



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:02 AM UTC

PDB ID : 6N6B / pdb_00006n6b
Title : The complex crystal structure of neuraminidase from A/Minnesota/11/2010 with B10 antibody.
Authors : Yang, H.; Stevens, J.
Deposited on : 2018-11-26
Resolution : 2.30 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

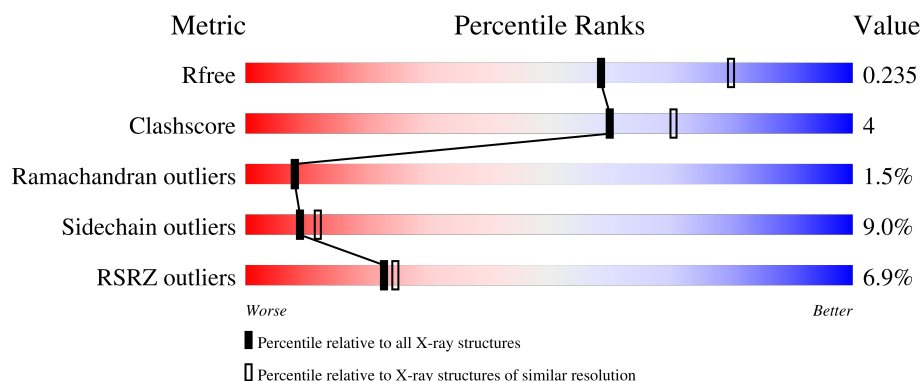
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	397	% 85% 11% ...
2	K	221	12% 75% 17% 6% .
3	L	214	13% 78% 14% 6% .
4	B	5	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6694 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	0	0
			3019	1876	536	584	23			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	GLY	-	expression tag	UNP A0A075ETL7
A	74	SER	-	expression tag	UNP A0A075ETL7
A	75	GLY	-	expression tag	UNP A0A075ETL7
A	76	ASP	-	expression tag	UNP A0A075ETL7
A	77	SER	-	expression tag	UNP A0A075ETL7
A	78	GLY	-	expression tag	UNP A0A075ETL7
A	79	SER	-	expression tag	UNP A0A075ETL7
A	80	PRO	-	expression tag	UNP A0A075ETL7
A	81	GLY	-	expression tag	UNP A0A075ETL7

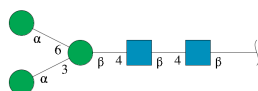
- Molecule 2 is a protein called B10 antibody Heavy Chain Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	221	Total	C	N	O	S	0	0	0
			1693	1072	274	341	6			

- Molecule 3 is a protein called B10 antibody Light Chain Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1671	1037	285	341	8			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.

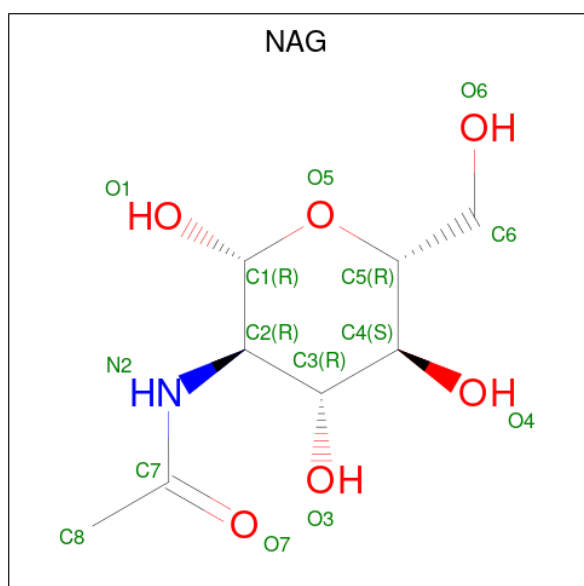


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	161	Total	O	0	0
			161	161		
7	K	44	Total	O	0	0
			44	44		

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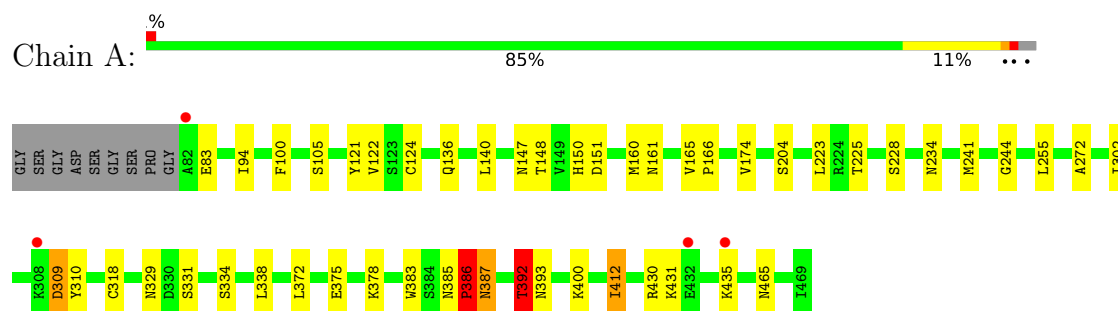
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	30	Total	O	0	0
			30	30		

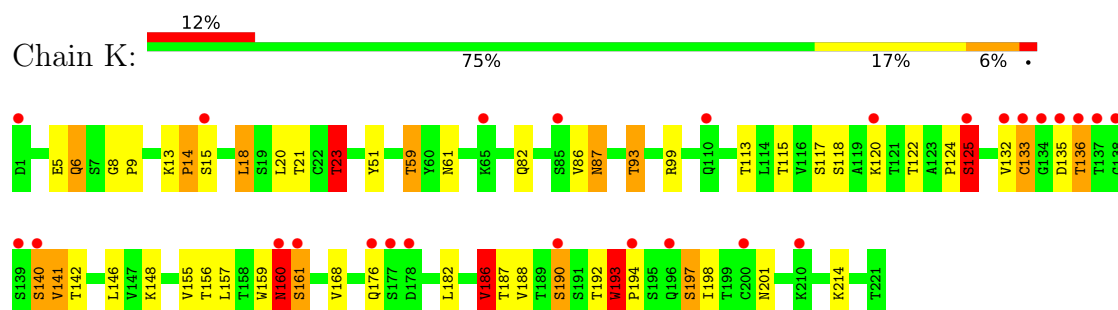
3 Residue-property plots [i](#)

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.

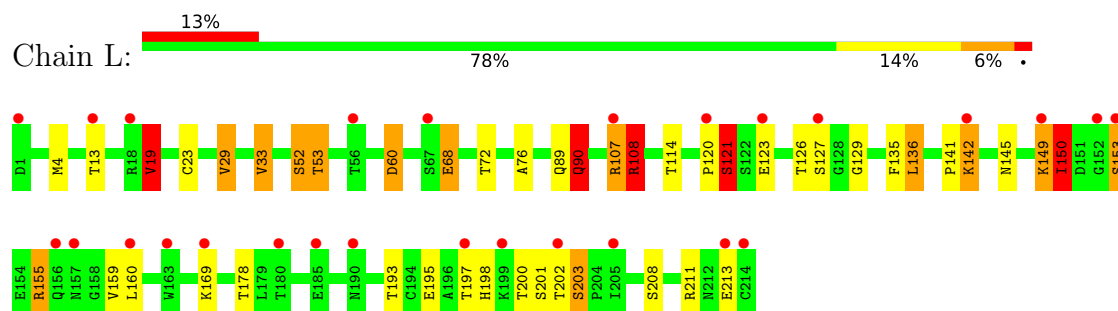
- Molecule 1: Neuraminidase



- Molecule 2: B10 antibody Heavy Chain Fab



- Molecule 3: B10 antibody Light Chain Fab



- Molecule 4: alpha-D-mannopyranose-(1-3)-[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



MAG1
MAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	188.47Å 188.47Å 136.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.30) 97.5 (50.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.220 , 0.245 0.207 , 0.235	Depositor DCC
R_{free} test set	5115 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 17.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6694	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN, CA

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	1.47	16/3091 (0.5%)	1.29	17/4190 (0.4%)
2	K	1.30	5/1739 (0.3%)	1.37	18/2384 (0.8%)
3	L	1.33	9/1710 (0.5%)	1.35	16/2325 (0.7%)
All	All	1.39	30/6540 (0.5%)	1.32	51/8899 (0.6%)

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
2	K	0	3
All	All	0	4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	ASN	N-CA	9.20	1.58	1.46
3	L	108	ARG	N-CA	7.73	1.56	1.46
3	L	108	ARG	CA-C	7.62	1.62	1.52
2	K	125	SER	N-CA	7.24	1.55	1.46
2	K	141	VAL	N-CA	7.06	1.55	1.46
1	A	160	MET	C-O	-6.96	1.15	1.23
1	A	148	THR	N-CA	-6.81	1.39	1.46
1	A	329	ASN	CA-CB	6.81	1.64	1.53
1	A	100	PHE	CA-C	6.07	1.58	1.52
1	A	94	ILE	C-O	-5.96	1.17	1.24
1	A	166	PRO	N-CA	5.96	1.54	1.47
1	A	386	PRO	N-CA	-5.79	1.40	1.47
3	L	129	GLY	N-CA	5.65	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	60	ASP	CB-CG	5.54	1.66	1.52
1	A	272	ALA	C-O	-5.51	1.17	1.23
3	L	127	SER	N-CA	5.42	1.53	1.46
3	L	150	ILE	CA-C	5.42	1.59	1.52
2	K	99	ARG	CD-NE	-5.38	1.38	1.46
1	A	234	ASN	CA-CB	5.34	1.61	1.53
1	A	204	SER	C-O	5.33	1.30	1.23
1	A	122	VAL	C-O	5.32	1.29	1.24
3	L	195	GLU	N-CA	5.31	1.52	1.46
1	A	147	ASN	CA-C	5.30	1.58	1.53
3	L	150	ILE	N-CA	5.30	1.52	1.46
1	A	375	GLU	C-O	-5.30	1.17	1.23
3	L	33	VAL	CA-C	-5.20	1.46	1.52
2	K	125	SER	CA-C	5.15	1.59	1.52
1	A	378	LYS	CA-C	-5.12	1.46	1.52
2	K	193	TRP	CA-C	-5.08	1.46	1.52
1	A	165	VAL	CA-CB	-5.07	1.48	1.53

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	ASP	N-CA-C	11.86	130.60	114.12
1	A	309	ASP	CA-C-N	10.58	140.75	121.70
1	A	309	ASP	C-N-CA	10.58	140.75	121.70
2	K	140	SER	N-CA-C	10.02	127.38	114.75
2	K	193	TRP	CA-C-N	-9.12	108.89	119.47
2	K	193	TRP	C-N-CA	-9.12	108.89	119.47
2	K	186	VAL	CB-CA-C	-8.97	96.69	110.50
1	A	309	ASP	O-C-N	-8.96	111.88	122.27
2	K	99	ARG	NE-CZ-NH2	-7.89	112.09	119.20
3	L	19	VAL	CB-CA-C	-7.53	98.83	110.95
3	L	29	VAL	N-CA-CB	-7.37	102.78	112.36
1	A	386	PRO	CA-C-N	-7.13	107.92	121.54
1	A	386	PRO	C-N-CA	-7.13	107.92	121.54
3	L	108	ARG	N-CA-C	7.11	125.94	110.80
3	L	107	ARG	N-CA-C	7.05	121.97	113.23
1	A	310	TYR	N-CA-C	-6.75	92.10	111.00
1	A	412	ILE	CB-CA-C	-6.74	100.12	110.50
3	L	149	LYS	N-CA-C	6.48	121.01	112.13
3	L	76	ALA	N-CA-C	6.48	121.26	113.23
3	L	29	VAL	CB-CA-C	6.41	117.98	110.93
2	K	13	LYS	CA-C-N	6.38	127.81	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	13	LYS	C-N-CA	6.38	127.81	119.84
1	A	392	THR	CB-CA-C	-6.30	96.63	110.67
2	K	141	VAL	N-CA-C	6.28	122.40	109.34
3	L	90	GLN	N-CA-CB	-6.27	100.59	110.69
2	K	93	THR	CB-CA-C	6.27	120.09	109.75
3	L	52	SER	N-CA-CB	-6.02	102.36	111.15
2	K	99	ARG	CG-CD-NE	-5.98	98.84	112.00
1	A	151	ASP	N-CA-C	5.86	118.62	111.82
1	A	161	ASN	CB-CA-C	-5.75	97.85	110.67
2	K	190	SER	N-CA-C	5.74	123.02	110.80
3	L	159	VAL	CB-CA-C	-5.71	104.05	110.96
2	K	8	GLY	CA-C-N	5.69	126.95	119.84
2	K	8	GLY	C-N-CA	5.69	126.95	119.84
2	K	136	THR	N-CA-C	5.65	118.61	109.40
2	K	14	PRO	CA-C-N	-5.62	113.22	121.99
2	K	14	PRO	C-N-CA	-5.62	113.22	121.99
1	A	244	GLY	CA-C-N	5.62	128.82	120.90
1	A	244	GLY	C-N-CA	5.62	128.82	120.90
3	L	153	SER	N-CA-C	5.50	118.51	109.72
2	K	23	THR	CB-CA-C	5.46	119.03	110.19
2	K	99	ARG	CD-NE-CZ	5.39	131.94	124.40
1	A	165	VAL	CA-C-N	-5.31	114.24	119.92
1	A	165	VAL	C-N-CA	-5.31	114.24	119.92
3	L	203	SER	CA-C-N	5.31	125.31	119.90
3	L	203	SER	C-N-CA	5.31	125.31	119.90
3	L	142	LYS	N-CA-C	5.25	117.68	111.33
1	A	150	HIS	N-CA-C	5.21	117.78	110.23
3	L	211	ARG	NE-CZ-NH1	-5.17	116.33	121.50
3	L	53	THR	CB-CA-C	5.15	118.25	109.80
1	A	465	ASN	N-CA-C	5.12	118.79	112.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	309	ASP	Peptide
2	K	136	THR	Peptide
2	K	160	ASN	Peptide
2	K	192	THR	Peptide

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	2863	14	0
2	K	1693	0	1636	24	0
3	L	1671	0	1583	16	0
4	B	61	0	52	0	0
5	A	1	0	0	0	0
6	A	14	0	13	0	0
7	A	161	0	0	3	0
7	K	44	0	0	2	0
7	L	30	0	0	0	0
All	All	6694	0	6147	53	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 (53) 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)
2:K:140:SER:O	2:K:188:VAL:O	1.97	0.81
2:K:6:GLN:HE21	2:K:6:GLN:H	1.39	0.71
1:A:223:LEU:HD11	1:A:241:MET:HE2	1.72	0.69
2:K:133:CYS:HB3	2:K:135:ASP:OD2	1.94	0.67
2:K:59:THR:HG21	7:K:337:HOH:O	1.96	0.66
2:K:6:GLN:H	2:K:6:GLN:NE2	1.93	0.66
3:L:120:PRO:O	3:L:121:SER:HB3	1.95	0.65
3:L:13:THR:HG23	3:L:19:VAL:HG13	1.79	0.65
3:L:13:THR:HG21	3:L:19:VAL:HG22	1.81	0.63
2:K:193:TRP:O	2:K:194:PRO:C	2.39	0.62
2:K:23:THR:HG23	7:K:308:HOH:O	1.98	0.62
2:K:124:PRO:O	2:K:148:LYS:O	2.19	0.61
3:L:149:LYS:O	3:L:153:SER:O	2.18	0.60
2:K:87:ASN:C	2:K:87:ASN:HD22	2.09	0.60
1:A:223:LEU:HD11	1:A:241:MET:CE	2.32	0.59
3:L:150:ILE:HD12	3:L:155:ARG:HG3	1.85	0.59
3:L:107:ARG:O	3:L:108:ARG:O	2.21	0.58
3:L:4:MET:HE3	3:L:23:CYS:SG	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:135:PHE:C	3:L:136:LEU:HD23	2.30	0.56
3:L:13:THR:CG2	3:L:19:VAL:HG13	2.36	0.56
2:K:142:THR:HG22	2:K:187:THR:OG1	2.08	0.54
2:K:18:LEU:CD1	2:K:20:LEU:HG	2.38	0.54
2:K:51:TYR:CE2	2:K:59:THR:HG23	2.43	0.53
1:A:392:THR:HB	1:A:393:ASN:OD1	2.11	0.51
1:A:318:CYS:O	1:A:386:PRO:O	2.29	0.50
1:A:334:SER:HA	1:A:387:ASN:HD21	1.76	0.50
1:A:255:LEU:N	1:A:255:LEU:HD12	2.27	0.50
2:K:159:TRP:CE2	2:K:186:VAL:HG22	2.48	0.49
1:A:435:LYS:HD2	7:A:755:HOH:O	2.14	0.47
1:A:430:ARG:HB3	1:A:431:LYS:HA	1.97	0.47
2:K:133:CYS:CB	2:K:135:ASP:OD2	2.62	0.47
3:L:33:VAL:HA	3:L:89:GLN:O	2.15	0.47
2:K:157:LEU:C	2:K:157:LEU:HD23	2.40	0.46
2:K:168:VAL:HG22	2:K:186:VAL:HG13	1.98	0.45
3:L:4:MET:SD	3:L:90:GLN:HB2	2.56	0.45
7:A:738:HOH:O	2:K:59:THR:HG22	2.17	0.45
1:A:140:LEU:C	1:A:140:LEU:HD23	2.43	0.43
7:A:738:HOH:O	2:K:59:THR:CG2	2.67	0.42
1:A:121:TYR:CG	1:A:228:SER:HA	2.54	0.42
1:A:385:ASN:O	1:A:386:PRO:C	2.61	0.42
3:L:135:PHE:O	3:L:136:LEU:HD23	2.18	0.42
1:A:302:ILE:HD13	1:A:383:TRP:CZ2	2.54	0.42
1:A:124:CYS:SG	1:A:412:ILE:HD11	2.60	0.42
2:K:132:VAL:HG12	2:K:133:CYS:HB2	2.01	0.41
2:K:160:ASN:HD21	2:K:198:ILE:HA	1.86	0.41
1:A:225:THR:HB	1:A:241:MET:HG2	2.02	0.41
2:K:160:ASN:HD22	2:K:160:ASN:HA	1.51	0.41
2:K:159:TRP:CZ2	2:K:186:VAL:HG22	2.56	0.41
2:K:176:GLN:HG3	3:L:160:LEU:HD13	2.03	0.41
3:L:198:HIS:HD2	3:L:200:THR:OG1	2.03	0.41
2:K:61:ASN:C	2:K:61:ASN:HD22	2.29	0.40
3:L:120:PRO:O	3:L:121:SER:CB	2.63	0.40
3:L:141:PRO:O	3:L:198:HIS:HE1	2.03	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 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	386/397 (97%)	367 (95%)	18 (5%)	1 (0%)	36	46
2	K	219/221 (99%)	199 (91%)	13 (6%)	7 (3%)	3	2
3	L	212/214 (99%)	201 (95%)	7 (3%)	4 (2%)	6	5
All	All	817/832 (98%)	767 (94%)	38 (5%)	12 (2%)	8	8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	108	ARG
2	K	190	SER
1	A	386	PRO
2	K	197	SER
3	L	121	SER
2	K	125	SER
2	K	161	SER
3	L	150	ILE
2	K	141	VAL
3	L	68	GLU
2	K	14	PRO
2	K	193	TRP

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 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	337/342 (98%)	327 (97%)	10 (3%)	36 53
2	K	195/195 (100%)	165 (85%)	30 (15%)	2 3
3	L	191/191 (100%)	166 (87%)	25 (13%)	4 4
All	All	723/728 (99%)	658 (91%)	65 (9%)	9 12

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	A	105	SER
1	A	136	GLN
1	A	174	VAL
1	A	331	SER
1	A	338	LEU
1	A	372	LEU
1	A	386	PRO
1	A	392	THR
1	A	400	LYS
2	K	5	GLU
2	K	6	GLN
2	K	9	PRO
2	K	15	SER
2	K	18	LEU
2	K	21	THR
2	K	23	THR
2	K	59	THR
2	K	82	GLN
2	K	86	VAL
2	K	87	ASN
2	K	93	THR
2	K	113	THR
2	K	115	THR
2	K	117	SER
2	K	118	SER
2	K	120	LYS
2	K	122	THR
2	K	125	SER
2	K	133	CYS
2	K	146	LEU

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Mol	Chain	Res	Type
2	K	155	VAL
2	K	156	THR
2	K	160	ASN
2	K	161	SER
2	K	182	LEU
2	K	186	VAL
2	K	197	SER
2	K	201	ASN
2	K	214	LYS
3	L	19	VAL
3	L	29	VAL
3	L	52	SER
3	L	53	THR
3	L	60	ASP
3	L	68	GLU
3	L	72	THR
3	L	90	GLN
3	L	114	THR
3	L	121	SER
3	L	123	GLU
3	L	126	THR
3	L	136	LEU
3	L	142	LYS
3	L	145	ASN
3	L	155	ARG
3	L	169	LYS
3	L	178	THR
3	L	193	THR
3	L	197	THR
3	L	201	SER
3	L	202	THR
3	L	203	SER
3	L	208	SER
3	L	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	147	ASN
1	A	150	HIS
1	A	168	HIS

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Mol	Chain	Res	Type
1	A	173	GLN
1	A	199	ASN
1	A	264	HIS
1	A	342	ASN
1	A	358	ASN
1	A	387	ASN
1	A	419	ASN
2	K	6	GLN
2	K	40	GLN
2	K	61	ASN
2	K	87	ASN
2	K	110	GLN
2	K	160	ASN
2	K	169	HIS
2	K	176	GLN
3	L	8	HIS
3	L	38	GLN
3	L	55	HIS
3	L	198	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

5 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	0.93	1 (7%)	17,19,21	1.53	2 (11%)
4	NAG	B	2	4	14,14,15	1.00	2 (14%)	17,19,21	1.65	5 (29%)
4	BMA	B	3	4	11,11,12	1.30	2 (18%)	15,15,17	2.22	5 (33%)
4	MAN	B	4	4	11,11,12	1.32	1 (9%)	15,15,17	1.61	5 (33%)
4	MAN	B	5	4	11,11,12	1.22	2 (18%)	15,15,17	3.67	9 (60%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4	MAN	O2-C2	2.73	1.49	1.43
4	B	5	MAN	O4-C4	2.72	1.49	1.43
4	B	5	MAN	O5-C5	2.54	1.48	1.43
4	B	1	NAG	C1-C2	2.53	1.55	1.52
4	B	3	BMA	O5-C5	2.34	1.48	1.43
4	B	2	NAG	C1-C2	2.25	1.55	1.52
4	B	3	BMA	C6-C5	2.15	1.59	1.51
4	B	2	NAG	C4-C5	2.01	1.57	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5	MAN	C1-C2-C3	6.89	119.67	109.64
4	B	5	MAN	C2-C3-C4	6.15	121.67	110.86
4	B	5	MAN	O4-C4-C5	5.84	123.72	109.32
4	B	5	MAN	O3-C3-C2	-5.16	99.53	110.05
4	B	3	BMA	C6-C5-C4	4.80	124.81	113.02
4	B	3	BMA	O4-C4-C3	-4.38	100.05	110.38
4	B	1	NAG	O5-C1-C2	-3.78	105.44	111.29
4	B	5	MAN	O5-C5-C4	3.64	119.69	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5	MAN	C3-C4-C5	-3.47	103.95	110.23
4	B	3	BMA	O4-C4-C5	2.93	116.53	109.32
4	B	2	NAG	C3-C4-C5	-2.85	105.06	110.23
4	B	5	MAN	O2-C2-C3	-2.84	104.27	110.15
4	B	1	NAG	C1-O5-C5	2.81	115.96	112.19
4	B	4	MAN	O2-C2-C1	2.78	115.60	109.22
4	B	3	BMA	O3-C3-C2	-2.77	104.40	110.05
4	B	2	NAG	C2-N2-C7	2.64	126.43	122.90
4	B	5	MAN	O4-C4-C3	-2.63	104.17	110.38
4	B	5	MAN	O5-C1-C2	2.56	116.89	110.79
4	B	4	MAN	O5-C5-C6	2.53	112.59	107.66
4	B	3	BMA	O5-C5-C4	-2.37	105.06	110.83
4	B	2	NAG	C1-O5-C5	-2.35	109.04	112.19
4	B	4	MAN	O2-C2-C3	2.23	114.76	110.15
4	B	2	NAG	O7-C7-C8	-2.22	118.10	122.05
4	B	4	MAN	C1-O5-C5	2.13	115.05	112.19
4	B	4	MAN	C2-C3-C4	2.06	114.49	110.86
4	B	2	NAG	O4-C4-C3	-2.02	105.61	110.38

There are no chirality outliers.

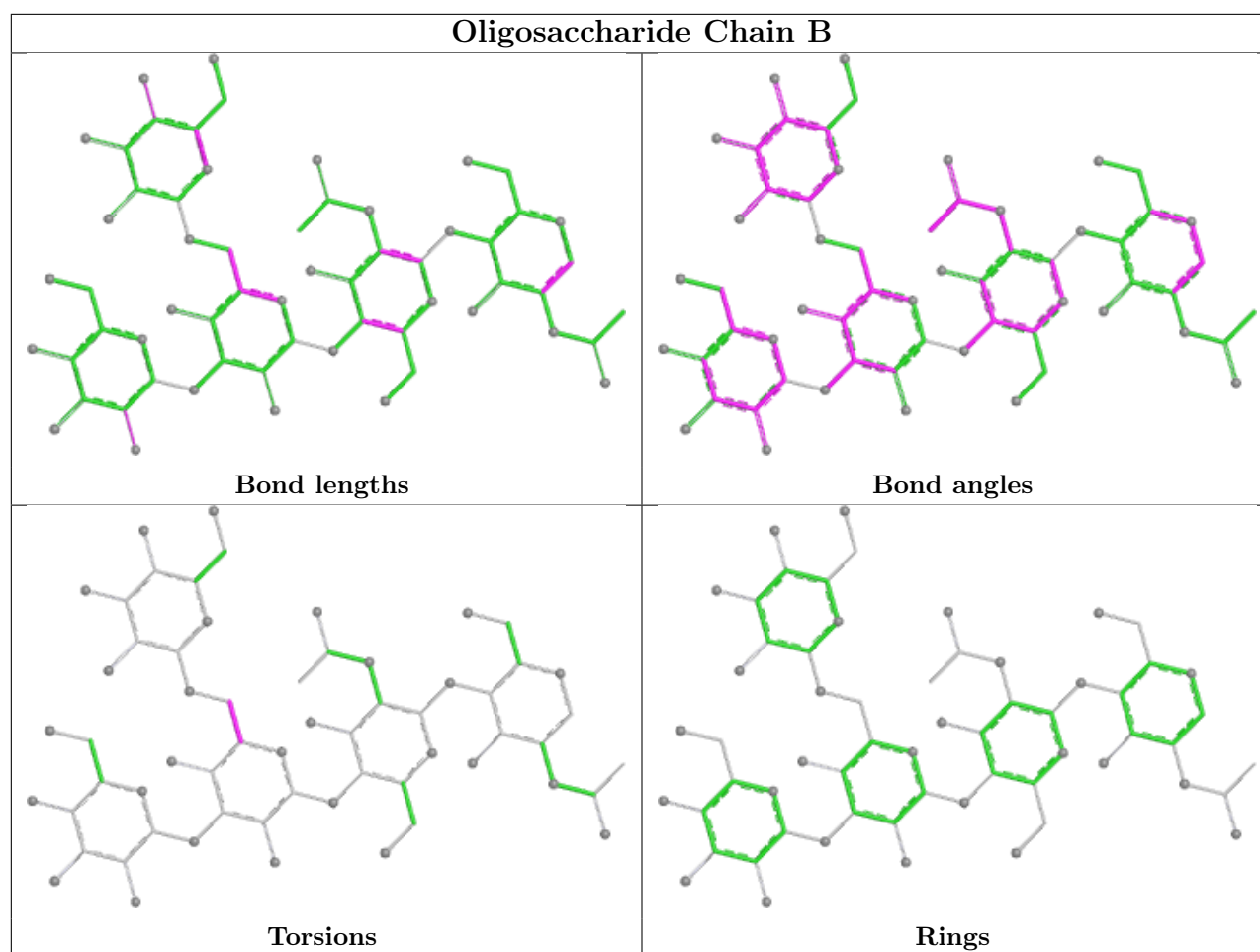
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3	BMA	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
6	NAG	A	507	1	14,14,15	1.37	2 (14%)	17,19,21	2.85	9 (52%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	507	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	507	NAG	O4-C4	3.28	1.51	1.43
6	A	507	NAG	O5-C1	-2.00	1.40	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	507	NAG	C3-C4-C5	-5.69	99.92	110.23
6	A	507	NAG	O4-C4-C5	4.52	120.45	109.32
6	A	507	NAG	C1-O5-C5	4.01	117.57	112.19
6	A	507	NAG	O5-C5-C6	-3.95	99.97	107.66
6	A	507	NAG	C6-C5-C4	3.38	121.33	113.02
6	A	507	NAG	C1-C2-N2	-3.28	105.27	110.43
6	A	507	NAG	O3-C3-C4	3.07	117.60	110.38
6	A	507	NAG	O4-C4-C3	2.58	116.46	110.38
6	A	507	NAG	O3-C3-C2	-2.51	104.19	109.40

There are no chirality outliers.

There are no torsion outliers.

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 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	388/397 (97%)	-0.41	4 (1%) 79 80	16, 25, 40, 67	0
2	K	221/221 (100%)	0.61	26 (11%) 9 10	22, 42, 69, 104	0
3	L	214/214 (100%)	0.66	27 (12%) 8 9	25, 43, 70, 100	0
All	All	823/832 (98%)	0.14	57 (6%) 23 25	16, 32, 65, 104	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	136	THR	7.4
2	K	137	THR	6.7
2	K	138	GLY	6.0
2	K	135	ASP	5.9
2	K	177	SER	5.6
3	L	214	CYS	5.1
3	L	157	ASN	5.1
2	K	196	GLN	4.4
2	K	134	GLY	4.2
1	A	82	ALA	4.1
2	K	133	CYS	4.0
3	L	213	GLU	3.9
2	K	176	GLN	3.9
3	L	169	LYS	3.9
3	L	152	GLY	3.9
2	K	1	ASP	3.7
2	K	65	LYS	3.6
2	K	210	LYS	3.6
3	L	202	THR	3.5
2	K	194	PRO	3.2
3	L	160	LEU	3.2
3	L	149	LYS	3.1
2	K	139	SER	3.1

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Mol	Chain	Res	Type	RSRZ
3	L	153	SER	3.1
2	K	120	LYS	3.0
3	L	123	GLU	3.0
3	L	197	THR	2.8
3	L	107	ARG	2.8
3	L	205	ILE	2.7
2	K	110	GLN	2.7
2	K	140	SER	2.7
3	L	190	ASN	2.7
3	L	67	SER	2.7
3	L	156	GLN	2.7
2	K	190	SER	2.6
3	L	56	THR	2.6
2	K	161	SER	2.5
2	K	15	SER	2.5
3	L	142	LYS	2.5
3	L	127	SER	2.5
3	L	163	TRP	2.4
3	L	120	PRO	2.3
1	A	308	LYS	2.3
2	K	125	SER	2.2
3	L	18	ARG	2.2
2	K	132	VAL	2.1
3	L	13	THR	2.1
2	K	178	ASP	2.1
1	A	432	GLU	2.1
1	A	435	LYS	2.0
2	K	85	SER	2.0
3	L	185	GLU	2.0
3	L	180	THR	2.0
2	K	200	CYS	2.0
2	K	160	ASN	2.0
3	L	1	ASP	2.0
3	L	199	LYS	2.0

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

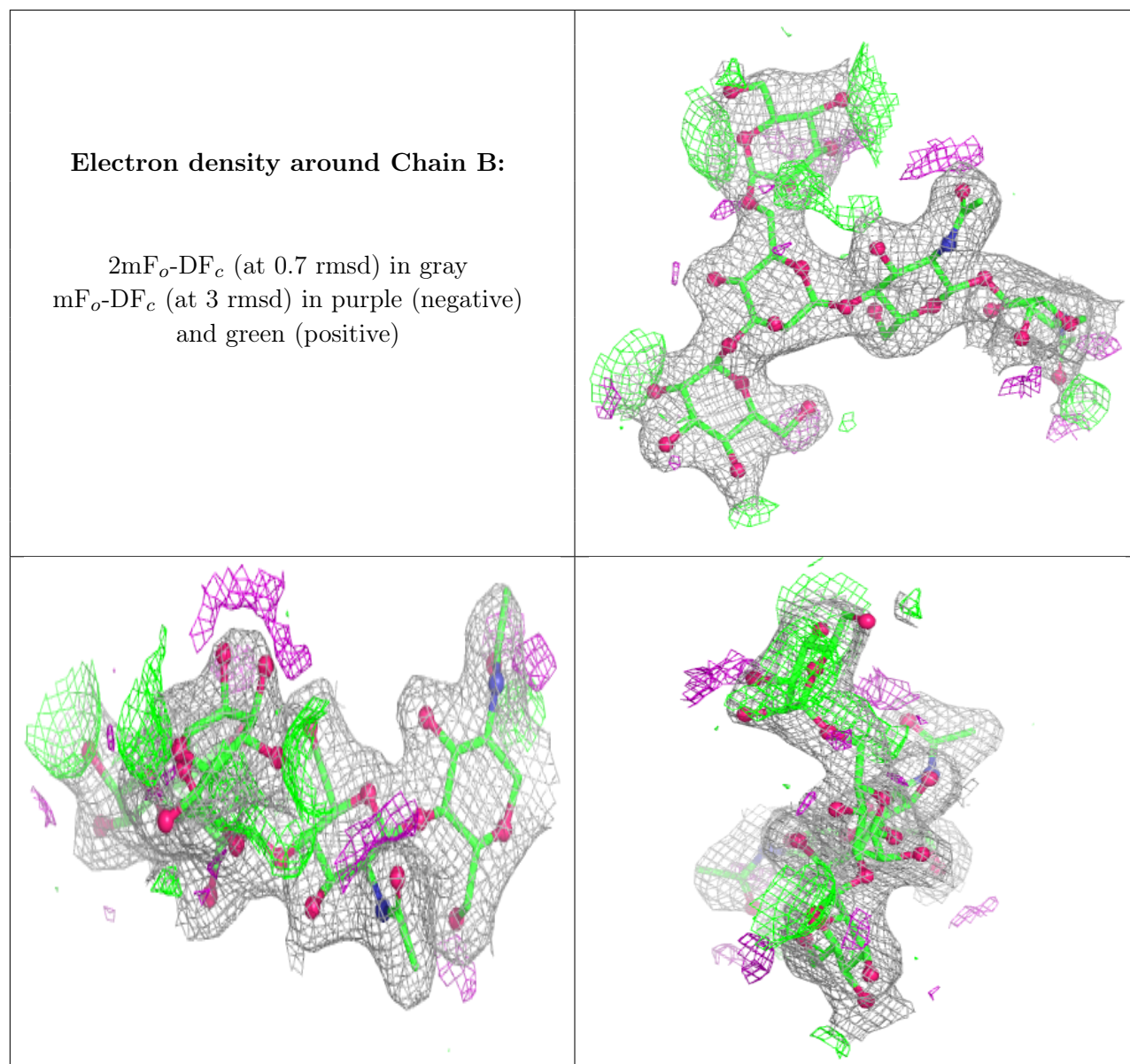
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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(Å ²)	Q<0.9
4	NAG	B	1	14/15	-	-	25,27,45,61	0
4	NAG	B	2	14/15	-	-	24,26,28,30	0
4	BMA	B	3	11/12	-	-	25,28,34,52	0
4	MAN	B	4	11/12	-	-	27,28,30,33	0
4	MAN	B	5	11/12	-	-	43,54,65,69	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 [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(Å ²)	Q<0.9
6	NAG	A	507	14/15	0.90	0.12	31,40,46,49	0
5	CA	A	501	1/1	0.99	0.02	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.