Full wwPDB EM Validation Report ⓘ

May 20, 2025 – 07:11 PM EDT

PDB ID	:	9BDF / pdb_00009bdf
EMDB ID	:	EMD-44451
Title	:	Influenza A virus Hemagglutinin H3/Darwin/6/2021 in complex with Fab ADI-85666
Authors	:	Ferreira Ramos, A.S.; Bajic, G.
Deposited on	:	2024-04-11
Resolution	:	3.01 Å(reported)

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

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

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

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

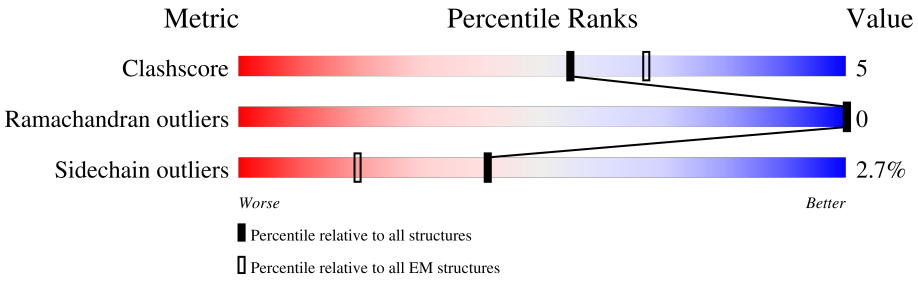
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.01 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	81% 12% 7%
1	G	514	80% 13% 7%
1	H	514	79% 13% 7%
2	B	240	45% 8% 47%
2	C	240	47% 48%
2	E	240	44% 8% 48%
3	D	214	40% 9% 51%
3	I	214	41% 8% 51%

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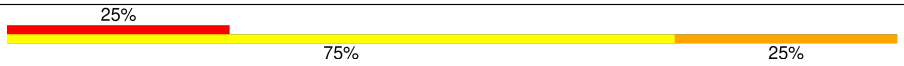
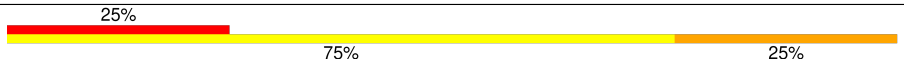
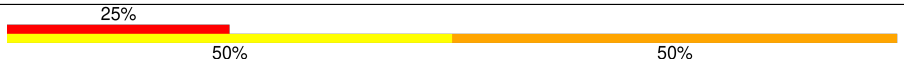
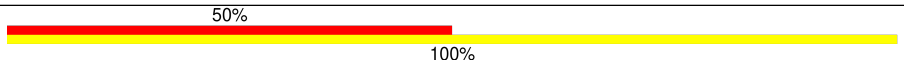
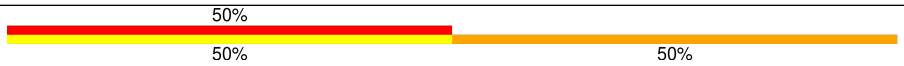
Mol	Chain	Length	Quality of chain
3	J	214	
4	F	4	
4	M	4	
4	R	4	
5	K	2	
5	N	2	
5	O	2	
5	P	2	
5	Q	2	
6	L	3	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17167 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	479	Total	C	N	O	S	0	0
			3778	2352	674	734	18		
1	G	479	Total	C	N	O	S	0	0
			3778	2352	674	734	18		
1	H	479	Total	C	N	O	S	0	0
			3778	2352	674	734	18		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ASN	ASP	conflict	UNP A0A8F5JT24
A	53	GLY	ASP	conflict	UNP A0A8F5JT24
A	355	TRP	HIS	conflict	UNP A0A8F5JT24
A	380	ILE	LYS	conflict	UNP A0A8F5JT24
A	432	ILE	GLU	conflict	UNP A0A8F5JT24
A	505	ALA	VAL	conflict	UNP A0A8F5JT24
A	506	GLY	-	expression tag	UNP A0A8F5JT24
A	507	SER	-	expression tag	UNP A0A8F5JT24
A	508	SER	-	expression tag	UNP A0A8F5JT24
A	509	LEU	-	expression tag	UNP A0A8F5JT24
A	510	GLU	-	expression tag	UNP A0A8F5JT24
A	511	VAL	-	expression tag	UNP A0A8F5JT24
A	512	LEU	-	expression tag	UNP A0A8F5JT24
A	513	PHE	-	expression tag	UNP A0A8F5JT24
A	514	GLN	-	expression tag	UNP A0A8F5JT24
G	31	ASN	ASP	conflict	UNP A0A8F5JT24
G	53	GLY	ASP	conflict	UNP A0A8F5JT24
G	355	TRP	HIS	conflict	UNP A0A8F5JT24
G	380	ILE	LYS	conflict	UNP A0A8F5JT24
G	432	ILE	GLU	conflict	UNP A0A8F5JT24
G	505	ALA	VAL	conflict	UNP A0A8F5JT24
G	506	GLY	-	expression tag	UNP A0A8F5JT24
G	507	SER	-	expression tag	UNP A0A8F5JT24
G	508	SER	-	expression tag	UNP A0A8F5JT24

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Chain	Residue	Modelled	Actual	Comment	Reference
G	509	LEU	-	expression tag	UNP A0A8F5JT24
G	510	GLU	-	expression tag	UNP A0A8F5JT24
G	511	VAL	-	expression tag	UNP A0A8F5JT24
G	512	LEU	-	expression tag	UNP A0A8F5JT24
G	513	PHE	-	expression tag	UNP A0A8F5JT24
G	514	GLN	-	expression tag	UNP A0A8F5JT24
H	31	ASN	ASP	conflict	UNP A0A8F5JT24
H	53	GLY	ASP	conflict	UNP A0A8F5JT24
H	355	TRP	HIS	conflict	UNP A0A8F5JT24
H	380	ILE	LYS	conflict	UNP A0A8F5JT24
H	432	ILE	GLU	conflict	UNP A0A8F5JT24
H	505	ALA	VAL	conflict	UNP A0A8F5JT24
H	506	GLY	-	expression tag	UNP A0A8F5JT24
H	507	SER	-	expression tag	UNP A0A8F5JT24
H	508	SER	-	expression tag	UNP A0A8F5JT24
H	509	LEU	-	expression tag	UNP A0A8F5JT24
H	510	GLU	-	expression tag	UNP A0A8F5JT24
H	511	VAL	-	expression tag	UNP A0A8F5JT24
H	512	LEU	-	expression tag	UNP A0A8F5JT24
H	513	PHE	-	expression tag	UNP A0A8F5JT24
H	514	GLN	-	expression tag	UNP A0A8F5JT24

- Molecule 2 is a protein called ADI-85666 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	128	Total	C	N	O	S	0	0
			979	621	164	189	5		
2	C	124	Total	C	N	O	S	0	0
			958	610	160	183	5		
2	E	125	Total	C	N	O	S	0	0
			964	613	161	185	5		

- Molecule 3 is a protein called ADI-85666 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	104	Total	C	N	O	S	0	0
			793	495	140	156	2		
3	I	104	Total	C	N	O	S	0	0
			793	495	140	156	2		
3	J	104	Total	C	N	O	S	0	0
			793	495	140	156	2		

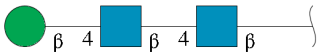
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	4	Total	C	N	O	0	0
			50	28	2	20		
4	M	4	Total	C	N	O	0	0
			50	28	2	20		
4	R	4	Total	C	N	O	0	0
			50	28	2	20		

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

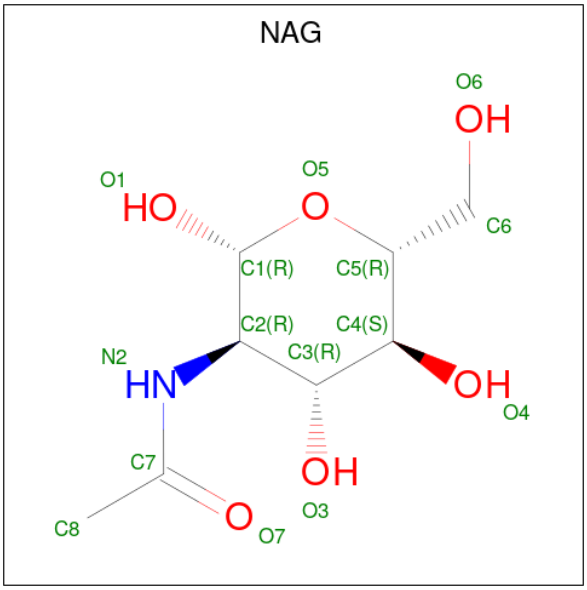
Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 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
6	L	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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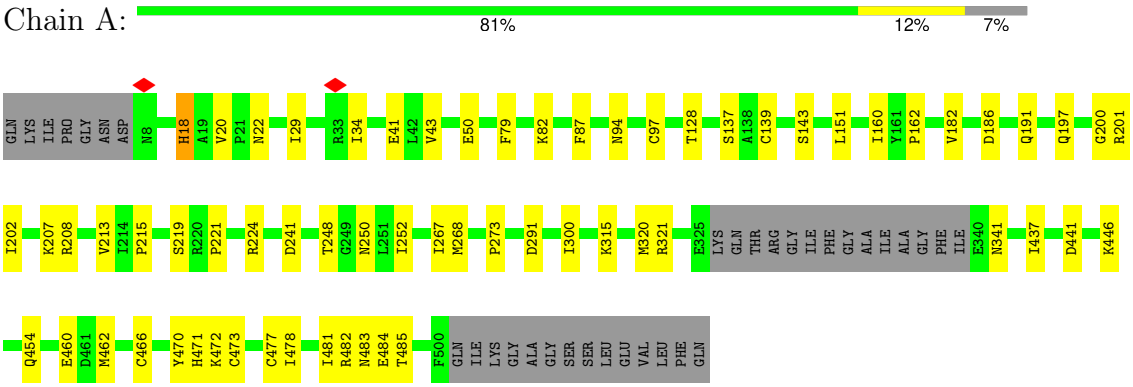
Mol	Chain	Residues	Atoms				AltConf
7	G	1	Total	C	N	O	0
			14	8	1	5	
7	H	1	Total	C	N	O	0
			14	8	1	5	
7	H	1	Total	C	N	O	0
			14	8	1	5	
7	H	1	Total	C	N	O	0
			14	8	1	5	
7	H	1	Total	C	N	O	0
			14	8	1	5	
7	H	1	Total	C	N	O	0
			14	8	1	5	

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.

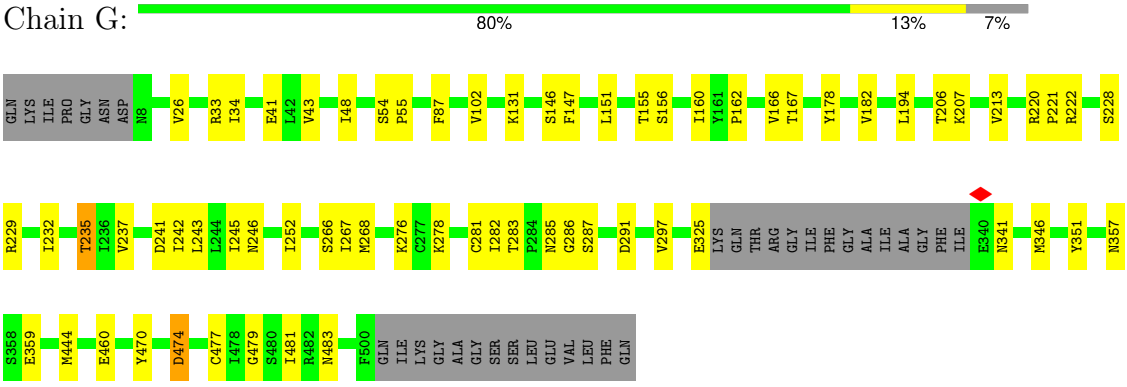
• Molecule 1: Hemagglutinin

Chain A:



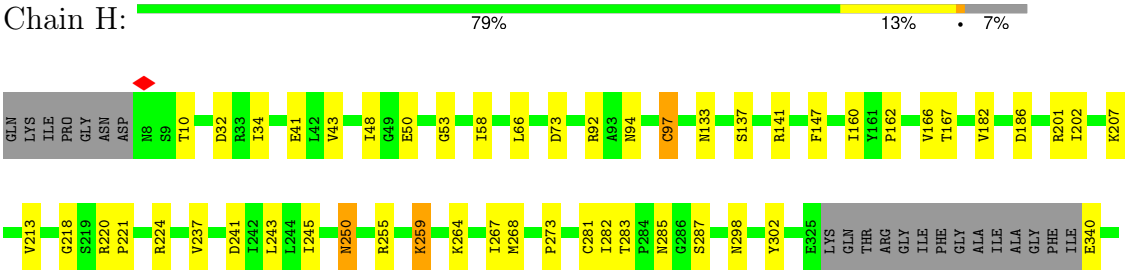
• Molecule 1: Hemagglutinin

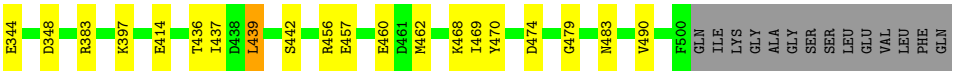
Chain G:



• Molecule 1: Hemagglutinin

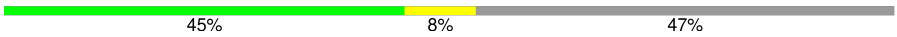
Chain H:

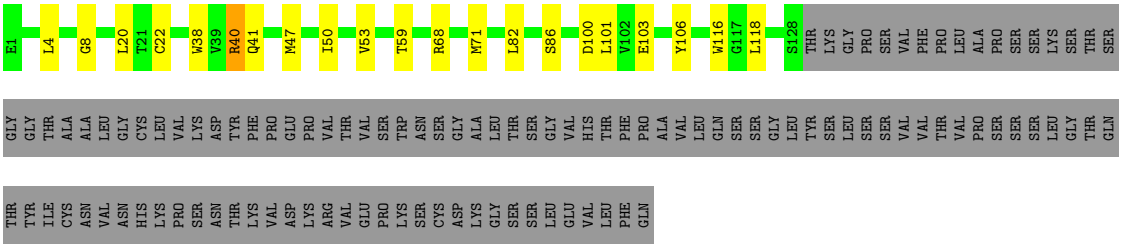




• Molecule 2: ADI-85666 Fab heavy chain

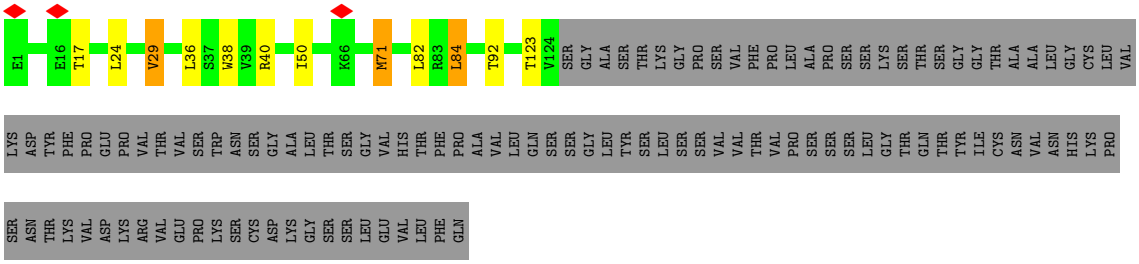
Chain B:





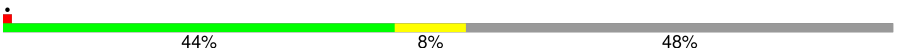
• Molecule 2: ADI-85666 Fab heavy chain

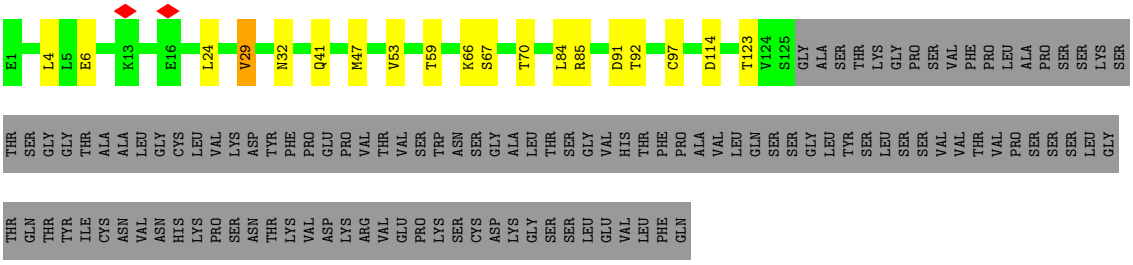
Chain C:



• Molecule 2: ADI-85666 Fab heavy chain

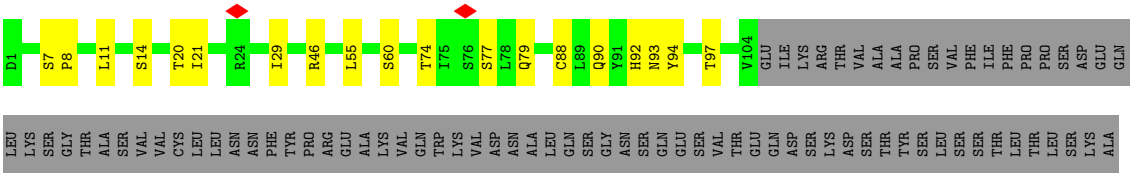
Chain E:





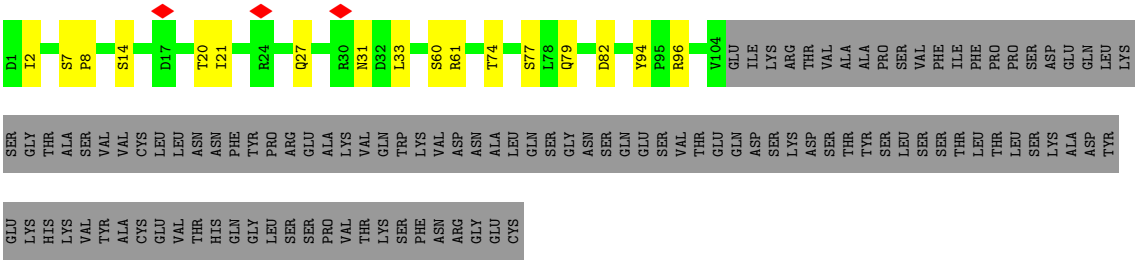
• Molecule 3: ADI-85666 Fab light chain

Chain D:



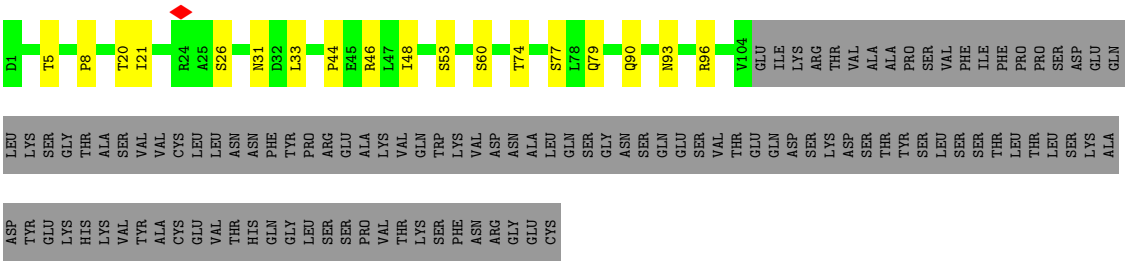
• Molecule 3: ADI-85666 Fab light chain

Chain I:



• Molecule 3: ADI-85666 Fab light chain

Chain J:



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

Chain M:

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

Chain R:

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

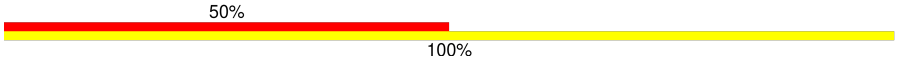
Chain K:

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

Chain N:

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

Chain O:



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

Chain P:

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

Chain Q:

• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:


NAG1
NAG2
BMA3

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	315433	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52.44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.673	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, 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	0.15	0/3853	0.30	0/5215
1	G	0.15	0/3853	0.31	0/5215
1	H	0.15	0/3853	0.30	0/5215
2	B	0.15	0/1003	0.34	0/1363
2	C	0.15	0/982	0.33	0/1335
2	E	0.14	0/988	0.31	0/1343
3	D	0.15	0/812	0.38	0/1103
3	I	0.16	0/812	0.42	0/1103
3	J	0.15	0/812	0.37	0/1103
All	All	0.15	0/16968	0.32	0/22995

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3778	0	3668	36	0
1	G	3778	0	3670	38	0
1	H	3778	0	3667	42	0
2	B	979	0	959	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	958	0	941	6	0
2	E	964	0	946	14	0
3	D	793	0	773	8	0
3	I	793	0	773	7	0
3	J	793	0	773	8	0
4	F	50	0	43	2	0
4	M	50	0	43	1	0
4	R	50	0	43	2	0
5	K	28	0	25	1	0
5	N	28	0	25	1	0
5	O	28	0	25	1	0
5	P	28	0	25	1	0
5	Q	28	0	25	2	0
6	L	39	0	34	0	0
7	A	70	0	65	0	0
7	G	84	0	78	0	0
7	H	70	0	65	0	0
All	All	17167	0	16666	164	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 5.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:479:GLY:O	1:H:483:ASN:HB2	1.89	0.72
1:H:250:ASN:N	1:H:250:ASN:OD1	2.25	0.69
1:A:182:VAL:HG21	1:A:213:VAL:HG11	1.76	0.68
2:C:71:MET:HE2	2:C:82:LEU:HD13	1.75	0.68
3:D:77:SER:OG	3:D:79:GLN:NE2	2.29	0.66
1:A:97:CYS:O	1:A:224:ARG:NH1	2.29	0.66
2:C:40:ARG:HB3	2:C:50:ILE:HD11	1.77	0.66
1:G:221:PRO:HA	4:F:2:NAG:H81	1.78	0.65
1:H:182:VAL:HG21	1:H:213:VAL:HG11	1.78	0.65
1:H:268:MET:HE1	1:H:282:ILE:HG22	1.79	0.65
1:H:221:PRO:HA	4:M:2:NAG:H81	1.78	0.65
1:H:97:CYS:O	1:H:224:ARG:NH1	2.31	0.64
1:H:201:ARG:HH21	5:Q:1:NAG:H83	1.62	0.64
1:H:50:GLU:HG2	1:H:273:PRO:HG2	1.79	0.64
2:B:68:ARG:NH1	2:B:86:SER:O	2.31	0.63
1:G:146:SER:OG	1:G:147:PHE:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:298:ASN:HA	5:O:2:NAG:H62	1.81	0.63
1:G:222:ARG:HG3	4:F:2:NAG:H82	1.81	0.61
1:G:283:THR:OG1	1:G:286:GLY:O	2.18	0.59
2:B:8:GLY:HA3	2:B:20:LEU:HD23	1.84	0.59
1:G:102:VAL:HG22	1:G:232:ILE:HB	1.84	0.59
1:G:55:PRO:HG3	1:G:278:LYS:HD2	1.82	0.59
1:A:268:MET:HE2	1:A:300:ILE:HG22	1.85	0.59
1:A:34:ILE:HD13	1:A:437:ILE:HD13	1.84	0.58
1:A:462:MET:HE2	1:A:466:CYS:HB2	1.83	0.58
3:D:90:GLN:OE1	3:D:97:THR:OG1	2.21	0.58
1:G:266:SER:OG	1:G:267:ILE:N	2.37	0.57
2:E:114:ASP:OD1	3:J:46:ARG:NH1	2.38	0.57
1:G:182:VAL:HG21	1:G:213:VAL:HG11	1.86	0.57
1:G:474:ASP:OD1	1:G:474:ASP:N	2.35	0.56
2:E:67:SER:O	2:E:85:ARG:NH2	2.39	0.56
1:A:50:GLU:HG2	1:A:273:PRO:HG2	1.88	0.56
3:D:90:GLN:NE2	3:D:93:ASN:OD1	2.39	0.56
3:J:90:GLN:NE2	3:J:93:ASN:OD1	2.39	0.55
1:A:29:ILE:O	1:H:383:ARG:NH2	2.41	0.54
1:H:283:THR:HG22	1:H:285:ASN:H	1.71	0.54
1:G:357:ASN:OD1	1:G:359:GLU:N	2.39	0.54
1:A:454:GLN:HE22	1:A:484:GLU:HA	1.73	0.53
3:I:77:SER:OG	3:I:79:GLN:OE1	2.26	0.53
2:B:71:MET:HE2	2:B:82:LEU:HD13	1.89	0.53
1:G:155:THR:OG1	1:G:156:SER:N	2.40	0.53
1:H:264:LYS:O	1:H:302:TYR:OH	2.24	0.53
1:A:291:ASP:OD1	1:A:291:ASP:N	2.42	0.53
2:E:53:VAL:HG23	2:E:59:THR:HG22	1.90	0.53
1:A:160:ILE:HG22	1:A:162:PRO:HD3	1.90	0.52
1:G:131:LYS:HB3	1:G:131:LYS:NZ	2.25	0.52
2:C:24:LEU:HD22	2:C:29:VAL:HG23	1.91	0.52
1:A:471:HIS:NE2	1:A:473:CYS:SG	2.80	0.52
1:A:483:ASN:HB3	1:A:485:THR:HG23	1.92	0.52
2:E:92:THR:HG23	2:E:123:THR:HA	1.91	0.52
1:H:201:ARG:HE	5:Q:1:NAG:H83	1.75	0.52
1:H:460:GLU:HB2	1:H:470:TYR:HE1	1.76	0.51
2:E:41:GLN:HB2	2:E:47:MET:HG2	1.91	0.51
1:H:166:VAL:HG23	1:H:245:ILE:HB	1.92	0.51
1:H:32:ASP:OD1	1:H:32:ASP:N	2.36	0.51
3:I:20:THR:HG23	3:I:74:THR:HG22	1.93	0.51
1:A:191:GLN:NE2	1:A:250:ASN:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:285:ASN:HD21	1:G:297:VAL:HG12	1.76	0.51
2:B:53:VAL:HG23	2:B:59:THR:HG22	1.93	0.50
3:J:20:THR:HG23	3:J:74:THR:HG22	1.92	0.50
1:A:460:GLU:HB2	1:A:470:TYR:HE2	1.76	0.50
2:B:40:ARG:HB3	2:B:50:ILE:HD11	1.94	0.50
1:A:186:ASP:OD1	1:A:186:ASP:N	2.41	0.50
1:G:477:CYS:O	1:G:481:ILE:HG13	2.12	0.50
1:G:281:CYS:O	1:G:287:SER:OG	2.26	0.49
1:G:268:MET:HE3	1:G:282:ILE:HG22	1.95	0.49
1:A:321:ARG:NH1	1:A:441:ASP:OD2	2.45	0.49
1:A:151:LEU:HD23	1:A:252:ILE:HG21	1.95	0.49
1:G:479:GLY:O	1:G:483:ASN:HB2	2.13	0.49
1:H:348:ASP:N	1:H:348:ASP:OD1	2.45	0.49
1:G:160:ILE:HG22	1:G:162:PRO:HD3	1.95	0.49
1:H:34:ILE:HD13	1:H:437:ILE:HD13	1.95	0.49
3:I:94:TYR:O	3:I:96:ARG:HG2	2.13	0.49
2:C:38:TRP:HB2	2:C:71:MET:HE1	1.94	0.48
1:A:454:GLN:NE2	1:A:484:GLU:HA	2.27	0.48
2:E:24:LEU:HD22	2:E:29:VAL:HG23	1.95	0.48
3:J:8:PRO:HG2	3:J:21:ILE:HG23	1.96	0.48
3:D:20:THR:HG23	3:D:74:THR:HG22	1.95	0.48
1:A:219:SER:OG	4:R:1:NAG:O7	2.18	0.47
1:G:166:VAL:HG23	1:G:245:ILE:HB	1.96	0.47
1:H:94:ASN:OD1	1:H:94:ASN:N	2.46	0.47
2:B:106:TYR:CZ	1:H:462:MET:HE1	2.48	0.47
2:E:4:LEU:HD21	2:E:24:LEU:HD12	1.96	0.47
1:G:341:ASN:N	1:G:341:ASN:OD1	2.48	0.47
3:I:61:ARG:NH2	3:I:82:ASP:OD2	2.37	0.47
1:G:291:ASP:N	1:G:291:ASP:OD1	2.46	0.47
1:A:460:GLU:OE1	1:H:456:ARG:NH2	2.34	0.46
1:G:54:SER:HB3	1:G:55:PRO:HD3	1.96	0.46
1:H:160:ILE:HG22	1:H:162:PRO:HD3	1.95	0.46
1:G:237:VAL:HG21	1:G:243:LEU:HB2	1.96	0.46
3:J:93:ASN:O	3:J:96:ARG:NH1	2.48	0.46
1:H:141:ARG:NH2	1:H:147:PHE:O	2.48	0.46
3:I:2:ILE:HG23	3:I:27:GLN:H	1.81	0.46
1:G:460:GLU:HB2	1:G:470:TYR:HE2	1.81	0.46
1:H:207:LYS:HB2	1:H:241:ASP:OD1	2.16	0.46
2:C:92:THR:HG23	2:C:123:THR:HA	1.96	0.46
3:D:8:PRO:HG2	3:D:21:ILE:HG23	1.98	0.46
2:E:6:GLU:HG2	2:E:97:CYS:SG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:THR:HG22	1:G:207:LYS:H	1.81	0.45
3:J:77:SER:OG	3:J:79:GLN:OE1	2.33	0.45
2:B:38:TRP:HB2	2:B:71:MET:HE1	1.98	0.45
1:G:87:PHE:HB3	1:G:267:ILE:HG13	1.97	0.45
1:H:41:GLU:HG3	1:H:43:VAL:H	1.82	0.45
1:A:94:ASN:OD1	1:A:94:ASN:N	2.50	0.45
1:H:10:THR:HG21	1:H:468:LYS:NZ	2.31	0.45
1:G:26:VAL:HG23	1:G:34:ILE:HG23	1.98	0.45
2:B:4:LEU:HB3	2:B:22:CYS:SG	2.57	0.44
1:H:53:GLY:HA2	1:H:58:ILE:HD12	1.99	0.44
1:A:41:GLU:HG3	1:A:43:VAL:H	1.82	0.44
2:E:66:LYS:H	2:E:66:LYS:HD2	1.82	0.44
1:G:167:THR:HB	1:G:242:ILE:HD11	2.00	0.44
1:H:133:ASN:OD1	1:H:255:ARG:NH2	2.51	0.44
2:E:47:MET:HE1	3:J:44:PRO:HG3	1.99	0.44
1:H:73:ASP:OD1	1:H:97:CYS:HB2	2.17	0.43
1:G:220:ARG:HD3	1:G:229:ARG:HG2	2.01	0.43
1:G:351:TYR:CD2	1:G:444:MET:HG2	2.53	0.43
2:E:84:LEU:HD12	2:E:84:LEU:HA	1.92	0.43
2:B:100:ASP:OD1	2:B:101:LEU:N	2.51	0.43
1:G:276:LYS:HE3	1:G:276:LYS:HB3	1.78	0.43
1:H:259:LYS:HE2	1:H:259:LYS:HB3	1.58	0.43
1:A:200:GLY:O	1:A:215:PRO:HD2	2.19	0.43
3:I:8:PRO:HG2	3:I:21:ILE:HG23	2.00	0.43
2:E:91:ASP:N	2:E:91:ASP:OD1	2.51	0.42
1:G:178:TYR:HB2	1:G:235:THR:HG23	2.01	0.42
2:C:17:THR:HA	2:C:84:LEU:O	2.19	0.42
2:B:47:MET:HE1	2:B:116:TRP:CZ3	2.55	0.42
1:H:92:ARG:HH21	5:P:1:NAG:H81	1.84	0.42
1:A:201:ARG:HE	5:K:1:NAG:H82	1.84	0.42
1:A:207:LYS:HB2	1:A:241:ASP:OD1	2.20	0.42
1:H:397:LYS:HZ3	1:H:414:GLU:CD	2.28	0.42
1:H:436:THR:HA	1:H:439:LEU:HD23	2.00	0.42
1:H:48:ILE:H	1:H:48:ILE:HG13	1.63	0.42
1:A:18:HIS:CE1	1:A:320:MET:HE3	2.55	0.42
2:B:103:GLU:OE2	1:H:344:GLU:N	2.48	0.42
1:H:237:VAL:HG21	1:H:243:LEU:HB2	2.02	0.42
1:H:202:ILE:HD11	1:H:250:ASN:O	2.20	0.41
1:A:341:ASN:N	1:A:341:ASN:OD1	2.52	0.41
1:A:221:PRO:HA	4:R:2:NAG:H81	2.00	0.41
2:E:66:LYS:HD2	2:E:66:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:186:ASP:OD1	1:H:186:ASP:N	2.45	0.41
1:G:246:ASN:HD22	5:N:1:NAG:C7	2.33	0.41
1:H:218:GLY:O	1:H:220:ARG:NH1	2.54	0.41
1:A:201:ARG:H	1:A:248:THR:HG22	1.86	0.41
1:A:477:CYS:O	1:A:481:ILE:HG13	2.20	0.41
3:D:46:ARG:NE	3:D:55:LEU:HD11	2.35	0.41
1:G:357:ASN:OD1	1:G:357:ASN:C	2.63	0.41
3:J:48:ILE:HG23	3:J:53:SER:H	1.86	0.41
3:D:7:SER:OG	3:D:8:PRO:HD3	2.21	0.41
1:G:41:GLU:HG3	1:G:43:VAL:H	1.85	0.41
1:H:237:VAL:HG13	1:H:241:ASP:HB3	2.02	0.41
1:A:20:VAL:HG23	1:A:22:ASN:O	2.21	0.41
1:A:87:PHE:HB3	1:A:267:ILE:HG13	2.02	0.41
2:B:41:GLN:HB2	2:B:47:MET:HG2	2.02	0.41
3:D:29:ILE:HG13	3:D:92:HIS:HB2	2.01	0.41
1:G:151:LEU:HD23	1:G:252:ILE:HG21	2.01	0.41
1:A:478:ILE:O	1:A:482:ARG:HG3	2.21	0.41
1:G:207:LYS:HB2	1:G:241:ASP:OD1	2.20	0.41
1:H:66:LEU:HD22	1:H:267:ILE:HD12	2.02	0.41
1:A:446:LYS:HB3	1:A:446:LYS:NZ	2.36	0.40
1:H:281:CYS:O	1:H:287:SER:OG	2.20	0.40
1:A:79:PHE:HA	1:A:82:LYS:HG3	2.02	0.40
2:E:32:ASN:HB3	1:G:325:GLU:HG2	2.03	0.40
3:I:7:SER:OG	3:I:8:PRO:HD3	2.21	0.40
1:A:182:VAL:HG22	1:A:202:ILE:HD12	2.04	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	475/514 (92%)	463 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	475/514 (92%)	460 (97%)	15 (3%)	0	100	100
1	H	475/514 (92%)	458 (96%)	17 (4%)	0	100	100
2	B	126/240 (52%)	121 (96%)	5 (4%)	0	100	100
2	C	122/240 (51%)	118 (97%)	4 (3%)	0	100	100
2	E	123/240 (51%)	121 (98%)	2 (2%)	0	100	100
3	D	102/214 (48%)	95 (93%)	7 (7%)	0	100	100
3	I	102/214 (48%)	96 (94%)	6 (6%)	0	100	100
3	J	102/214 (48%)	94 (92%)	8 (8%)	0	100	100
All	All	2102/2904 (72%)	2026 (96%)	76 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	420/446 (94%)	411 (98%)	9 (2%)	48	76
1	G	420/446 (94%)	413 (98%)	7 (2%)	56	80
1	H	420/446 (94%)	408 (97%)	12 (3%)	37	69
2	B	108/206 (52%)	106 (98%)	2 (2%)	52	78
2	C	106/206 (52%)	102 (96%)	4 (4%)	28	61
2	E	107/206 (52%)	105 (98%)	2 (2%)	52	78
3	D	88/187 (47%)	83 (94%)	5 (6%)	17	47
3	I	88/187 (47%)	84 (96%)	4 (4%)	23	56
3	J	88/187 (47%)	83 (94%)	5 (6%)	17	47
All	All	1845/2517 (73%)	1795 (97%)	50 (3%)	41	70

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	128	THR
1	A	137	SER
1	A	139	CYS
1	A	143	SER
1	A	197	GLN
1	A	208	ARG
1	A	315	LYS
1	A	472	LYS
2	B	40	ARG
2	B	118	LEU
2	C	29	VAL
2	C	36	LEU
2	C	71	MET
2	C	84	LEU
3	D	11	LEU
3	D	14	SER
3	D	60	SER
3	D	88	CYS
3	D	94	TYR
2	E	29	VAL
2	E	70	THR
1	G	33	ARG
1	G	48	ILE
1	G	194	LEU
1	G	228	SER
1	G	235	THR
1	G	346	MET
1	G	474	ASP
1	H	97	CYS
1	H	137	SER
1	H	167	THR
1	H	250	ASN
1	H	259	LYS
1	H	340	GLU
1	H	439	LEU
1	H	442	SER
1	H	457	GLU
1	H	469	ILE
1	H	474	ASP
1	H	490	VAL
3	I	14	SER
3	I	31	ASN

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Mol	Chain	Res	Type
3	I	33	LEU
3	I	60	SER
3	J	5	THR
3	J	26	SER
3	J	31	ASN
3	J	33	LEU
3	J	60	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	122	ASN
1	A	389	ASN
1	A	497	ASN
2	C	55	HIS
3	D	79	GLN
1	G	75	GLN
1	G	158	ASN
1	G	197	GLN
1	G	376	GLN
1	G	382	ASN
1	G	389	ASN
1	H	56	HIS
1	H	96	ASN
1	H	132	GLN
1	H	382	ASN
1	H	389	ASN
1	H	454	GLN
3	I	27	GLN
3	J	92	HIS

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)

25 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	F	1	4,1	14,14,15	0.76	0	17,19,21	0.94	1 (5%)
4	NAG	F	2	4	14,14,15	0.76	0	17,19,21	1.08	1 (5%)
4	BMA	F	3	4	11,11,12	0.79	0	15,15,17	2.50	5 (33%)
4	MAN	F	4	4	11,11,12	0.68	0	15,15,17	1.22	1 (6%)
5	NAG	K	1	1,5	14,14,15	0.66	0	17,19,21	1.66	2 (11%)
5	NAG	K	2	5	14,14,15	0.73	0	17,19,21	0.97	0
6	NAG	L	1	6,1	14,14,15	0.71	0	17,19,21	0.89	0
6	NAG	L	2	6	14,14,15	0.72	0	17,19,21	0.95	1 (5%)
6	BMA	L	3	6	11,11,12	0.91	1 (9%)	15,15,17	2.12	4 (26%)
4	NAG	M	1	4,1	14,14,15	0.74	0	17,19,21	1.00	2 (11%)
4	NAG	M	2	4	14,14,15	0.75	0	17,19,21	1.01	2 (11%)
4	BMA	M	3	4	11,11,12	0.80	0	15,15,17	2.50	6 (40%)
4	MAN	M	4	4	11,11,12	0.69	0	15,15,17	1.04	1 (6%)
5	NAG	N	1	1,5	14,14,15	0.72	0	17,19,21	0.83	1 (5%)
5	NAG	N	2	5	14,14,15	0.73	0	17,19,21	0.95	0
5	NAG	O	1	1,5	14,14,15	0.69	0	17,19,21	1.31	2 (11%)
5	NAG	O	2	5	14,14,15	0.70	0	17,19,21	0.79	0
5	NAG	P	1	1,5	14,14,15	0.71	0	17,19,21	1.49	3 (17%)
5	NAG	P	2	5	14,14,15	0.81	0	17,19,21	1.24	2 (11%)
5	NAG	Q	1	1,5	14,14,15	0.71	0	17,19,21	0.93	1 (5%)
5	NAG	Q	2	5	14,14,15	0.73	0	17,19,21	0.90	0
4	NAG	R	1	4,1	14,14,15	0.70	0	17,19,21	1.31	2 (11%)
4	NAG	R	2	4	14,14,15	0.73	0	17,19,21	1.15	1 (5%)
4	BMA	R	3	4	11,11,12	0.79	0	15,15,17	2.55	5 (33%)
4	MAN	R	4	4	11,11,12	0.68	0	15,15,17	1.18	1 (6%)

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	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
6	NAG	L	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	1/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
4	MAN	M	4	4	-	1/2/19/22	1/1/1/1
5	NAG	N	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
5	NAG	Q	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	3/6/23/26	0/1/1/1
4	BMA	R	3	4	-	0/2/19/22	0/1/1/1
4	MAN	R	4	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	3	BMA	C2-C3	2.03	1.55	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	3	BMA	C1-O5-C5	7.69	122.49	112.19
4	F	3	BMA	C1-O5-C5	7.54	122.28	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	3	BMA	C1-O5-C5	7.42	122.12	112.19
6	L	3	BMA	C1-O5-C5	5.48	119.53	112.19
5	K	1	NAG	C2-N2-C7	4.39	128.78	122.90
5	O	1	NAG	C2-N2-C7	3.79	127.98	122.90
4	F	4	MAN	C1-O5-C5	3.63	117.05	112.19
5	K	1	NAG	O5-C1-C2	-3.62	105.68	111.29
4	R	1	NAG	C2-N2-C7	3.60	127.73	122.90
4	M	3	BMA	C3-C4-C5	3.45	116.49	110.23
4	R	3	BMA	C3-C4-C5	3.43	116.45	110.23
4	R	4	MAN	C1-O5-C5	3.42	116.77	112.19
5	P	2	NAG	C2-N2-C7	3.41	127.47	122.90
6	L	3	BMA	C2-C3-C4	3.32	116.69	110.86
4	F	3	BMA	C3-C4-C5	3.30	116.22	110.23
5	P	1	NAG	C2-N2-C7	3.16	127.13	122.90
4	M	4	MAN	C1-O5-C5	2.88	116.05	112.19
5	Q	1	NAG	O5-C1-C2	-2.86	106.87	111.29
4	R	2	NAG	C1-O5-C5	2.84	115.99	112.19
4	F	2	NAG	C2-N2-C7	2.72	126.55	122.90
5	P	1	NAG	O4-C4-C3	-2.63	104.18	110.38
5	N	1	NAG	O5-C1-C2	-2.62	107.24	111.29
5	P	2	NAG	O5-C1-C2	-2.62	107.24	111.29
6	L	3	BMA	C3-C4-C5	2.62	114.98	110.23
5	O	1	NAG	O5-C1-C2	-2.46	107.48	111.29
6	L	2	NAG	O5-C1-C2	-2.39	107.60	111.29
4	F	3	BMA	O4-C4-C3	-2.36	104.82	110.38
4	R	3	BMA	O4-C4-C3	-2.35	104.83	110.38
4	R	3	BMA	C2-C3-C4	2.32	114.94	110.86
4	M	3	BMA	O4-C4-C3	-2.31	104.92	110.38
4	R	3	BMA	O5-C5-C4	2.31	116.46	110.83
4	F	3	BMA	C2-C3-C4	2.30	114.90	110.86
4	M	3	BMA	O5-C5-C4	2.23	116.24	110.83
4	M	3	BMA	C2-C3-C4	2.20	114.73	110.86
4	R	1	NAG	O5-C1-C2	-2.18	107.92	111.29
4	M	1	NAG	O5-C1-C2	-2.17	107.93	111.29
6	L	3	BMA	O4-C4-C3	-2.16	105.28	110.38
4	F	3	BMA	O5-C5-C4	2.13	116.01	110.83
4	M	3	BMA	O3-C3-C2	-2.08	105.80	110.05
4	F	1	NAG	C2-N2-C7	2.08	125.69	122.90
4	M	2	NAG	C2-N2-C7	2.06	125.66	122.90
4	M	1	NAG	C2-N2-C7	2.05	125.65	122.90
5	P	1	NAG	O5-C1-C2	-2.02	108.17	111.29
4	M	2	NAG	O4-C4-C3	-2.01	105.64	110.38

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	NAG	C1-C2-N2-C7
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	N	2	NAG	C8-C7-N2-C2
5	N	2	NAG	O7-C7-N2-C2
5	P	2	NAG	C8-C7-N2-C2
5	P	2	NAG	O7-C7-N2-C2
6	L	1	NAG	C8-C7-N2-C2
6	L	1	NAG	O7-C7-N2-C2
4	M	1	NAG	O5-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	M	4	MAN	O5-C5-C6-O6
5	P	1	NAG	C1-C2-N2-C7
4	R	1	NAG	C3-C2-N2-C7
5	O	1	NAG	C3-C2-N2-C7
5	P	1	NAG	C3-C2-N2-C7
6	L	3	BMA	O5-C5-C6-O6
4	R	1	NAG	C1-C2-N2-C7
5	O	1	NAG	C1-C2-N2-C7
5	K	1	NAG	C3-C2-N2-C7

All (1) ring outliers are listed below:

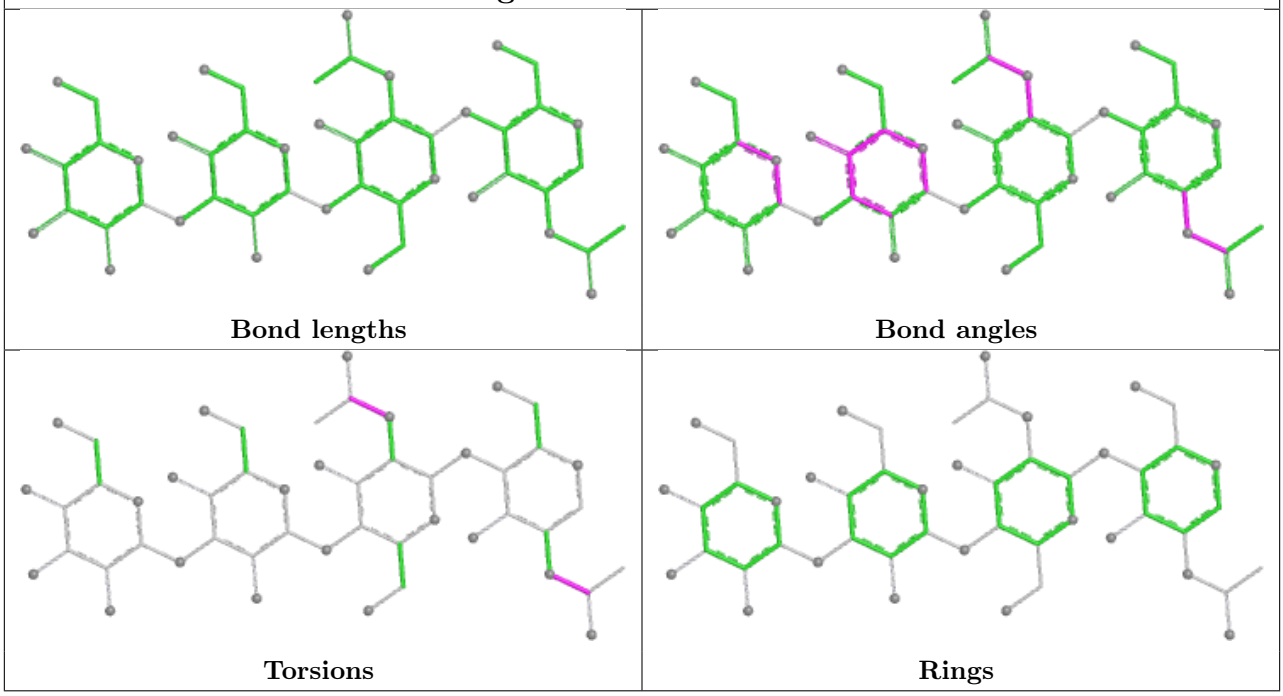
Mol	Chain	Res	Type	Atoms
4	M	4	MAN	C1-C2-C3-C4-C5-O5

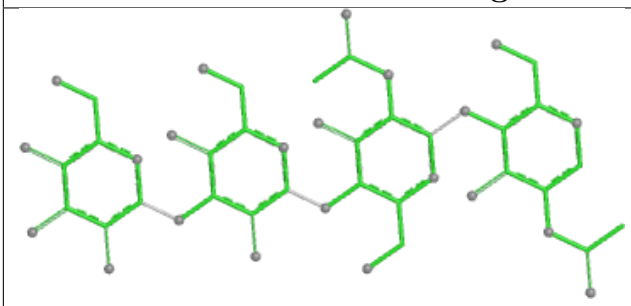
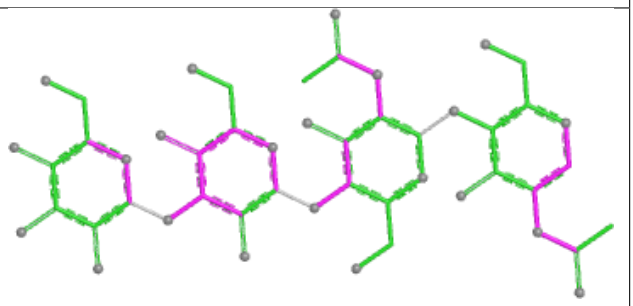
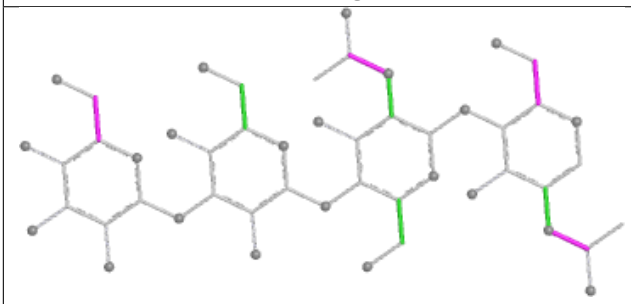
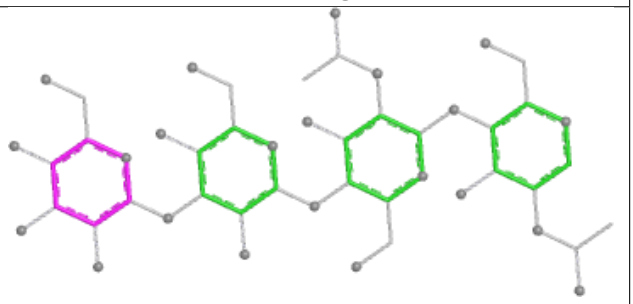
9 monomers are involved in 11 short contacts:

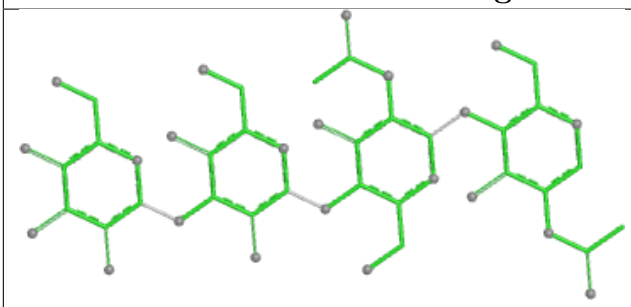
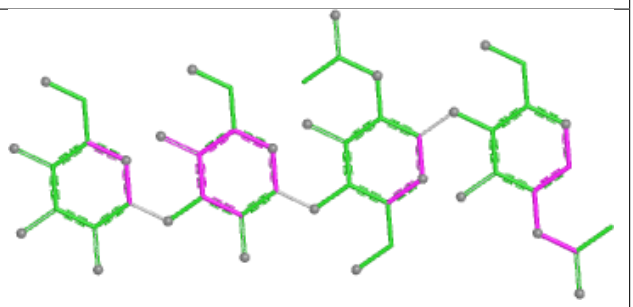
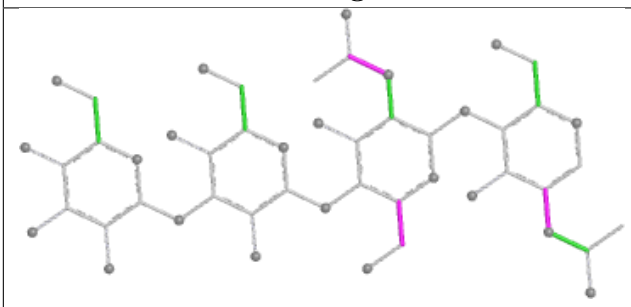
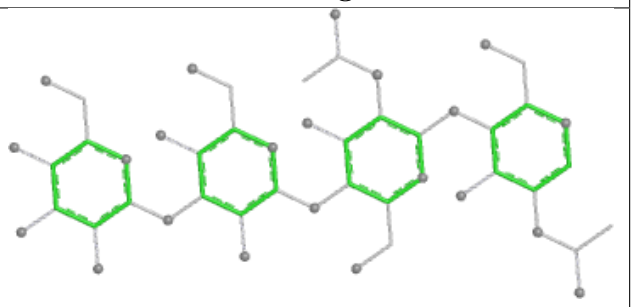
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	1	NAG	1	0
5	Q	1	NAG	2	0
5	K	1	NAG	1	0
5	O	2	NAG	1	0
4	M	2	NAG	1	0
4	F	2	NAG	2	0
4	R	1	NAG	1	0
4	R	2	NAG	1	0
5	P	1	NAG	1	0

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

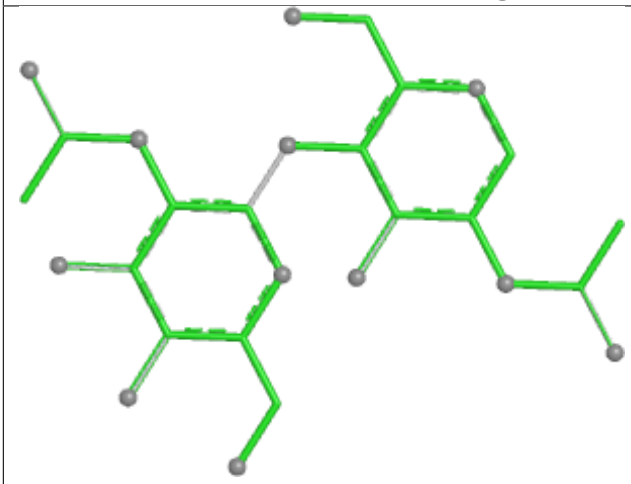
Oligosaccharide Chain F



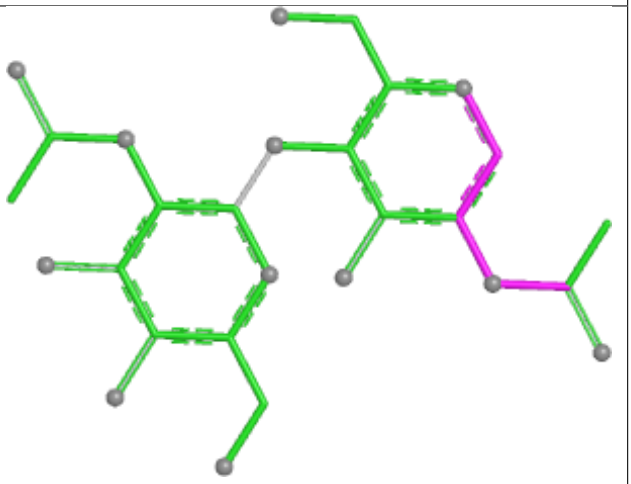
Oligosaccharide Chain M	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain R	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

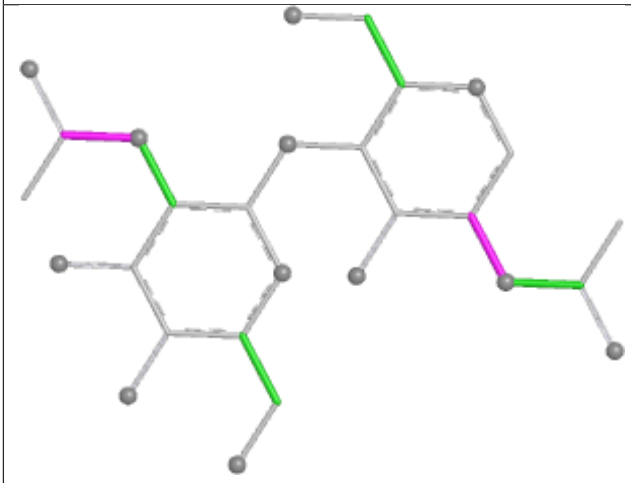
Oligosaccharide Chain K



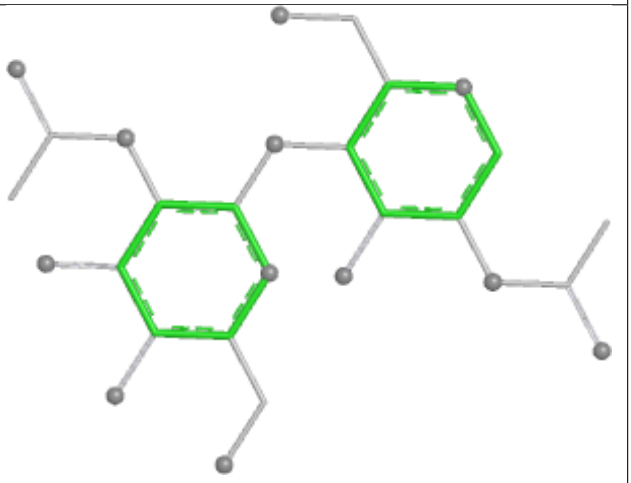
Bond lengths



Bond angles

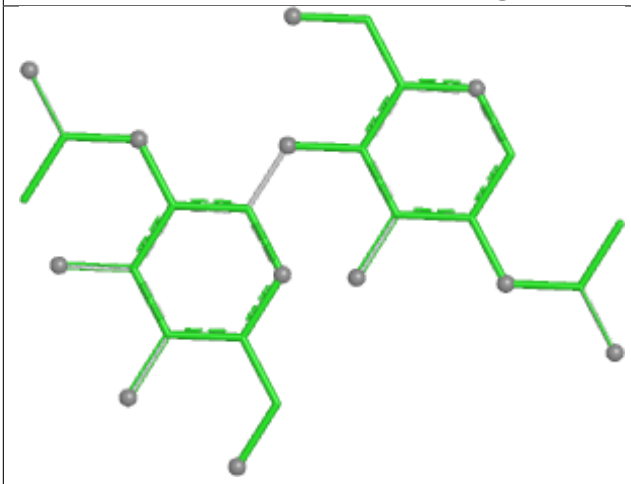


Torsions

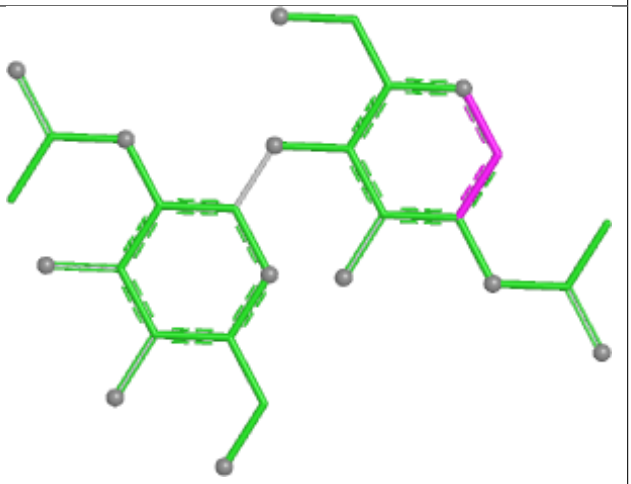


Rings

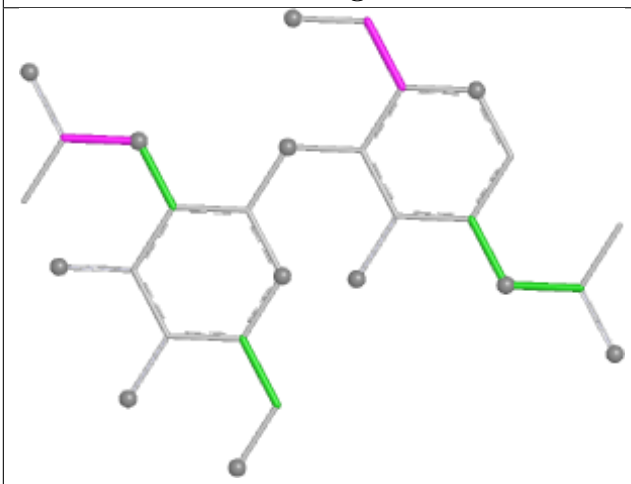
Oligosaccharide Chain N



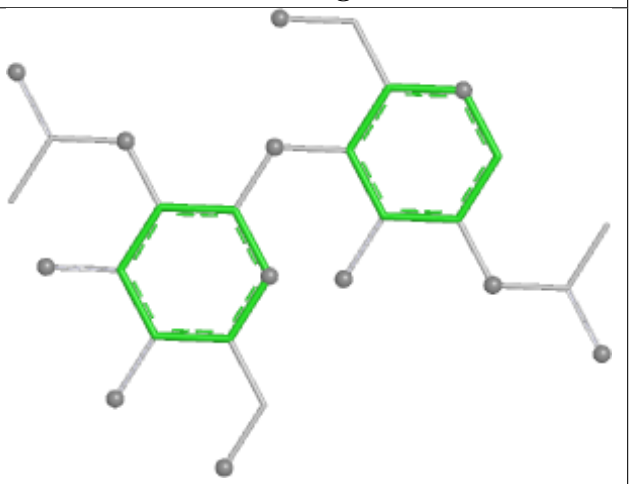
Bond lengths



Bond angles

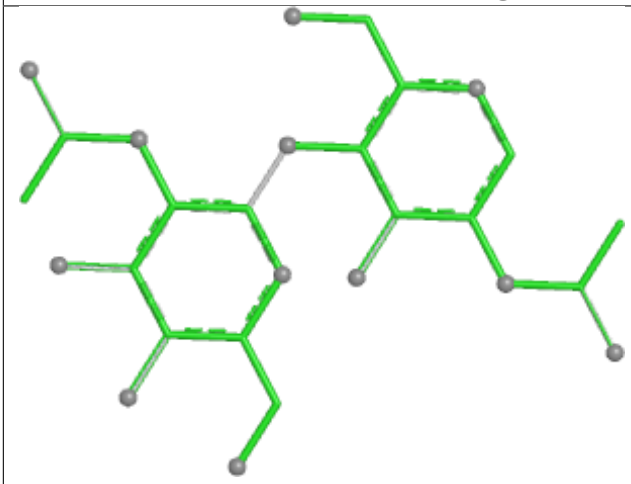


Torsions

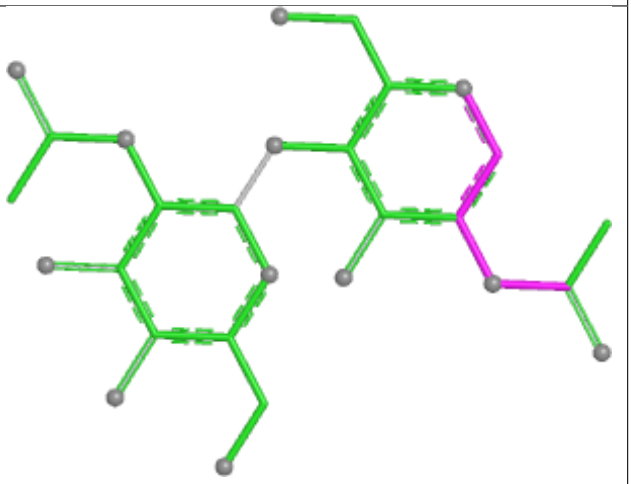


Rings

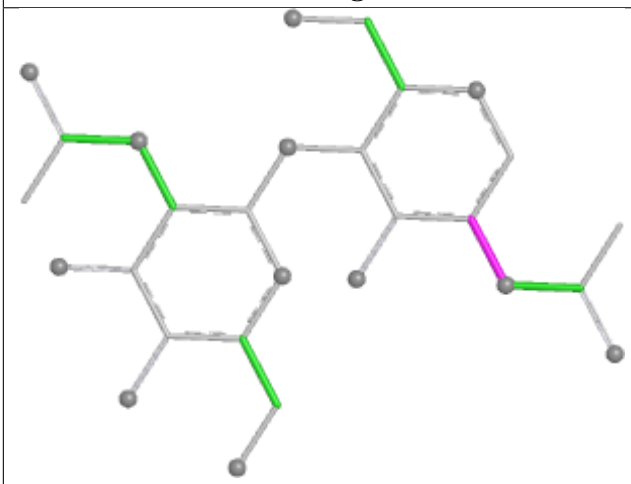
Oligosaccharide Chain O



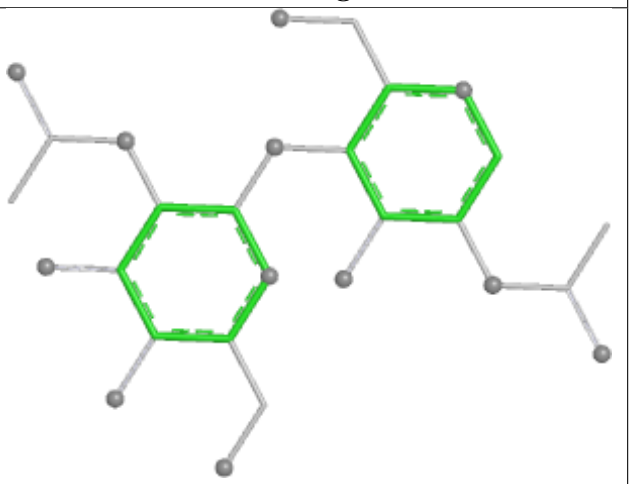
Bond lengths



Bond angles

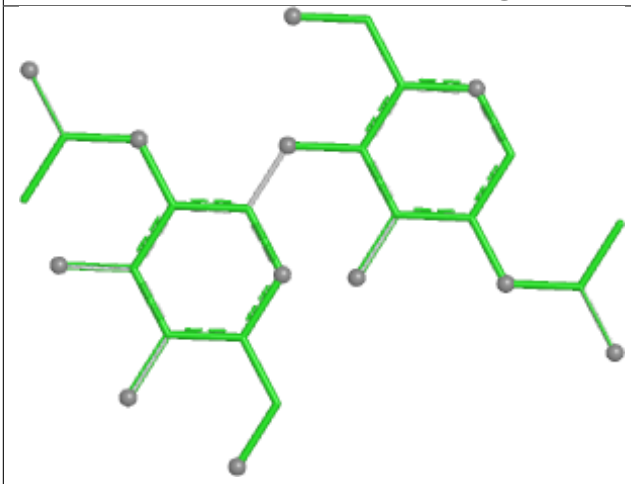


Torsions

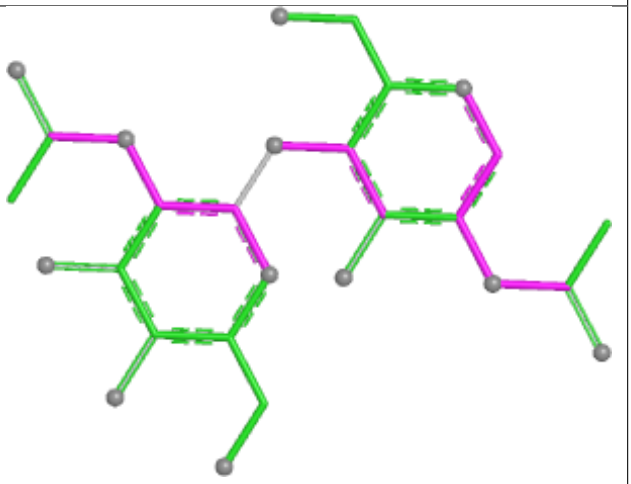


Rings

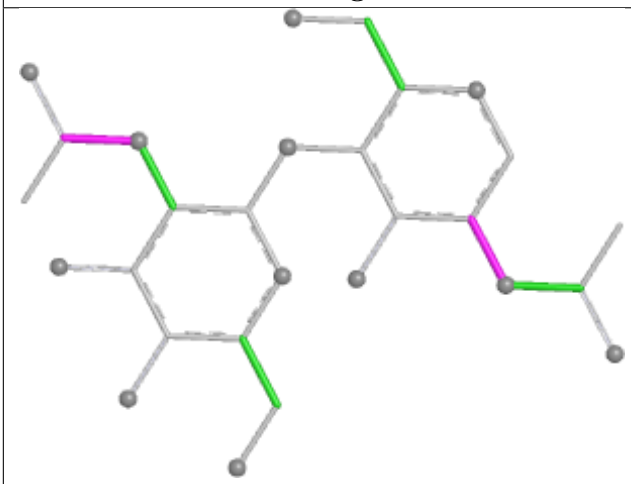
Oligosaccharide Chain P



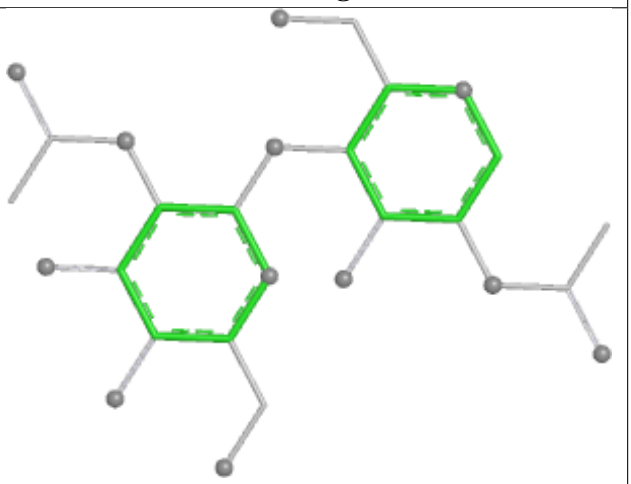
Bond lengths



Bond angles

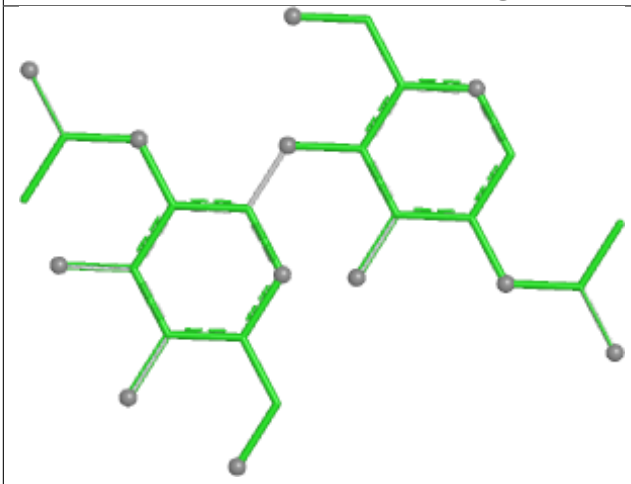


Torsions

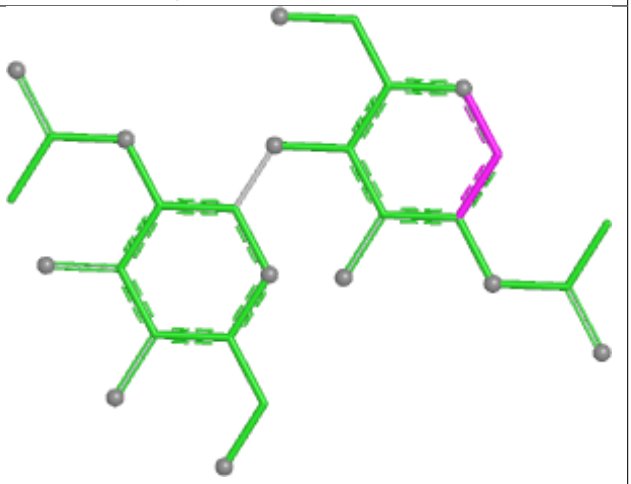


Rings

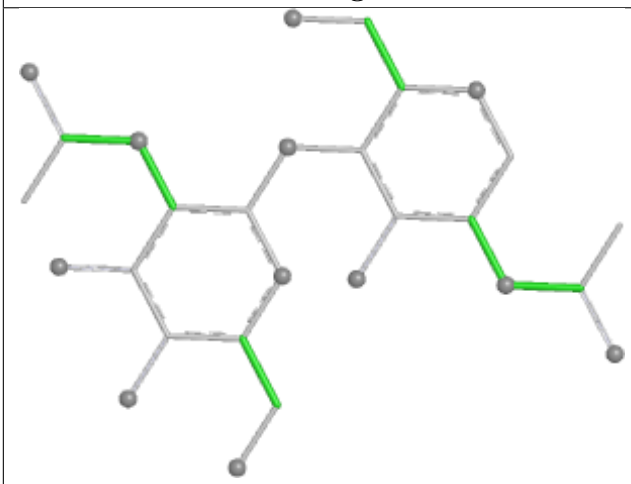
Oligosaccharide Chain Q



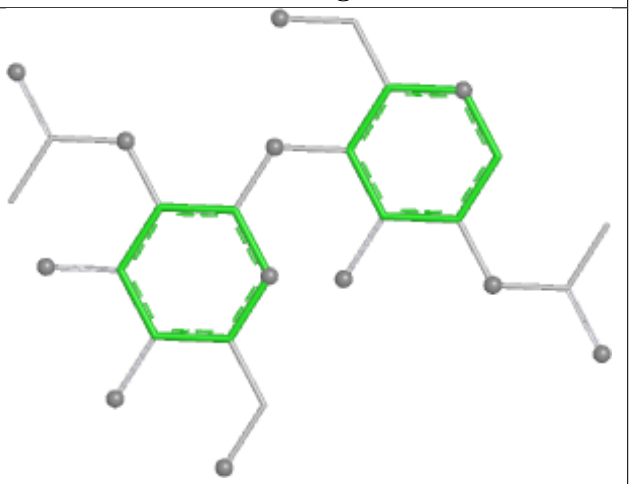
Bond lengths



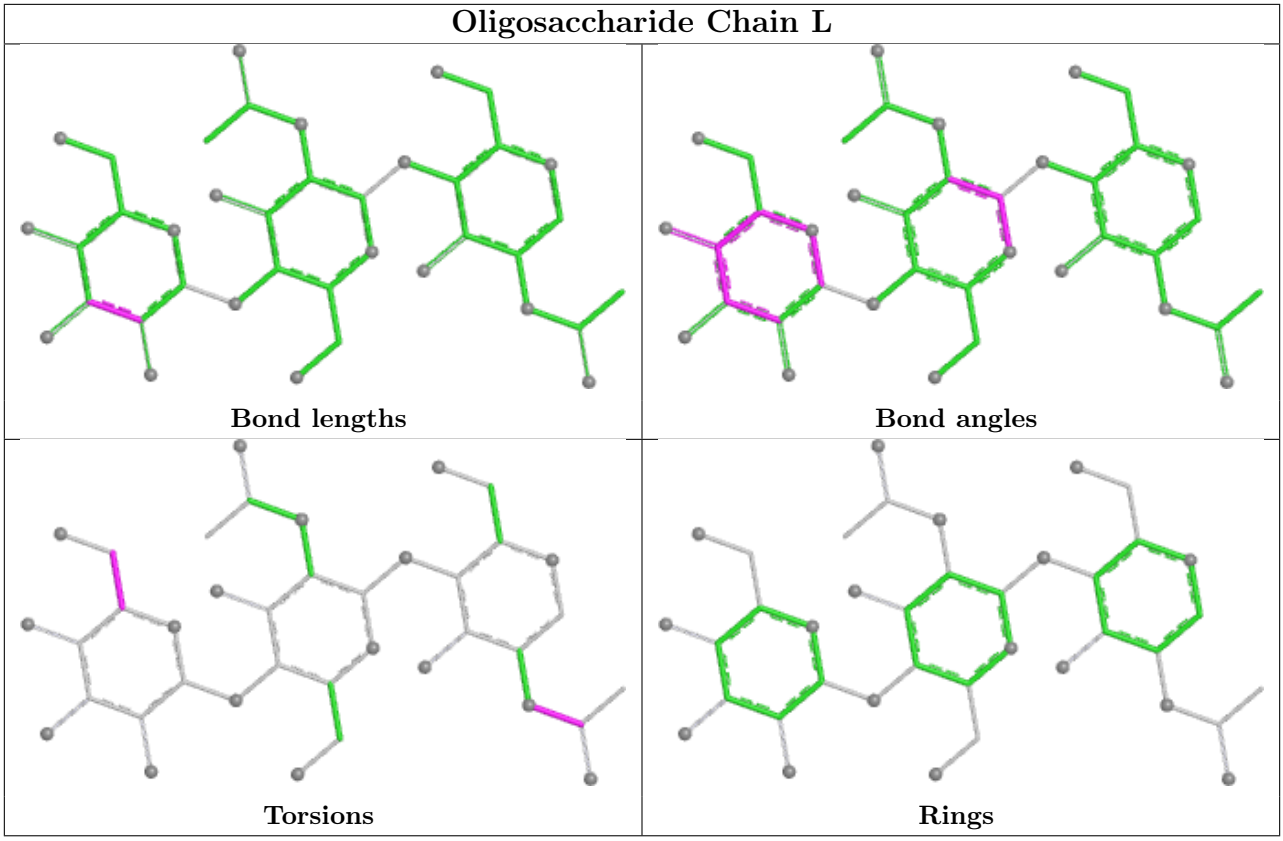
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
7	NAG	G	606	1	14,14,15	0.73	0	17,19,21	1.01	1 (5%)
7	NAG	G	605	1	14,14,15	0.73	0	17,19,21	0.92	1 (5%)
7	NAG	H	601	1	14,14,15	0.75	0	17,19,21	0.97	2 (11%)
7	NAG	A	604	1	14,14,15	0.72	0	17,19,21	0.87	0
7	NAG	H	603	1	14,14,15	0.72	0	17,19,21	0.77	0
7	NAG	G	601	1	14,14,15	0.71	0	17,19,21	0.77	0
7	NAG	H	602	1	14,14,15	0.72	0	17,19,21	0.95	0
7	NAG	A	605	1	14,14,15	0.70	0	17,19,21	1.13	1 (5%)
7	NAG	H	604	1	14,14,15	0.73	0	17,19,21	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	G	602	1	14,14,15	0.72	0	17,19,21	0.87	0
7	NAG	G	603	1	14,14,15	0.74	0	17,19,21	0.99	2 (11%)
7	NAG	A	602	1	14,14,15	0.72	0	17,19,21	0.93	0
7	NAG	G	604	1	14,14,15	0.75	0	17,19,21	0.86	0
7	NAG	A	603	1	14,14,15	0.75	0	17,19,21	1.37	1 (5%)
7	NAG	A	601	1	14,14,15	0.76	0	17,19,21	1.01	2 (11%)
7	NAG	H	605	1	14,14,15	0.71	0	17,19,21	0.79	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
7	NAG	G	606	1	-	3/6/23/26	0/1/1/1
7	NAG	G	605	1	-	2/6/23/26	0/1/1/1
7	NAG	H	601	1	-	2/6/23/26	0/1/1/1
7	NAG	A	604	1	-	2/6/23/26	0/1/1/1
7	NAG	H	603	1	-	0/6/23/26	0/1/1/1
7	NAG	G	601	1	-	0/6/23/26	0/1/1/1
7	NAG	H	602	1	-	2/6/23/26	0/1/1/1
7	NAG	A	605	1	-	2/6/23/26	0/1/1/1
7	NAG	H	604	1	-	2/6/23/26	0/1/1/1
7	NAG	G	602	1	-	1/6/23/26	0/1/1/1
7	NAG	G	603	1	-	2/6/23/26	0/1/1/1
7	NAG	A	602	1	-	2/6/23/26	0/1/1/1
7	NAG	G	604	1	-	0/6/23/26	0/1/1/1
7	NAG	A	603	1	-	1/6/23/26	0/1/1/1
7	NAG	A	601	1	-	2/6/23/26	0/1/1/1
7	NAG	H	605	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	603	NAG	C1-O5-C5	4.47	118.18	112.19
7	A	605	NAG	C2-N2-C7	3.16	127.14	122.90
7	A	601	NAG	C2-N2-C7	2.19	125.83	122.90
7	G	603	NAG	C2-N2-C7	2.13	125.75	122.90

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	601	NAG	C1-O5-C5	2.12	115.03	112.19
7	G	606	NAG	C2-N2-C7	2.11	125.72	122.90
7	H	601	NAG	C2-N2-C7	2.03	125.62	122.90
7	G	605	NAG	C2-N2-C7	2.02	125.61	122.90
7	G	603	NAG	C1-O5-C5	2.02	114.90	112.19
7	H	601	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	601	NAG	C8-C7-N2-C2
7	A	601	NAG	O7-C7-N2-C2
7	A	602	NAG	C8-C7-N2-C2
7	A	602	NAG	O7-C7-N2-C2
7	A	604	NAG	C8-C7-N2-C2
7	A	604	NAG	O7-C7-N2-C2
7	G	603	NAG	C8-C7-N2-C2
7	G	603	NAG	O7-C7-N2-C2
7	G	605	NAG	C8-C7-N2-C2
7	G	605	NAG	O7-C7-N2-C2
7	G	606	NAG	C8-C7-N2-C2
7	G	606	NAG	O7-C7-N2-C2
7	H	601	NAG	C8-C7-N2-C2
7	H	601	NAG	O7-C7-N2-C2
7	H	602	NAG	C8-C7-N2-C2
7	H	602	NAG	O7-C7-N2-C2
7	H	604	NAG	C8-C7-N2-C2
7	H	604	NAG	O7-C7-N2-C2
7	G	606	NAG	O5-C5-C6-O6
7	G	602	NAG	O5-C5-C6-O6
7	A	603	NAG	O5-C5-C6-O6
7	H	605	NAG	O5-C5-C6-O6
7	A	605	NAG	C1-C2-N2-C7
7	A	605	NAG	C3-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.

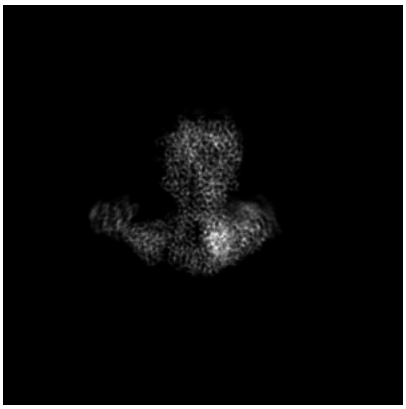
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44451. 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

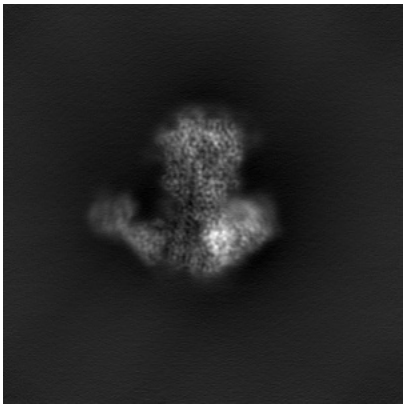


X

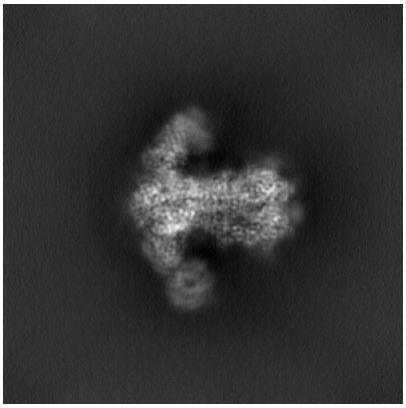
Y

Z

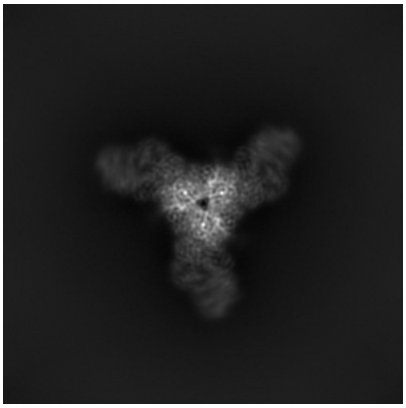
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

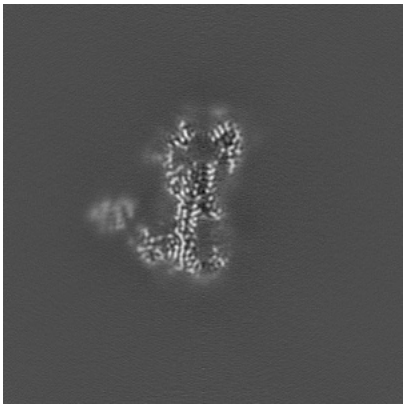
6.2.1 Primary map

X Index: 200

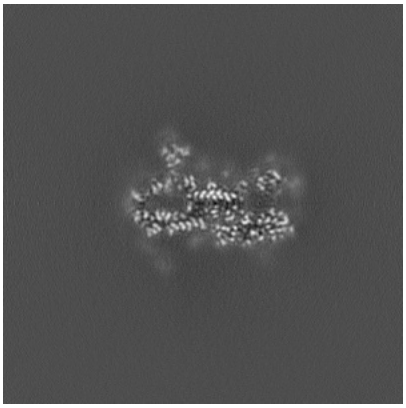
Y Index: 200

Z Index: 200

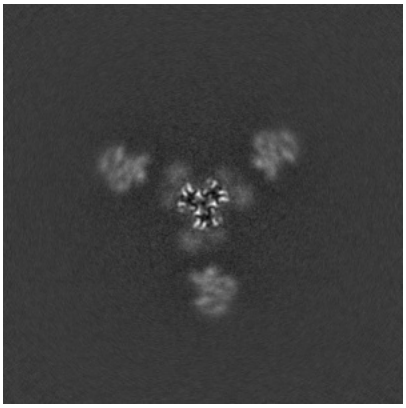
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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

6.3 Largest variance slices (i)

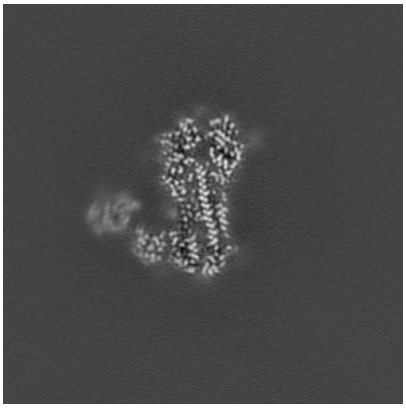
6.3.1 Primary map

X Index: 207

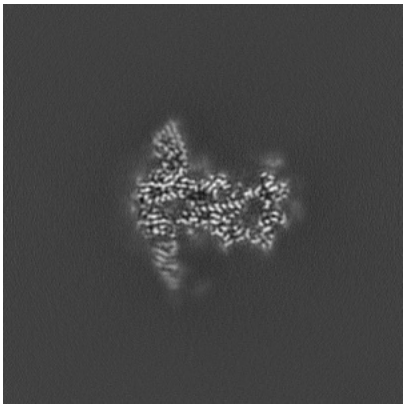
Y Index: 210

Z Index: 170

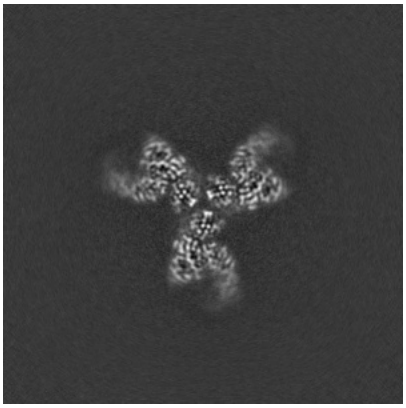
6.3.2 Raw map



X Index: 208



Y Index: 210

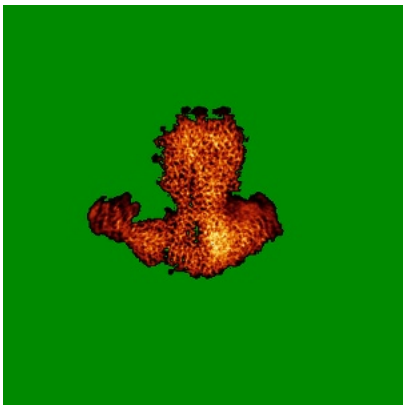


Z Index: 166

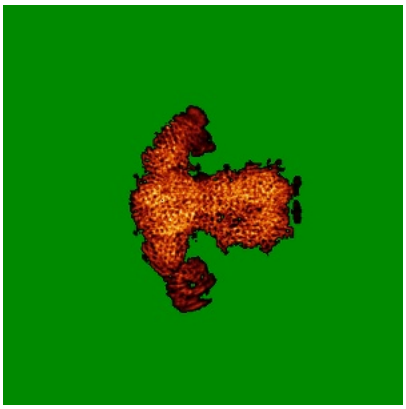
The images above show the largest variance slices of the map in three orthogonal directions.

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

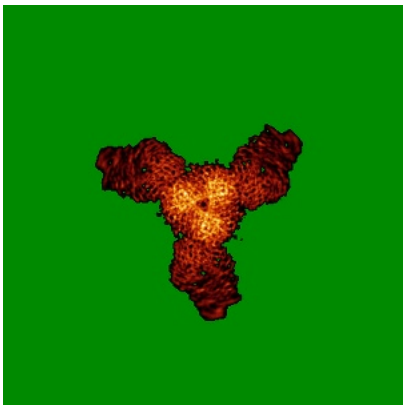
6.4.1 Primary map



X

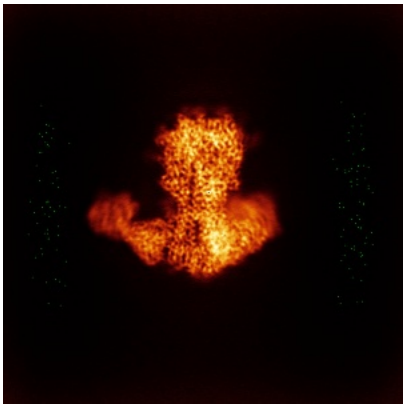


Y

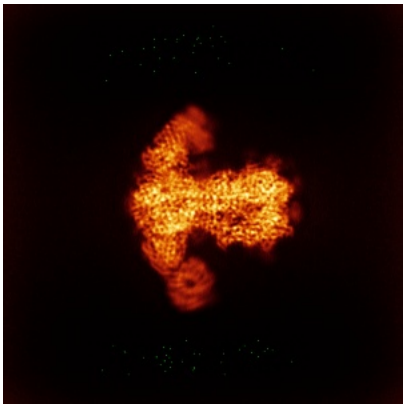


Z

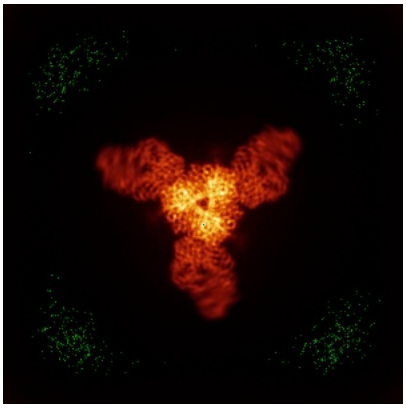
6.4.2 Raw map



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 0.16. 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.

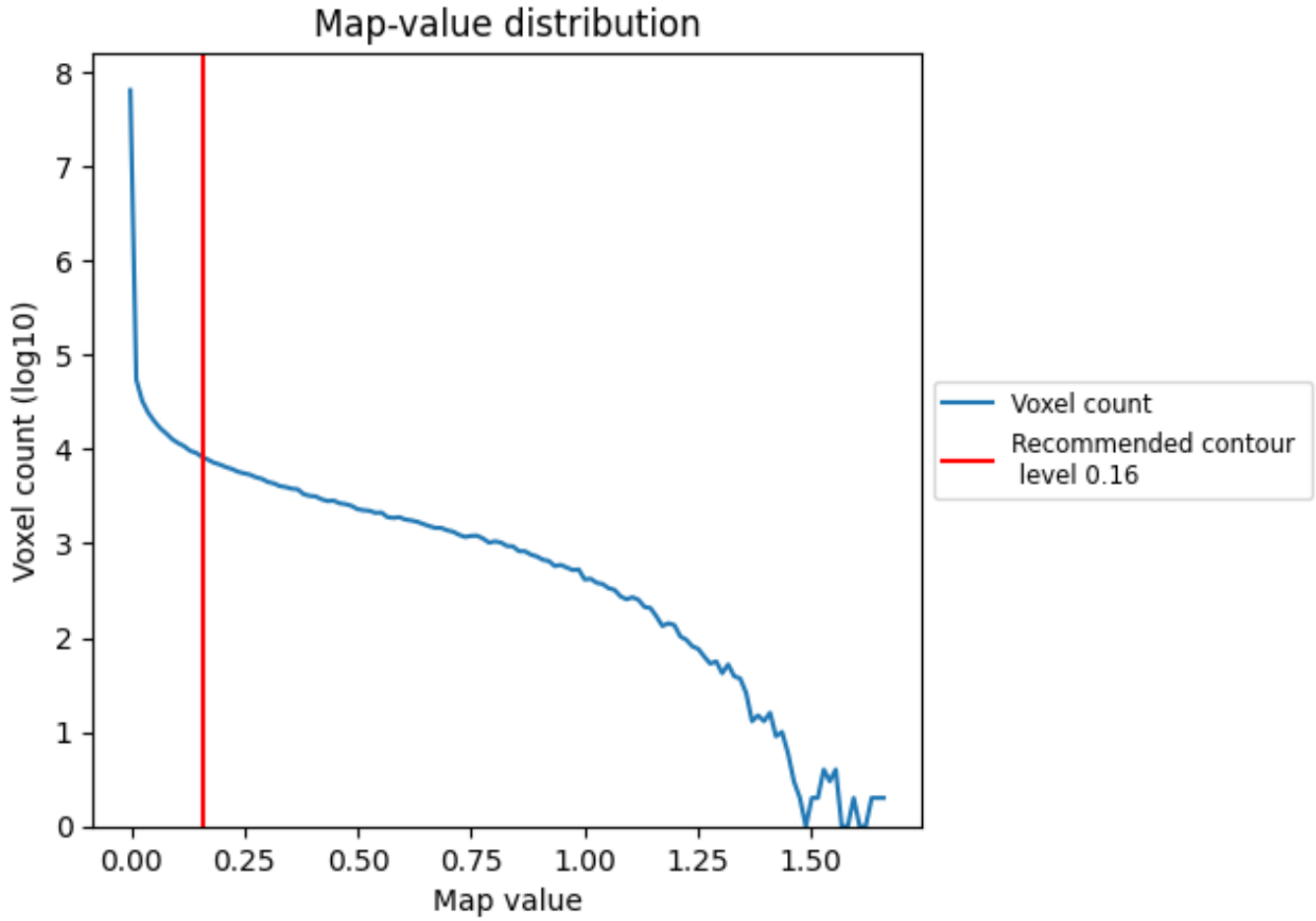
6.6 Mask visualisation (i)

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

7 Map analysis

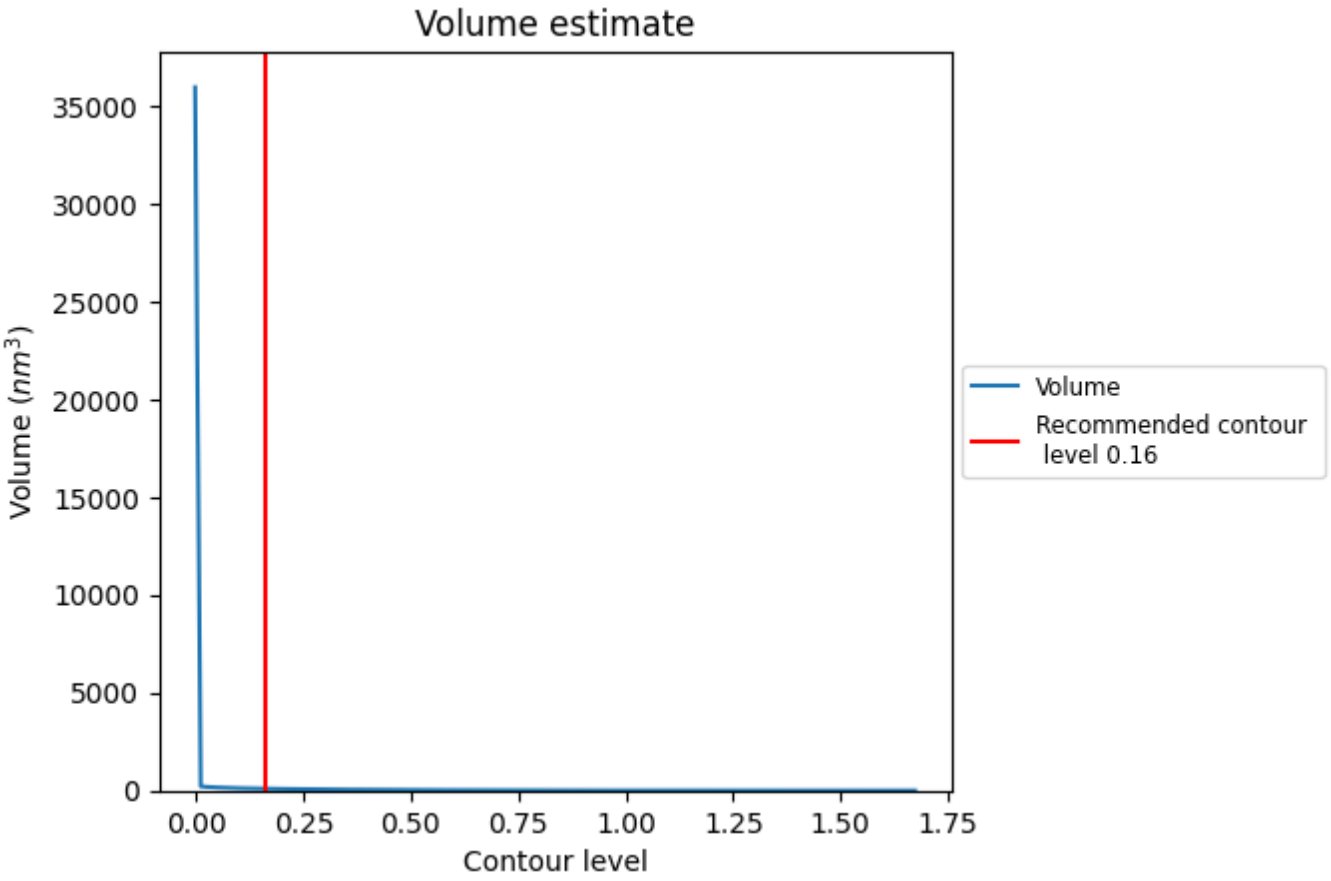
This section contains the results of statistical analysis of the map.

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.

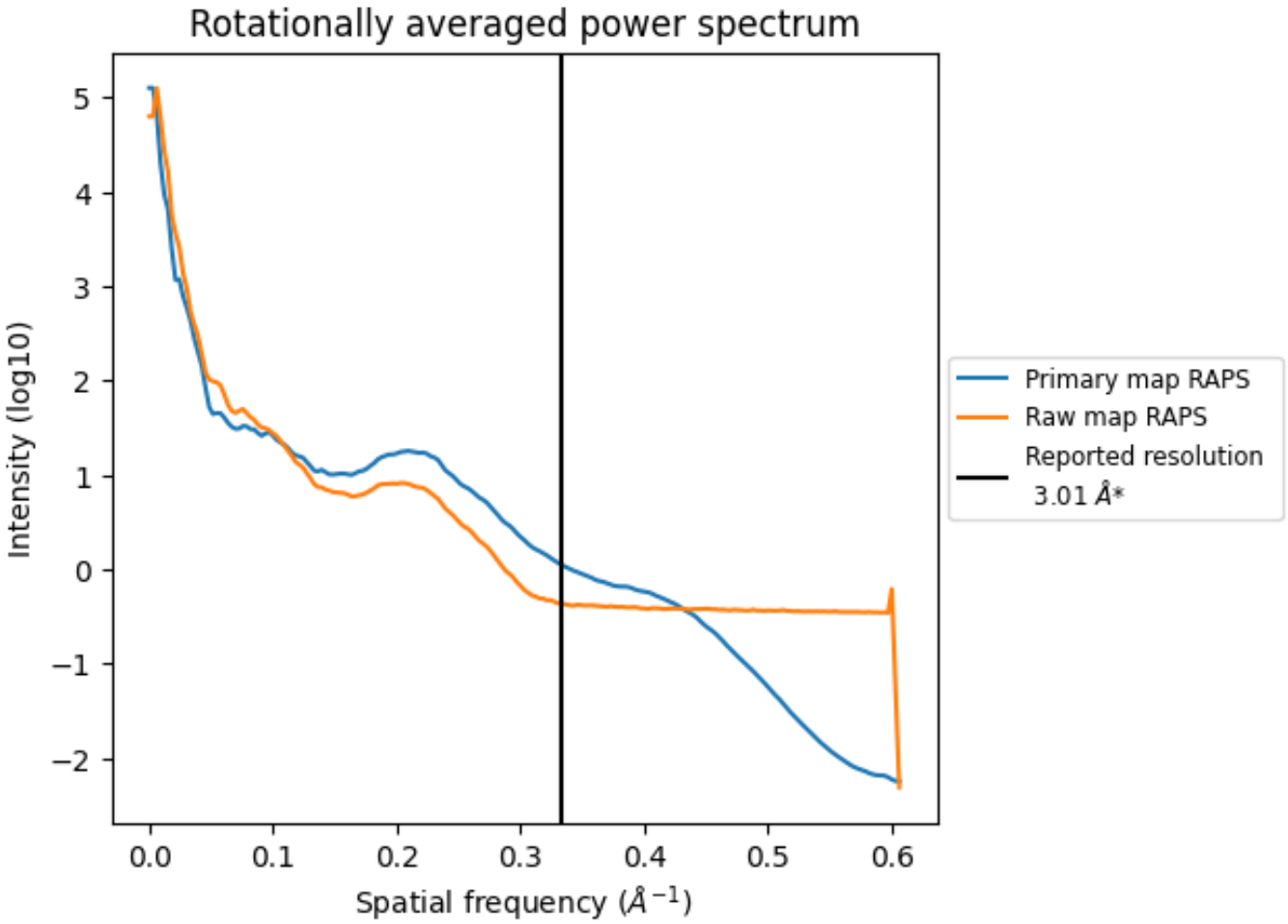
7.2 Volume estimate



The volume at the recommended contour level is 96 nm^3; this corresponds to an approximate mass of 87 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)

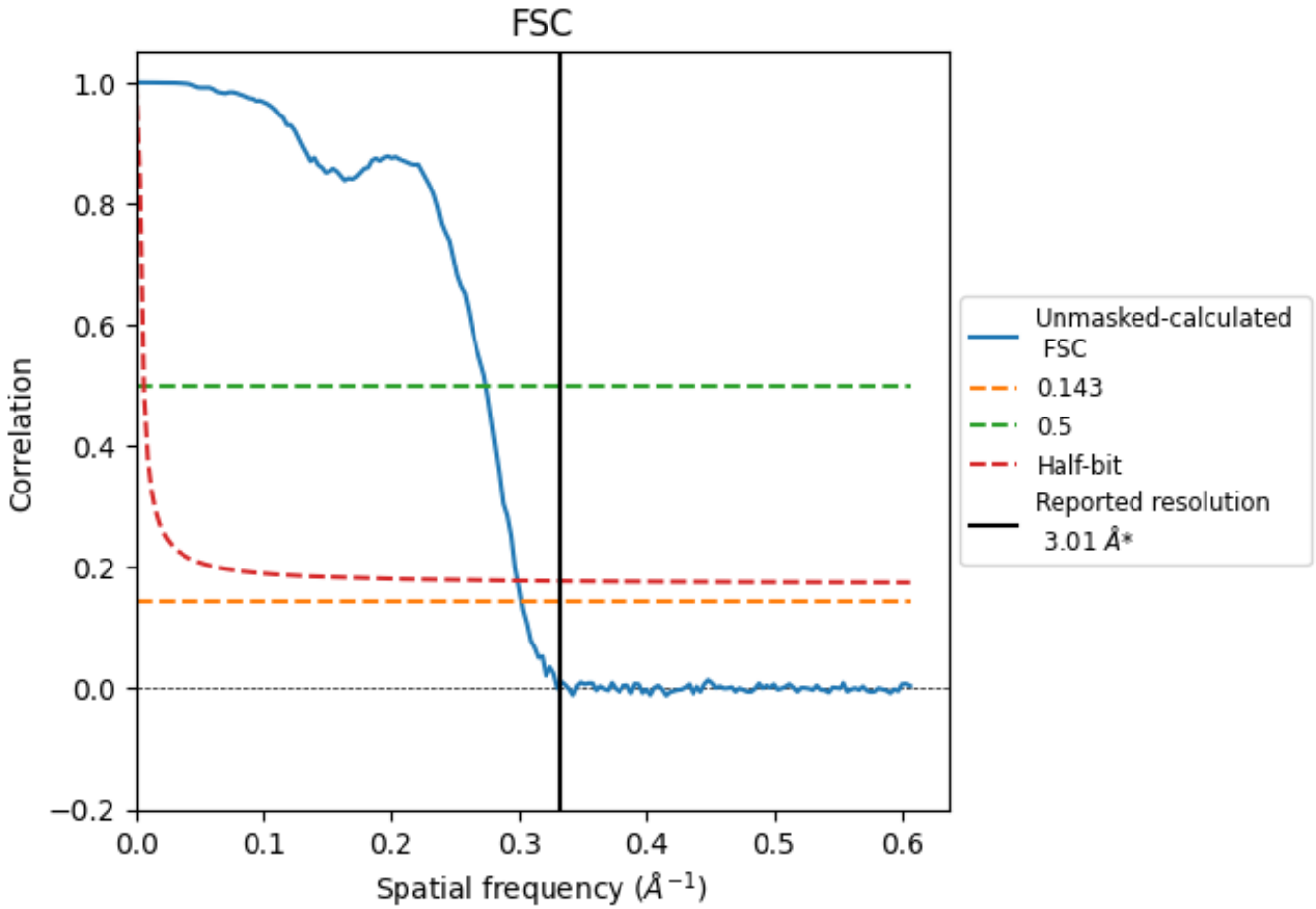


*Reported resolution corresponds to spatial frequency of 0.332 Å^{-1}

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 0.332 Å^{-1}

8.2 Resolution estimates (i)

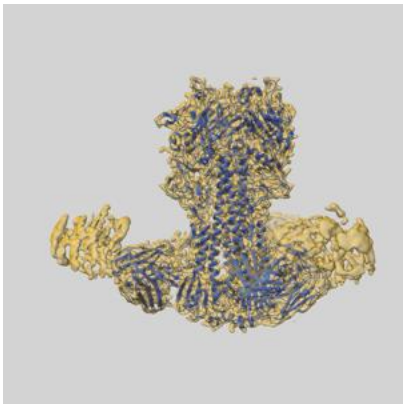
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.31	3.65	3.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

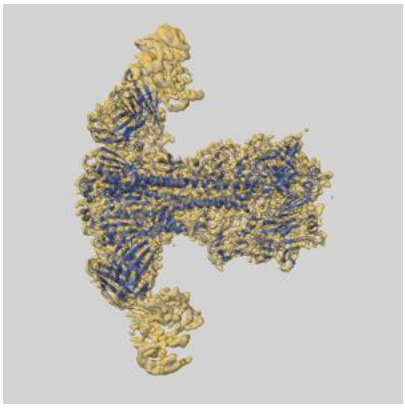
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44451 and PDB model 9BDF. Per-residue inclusion information can be found in section 3 on page 9.

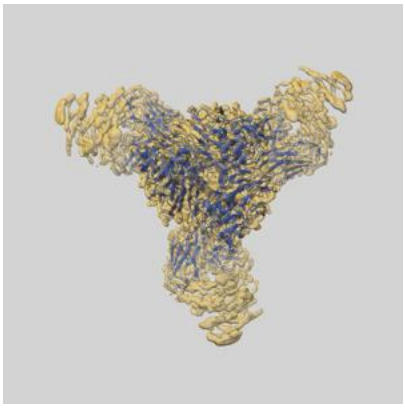
9.1 Map-model overlay



X



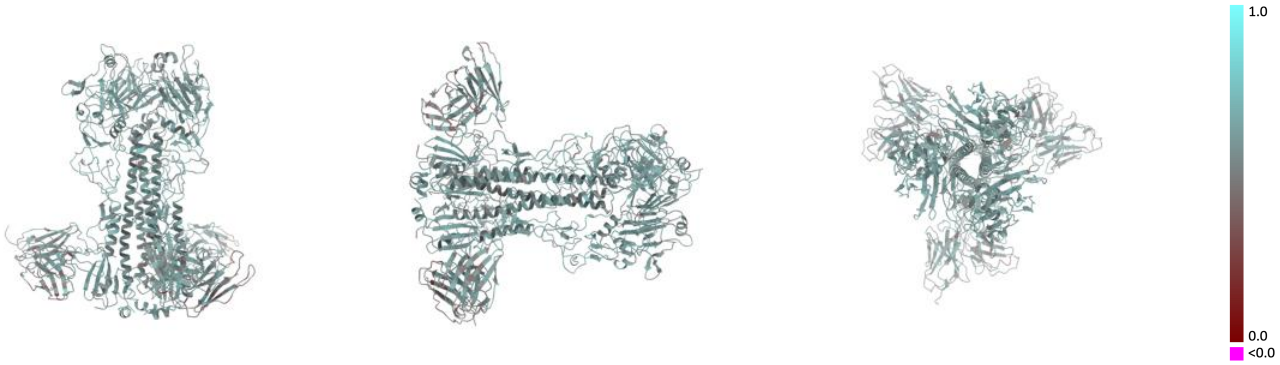
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 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.

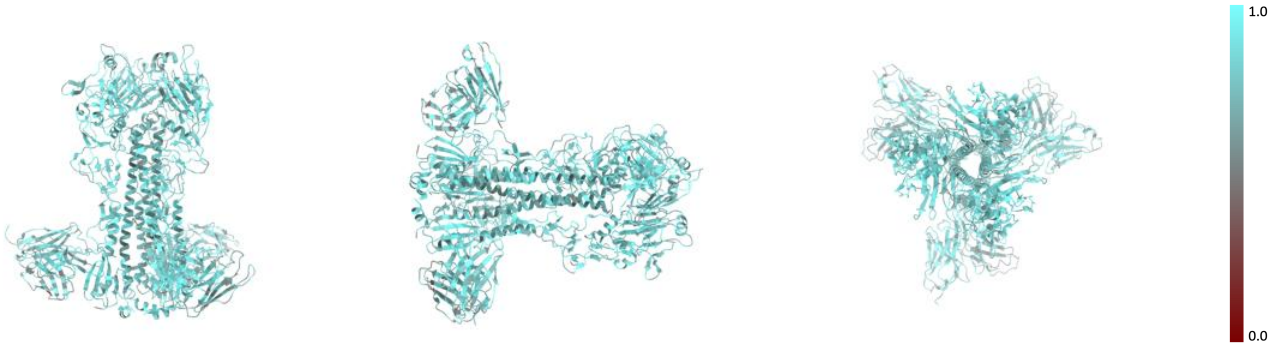
9.2 Q-score mapped to coordinate model (i)



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.

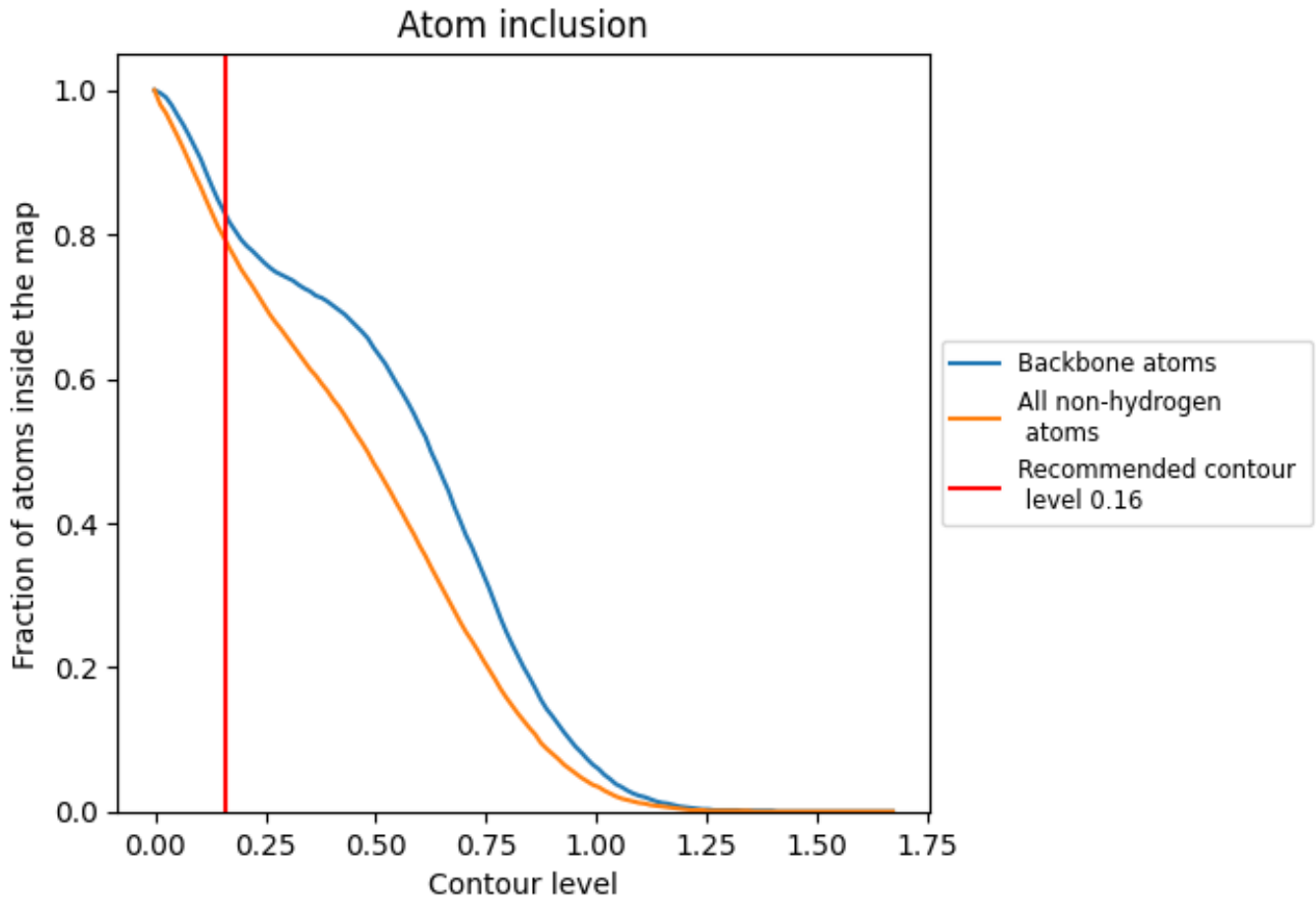
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 79% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7910	0.5630
A	0.8140	0.5830
B	0.7970	0.5480
C	0.7890	0.5460
D	0.7250	0.4970
E	0.7900	0.5500
F	0.5800	0.4880
G	0.8120	0.5840
H	0.8150	0.5850
I	0.7080	0.4960
J	0.7130	0.4970
K	0.6430	0.5400
L	0.3080	0.4080
M	0.5800	0.4690
N	0.6790	0.5540
O	0.4290	0.2220
P	0.2140	0.2900
Q	0.6430	0.5460
R	0.6200	0.4520