:d:177:LEU:HB3	3:d:187:ILE:HG23	1.97	0.46
3:d:394:ILE:HG23	3:d:395:THR:HG23	1.98	0.46
3:b:174:ASP:OD1	3:b:175:HIS:N	2.48	0.46
1:B:305:THR:HG23	1:B:317:ALA:HA	1.97	0.46
1:A:140:VAL:O	1:A:141:SER:OG	2.31	0.46
3:d:34:GLU:O	3:d:48:GLN:HB3	2.16	0.46
3:a:198:TYR:HB3	3:a:224:ARG:HE	1.81	0.46
1:B:265:GLU:HB3	1:B:266:PRO:HD2	1.98	0.45
3:c:399:LEU:HD12	3:c:400:ALA:N	2.30	0.45
3:a:342:GLU:HB2	3:a:355:TYR:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:THR:HA	1:B:142:TRP:HA	1.98	0.45
2:Q:195:TYR:HD2	2:Q:199:ARG:H	1.64	0.45
3:c:286:PRO:HD2	3:c:311:PRO:HA	1.97	0.45
3:d:394:ILE:HG13	3:d:413:CYS:HB3	1.98	0.45
1:D:332:HIS:HA	1:D:340:ILE:HD11	1.98	0.45
1:B:86:PRO:O	1:B:92:ALA:HA	2.16	0.45
1:B:156:LYS:HA	1:B:161:LYS:HA	1.97	0.45
3:a:31:ILE:HG22	3:a:51:ALA:HB2	1.97	0.45
1:D:30:GLN:HB3	1:D:136:THR:HB	1.98	0.45
1:D:59:VAL:HB	1:D:103:MET:HG3	1.98	0.45
1:B:180:VAL:HG22	1:B:185:VAL:HG12	1.99	0.45
1:A:33:LEU:HG	1:A:133:VAL:HG12	1.98	0.45
2:R:216:ILE:C	2:R:217:LEU:HD12	2.42	0.45
3:c:125:ALA:HB2	3:d:140:HIS:CD2	2.52	0.45
3:d:266:THR:OG1	3:d:267:LEU:N	2.49	0.45
1:C:403:ILE:H	1:C:403:ILE:HG13	1.65	0.45
1:D:114:CYS:O	1:D:118:HIS:ND1	2.49	0.45
1:D:304:ILE:HA	1:D:317:ALA:HA	1.98	0.45
1:D:388:ILE:HG12	1:D:389:VAL:N	2.30	0.45
1:A:323:SER:HB3	1:A:350:SER:H	1.81	0.45
3:c:163:TYR:HB3	3:c:251:LYS:HB2	1.99	0.45
3:a:187:ILE:HG23	3:a:211:SER:HB3	1.98	0.45
3:c:1:ASP:O	3:c:4:THR:OG1	2.25	0.45
3:b:185:VAL:HG23	3:b:214:THR:OG1	2.16	0.45
1:D:297:VAL:HG12	1:D:323:SER:HB2	1.97	0.45
1:A:8:PRO:HB2	1:A:10:LYS:HD3	1.99	0.45
3:d:281:ILE:HG12	5:d:501:NAG:H81	1.98	0.45
3:b:41:HIS:CE1	3:b:133:VAL:HG13	2.52	0.45
1:B:143:ARG:HH22	1:B:160:ALA:N	2.15	0.45
1:B:309:TYR:O	1:B:309:TYR:CG	2.70	0.44
2:Q:138:HIS:HB3	2:Q:261:TRP:CZ3	2.51	0.44
3:d:140:HIS:CG	3:d:141:PRO:HD2	2.52	0.44
2:R:218:ASP:OD1	2:R:219:ASN:N	2.50	0.44
1:B:19:VAL:HB	1:B:27:VAL:HB	2.00	0.44
3:a:371:CYS:HA	3:a:374:ILE:HG12	1.99	0.44
3:c:138:TYR:HD2	3:c:266:THR:HB	1.82	0.44
3:d:127:LYS:HA	3:d:127:LYS:HZ2	1.82	0.44
3:b:267:LEU:HD13	3:b:268:ALA:O	2.18	0.44
3:a:200:LYS:HB3	3:a:217:CYS:SG	2.58	0.44
1:B:96:CYS:HB3	1:B:99:GLU:HB2	1.98	0.44
3:c:336:TRP:CG	3:c:337:ALA:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:193:ALA:HB3	3:d:228:ILE:HB	1.99	0.44
3:a:198:TYR:HE1	3:a:203:ASP:H	1.65	0.44
1:C:298:SER:O	1:C:299:ASP:C	2.59	0.44
1:B:171:TRP:CD1	1:B:171:TRP:H	2.35	0.44
1:A:234:PHE:CE2	1:A:236:GLN:HB2	2.52	0.44
2:S:137:LEU:HB3	2:S:160:ASP:OD1	2.17	0.44
3:d:281:ILE:HD13	5:d:501:NAG:C8	2.47	0.44
3:d:371:CYS:HA	3:d:374:ILE:HG12	2.00	0.44
3:b:282:LEU:HD13	3:b:325:TYR:CZ	2.53	0.44
3:a:95:HIS:CE1	3:a:157:ARG:HD3	2.53	0.44
3:b:181:HIS:O	3:b:182:SER:OG	2.24	0.44
1:B:321:TYR:HE1	1:B:353:PHE:N	2.15	0.44
3:c:162:HIS:CE1	3:c:254:VAL:HB	2.53	0.44
3:d:135:ARG:HD2	3:d:291:LEU:HD11	1.99	0.44
1:A:24:TYR:HD1	1:A:290:ARG:HA	1.83	0.43
3:c:235:TYR:CE2	3:c:237:SER:HB2	2.53	0.43
1:C:34:VAL:HG12	1:C:35:ASN:HD22	1.82	0.43
1:D:84:VAL:HG22	1:D:86:PRO:HD3	2.01	0.43
1:A:322:LYS:HA	1:A:350:SER:HA	2.00	0.43
3:d:166:MET:HE3	3:d:235:TYR:HB2	2.00	0.43
3:b:294:THR:HG22	3:b:304:THR:HB	2.00	0.43
1:C:363:HIS:HD2	1:C:405:ALA:HB2	1.78	0.43
1:C:394:GLN:HB2	1:C:396:THR:HG22	2.00	0.43
1:B:15:TYR:HB3	1:B:31:ILE:HG23	2.00	0.43
2:P:197:ASN:CG	2:P:198:ASN:N	2.76	0.43
1:C:6:VAL:HA	1:C:278:PRO:HA	1.99	0.43
3:d:200:LYS:O	3:d:203:ASP:N	2.44	0.43
1:B:19:VAL:N	1:B:27:VAL:O	2.26	0.43
1:B:366:PHE:CZ	1:B:377:CYS:HB2	2.54	0.43
1:A:293:GLU:O	1:A:325:LYS:NZ	2.43	0.43
3:c:150:CYS:N	3:c:261:ALA:O	2.41	0.43
3:a:418:THR:O	3:a:420:ALA:N	2.52	0.43
1:A:31:ILE:HG13	1:A:135:ILE:HD12	2.00	0.43
3:d:14:PRO:HD3	3:d:52:MET:HE2	2.00	0.43
1:B:85:TYR:HD1	1:B:85:TYR:HA	1.75	0.43
1:A:406:THR:HG21	3:a:346:HIS:HB3	2.01	0.43
3:b:98:TYR:HD2	3:b:255:PRO:HD2	1.83	0.43
3:c:92:VAL:HG23	3:c:101:ALA:HA	2.00	0.43
3:b:185:VAL:HG22	3:b:218:THR:HA	2.00	0.43
1:B:285:ASP:OD1	1:B:286:ALA:N	2.52	0.42
1:B:391:TYR:CD2	1:B:392:PRO:CD	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:HIS:CG	1:A:19:VAL:HG12	2.53	0.42
1:A:95:PHE:HD1	3:a:224:ARG:HD3	1.83	0.42
3:b:56:LYS:H	3:b:61:ASP:HB2	1.84	0.42
3:b:153:TYR:HA	3:b:258:PRO:HA	2.01	0.42
3:a:15:TYR:CE2	3:a:17:ALA:HB2	2.53	0.42
1:C:362:ILE:HG21	1:C:404:SER:HA	2.00	0.42
1:D:214:LEU:C	1:D:214:LEU:HD12	2.44	0.42
1:A:9:ASN:C	1:A:10:LYS:HD2	2.44	0.42
1:A:220:LEU:HB3	1:A:234:PHE:HE1	1.84	0.42
3:b:345:PRO:HD3	3:b:355:TYR:HB3	2.01	0.42
3:b:345:PRO:HD3	3:b:355:TYR:CB	2.49	0.42
1:B:17:ALA:O	1:B:29:LEU:N	2.40	0.42
1:B:175:ASP:OD1	1:B:175:ASP:N	2.52	0.42
1:A:394:GLN:HB2	1:A:396:THR:HG22	2.01	0.42
2:R:166:VAL:HG13	2:R:167:PRO:HD2	2.01	0.42
3:d:89:CYS:HB3	3:d:102:GLN:O	2.19	0.42
1:D:361:ASN:HB2	1:D:406:THR:HG21	2.01	0.42
1:A:410:TRP:CZ2	3:a:349:PRO:HB3	2.55	0.42
3:a:200:LYS:HE3	3:a:217:CYS:SG	2.60	0.42
3:d:186:LYS:HA	3:d:213:HIS:HD2	1.83	0.42
3:b:177:LEU:HD12	3:b:178:LEU:N	2.35	0.42
1:B:133:VAL:O	1:B:144:SER:OG	2.33	0.42
1:B:192:GLU:O	1:B:193:TYR:C	2.63	0.42
1:B:300:LEU:HD12	1:B:300:LEU:H	1.85	0.42
1:A:61:LYS:HG2	1:A:64:GLY:O	2.20	0.42
1:A:271:ASN:ND2	1:A:271:ASN:O	2.52	0.42
2:S:231:VAL:HG22	2:S:232:ASN:H	1.83	0.42
3:c:394:ILE:C	3:c:394:ILE:HD12	2.45	0.42
3:d:201:CYS:O	3:d:202:PRO:C	2.62	0.42
1:C:1:TYR:CD1	1:C:1:TYR:N	2.81	0.42
1:D:184:GLU:HB3	1:D:251:PRO:HB3	2.02	0.42
1:A:296:THR:O	1:A:323:SER:HA	2.20	0.42
3:c:165:GLU:OE1	3:c:165:GLU:N	2.46	0.42
1:A:12:GLY:O	1:A:32:GLN:NE2	2.52	0.42
1:A:361:ASN:HD21	1:A:402:ALA:H	1.68	0.42
2:S:143:ILE:HG22	2:S:144:ASP:N	2.34	0.42
3:c:392:LEU:C	3:c:394:ILE:H	2.28	0.42
1:D:321:TYR:HE2	1:D:353:PHE:HD2	1.67	0.42
3:d:78:ILE:O	3:d:81:LEU:HD12	2.20	0.42
3:a:181:HIS:C	3:a:183:ALA:H	2.28	0.42
3:a:284:LEU:C	3:a:285:HIS:CG	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:CYS:HA	1:C:315:GLY:HA2	2.02	0.41
1:D:123:LYS:HA	1:D:177:LYS:HA	2.01	0.41
1:B:112:GLU:HB3	3:b:162:HIS:CD2	2.54	0.41
1:B:146:ASP:OD1	1:B:146:ASP:N	2.53	0.41
1:A:143:ARG:HD2	1:A:158:GLY:HA3	2.02	0.41
2:Q:125:TYR:CD1	2:Q:214:ARG:HD3	2.55	0.41
3:b:151:ASN:OD1	3:b:151:ASN:N	2.52	0.41
3:a:216:THR:O	3:a:217:CYS:C	2.62	0.41
1:D:50:LYS:HG2	1:D:51:TYR:H	1.84	0.41
1:C:368:LEU:H	1:C:368:LEU:HD23	1.85	0.41
1:A:321:TYR:HD1	1:A:352:SER:HA	1.85	0.41
3:d:138:TYR:HD1	3:d:139:ARG:H	1.66	0.41
3:b:292:LEU:HB2	3:b:327:TRP:CE3	2.54	0.41
3:b:397:TYR:C	3:b:399:LEU:N	2.78	0.41
1:C:243:ARG:HA	1:C:247:ASP:OD1	2.21	0.41
1:B:88:MET:C	1:B:90:GLY:H	2.29	0.41
1:A:86:PRO:HB3	1:A:230:VAL:HG22	2.02	0.41
3:c:136:GLU:OE1	3:c:329:ASN:ND2	2.54	0.41
1:D:387:HIS:CE1	3:d:340:SER:HA	2.56	0.41
1:A:114:CYS:O	1:A:118:HIS:ND1	2.53	0.41
3:d:67:PHE:HE2	3:d:69:ASN:HB2	1.85	0.41
3:d:372:VAL:HG12	3:d:376:MET:HE2	2.03	0.41
1:C:1:TYR:HD1	1:C:1:TYR:N	2.16	0.41
1:B:305:THR:OG1	1:B:316:ILE:O	2.30	0.41
2:Q:154:LYS:HB2	2:Q:163:TYR:CE2	2.56	0.41
3:c:197:TYR:CE2	3:c:207:GLY:HA2	2.54	0.41
3:d:118:ASN:HB3	3:d:120:HIS:CE1	2.56	0.41
3:a:392:LEU:C	3:a:394:ILE:H	2.29	0.41
1:C:88:MET:HE1	1:C:89:TRP:CE2	2.55	0.41
1:C:129:VAL:HG22	1:C:149:VAL:HB	2.02	0.41
1:C:247:ASP:OD1	1:C:247:ASP:N	2.45	0.41
1:D:100:ASN:OD1	1:D:100:ASN:N	2.51	0.41
1:D:318:THR:HG22	1:D:354:THR:HB	2.01	0.41
3:c:77:LYS:HB2	3:c:77:LYS:NZ	2.36	0.41
1:D:81:PHE:CD1	1:D:224:ARG:HB3	2.56	0.41
1:D:243:ARG:C	1:D:245:LYS:H	2.28	0.41
1:B:302:CYS:SG	1:B:303:LYS:N	2.94	0.41
2:S:195:TYR:CG	2:S:196:GLU:N	2.88	0.41
2:P:138:HIS:HB3	2:P:261:TRP:CZ3	2.56	0.41
3:c:400:ALA:HB1	3:c:402:ASN:ND2	2.36	0.41
3:d:395:THR:N	3:d:396:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:240:LEU:HD22	3:a:241:PRO:HD2	2.03	0.41
1:C:329:CYS:SG	1:C:330:PRO:HD2	2.61	0.41
1:B:298:SER:O	1:B:322:LYS:HB3	2.21	0.41
3:b:136:GLU:HG2	3:b:290:THR:HG23	2.03	0.41
2:S:188:TRP:CH2	2:S:193:VAL:HB	2.56	0.41
3:b:394:ILE:HG13	3:b:395:THR:H	1.86	0.41
1:A:369:GLN:HG2	1:A:374:ALA:HB2	2.02	0.40
3:a:266:THR:OG1	3:a:267:LEU:N	2.54	0.40
1:D:323:SER:OG	1:D:324:SER:N	2.53	0.40
3:d:11:LEU:O	3:d:232:LYS:HB3	2.20	0.40
3:b:181:HIS:C	3:b:183:ALA:H	2.29	0.40
3:a:274:GLU:HB3	3:a:281:ILE:HG13	2.03	0.40
3:a:319:THR:HG23	3:a:322:GLY:H	1.86	0.40
1:B:84:VAL:HG23	1:B:100:ASN:HB3	2.02	0.40
3:c:11:LEU:HD11	3:c:233:TRP:CE3	2.56	0.40
1:B:87:PHE:CD2	1:B:91:GLY:HA2	2.55	0.40
1:A:51:TYR:OH	1:A:237:ALA:O	2.40	0.40
2:R:261:TRP:CD1	2:R:261:TRP:N	2.89	0.40
3:d:129:GLU:HB3	3:d:131:ARG:NH1	2.32	0.40
1:D:67:GLN:OE1	1:D:67:GLN:N	2.55	0.40
1:D:203:ASP:OD1	1:D:203:ASP:N	2.53	0.40
1:B:295:PRO:HB3	1:B:325:LYS:HG2	2.03	0.40
1:A:236:GLN:HG2	1:A:237:ALA:O	2.20	0.40
2:P:243:THR:HG23	2:P:251:VAL:HG23	2.02	0.40
3:b:163:TYR:CZ	3:b:253:HIS:CE1	3.09	0.40
3:b:179:SER:N	3:b:186:LYS:O	2.49	0.40
3:b:418:THR:O	3:b:419:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/437 (100%)	400 (92%)	35 (8%)	0	100	100
1	B	435/437 (100%)	397 (91%)	35 (8%)	3 (1%)	18	55
1	C	435/437 (100%)	403 (93%)	31 (7%)	1 (0%)	43	76
1	D	435/437 (100%)	397 (91%)	34 (8%)	4 (1%)	14	49
2	P	158/160 (99%)	142 (90%)	15 (10%)	1 (1%)	21	58
2	Q	158/160 (99%)	141 (89%)	17 (11%)	0	100	100
2	R	157/160 (98%)	141 (90%)	16 (10%)	0	100	100
2	S	158/160 (99%)	142 (90%)	15 (10%)	1 (1%)	21	58
3	a	418/420 (100%)	377 (90%)	39 (9%)	2 (0%)	24	61
3	b	418/420 (100%)	378 (90%)	38 (9%)	2 (0%)	24	61
3	c	418/420 (100%)	368 (88%)	48 (12%)	2 (0%)	24	61
3	d	418/420 (100%)	367 (88%)	48 (12%)	3 (1%)	18	55
All	All	4043/4068 (99%)	3653 (90%)	371 (9%)	19 (0%)	26	61

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	388	ILE
1	B	265	GLU
3	d	202	PRO
3	a	419	ARG
1	D	389	VAL
3	a	415	ILE
2	P	172	SER
3	b	398	LYS
1	D	89	TRP
3	c	417	PRO
1	B	389	VAL
3	d	395	THR
1	C	385	LYS
1	D	391	TYR
1	B	264	LEU
3	c	406	PRO
3	b	415	ILE
2	S	234	GLY
3	d	406	PRO

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	366/366 (100%)	337 (92%)	29 (8%)	11	34
1	B	366/366 (100%)	333 (91%)	33 (9%)	9	30
1	C	366/366 (100%)	336 (92%)	30 (8%)	10	33
1	D	366/366 (100%)	342 (93%)	24 (7%)	15	39
2	P	134/134 (100%)	130 (97%)	4 (3%)	36	57
2	Q	134/134 (100%)	134 (100%)	0	100	100
2	R	133/134 (99%)	126 (95%)	7 (5%)	20	44
2	S	134/134 (100%)	132 (98%)	2 (2%)	57	70
3	a	367/367 (100%)	340 (93%)	27 (7%)	13	35
3	b	367/367 (100%)	338 (92%)	29 (8%)	11	34
3	c	367/367 (100%)	340 (93%)	27 (7%)	13	35
3	d	367/367 (100%)	336 (92%)	31 (8%)	10	32
All	All	3467/3468 (100%)	3224 (93%)	243 (7%)	16	38

All (243) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	TYR
1	C	18	LEU
1	C	29	LEU
1	C	30	GLN
1	C	62	CYS
1	C	63	CYS
1	C	66	THR
1	C	67	GLN
1	C	68	CYS
1	C	77	GLN
1	C	82	THR
1	C	95	PHE
1	C	104	SER
1	C	109	GLU

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Mol	Chain	Res	Type
1	C	129	VAL
1	C	132	MET
1	C	149	VAL
1	C	218	THR
1	C	219	ASN
1	C	264	LEU
1	C	283	ILE
1	C	300	LEU
1	C	319	VAL
1	C	340	ILE
1	C	341	LYS
1	C	371	CYS
1	C	380	ASP
1	C	384	PRO
1	C	408	TRP
1	C	436	LEU
1	D	35	ASN
1	D	44	LEU
1	D	52	LYS
1	D	84	VAL
1	D	85	TYR
1	D	100	ASN
1	D	113	GLU
1	D	134	ASN
1	D	135	ILE
1	D	162	LEU
1	D	239	SER
1	D	243	ARG
1	D	244	TRP
1	D	247	ASP
1	D	291	ILE
1	D	293	GLU
1	D	300	LEU
1	D	305	THR
1	D	319	VAL
1	D	328	ASN
1	D	371	CYS
1	D	382	LYS
1	D	387	HIS
1	D	406	THR
1	B	6	VAL
1	B	11	VAL

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Mol	Chain	Res	Type
1	B	16	LYS
1	B	18	LEU
1	B	28	HIS
1	B	31	ILE
1	B	53	THR
1	B	85	TYR
1	B	93	TYR
1	B	157	ILE
1	B	159	ASP
1	B	162	LEU
1	B	171	TRP
1	B	175	ASP
1	B	185	VAL
1	B	214	LEU
1	B	223	GLN
1	B	224	ARG
1	B	241	PHE
1	B	245	LYS
1	B	277	ILE
1	B	282	ASP
1	B	304	ILE
1	B	322	LYS
1	B	323	SER
1	B	343	ASN
1	B	353	PHE
1	B	359	THR
1	B	371	CYS
1	B	372	THR
1	B	391	TYR
1	B	429	THR
1	B	434	LEU
1	A	6	VAL
1	A	13	ILE
1	A	27	VAL
1	A	28	HIS
1	A	80	VAL
1	A	85	TYR
1	A	100	ASN
1	A	103	MET
1	A	129	VAL
1	A	134	ASN
1	A	136	THR

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Mol	Chain	Res	Type
1	A	142	TRP
1	A	149	VAL
1	A	153	THR
1	A	167	LEU
1	A	176	ASN
1	A	212	ASN
1	A	234	PHE
1	A	244	TRP
1	A	267	LEU
1	A	291	ILE
1	A	294	THR
1	A	303	LYS
1	A	340	ILE
1	A	370	VAL
1	A	375	VAL
1	A	387	HIS
1	A	394	GLN
1	A	406	THR
2	R	161	LEU
2	R	181	LYS
2	R	193	VAL
2	R	194	GLN
2	R	195	TYR
2	R	231	VAL
2	R	232	ASN
2	S	125	TYR
2	S	174	THR
2	P	177	TYR
2	P	181	LYS
2	P	251	VAL
2	P	252	LYS
3	c	9	TYR
3	c	18	ASP
3	c	22	CYS
3	c	24	HIS
3	c	27	CYS
3	c	31	ILE
3	c	77	LYS
3	c	85	THR
3	c	99	ILE
3	c	115	ASP
3	c	118	ASN

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Mol	Chain	Res	Type
3	c	135	ARG
3	c	157	ARG
3	c	177	LEU
3	c	184	LYS
3	c	195	VAL
3	c	252	LEU
3	c	278	ARG
3	c	283	HIS
3	c	310	ARG
3	c	359	ARG
3	c	363	THR
3	c	364	THR
3	c	386	LEU
3	c	390	ARG
3	c	402	ASN
3	c	411	LEU
3	d	15	TYR
3	d	39	ASP
3	d	55	LEU
3	d	81	LEU
3	d	115	ASP
3	d	127	LYS
3	d	133	VAL
3	d	156	LYS
3	d	157	ARG
3	d	174	ASP
3	d	196	LYS
3	d	201	CYS
3	d	217	CYS
3	d	239	ARG
3	d	242	ARG
3	d	247	THR
3	d	259	VAL
3	d	280	LEU
3	d	282	LEU
3	d	291	LEU
3	d	293	THR
3	d	307	TRP
3	d	325	TYR
3	d	326	THR
3	d	344	ASN
3	d	360	TYR

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Mol	Chain	Res	Type
3	d	378	SER
3	d	388	ARG
3	d	397	TYR
3	d	404	GLN
3	d	419	ARG
3	b	4	THR
3	b	22	CYS
3	b	24	HIS
3	b	27	CYS
3	b	41	HIS
3	b	46	ARG
3	b	53	PHE
3	b	61	ASP
3	b	71	LYS
3	b	110	THR
3	b	138	TYR
3	b	178	LEU
3	b	201	CYS
3	b	221	LYS
3	b	239	ARG
3	b	242	ARG
3	b	247	THR
3	b	248	PHE
3	b	266	THR
3	b	267	LEU
3	b	283	HIS
3	b	284	LEU
3	b	292	LEU
3	b	310	ARG
3	b	336	TRP
3	b	364	THR
3	b	368	LEU
3	b	397	TYR
3	b	404	GLN
3	a	3	ASP
3	a	16	ILE
3	a	27	CYS
3	a	37	ARG
3	a	66	SER
3	a	76	ILE
3	a	114	HIS
3	a	139	ARG

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Mol	Chain	Res	Type
3	a	157	ARG
3	a	172	VAL
3	a	184	LYS
3	a	187	ILE
3	a	214	THR
3	a	220	VAL
3	a	240	LEU
3	a	247	THR
3	a	296	SER
3	a	315	ASN
3	a	346	HIS
3	a	348	TRP
3	a	352	VAL
3	a	357	TYR
3	a	395	THR
3	a	397	TYR
3	a	399	LEU
3	a	404	GLN
3	a	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	43	ASN
1	C	236	GLN
1	C	253	ASN
1	C	328	ASN
1	D	43	ASN
1	D	125	HIS
1	D	134	ASN
1	D	253	ASN
1	D	332	HIS
1	B	9	ASN
1	B	30	GLN
1	B	35	ASN
1	B	125	HIS
1	B	217	ASN
1	B	271	ASN
1	B	356	HIS
1	B	361	ASN
1	B	395	HIS
1	A	3	HIS

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Mol	Chain	Res	Type
1	A	43	ASN
1	A	236	GLN
1	A	328	ASN
2	R	147	GLN
2	S	198	ASN
2	Q	121	GLN
2	P	197	ASN
3	c	73	GLN
3	c	151	ASN
3	c	162	HIS
3	c	302	ASN
3	c	358	ASN
3	d	69	ASN
3	d	338	GLN
3	d	404	GLN
3	b	358	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	$\#\|Z\| > 2$
4	NAG	E	1	1,4	14,14,15	0.37	0	17,19,21	0.55	0
4	NAG	E	2	4	14,14,15	0.38	0	17,19,21	1.09	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BMA	E	3	4	11,11,12	0.30	0	15,15,17	0.43	0
4	NAG	F	1	4	14,14,15	0.35	0	17,19,21	0.56	0
4	NAG	F	2	4	14,14,15	0.36	0	17,19,21	1.08	2 (11%)
4	BMA	F	3	4	11,11,12	0.30	0	15,15,17	0.43	0
4	NAG	G	1	4	14,14,15	0.37	0	17,19,21	0.56	0
4	NAG	G	2	4	14,14,15	0.38	0	17,19,21	1.09	2 (11%)
4	BMA	G	3	4	11,11,12	0.29	0	15,15,17	0.44	0
4	NAG	H	1	4	14,14,15	0.36	0	17,19,21	0.56	0
4	NAG	H	2	4	14,14,15	0.36	0	17,19,21	1.08	2 (11%)
4	BMA	H	3	4	11,11,12	0.29	0	15,15,17	0.43	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
4	NAG	E	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	3/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	NAG	H	1	4	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	3/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	2	NAG	C2-N2-C7	2.87	126.74	122.90
4	E	2	NAG	C1-C2-N2	2.86	114.94	110.43
4	F	2	NAG	C2-N2-C7	2.85	126.72	122.90
4	H	2	NAG	C2-N2-C7	2.85	126.71	122.90
4	E	2	NAG	C2-N2-C7	2.84	126.70	122.90
4	G	2	NAG	C1-C2-N2	2.81	114.86	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	2	NAG	C1-C2-N2	2.80	114.84	110.43
4	F	2	NAG	C1-C2-N2	2.79	114.84	110.43

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C1-C2-N2-C7
4	F	2	NAG	C1-C2-N2-C7
4	G	2	NAG	C1-C2-N2-C7
4	H	2	NAG	C1-C2-N2-C7
4	E	2	NAG	O7-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	E	2	NAG	C8-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	E	1	NAG	C3-C2-N2-C7
4	F	1	NAG	C3-C2-N2-C7
4	G	1	NAG	C3-C2-N2-C7
4	H	1	NAG	C3-C2-N2-C7

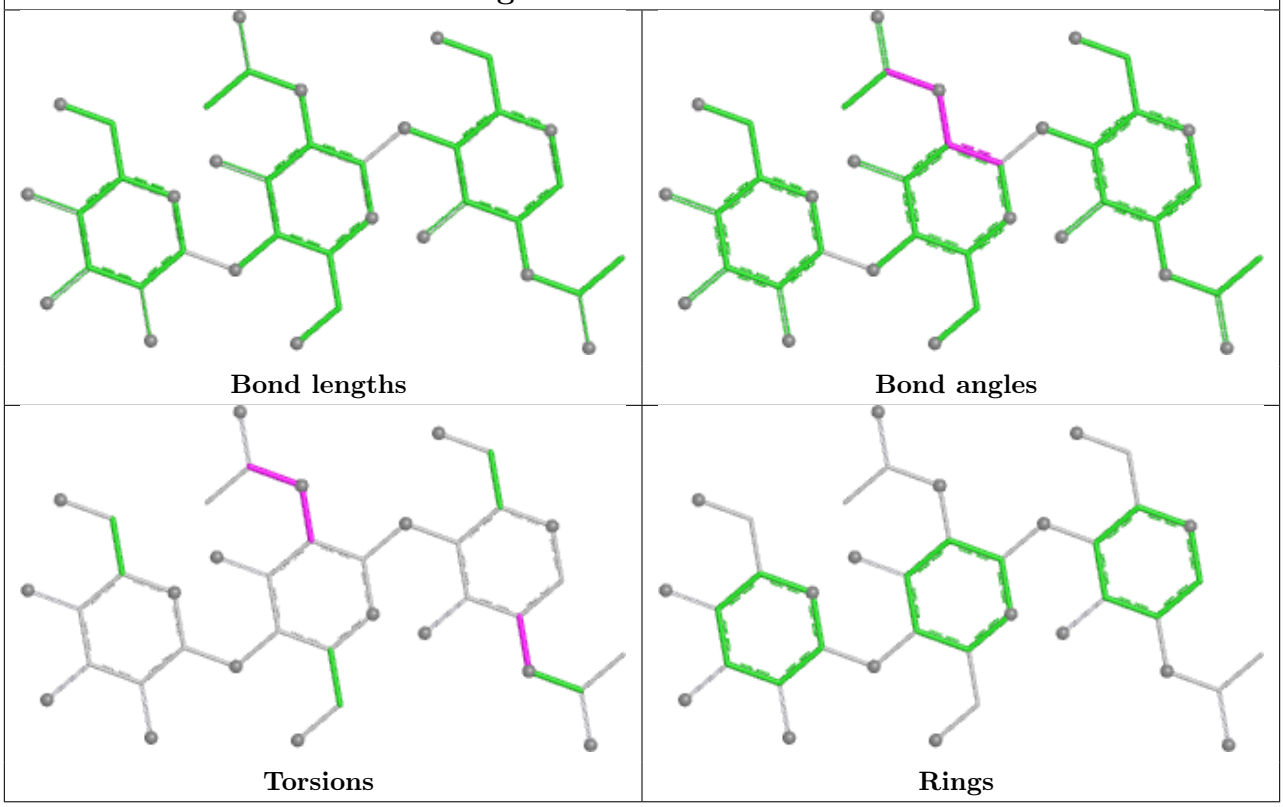
There are no ring outliers.

2 monomers are involved in 2 short contacts:

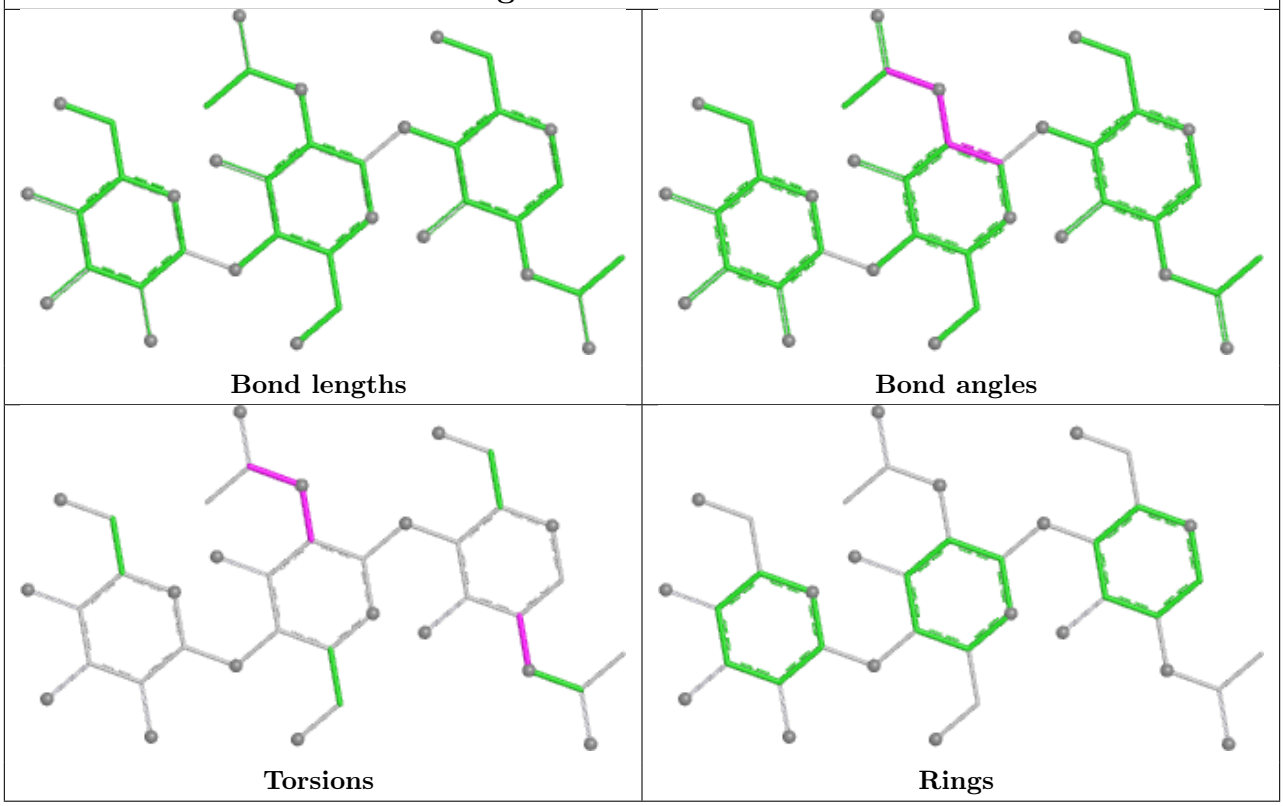
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	1	0
4	F	1	NAG	1	0

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

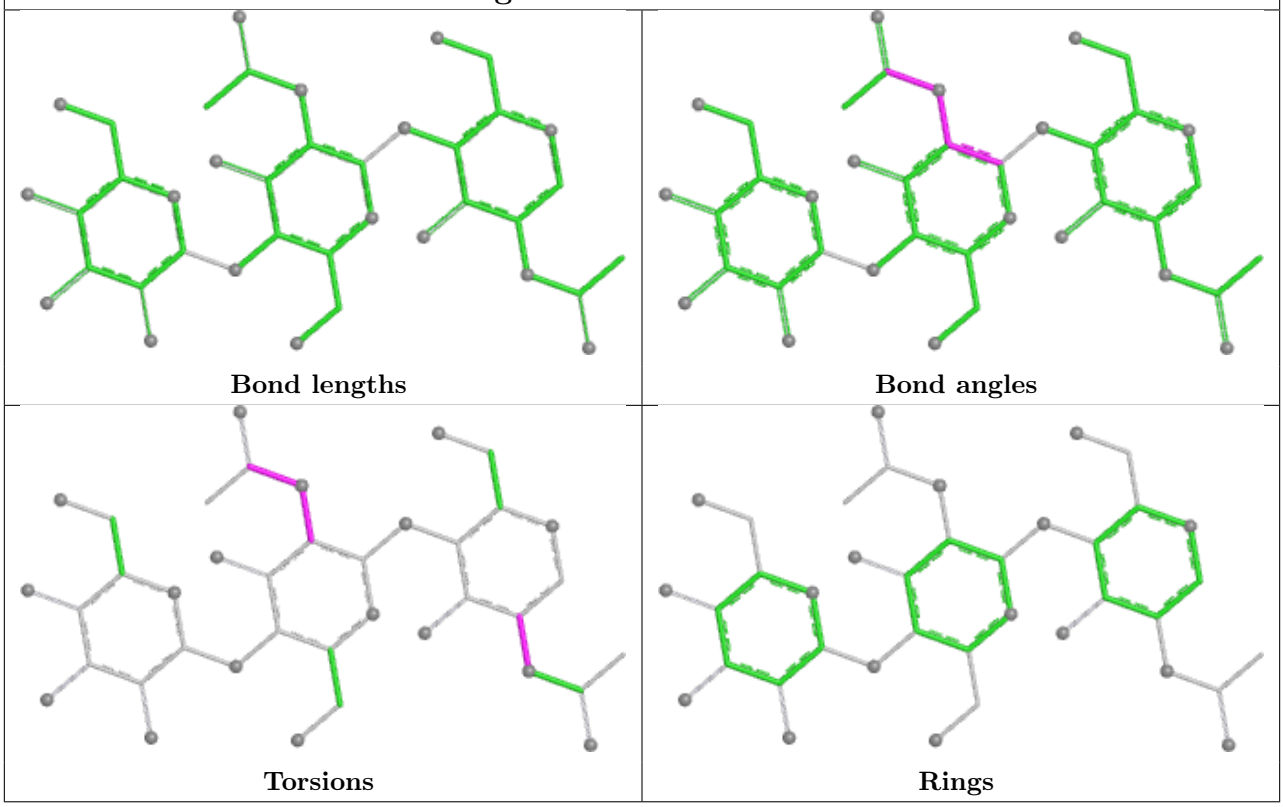
Oligosaccharide Chain E



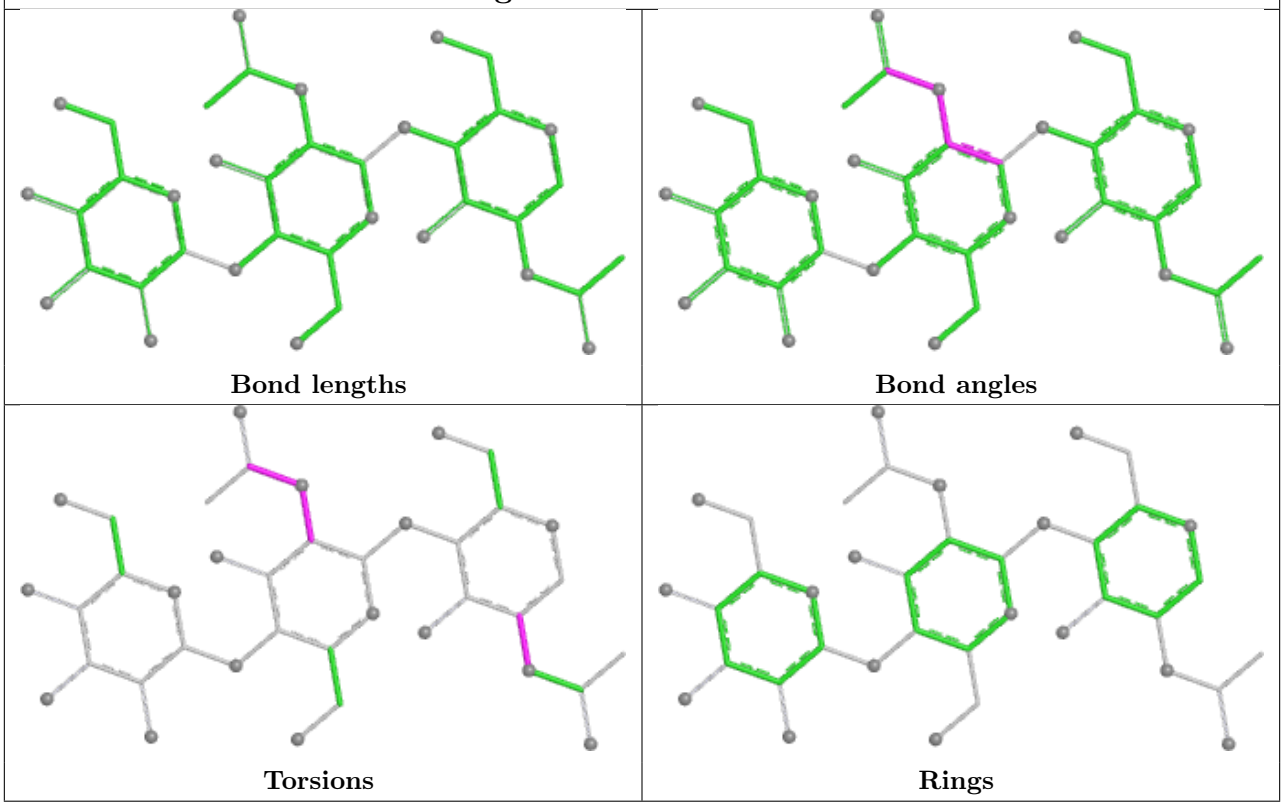
Oligosaccharide Chain F



Oligosaccharide Chain G



Oligosaccharide Chain H



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	$\#\|Z\| > 2$
5	NAG	a	501	3	14,14,15	0.79	0	17,19,21	0.74	0
5	NAG	b	501	3	14,14,15	0.84	0	17,19,21	0.94	1 (5%)
5	NAG	c	501	3	14,14,15	1.11	1 (7%)	17,19,21	1.38	4 (23%)
5	NAG	d	501	-	14,14,15	1.13	1 (7%)	17,19,21	1.38	4 (23%)

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	a	501	3	-	4/6/23/26	0/1/1/1
5	NAG	b	501	3	-	4/6/23/26	0/1/1/1
5	NAG	c	501	3	-	2/6/23/26	0/1/1/1
5	NAG	d	501	-	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	d	501	NAG	O5-C1	-2.82	1.39	1.43
5	c	501	NAG	O5-C1	-2.77	1.39	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	501	NAG	C1-C2-N2	3.42	115.82	110.43
5	d	501	NAG	C1-C2-N2	3.40	115.80	110.43
5	c	501	NAG	O5-C1-C2	2.48	115.12	111.29
5	d	501	NAG	O5-C1-C2	2.45	115.09	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	b	501	NAG	C1-O5-C5	2.44	115.46	112.19
5	d	501	NAG	C2-N2-C7	2.09	125.70	122.90
5	d	501	NAG	C1-O5-C5	2.07	114.96	112.19
5	c	501	NAG	C1-O5-C5	2.04	114.92	112.19
5	c	501	NAG	C2-N2-C7	2.04	125.64	122.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	b	501	NAG	C4-C5-C6-O6
5	a	501	NAG	O5-C5-C6-O6
5	b	501	NAG	O5-C5-C6-O6
5	a	501	NAG	C4-C5-C6-O6
5	c	501	NAG	C1-C2-N2-C7
5	d	501	NAG	C1-C2-N2-C7
5	b	501	NAG	C1-C2-N2-C7
5	b	501	NAG	C3-C2-N2-C7
5	a	501	NAG	C1-C2-N2-C7
5	c	501	NAG	C3-C2-N2-C7
5	d	501	NAG	C3-C2-N2-C7
5	a	501	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	d	501	NAG	7	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.

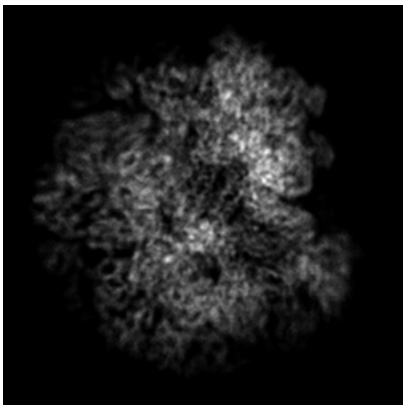
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-72746. These allow visual inspection of the internal detail of the map and identification of artifacts.

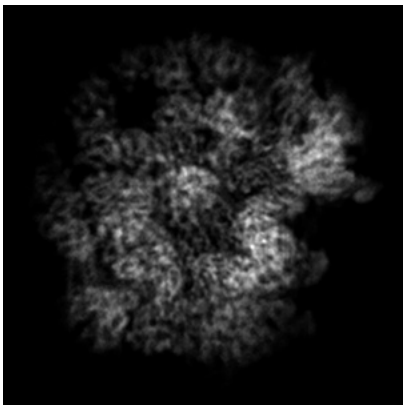
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

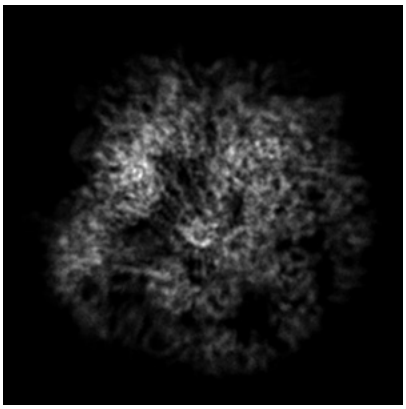
6.1.1 Primary map



X

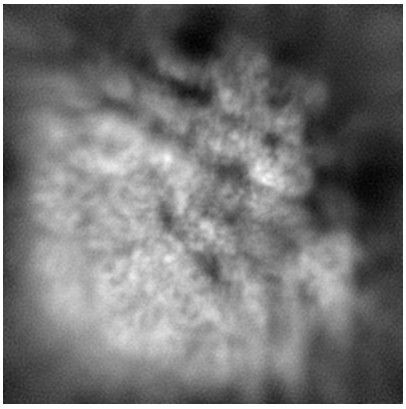


Y

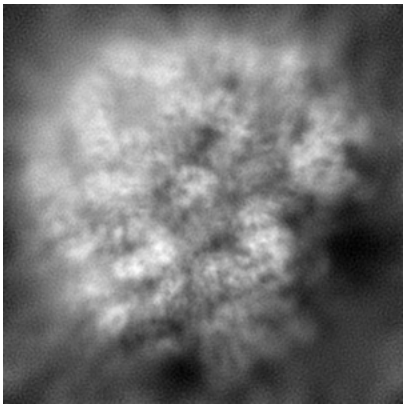


Z

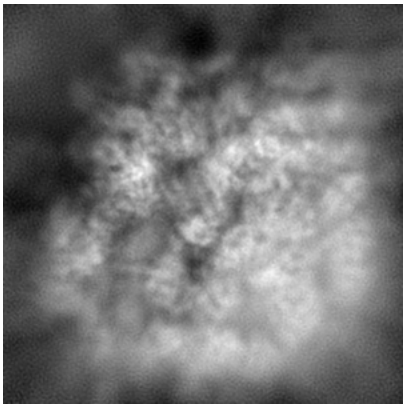
6.1.2 Raw map



X



Y

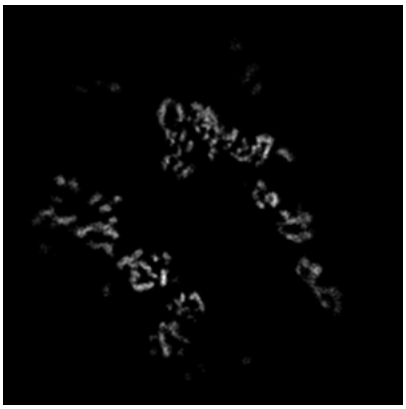


Z

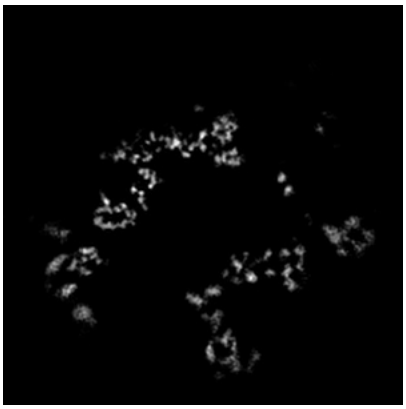
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

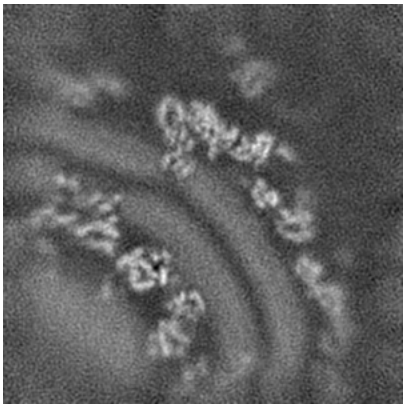
6.2.1 Primary map

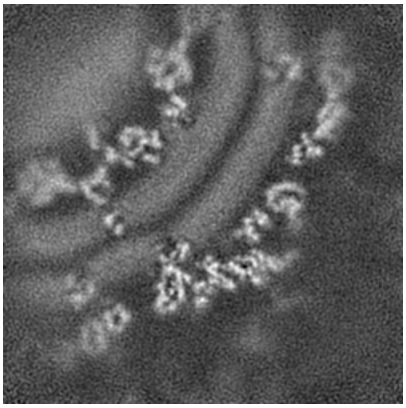

X Index: 110

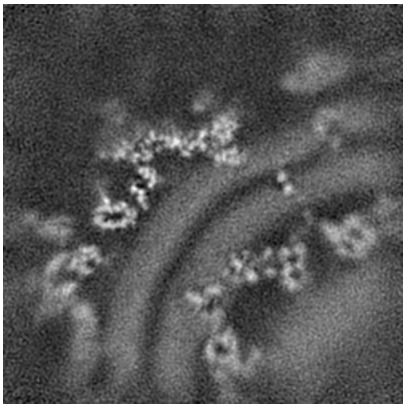
Y Index: 110


Z Index: 110

6.2.2 Raw map


X Index: 110

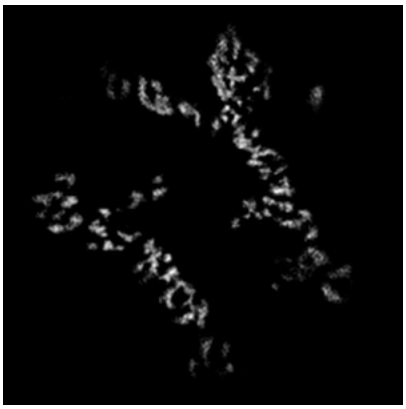

Y Index: 110


Z Index: 110

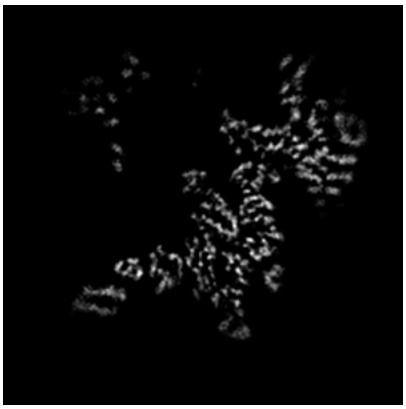
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

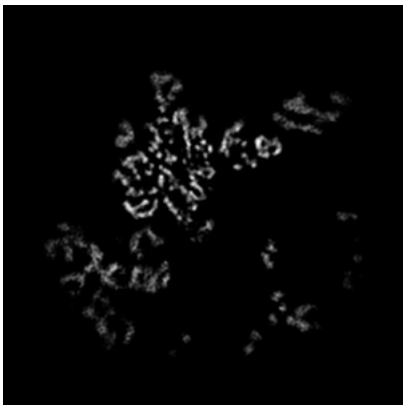
6.3.1 Primary map



X Index: 122

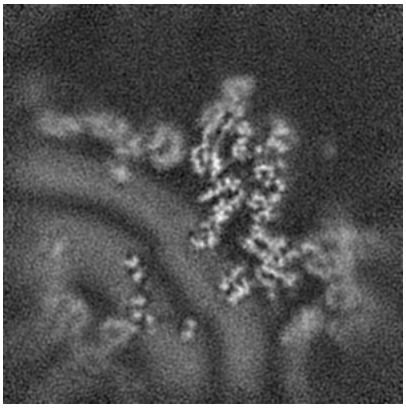


Y Index: 140

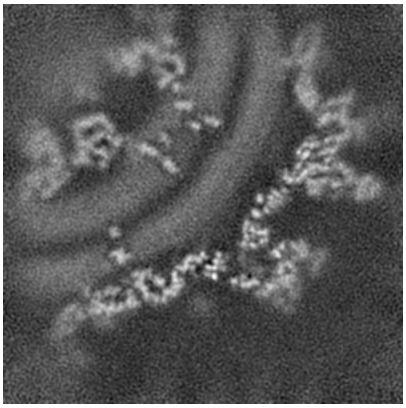


Z Index: 138

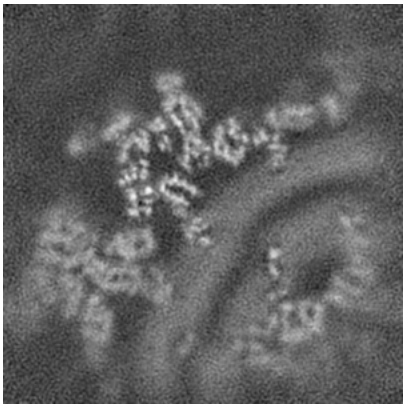
6.3.2 Raw map



X Index: 80



Y Index: 121

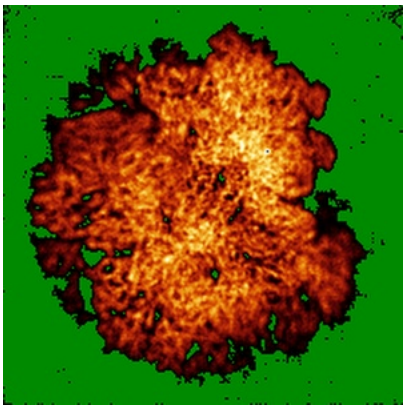


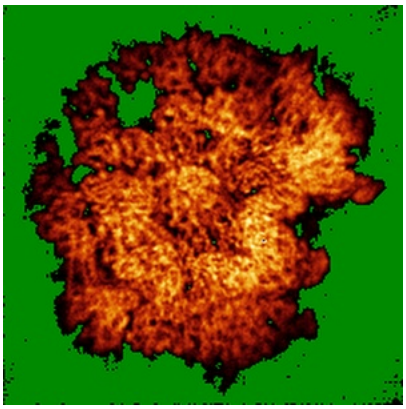
Z Index: 133

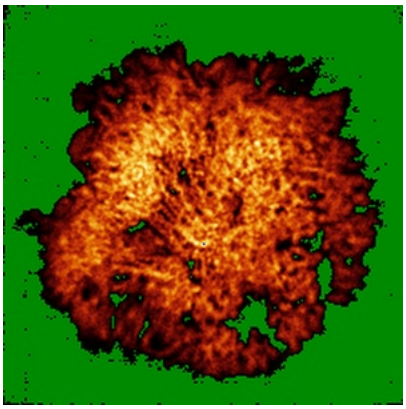
The images above show the largest variance slices of the map in three orthogonal directions.

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

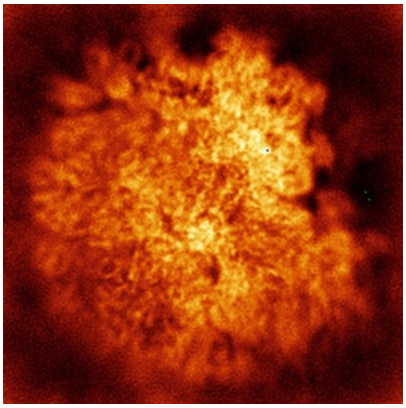
6.4.1 Primary map

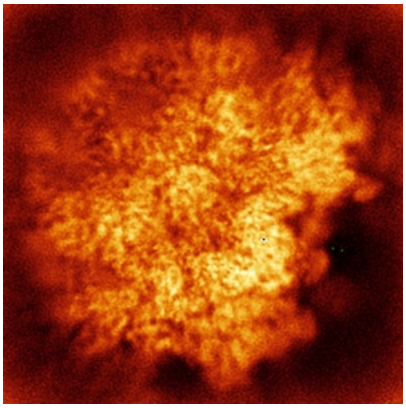

X

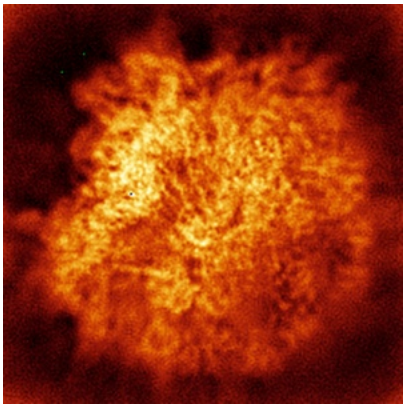

Y


Z

6.4.2 Raw map


X

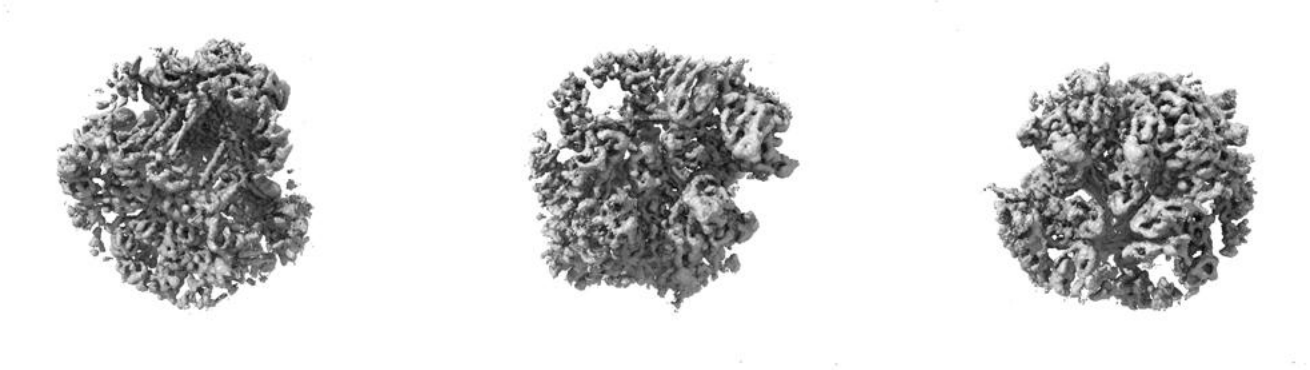

Y


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.

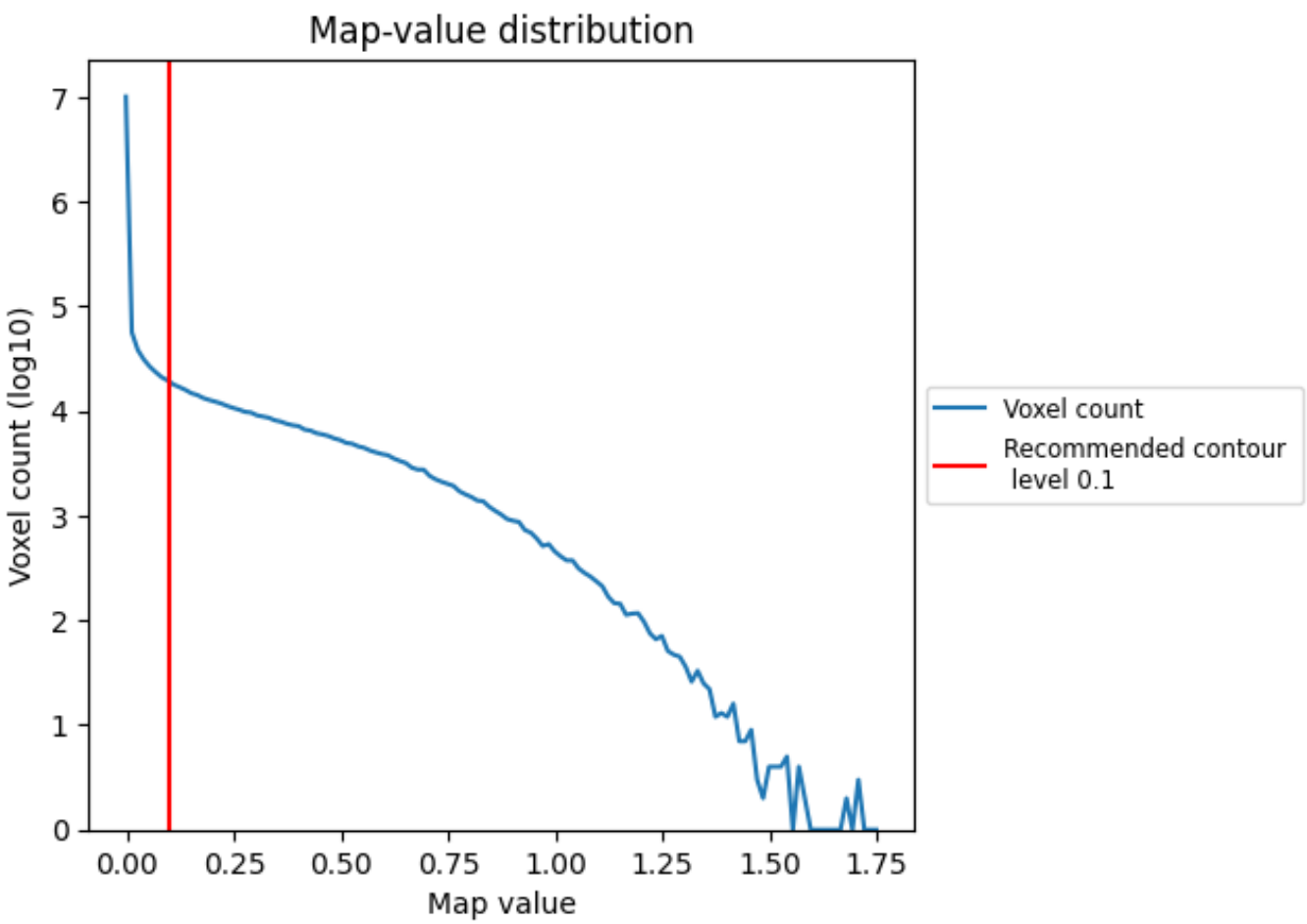
6.6 Mask visualisation (i)

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

7 Map analysis (i)

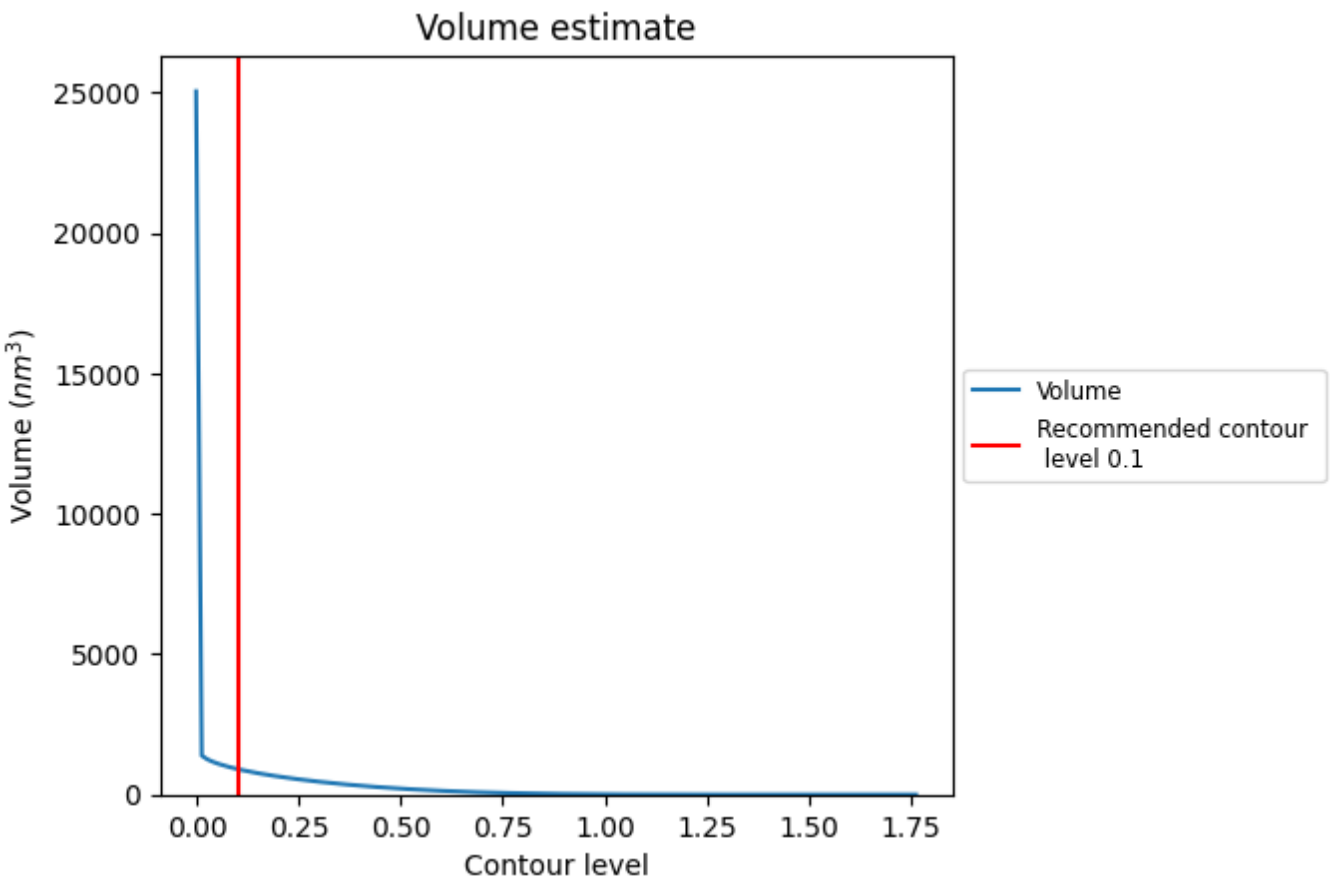
This section contains the results of statistical analysis of the map.

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.

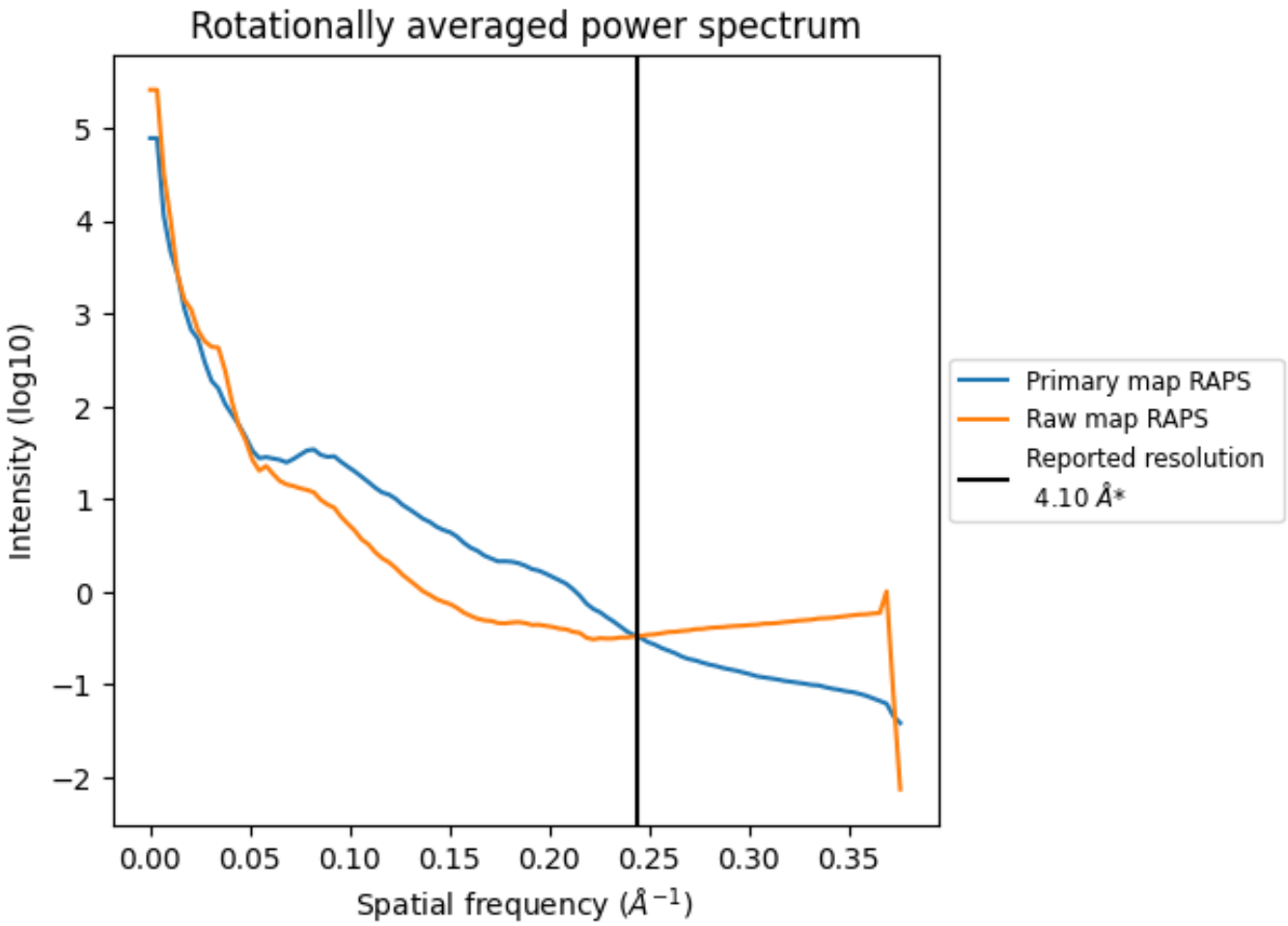
7.2 Volume estimate (i)



The volume at the recommended contour level is 908 nm^3; this corresponds to an approximate mass of 820 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)

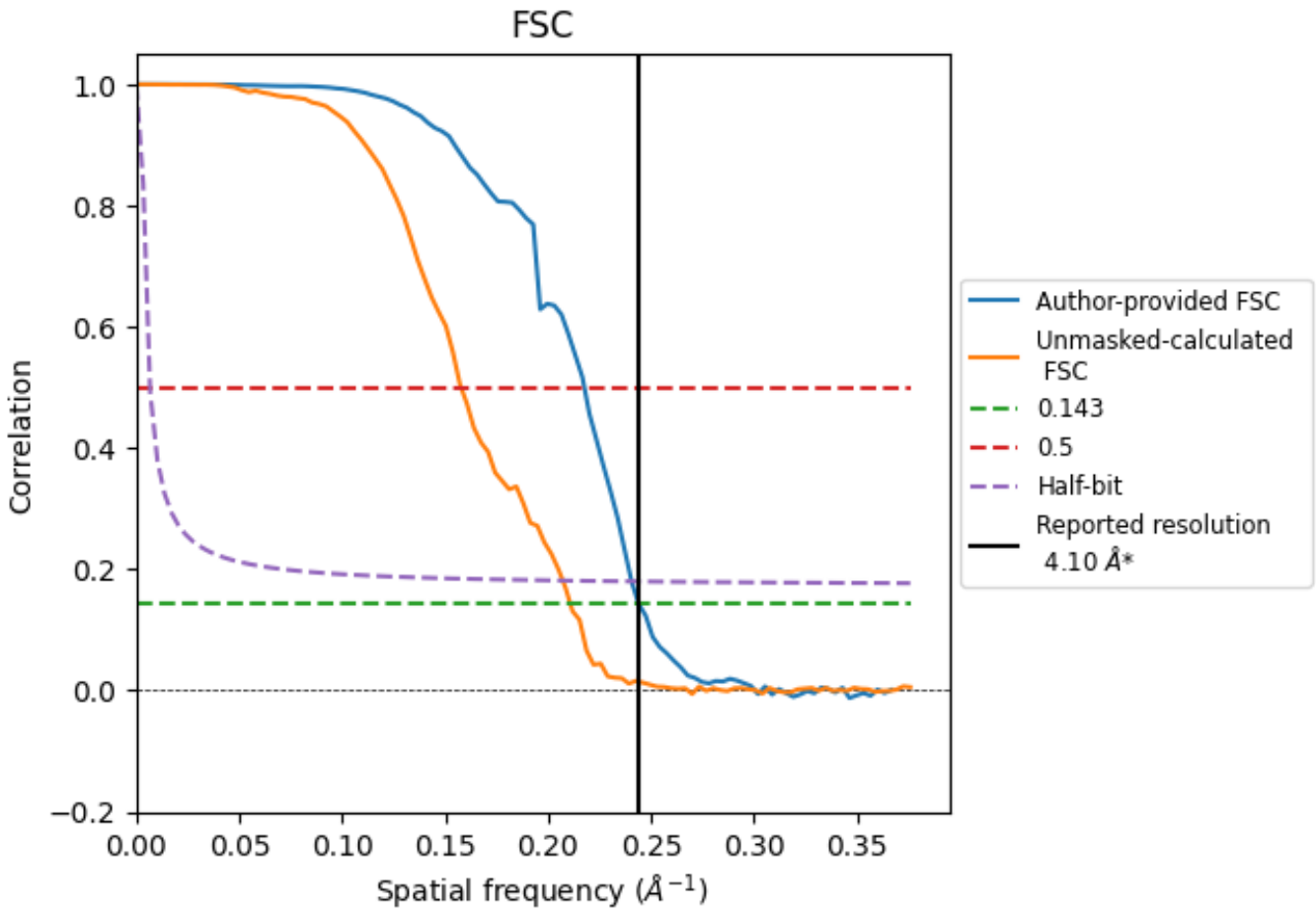


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

8.2 Resolution estimates (i)

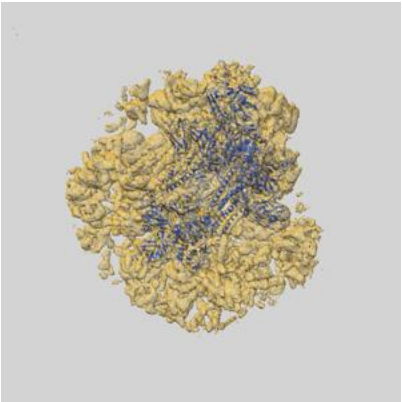
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.10	4.60	4.16
Unmasked-calculated*	4.74	6.34	4.83

*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 4.74 differs from the reported value 4.1 by more than 10 %

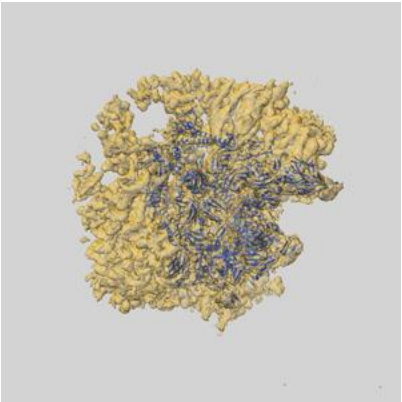
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-72746 and PDB model 9YB2. Per-residue inclusion information can be found in section 3 on page 6.

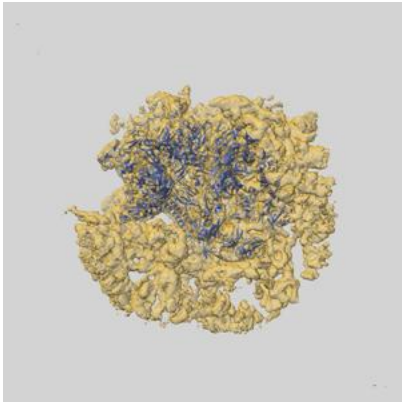
9.1 Map-model overlay (i)



X



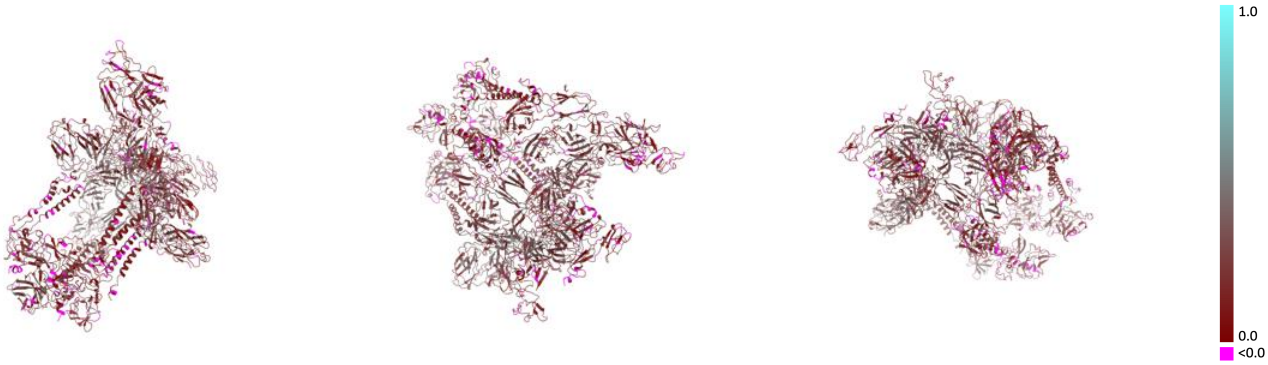
Y



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.

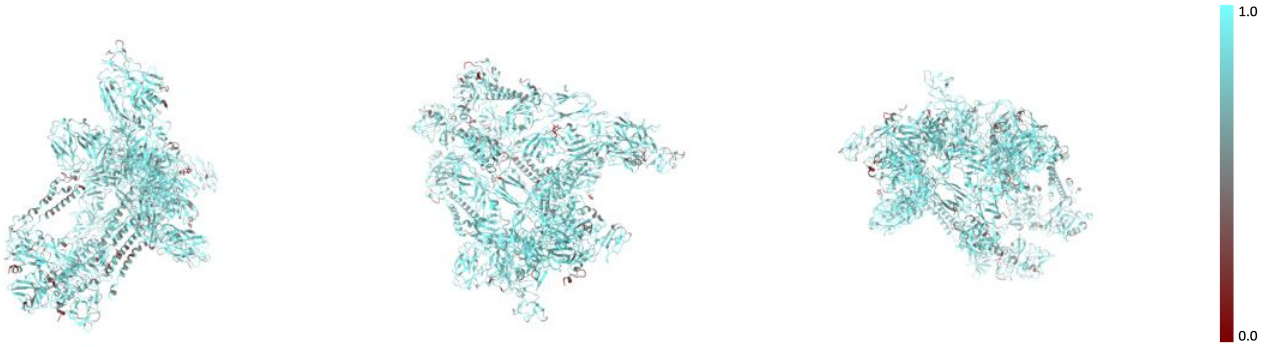
9.2 Q-score mapped to coordinate model (i)



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.

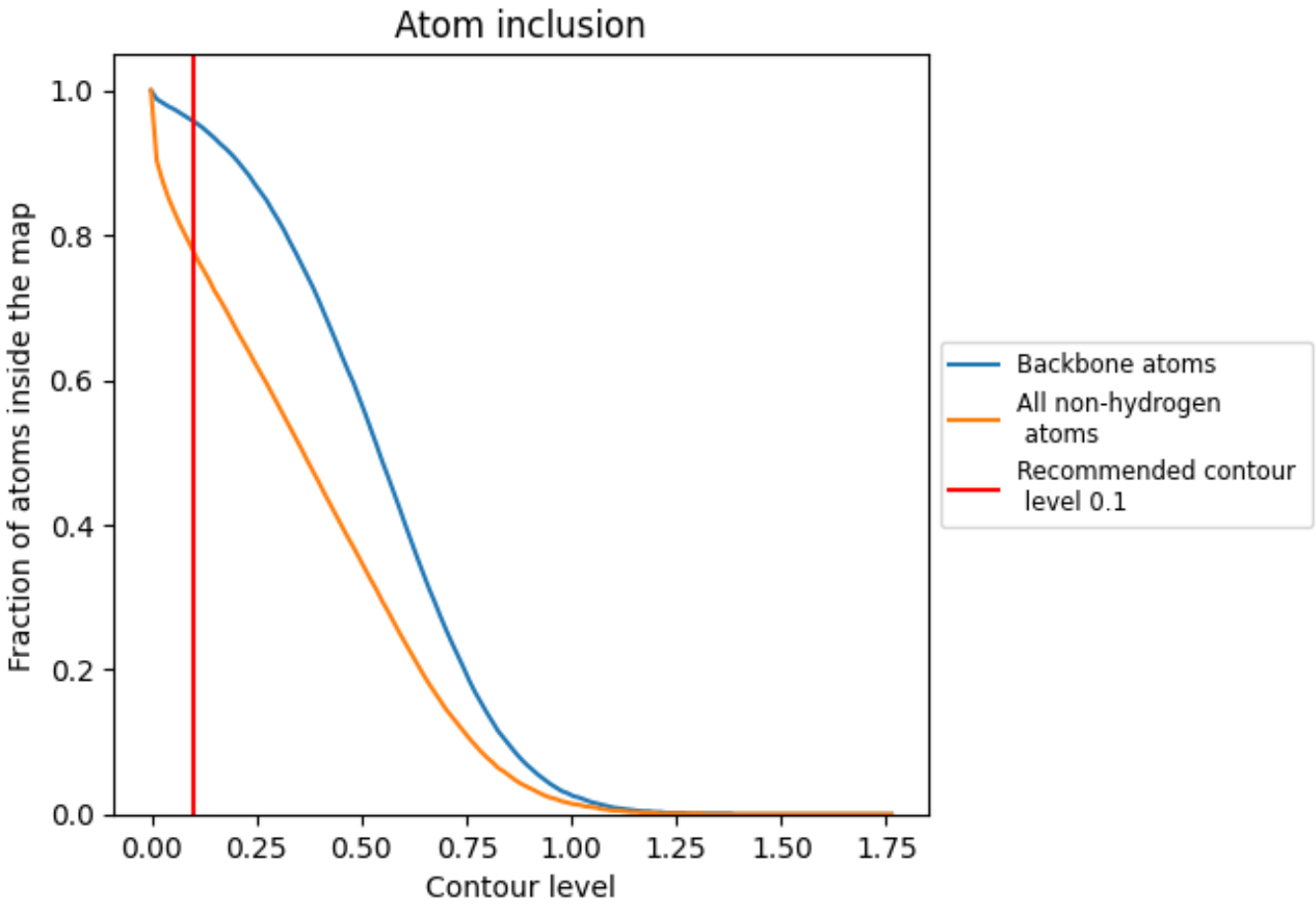
9.3 Atom inclusion mapped to coordinate model (i)



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, 96% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7770	0.2190
A	0.8070	0.2250
B	0.7990	0.2310
C	0.8370	0.2940
D	0.8020	0.2400
E	0.5900	0.2290
F	0.6410	0.1770
G	0.4870	0.2110
H	0.2820	0.1170
P	0.7330	0.1650
Q	0.7180	0.1690
R	0.7770	0.2160
S	0.7260	0.1610
a	0.7490	0.1690
b	0.7500	0.2130
c	0.7850	0.2330
d	0.7580	0.2090