



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:51 PM UTC

PDB ID : 2AEP / pdb_00002aep
Title : An epidemiologically significant epitope of a 1998 influenza virus neuraminidase forms a highly hydrated interface in the NA-antibody complex.
Authors : Venkatramani, L.; Bochkareva, E.; Lee, J.T.; Gulati, U.; Laver, W.G.; Bochkarev, A.; Air, G.M.
Deposited on : 2005-07-23
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

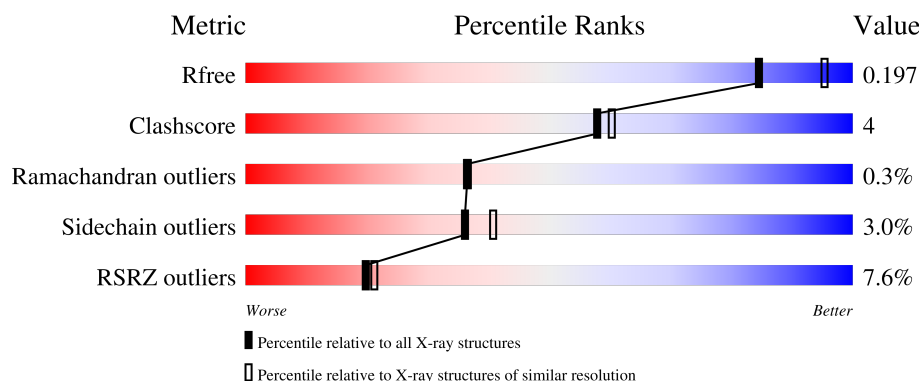
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	395	91% 7%
2	H	217	16% 56% 10% 34%
3	L	214	7% 52% 7% 40%
4	B	7	57% 43%

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
4	MAN	B	6	-	-	X	-
5	GLC	A	702	X	-	-	-
5	GLC	H	701	X	-	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5812 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	1	0
			3019	1876	537	584	22			

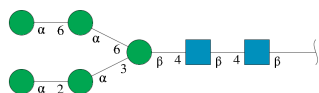
- Molecule 2 is a protein called FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	143	Total	C	N	O	S	0	0	0
			1102	701	179	217	5			

- Molecule 3 is a protein called FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	129	Total	C	N	O	S	0	0	0
			1005	628	169	204	4			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]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				ZeroOcc	AltConf	Trace
4	B	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 5 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	6	6		
5	H	1	Total	C	O	0	0
			12	6	6		

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



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

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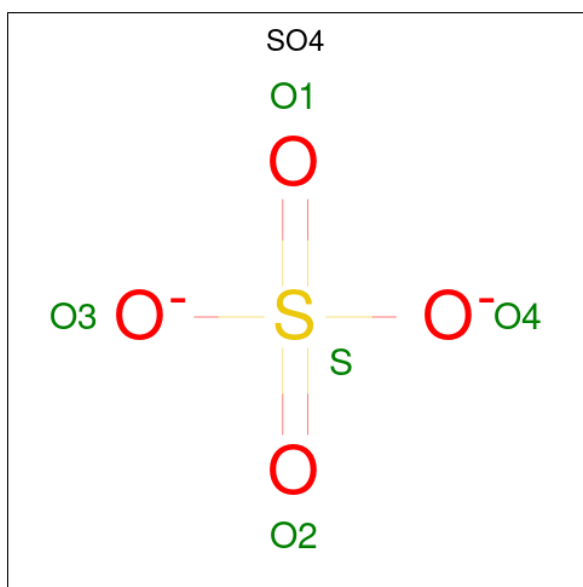
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

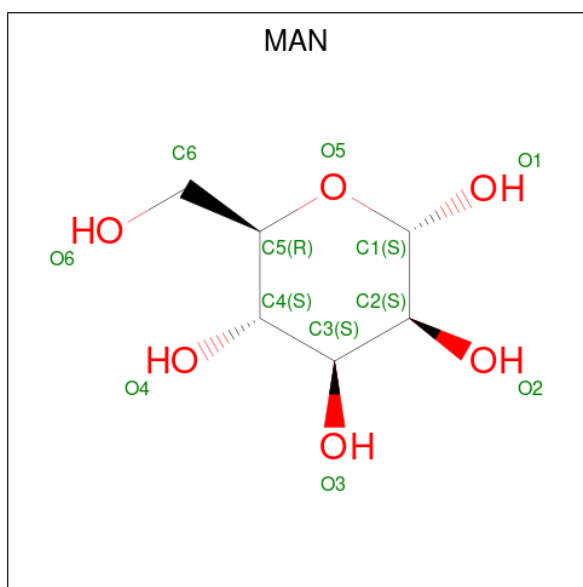
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	0
			11	6	5		

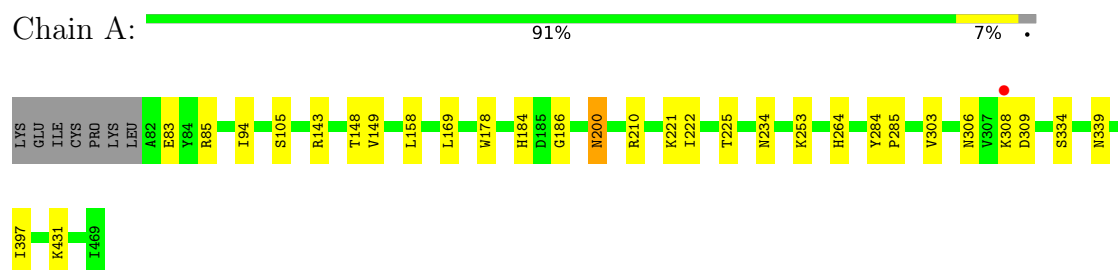
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	347	Total	O	0	0
			347	347		
10	H	75	Total	O	0	0
			75	75		
10	L	84	Total	O	0	0
			84	84		

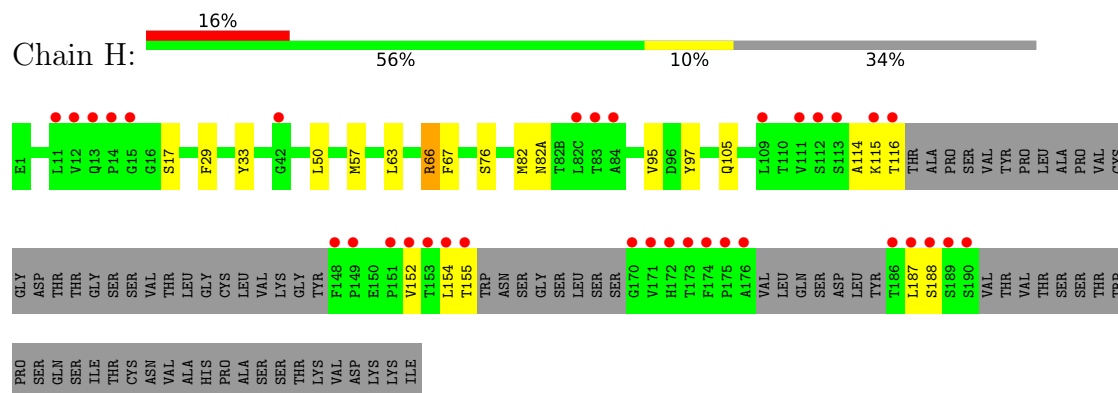
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

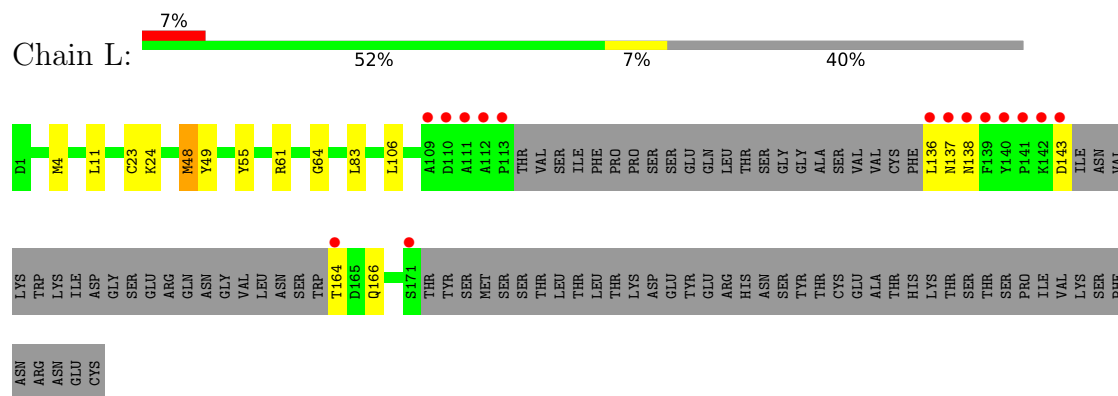
• Molecule 1: neuraminidase



• Molecule 2: FAB heavy chain



• Molecule 3: FAB light chain



- Molecule 4: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain B:



MAG1
MAG2
EMA3
MAN4
MAN5
MAN6
MAN7

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.06Å 155.06Å 102.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.10) 92.1 (20.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.188 , 0.224 0.196 , 0.197	Depositor DCC
R_{free} test set	7413 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5812	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: NAG, BMA, CA, MAN, SO4, GLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.37	10/3099 (0.3%)	1.12	3/4197 (0.1%)
2	H	1.26	1/1128 (0.1%)	1.11	0/1530
3	L	1.40	2/1025 (0.2%)	1.10	0/1384
All	All	1.35	13/5252 (0.2%)	1.11	3/7111 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	48	MET	SD-CE	-18.19	1.34	1.79
2	H	82	MET	SD-CE	-8.66	1.57	1.79
1	A	149	VAL	CA-CB	5.88	1.62	1.54
1	A	303	VAL	CA-CB	-5.67	1.47	1.54
1	A	186	GLY	C-O	-5.43	1.16	1.24
1	A	339	ASN	N-CA	-5.26	1.39	1.45
1	A	253	LYS	N-CA	-5.21	1.39	1.45
1	A	225	THR	CA-CB	5.11	1.61	1.54
1	A	210	ARG	NE-CZ	5.11	1.38	1.33
1	A	184	HIS	CA-C	5.06	1.58	1.52
1	A	85	ARG	CD-NE	-5.05	1.39	1.46
1	A	158	LEU	C-O	-5.02	1.18	1.24
3	L	61	ARG	NE-CZ	-5.00	1.27	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	ILE	N-CA-C	-6.49	106.23	111.81
1	A	105	SER	N-CA-C	5.86	118.62	111.82
1	A	334	SER	N-CA-C	5.63	116.82	108.60

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	3019	0	2854	20	0
2	H	1102	0	1053	11	0
3	L	1005	0	962	7	0
4	B	83	0	71	10	0
5	A	12	0	12	1	0
5	H	12	0	12	0	0
6	A	56	0	52	6	0
7	A	1	0	0	0	0
8	A	5	0	0	0	0
9	L	11	0	10	3	0
10	A	347	0	0	6	0
10	H	75	0	0	1	0
10	L	84	0	0	2	0
All	All	5812	0	5026	45	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 4.

All (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASN:HD21	1:A:308:LYS:HE2	1.40	0.86
6:A:686:NAG:H81	6:A:634:NAG:H5	1.57	0.85
1:A:200:ASN:HD22	4:B:1:NAG:H83	1.48	0.79
1:A:306:ASN:OD1	1:A:308:LYS:HG2	1.83	0.78
1:A:264:HIS:HD2	10:A:995:HOH:O	1.75	0.69
10:A:858:HOH:O	4:B:1:NAG:H81	1.94	0.68
5:A:702:GLC:O6	6:A:634:NAG:H81	1.94	0.67
4:B:3:BMA:HO6	4:B:6:MAN:C1	2.10	0.63
9:L:217(H):MAN:C1	4:B:6:MAN:O3	2.49	0.60
1:A:222:ILE:HD12	2:H:97:TYR:CD2	2.37	0.60
1:A:222:ILE:HD12	2:H:97:TYR:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ASN:ND2	4:B:1:NAG:H83	2.18	0.59
1:A:306:ASN:ND2	1:A:308:LYS:HE2	2.16	0.58
4:B:3:BMA:C6	4:B:6:MAN:C1	2.85	0.54
3:L:106:LEU:O	3:L:166:GLN:NE2	2.36	0.54
2:H:33:TYR:HB2	2:H:95:VAL:HB	1.89	0.53
1:A:264:HIS:HE1	10:A:840:HOH:O	1.91	0.53
1:A:308:LYS:HD3	10:A:980:HOH:O	2.11	0.50
1:A:234:ASN:HD22	6:A:634:NAG:H83	1.77	0.50
1:A:143:ARG:NH2	6:A:646:NAG:C8	2.75	0.49
1:A:308:LYS:CG	1:A:309:ASP:N	2.76	0.49
1:A:431:LYS:HD2	10:A:1045:HOH:O	2.12	0.48
2:H:50:LEU:C	2:H:50:LEU:HD12	2.38	0.48
2:H:63:LEU:HD13	2:H:67:PHE:CD1	2.48	0.48
2:H:154:LEU:C	2:H:154:LEU:HD23	2.38	0.48
1:A:284:TYR:CG	1:A:285:PRO:HA	2.49	0.48
10:A:858:HOH:O	4:B:1:NAG:C8	2.58	0.47
3:L:4:MET:HE3	3:L:23:CYS:SG	2.53	0.47
1:A:143:ARG:HH21	6:A:646:NAG:H83	1.80	0.47
3:L:24:LYS:HE2	10:L:295:HOH:O	2.14	0.47
3:L:24:LYS:CE	10:L:295:HOH:O	2.63	0.46
9:L:217(H):MAN:H5	4:B:6:MAN:O3	2.15	0.46
2:H:116:THR:O	10:H:759:HOH:O	2.21	0.45
1:A:143:ARG:HH21	6:A:646:NAG:C8	2.31	0.44
1:A:308:LYS:HG3	1:A:309:ASP:N	2.33	0.44
3:L:48:MET:HE2	3:L:64:GLY:HA3	1.98	0.44
2:H:29:PHE:CD2	2:H:76:SER:HA	2.53	0.44
4:B:3:BMA:O6	4:B:6:MAN:O5	2.33	0.43
2:H:66:ARG:HG2	2:H:82(A):ASN:O	2.18	0.43
2:H:154:LEU:HD23	2:H:155:THR:N	2.33	0.43
3:L:137:ASN:HB3	3:L:138:ASN:ND2	2.34	0.43
9:L:217(H):MAN:H3	4:B:6:MAN:O3	2.19	0.43
3:L:49:TYR:HB3	3:L:55:TYR:CE1	2.55	0.42
1:A:221:LYS:HA	2:H:97:TYR:O	2.20	0.41
1:A:169:LEU:HD23	1:A:169:LEU:HA	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	386/395 (98%)	369 (96%)	16 (4%)	1 (0%)	36	36
2	H	135/217 (62%)	127 (94%)	7 (5%)	1 (1%)	18	15
3	L	123/214 (58%)	117 (95%)	6 (5%)	0	100	100
All	All	644/826 (78%)	613 (95%)	29 (4%)	2 (0%)	36	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	114	ALA
1	A	200	ASN

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	338/344 (98%)	334 (99%)	4 (1%)	63	72
2	H	120/185 (65%)	112 (93%)	8 (7%)	15	12
3	L	113/192 (59%)	108 (96%)	5 (4%)	25	26
All	All	571/721 (79%)	554 (97%)	17 (3%)	36	41

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLU

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Mol	Chain	Res	Type
1	A	94	ILE
1	A	148	THR
1	A	178	TRP
2	H	17	SER
2	H	57	MET
2	H	66	ARG
2	H	105	GLN
2	H	115	LYS
2	H	152	VAL
2	H	187	LEU
2	H	188	SER
3	L	11	LEU
3	L	83	LEU
3	L	136	LEU
3	L	143	ASP
3	L	164	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	264	HIS
1	A	336	HIS
1	A	342	ASN
1	A	358	ASN
1	A	391	GLN
1	A	393	ASN
1	A	432	GLN
3	L	79	GLN
3	L	89	GLN
3	L	137	ASN
3	L	138	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

7 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	B	1	4,1	14,14,15	1.81	3 (21%)	17,19,21	2.53	6 (35%)
4	NAG	B	2	4	14,14,15	1.46	2 (14%)	17,19,21	1.67	6 (35%)
4	BMA	B	3	4	11,11,12	0.93	2 (18%)	15,15,17	1.60	2 (13%)
4	MAN	B	4	4	11,11,12	1.16	2 (18%)	15,15,17	1.71	5 (33%)
4	MAN	B	5	4	11,11,12	0.67	0	15,15,17	1.76	3 (20%)
4	MAN	B	6	4	11,11,12	0.92	1 (9%)	15,15,17	2.49	6 (40%)
4	MAN	B	7	4	11,11,12	0.54	0	15,15,17	1.26	2 (13%)

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	B	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1
4	MAN	B	4	4	-	0/2/19/22	0/1/1/1
4	MAN	B	5	4	-	2/2/19/22	0/1/1/1
4	MAN	B	6	4	-	0/2/19/22	0/1/1/1
4	MAN	B	7	4	-	1/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	NAG	C8-C7	-4.32	1.41	1.50
4	B	2	NAG	C8-C7	-4.02	1.42	1.50
4	B	1	NAG	O7-C7	3.73	1.31	1.23
4	B	4	MAN	O5-C1	-2.51	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4	MAN	C2-C3	2.33	1.56	1.52
4	B	6	MAN	O2-C2	-2.13	1.38	1.43
4	B	3	BMA	O5-C1	-2.11	1.40	1.43
4	B	1	NAG	C4-C5	2.05	1.57	1.53
4	B	3	BMA	O5-C5	2.04	1.47	1.43
4	B	2	NAG	O7-C7	2.02	1.27	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	6	MAN	C1-O5-C5	6.47	120.86	112.19
4	B	1	NAG	C2-N2-C7	5.41	130.15	122.90
4	B	1	NAG	C1-O5-C5	4.12	117.70	112.19
4	B	5	MAN	O5-C5-C6	4.03	115.50	107.66
4	B	1	NAG	C4-C3-C2	-3.97	105.19	111.02
4	B	3	BMA	C1-O5-C5	-3.97	106.86	112.19
4	B	1	NAG	O7-C7-N2	3.91	128.88	121.98
4	B	6	MAN	O2-C2-C1	-3.81	100.49	109.22
4	B	1	NAG	O7-C7-C8	-3.45	115.92	122.05
4	B	6	MAN	O5-C1-C2	3.41	118.92	110.79
4	B	5	MAN	O2-C2-C3	3.07	116.52	110.15
4	B	2	NAG	C2-N2-C7	3.06	127.00	122.90
4	B	2	NAG	O5-C1-C2	-3.03	106.60	111.29
4	B	6	MAN	O3-C3-C2	2.90	115.97	110.05
4	B	1	NAG	O5-C1-C2	-2.89	106.81	111.29
4	B	4	MAN	C1-O5-C5	2.85	116.01	112.19
4	B	3	BMA	C6-C5-C4	-2.77	106.22	113.02
4	B	4	MAN	O5-C5-C6	-2.72	102.36	107.66
4	B	2	NAG	O7-C7-C8	-2.70	117.24	122.05
4	B	4	MAN	C1-C2-C3	2.69	113.56	109.64
4	B	4	MAN	O4-C4-C3	-2.64	104.15	110.38
4	B	7	MAN	O5-C5-C6	2.62	112.77	107.66
4	B	2	NAG	O4-C4-C3	-2.54	104.39	110.38
4	B	6	MAN	C1-C2-C3	2.42	113.17	109.64
4	B	4	MAN	O4-C4-C5	2.17	114.67	109.32
4	B	2	NAG	O5-C5-C4	-2.17	105.55	110.83
4	B	5	MAN	C3-C4-C5	-2.11	106.41	110.23
4	B	6	MAN	O4-C4-C3	-2.02	105.61	110.38
4	B	2	NAG	O7-C7-N2	2.02	125.54	121.98
4	B	7	MAN	O2-C2-C3	2.00	114.30	110.15

There are no chirality outliers.

All (7) torsion outliers are listed below:

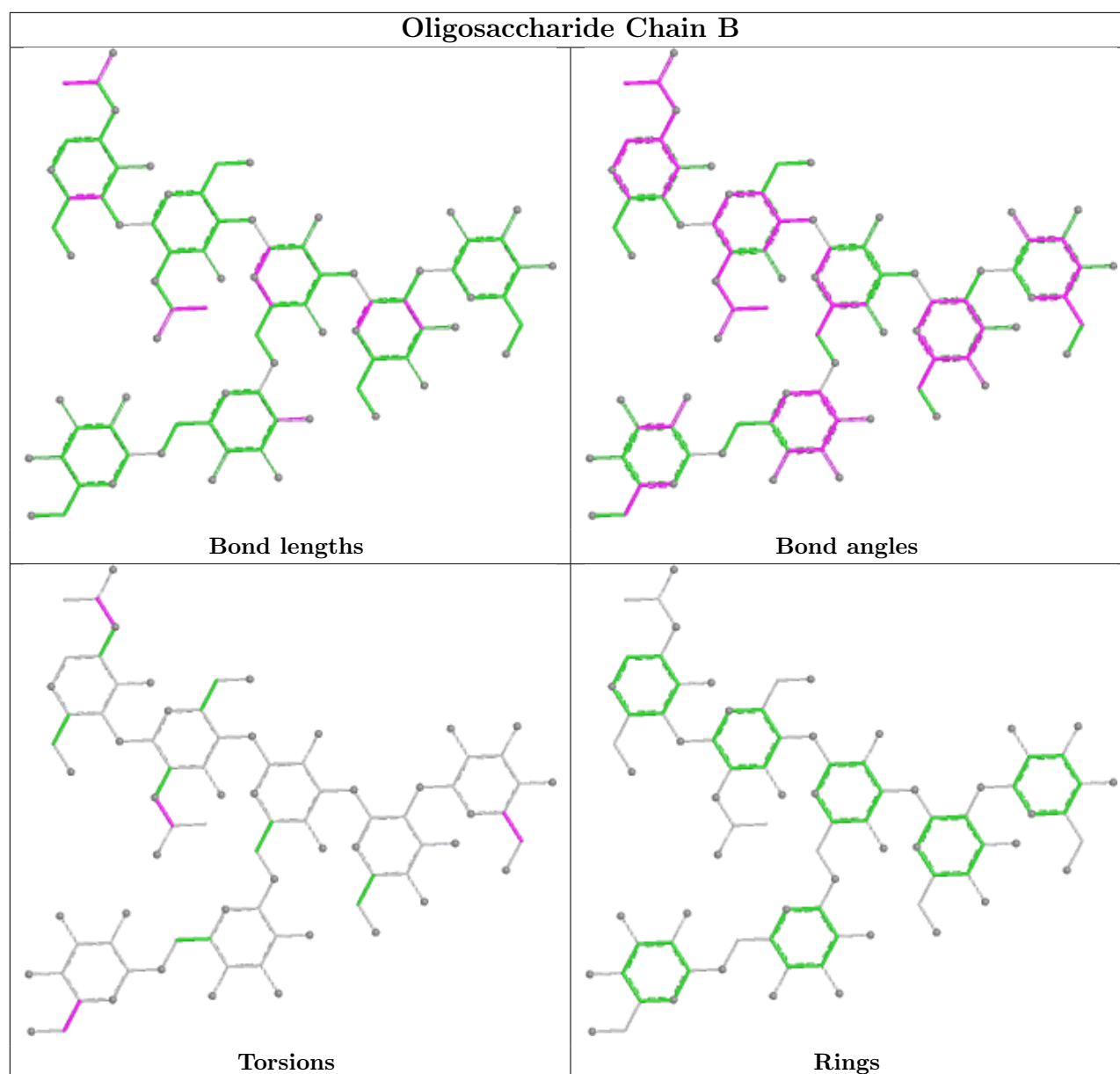
Mol	Chain	Res	Type	Atoms
4	B	5	MAN	C4-C5-C6-O6
4	B	5	MAN	O5-C5-C6-O6
4	B	2	NAG	C8-C7-N2-C2
4	B	1	NAG	C8-C7-N2-C2
4	B	1	NAG	O7-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
4	B	7	MAN	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	6	MAN	6	0
4	B	3	BMA	3	0
4	B	1	NAG	4	0

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



5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GLC	A	702	-	12,12,12	0.75	0	17,17,17	1.38	3 (17%)
6	NAG	A	634	1	14,14,15	1.68	3 (21%)	17,19,21	2.00	7 (41%)
6	NAG	A	646	1	14,14,15	1.13	1 (7%)	17,19,21	1.68	5 (29%)
6	NAG	A	686	1	14,14,15	1.03	0	17,19,21	2.03	3 (17%)
9	MAN	L	217(H)	-	11,11,12	0.52	0	15,15,17	2.18	4 (26%)
5	GLC	H	701	-	12,12,12	0.94	0	17,17,17	1.18	2 (11%)
6	NAG	A	629	1	14,14,15	0.78	0	17,19,21	1.79	7 (41%)
8	SO4	A	602	-	4,4,4	0.76	0	6,6,6	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
5	GLC	A	702	-	1/1/5/5	0/2/22/22	0/1/1/1
6	NAG	A	634	1	-	2/6/23/26	0/1/1/1
6	NAG	A	646	1	-	2/6/23/26	0/1/1/1
6	NAG	A	686	1	-	4/6/23/26	0/1/1/1
9	MAN	L	217(H)	-	-	0/2/19/22	0/1/1/1
5	GLC	H	701	-	1/1/5/5	1/2/22/22	0/1/1/1
6	NAG	A	629	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	634	NAG	O7-C7	4.05	1.32	1.23
6	A	646	NAG	C8-C7	-2.48	1.45	1.50
6	A	634	NAG	C1-C2	2.42	1.55	1.52
6	A	634	NAG	O4-C4	2.05	1.48	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	686	NAG	C1-O5-C5	6.50	120.90	112.19
9	L	217(H)	MAN	C1-O5-C5	6.13	120.40	112.19
9	L	217(H)	MAN	C1-C2-C3	4.08	115.59	109.64
6	A	634	NAG	O7-C7-N2	3.27	127.75	121.98
6	A	634	NAG	O4-C4-C5	3.19	117.19	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	634	NAG	C2-N2-C7	3.13	127.09	122.90
6	A	629	NAG	C8-C7-N2	3.12	121.29	116.12
6	A	634	NAG	C8-C7-N2	-2.97	111.19	116.12
6	A	686	NAG	C2-N2-C7	2.89	126.77	122.90
5	A	702	GLC	O5-C1-C2	-2.87	105.25	110.30
6	A	646	NAG	O6-C6-C5	-2.87	101.57	111.33
6	A	629	NAG	C2-N2-C7	2.84	126.70	122.90
6	A	629	NAG	O7-C7-N2	-2.81	117.01	121.98
6	A	634	NAG	O4-C4-C3	2.80	116.97	110.38
6	A	629	NAG	O4-C4-C5	2.74	116.07	109.32
6	A	634	NAG	C1-O5-C5	2.74	115.86	112.19
6	A	646	NAG	O5-C1-C2	-2.71	107.09	111.29
6	A	646	NAG	C3-C4-C5	-2.61	105.50	110.23
5	H	701	GLC	C1-O5-C5	2.60	118.69	113.65
9	L	217(H)	MAN	O5-C1-C2	2.50	116.75	110.79
9	L	217(H)	MAN	O2-C2-C1	-2.49	103.53	109.22
6	A	629	NAG	O5-C1-C2	-2.43	107.53	111.29
5	A	702	GLC	C3-C4-C5	-2.40	105.88	110.23
6	A	686	NAG	O5-C1-C2	-2.32	107.70	111.29
6	A	646	NAG	C4-C3-C2	-2.24	107.74	111.02
6	A	634	NAG	C3-C4-C5	-2.20	106.25	110.23
6	A	629	NAG	C4-C3-C2	-2.19	107.81	111.02
5	A	702	GLC	O4-C4-C3	2.10	115.33	110.38
6	A	629	NAG	C3-C4-C5	-2.07	106.48	110.23
5	H	701	GLC	O2-C2-C3	2.05	115.21	110.38
6	A	646	NAG	O3-C3-C4	2.03	115.16	110.38

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	702	GLC	C1
5	H	701	GLC	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	686	NAG	C4-C5-C6-O6
6	A	686	NAG	O5-C5-C6-O6
6	A	686	NAG	C8-C7-N2-C2
6	A	686	NAG	O7-C7-N2-C2
6	A	646	NAG	C8-C7-N2-C2
6	A	646	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	A	634	NAG	C8-C7-N2-C2
6	A	634	NAG	O7-C7-N2-C2
6	A	629	NAG	C8-C7-N2-C2
6	A	629	NAG	O7-C7-N2-C2
5	H	701	GLC	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	702	GLC	1	0
6	A	634	NAG	3	0
6	A	646	NAG	3	0
6	A	686	NAG	1	0
9	L	217(H)	MAN	3	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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/395 (98%)	-0.39	1 (0%) 90 91	23, 29, 40, 52	0
2	H	143/217 (65%)	1.13	34 (23%) 2 2	26, 44, 90, 94	0
3	L	129/214 (60%)	0.50	15 (11%) 9 10	26, 37, 71, 80	0
All	All	660/826 (79%)	0.12	50 (7%) 20 21	23, 32, 69, 94	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	112	SER	6.8
3	L	136	LEU	6.2
2	H	176	ALA	6.1
3	L	113	PRO	5.8
2	H	154	LEU	5.6
2	H	190	SER	5.0
2	H	155	THR	4.8
2	H	174	PHE	4.8
2	H	186	THR	4.8
2	H	148	PHE	4.6
2	H	187	LEU	4.3
2	H	152	VAL	4.3
2	H	171	VAL	4.2
2	H	149	PRO	4.2
3	L	164	THR	4.1
2	H	173	THR	3.9
2	H	111	VAL	3.8
2	H	153	THR	3.7
3	L	112	ALA	3.6
2	H	175	PRO	3.6
2	H	188	SER	3.6
2	H	116	THR	3.5
3	L	137	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
3	L	139	PHE	3.4
2	H	113	SER	3.3
3	L	111	ALA	3.2
2	H	170	GLY	3.1
3	L	109	ALA	3.1
2	H	151	PRO	3.0
3	L	141	PRO	3.0
2	H	189	SER	2.9
2	H	172	HIS	2.9
3	L	142	LYS	2.9
2	H	115	LYS	2.8
2	H	84	ALA	2.7
1	A	308	LYS	2.7
2	H	13	GLN	2.7
3	L	171	SER	2.7
2	H	12	VAL	2.4
3	L	110	ASP	2.4
2	H	109	LEU	2.4
2	H	83	THR	2.3
3	L	143	ASP	2.3
2	H	15	GLY	2.3
2	H	42	GLY	2.3
3	L	138	ASN	2.2
3	L	140	TYR	2.2
2	H	14	PRO	2.1
2	H	11	LEU	2.1
2	H	82(C)	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

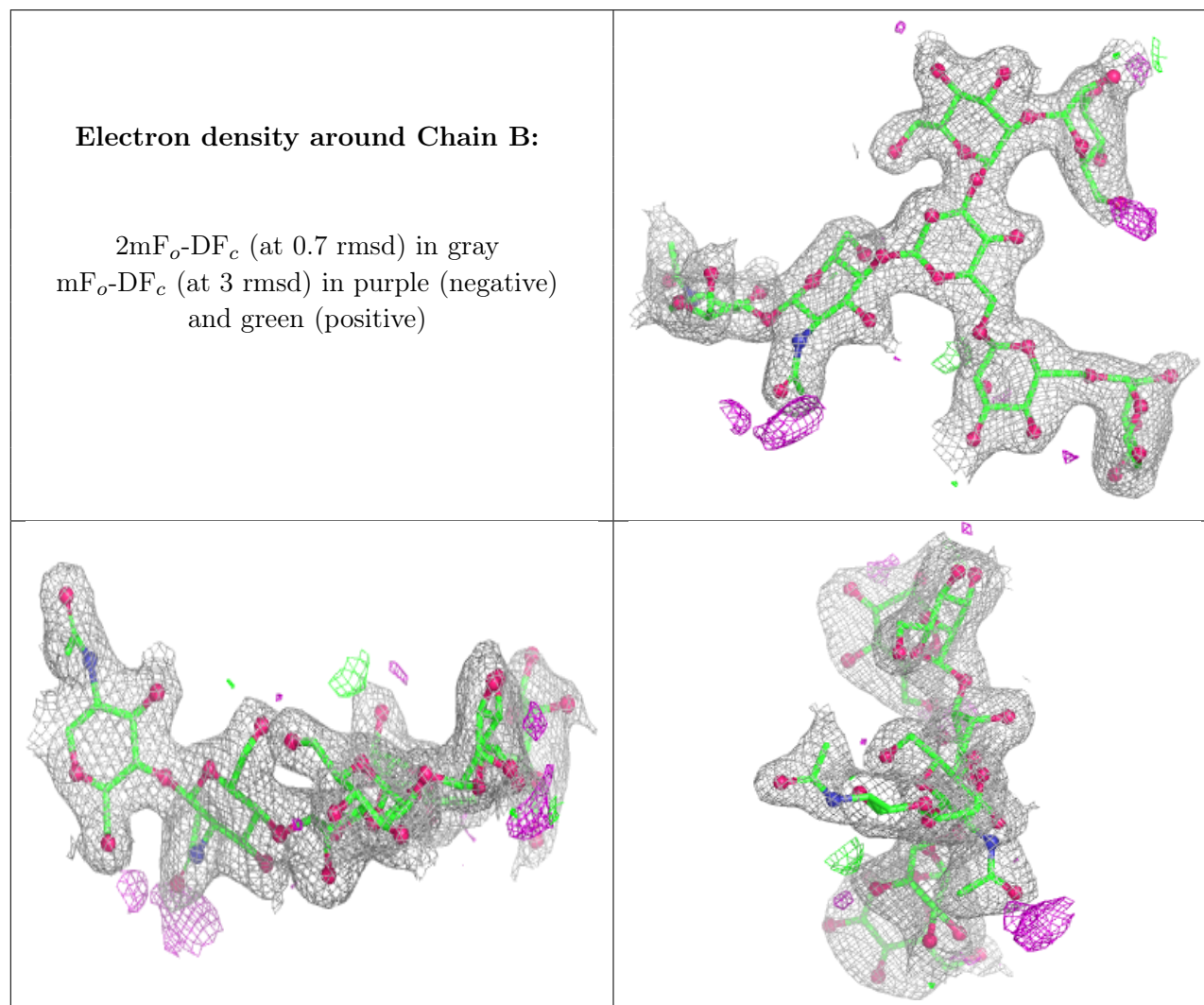
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	1	14/15	-	-	20,29,31,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	2	14/15	-	-	27,31,37,45	0
4	BMA	B	3	11/12	-	-	29,33,35,36	0
4	MAN	B	4	11/12	-	-	34,37,42,46	0
4	MAN	B	5	11/12	-	-	50,55,57,58	0
4	MAN	B	6	11/12	-	-	38,46,53,61	0
4	MAN	B	7	11/12	-	-	67,71,73,75	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	A	629	14/15	0.66	0.16	64,72,75,76	0
9	MAN	L	217(H)	11/12	0.75	0.19	75,79,80,81	0
6	NAG	A	686	14/15	0.79	0.13	53,59,67,68	0
6	NAG	A	634	14/15	0.80	0.12	44,52,57,62	0
6	NAG	A	646	14/15	0.81	0.14	40,48,53,57	0
5	GLC	A	702	12/12	0.85	0.11	46,58,61,63	0
5	GLC	H	701	12/12	0.93	0.09	32,41,51,52	0
8	SO4	A	602	5/5	0.99	0.05	26,31,34,35	0
7	CA	A	601	1/1	0.99	0.06	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.