



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:16 AM UTC

PDB ID : 3NN9 / pdb_00003nn9
Title : REFINED ATOMIC STRUCTURES OF N9 SUBTYPE INFLUENZA VIRUS
NEURAMINIDASE AND ESCAPE MUTANTS
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Deposited on : 1991-03-28
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

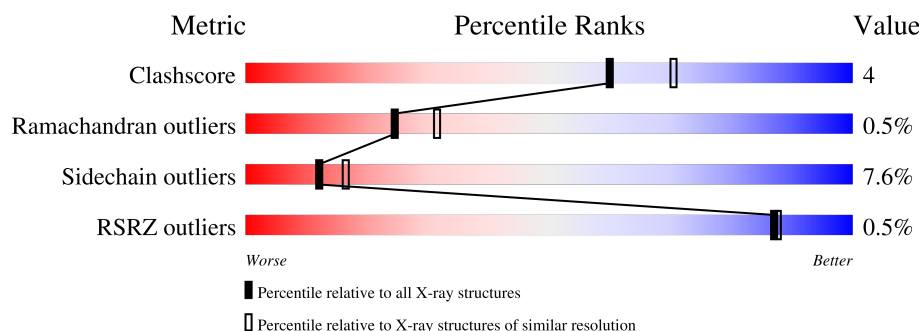
1 Overall quality at a glance

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))
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	388	57% 36% 5%
2	B	7	14% 86%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3268 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.

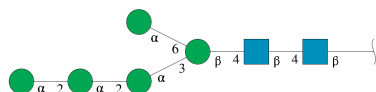
- Molecule 1 is a protein called NEURAMINIDASE N9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3067	1914	537	593	23			

There is a discrepancy between the modelled and reference sequences:

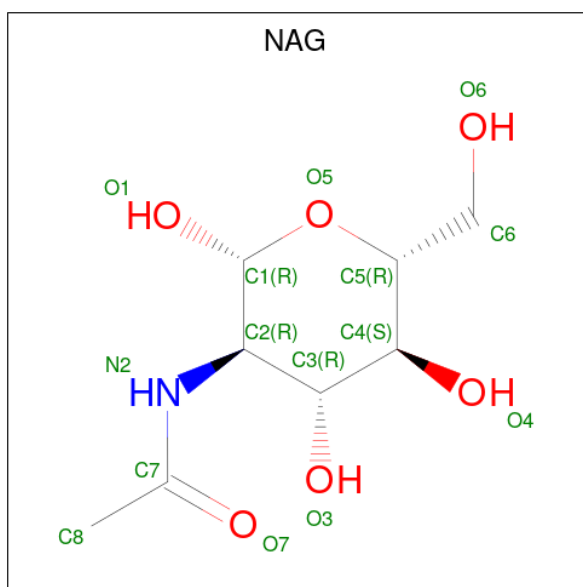
Chain	Residue	Modelled	Actual	Comment	Reference
A	329	ASP	ASN	conflict	UNP P03472

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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
2	B	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

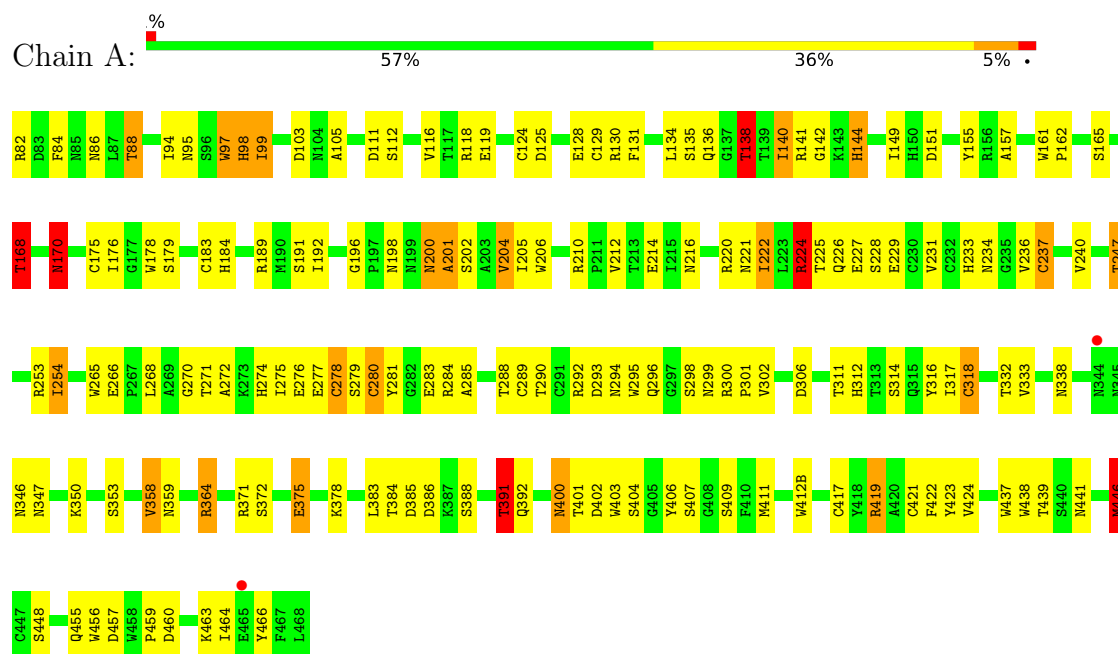
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	89	Total	O	0	0
			89	89		

3 Residue-property plots

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 N9



• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	185.10Å 185.10Å 185.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30 6.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.30) 65.5 (6.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.178 , (Not available) 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.8	EDS
L-test for twinning ¹	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3268	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: MAN, BMA, CA, 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	1.37	14/3150 (0.4%)	2.39	208/4290 (4.8%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	VAL	CA-CB	9.51	1.66	1.54
1	A	278	CYS	CA-CB	-8.52	1.39	1.53
1	A	161	TRP	CA-CB	7.87	1.64	1.53
1	A	184	HIS	CD2-NE2	-7.76	1.29	1.37
1	A	254	ILE	CA-CB	7.18	1.62	1.53
1	A	278	CYS	CB-SG	6.19	2.01	1.81
1	A	274	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	144	HIS	CD2-NE2	-6.07	1.31	1.37
1	A	233	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	317	ILE	CA-CB	5.94	1.61	1.54
1	A	98	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	312	HIS	CD2-NE2	-5.64	1.31	1.37
1	A	184	HIS	CG-ND1	-5.59	1.32	1.38
1	A	210	ARG	C-N	5.53	1.40	1.33

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ASN	OD1-CG-ND2	-12.50	110.10	122.60
1	A	359	ASN	OD1-CG-ND2	-12.02	110.58	122.60
1	A	170	ASN	OD1-CG-ND2	-11.59	111.01	122.60
1	A	99	ILE	CB-CA-C	-11.16	93.14	111.32
1	A	277	GLU	N-CA-C	10.21	125.34	111.24
1	A	359	ASN	CB-CG-ND2	10.18	131.67	116.40
1	A	220	ARG	N-CA-C	10.08	125.25	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ALA	N-CA-C	9.79	121.94	111.28
1	A	419	ARG	NE-CZ-NH1	9.01	130.51	121.50
1	A	265	TRP	CG-CD2-CE3	8.78	142.68	133.90
1	A	437	TRP	CG-CD2-CE3	8.58	142.48	133.90
1	A	84	PHE	CA-CB-CG	8.24	122.04	113.80
1	A	285	ALA	N-CA-C	8.22	122.75	111.90
1	A	99	ILE	N-CA-CB	8.15	123.82	110.13
1	A	216	ASN	CB-CG-ND2	8.08	128.52	116.40
1	A	198	ASN	OD1-CG-ND2	-8.00	114.60	122.60
1	A	392	GLN	CG-CD-NE2	8.00	128.41	116.40
1	A	358	VAL	N-CA-CB	-8.00	96.98	110.65
1	A	253	ARG	NE-CZ-NH1	7.97	129.47	121.50
1	A	391	THR	CA-CB-OG1	-7.90	97.75	109.60
1	A	253	ARG	NH1-CZ-NH2	-7.89	109.04	119.30
1	A	178	TRP	CG-CD2-CE3	7.84	141.74	133.90
1	A	318	CYS	N-CA-C	7.76	119.74	111.28
1	A	184	HIS	CB-CG-CD2	-7.73	121.16	131.20
1	A	170	ASN	CA-CB-CG	7.71	120.31	112.60
1	A	392	GLN	OE1-CD-NE2	-7.68	114.92	122.60
1	A	88	THR	N-CA-CB	-7.66	98.85	110.26
1	A	131	PHE	CA-CB-CG	7.63	121.43	113.80
1	A	165	SER	CA-C-N	7.44	128.04	120.38
1	A	165	SER	C-N-CA	7.44	128.04	120.38
1	A	138	THR	CB-CA-C	-7.33	96.98	110.62
1	A	119	GLU	CA-C-N	7.32	127.27	120.03
1	A	119	GLU	C-N-CA	7.32	127.27	120.03
1	A	333	VAL	N-CA-C	-7.29	96.97	108.86
1	A	88	THR	CA-CB-OG1	-7.22	98.78	109.60
1	A	226	GLN	N-CA-C	7.16	119.16	111.36
1	A	298	SER	CA-C-O	7.10	127.66	119.35
1	A	456	TRP	CG-CD2-CE3	7.07	140.97	133.90
1	A	463	LYS	CG-CD-CE	-7.06	95.06	111.30
1	A	353	SER	CA-C-O	-7.05	113.35	121.10
1	A	403	TRP	CE2-CD2-CG	-6.98	98.83	107.20
1	A	224	ARG	CA-CB-CG	6.92	127.94	114.10
1	A	179	SER	O-C-N	-6.91	115.32	123.41
1	A	438	TRP	CB-CG-CD1	-6.91	116.53	126.90
1	A	88	THR	N-CA-C	6.87	122.00	112.45
1	A	265	TRP	CB-CG-CD1	-6.79	116.71	126.90
1	A	338	ASN	CB-CG-ND2	6.69	126.43	116.40
1	A	138	THR	N-CA-CB	6.68	121.92	111.56
1	A	224	ARG	N-CA-C	6.66	119.53	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	125	ASP	CA-C-N	6.63	126.58	119.28
1	A	125	ASP	C-N-CA	6.63	126.58	119.28
1	A	142	GLY	CA-C-N	6.58	129.75	120.28
1	A	142	GLY	C-N-CA	6.58	129.75	120.28
1	A	317	ILE	N-CA-C	-6.52	100.28	108.89
1	A	200	ASN	CA-CB-CG	6.51	119.11	112.60
1	A	212	VAL	N-CA-CB	-6.51	100.48	111.23
1	A	189	ARG	N-CA-C	6.49	119.82	109.24
1	A	406	TYR	CB-CG-CD2	-6.48	111.08	120.80
1	A	400	ASN	N-CA-C	6.46	120.27	112.38
1	A	441	ASN	N-CA-C	6.46	118.59	108.96
1	A	131	PHE	CA-C-N	6.43	132.89	122.29
1	A	131	PHE	C-N-CA	6.43	132.89	122.29
1	A	221	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	A	224	ARG	CA-C-O	-6.39	114.17	121.58
1	A	247	THR	CA-C-O	6.38	125.97	119.97
1	A	306	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	135	SER	O-C-N	-6.36	115.53	122.79
1	A	284	ARG	NE-CZ-NH2	-6.35	113.49	119.20
1	A	296	GLN	N-CA-C	6.31	123.91	113.50
1	A	140	ILE	N-CA-C	6.29	117.04	110.62
1	A	206	TRP	CE2-CD2-CG	-6.28	99.67	107.20
1	A	437	TRP	CE2-CD2-CG	-6.25	99.70	107.20
1	A	95	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	A	271	THR	N-CA-C	6.21	120.47	113.02
1	A	456	TRP	N-CA-C	-6.21	99.88	109.14
1	A	456	TRP	CE2-CD2-CG	-6.20	99.76	107.20
1	A	441	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	A	460	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	176	ILE	O-C-N	-6.18	115.91	122.95
1	A	407	SER	CA-C-O	-6.17	114.08	120.99
1	A	118	ARG	NH1-CZ-NH2	-6.15	111.31	119.30
1	A	400	ASN	CB-CG-ND2	6.15	125.62	116.40
1	A	183	CYS	CA-C-O	-6.13	114.71	121.33
1	A	403	TRP	CG-CD2-CE3	6.12	140.02	133.90
1	A	417	CYS	O-C-N	-6.11	116.43	123.33
1	A	247	THR	N-CA-CB	-6.08	100.78	111.42
1	A	228	SER	CA-CB-OG	6.08	123.26	111.10
1	A	347	ASN	O-C-N	-6.06	117.46	123.46
1	A	459	PRO	O-C-N	-6.06	115.77	123.04
1	A	265	TRP	CE2-CD2-CG	-6.05	99.94	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	CYS	CA-C-N	6.04	125.80	119.76
1	A	237	CYS	C-N-CA	6.04	125.80	119.76
1	A	198	ASN	CB-CG-ND2	6.03	125.44	116.40
1	A	439	THR	CA-C-O	-6.02	113.63	120.32
1	A	97	TRP	CE2-CD2-CG	-6.01	99.98	107.20
1	A	175	CYS	CA-C-O	-5.94	114.93	121.28
1	A	161	TRP	CA-CB-CG	5.92	124.85	113.60
1	A	231	VAL	CA-C-N	-5.91	113.53	122.81
1	A	231	VAL	C-N-CA	-5.91	113.53	122.81
1	A	391	THR	N-CA-CB	-5.91	103.04	110.90
1	A	206	TRP	CD1-CG-CD2	5.91	115.75	106.30
1	A	184	HIS	CB-CG-ND1	5.90	131.55	122.70
1	A	290	THR	N-CA-C	-5.89	99.59	109.07
1	A	338	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	A	457	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	293	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	438	TRP	CG-CD2-CE3	5.85	139.75	133.90
1	A	385	ASP	CA-CB-CG	5.83	118.42	112.60
1	A	279	SER	CA-CB-OG	5.82	122.74	111.10
1	A	97	TRP	CD1-CG-CD2	5.82	115.61	106.30
1	A	350	LYS	CA-C-O	-5.81	114.29	120.92
1	A	278	CYS	N-CA-C	5.81	118.76	110.10
1	A	404	SER	O-C-N	-5.81	117.79	122.03
1	A	358	VAL	CB-CA-C	5.80	121.15	112.16
1	A	98	HIS	CA-C-O	-5.79	114.61	121.16
1	A	419	ARG	CB-CG-CD	-5.79	97.99	111.30
1	A	170	ASN	CB-CG-ND2	5.77	125.06	116.40
1	A	423	TYR	N-CA-C	-5.77	100.58	109.52
1	A	206	TRP	CB-CG-CD1	-5.76	118.25	126.90
1	A	220	ARG	NE-CZ-NH2	-5.75	114.03	119.20
1	A	178	TRP	CE2-CD2-CG	-5.75	100.31	107.20
1	A	170	ASN	N-CA-C	5.73	120.98	113.30
1	A	227	GLU	CB-CG-CD	5.71	122.30	112.60
1	A	175	CYS	CA-CB-SG	5.68	127.47	114.40
1	A	210	ARG	CA-C-N	5.67	125.86	119.90
1	A	210	ARG	C-N-CA	5.67	125.86	119.90
1	A	375	GLU	O-C-N	5.67	129.74	123.33
1	A	236	VAL	CG1-CB-CG2	-5.66	98.34	110.80
1	A	402	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	455	GLN	CG-CD-NE2	-5.64	107.94	116.40
1	A	88	THR	CA-CB-CG2	5.63	120.08	110.50
1	A	299	ASN	CA-CB-CG	5.62	118.22	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ASP	N-CA-C	5.62	120.20	113.23
1	A	312	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	A	97	TRP	CG-CD1-NE1	-5.61	102.90	110.20
1	A	391	THR	CA-CB-CG2	5.61	120.03	110.50
1	A	421	CYS	CA-CB-SG	5.59	127.27	114.40
1	A	97	TRP	CA-C-O	-5.57	114.25	120.66
1	A	316	TYR	N-CA-C	-5.57	101.05	109.85
1	A	275	ILE	CB-CG1-CD1	5.56	125.47	113.80
1	A	206	TRP	O-C-N	-5.55	117.00	123.27
1	A	288	THR	CA-CB-OG1	-5.55	101.28	109.60
1	A	103	ASP	N-CA-C	5.52	121.04	113.97
1	A	422	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	371	ARG	NE-CZ-NH1	5.48	126.98	121.50
1	A	403	TRP	CD1-CG-CD2	5.47	115.06	106.30
1	A	136	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	A	456	TRP	CG-CD1-NE1	-5.46	103.10	110.20
1	A	95	ASN	CA-CB-CG	-5.45	107.15	112.60
1	A	332	THR	OG1-CB-CG2	-5.44	98.42	109.30
1	A	229	GLU	CA-CB-CG	5.43	124.96	114.10
1	A	116	VAL	N-CA-C	-5.43	101.72	108.89
1	A	301	PRO	N-CA-CB	5.42	108.07	103.35
1	A	162	PRO	N-CA-C	5.41	119.69	111.15
1	A	119	GLU	CA-CB-CG	5.40	124.91	114.10
1	A	161	TRP	CA-C-O	-5.39	115.38	120.34
1	A	202	SER	O-C-N	5.36	129.59	123.48
1	A	295	TRP	N-CA-C	5.36	116.81	110.97
1	A	409	SER	O-C-N	-5.34	116.43	123.21
1	A	111	ASP	O-C-N	-5.32	116.92	122.18
1	A	276	GLU	N-CA-C	-5.29	99.70	108.75
1	A	98	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	A	424	VAL	N-CA-C	-5.28	100.46	108.17
1	A	204	VAL	CA-C-N	5.26	129.63	122.90
1	A	204	VAL	C-N-CA	5.26	129.63	122.90
1	A	170	ASN	CA-C-N	5.25	131.05	122.07
1	A	170	ASN	C-N-CA	5.25	131.05	122.07
1	A	272	ALA	CA-C-O	-5.25	114.78	120.81
1	A	270	GLY	CA-C-O	-5.24	117.06	122.25
1	A	437	TRP	NE1-CE2-CZ2	-5.24	122.24	130.10
1	A	459	PRO	CA-C-O	-5.22	115.26	122.15
1	A	386	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	168	THR	CA-CB-OG1	-5.21	101.78	109.60
1	A	206	TRP	CG-CD1-NE1	-5.21	103.43	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CYS	N-CA-C	5.21	118.08	109.85
1	A	412(B)	TRP	CE2-CD2-CG	-5.20	100.97	107.20
1	A	155	TYR	N-CA-CB	-5.18	102.82	110.49
1	A	144	HIS	CA-CB-CG	5.18	118.98	113.80
1	A	157	ALA	CA-C-O	-5.17	115.20	120.99
1	A	201	ALA	O-C-N	5.17	128.73	122.68
1	A	446	MET	CG-SD-CE	-5.16	89.54	100.90
1	A	295	TRP	CG-CD2-CE3	5.15	139.05	133.90
1	A	456	TRP	CD1-CG-CD2	5.14	114.53	106.30
1	A	388	SER	N-CA-C	5.14	117.61	109.96
1	A	403	TRP	CB-CG-CD1	-5.13	119.20	126.90
1	A	247	THR	CA-CB-OG1	-5.12	101.92	109.60
1	A	175	CYS	N-CA-C	5.11	115.91	108.14
1	A	265	TRP	NE1-CE2-CZ2	-5.11	122.43	130.10
1	A	191	SER	O-C-N	-5.11	116.95	123.24
1	A	274	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	A	300	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A	225	THR	CA-C-N	5.09	127.52	120.29
1	A	225	THR	C-N-CA	5.09	127.52	120.29
1	A	161	TRP	O-C-N	-5.08	117.94	121.65
1	A	266	GLU	CA-C-N	5.08	125.29	120.31
1	A	266	GLU	C-N-CA	5.08	125.29	120.31
1	A	168	THR	N-CA-CB	-5.07	102.36	110.46
1	A	318	CYS	CB-CA-C	-5.05	102.40	110.79
1	A	293	ASP	CA-C-O	-5.04	114.90	120.60
1	A	346	ASN	N-CA-C	5.04	118.68	111.92
1	A	372	SER	CA-CB-OG	5.03	121.16	111.10
1	A	306	ASP	CA-C-N	5.02	124.68	119.56
1	A	306	ASP	C-N-CA	5.02	124.68	119.56
1	A	112	SER	CA-CB-OG	-5.01	101.07	111.10
1	A	216	ASN	CA-CB-CG	5.01	117.61	112.60
1	A	412(B)	TRP	CA-C-N	5.00	128.58	121.42
1	A	412(B)	TRP	C-N-CA	5.00	128.58	121.42

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	3067	0	2891	26	0
2	B	83	0	70	0	0
3	A	28	0	26	0	0
4	A	1	0	0	0	0
5	A	89	0	0	2	0
All	All	3268	0	2987	26	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 (26) 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:278:CYS:CB	1:A:278:CYS:SG	2.01	1.46
1:A:466:TYR:OH	5:A:484:HOH:O	1.97	0.81
1:A:98:HIS:CE1	1:A:419:ARG:HH21	2.15	0.65
1:A:292:ARG:HH21	1:A:294:ASN:ND2	1.97	0.63
1:A:378:LYS:HD3	1:A:391:THR:HG22	1.81	0.62
1:A:168:THR:HG22	1:A:170:ASN:H	1.69	0.57
1:A:94:ILE:HG23	1:A:448:SER:HB2	1.88	0.55
1:A:138:THR:HG23	1:A:144:HIS:HB2	1.89	0.53
1:A:318:CYS:SG	1:A:383:LEU:O	2.67	0.53
1:A:138:THR:CG2	1:A:144:HIS:HB2	2.42	0.50
1:A:124:CYS:HA	1:A:129:CYS:HA	1.94	0.50
1:A:128:GLU:OE2	1:A:130:ARG:HD2	2.12	0.49
1:A:364:ARG:HD2	1:A:375:GLU:OE2	2.14	0.47
1:A:140:ILE:HD11	5:A:496:HOH:O	2.15	0.47
1:A:192:ILE:HG12	1:A:205:ILE:HG13	1.96	0.47
1:A:168:THR:H	1:A:170:ASN:ND2	2.14	0.46
1:A:222:ILE:O	1:A:224:ARG:HG3	2.16	0.44
1:A:86:ASN:OD1	1:A:234:ASN:HB2	2.17	0.44
1:A:97:TRP:HB3	1:A:446:MET:HG2	1.99	0.44
1:A:168:THR:HB	1:A:170:ASN:ND2	2.34	0.42
1:A:302:VAL:O	1:A:314:SER:HA	2.20	0.42
1:A:278:CYS:HB3	1:A:289:CYS:HB3	2.02	0.41
1:A:281:TYR:HB2	1:A:411:MET:HE2	2.02	0.41
1:A:98:HIS:HE1	1:A:419:ARG:HH21	1.66	0.41
1:A:240:VAL:HG22	1:A:254:ILE:HG13	2.04	0.40
1:A:196:GLY:HA3	1:A:201:ALA:HA	2.02	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	386/388 (100%)	362 (94%)	22 (6%)	2 (0%)	24	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	ILE
1	A	200	ASN

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	341/341 (100%)	315 (92%)	26 (8%)	12	16

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	88	THR
1	A	99	ILE
1	A	134	LEU
1	A	138	THR
1	A	141	ARG

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Mol	Chain	Res	Type
1	A	149	ILE
1	A	168	THR
1	A	170	ASN
1	A	204	VAL
1	A	214	GLU
1	A	224	ARG
1	A	237	CYS
1	A	247	THR
1	A	268	LEU
1	A	280	CYS
1	A	283	GLU
1	A	311	THR
1	A	358	VAL
1	A	364	ARG
1	A	384	THR
1	A	391	THR
1	A	400	ASN
1	A	401	THR
1	A	446	MET
1	A	464	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	98	HIS
1	A	150	HIS
1	A	170	ASN
1	A	221	ASN
1	A	233	HIS
1	A	294	ASN
1	A	325	ASN
1	A	346	ASN
1	A	381	ASN
1	A	392	GLN
1	A	395	GLN
1	A	400	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
2	NAG	B	1	2,1	14,14,15	0.98	0	17,19,21	2.68	5 (29%)
2	NAG	B	2	2	14,14,15	0.92	0	17,19,21	1.82	3 (17%)
2	BMA	B	3	2	11,11,12	0.96	0	15,15,17	1.50	4 (26%)
2	MAN	B	4	2	11,11,12	0.76	0	15,15,17	1.63	4 (26%)
2	MAN	B	5	2	11,11,12	1.15	1 (9%)	15,15,17	0.83	0
2	MAN	B	6	2	11,11,12	0.88	0	15,15,17	2.15	3 (20%)
2	MAN	B	7	2	11,11,12	0.64	0	15,15,17	1.02	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
2	NAG	B	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1
2	MAN	B	7	2	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	MAN	O5-C1	2.35	1.47	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C2-N2-C7	6.85	132.08	122.90
2	B	1	NAG	C1-C2-N2	5.81	119.59	110.43
2	B	6	MAN	C1-O5-C5	5.62	119.72	112.19
2	B	2	NAG	C8-C7-N2	5.17	124.68	116.12
2	B	1	NAG	O7-C7-N2	3.59	128.32	121.98
2	B	4	MAN	C1-O5-C5	3.22	116.50	112.19
2	B	6	MAN	O3-C3-C2	-3.22	103.48	110.05
2	B	1	NAG	C1-O5-C5	3.17	116.44	112.19
2	B	6	MAN	C3-C4-C5	-3.09	104.62	110.23
2	B	4	MAN	C2-C3-C4	-3.09	105.43	110.86
2	B	2	NAG	O7-C7-N2	-3.01	116.66	121.98
2	B	3	BMA	C6-C5-C4	2.83	119.96	113.02
2	B	3	BMA	O2-C2-C1	2.68	115.36	109.22
2	B	4	MAN	O3-C3-C2	2.61	115.39	110.05
2	B	1	NAG	C8-C7-N2	-2.53	111.92	116.12
2	B	3	BMA	O4-C4-C3	-2.45	104.61	110.38
2	B	4	MAN	O2-C2-C1	-2.32	103.92	109.22
2	B	2	NAG	C4-C3-C2	-2.26	107.71	111.02
2	B	3	BMA	O3-C3-C2	-2.25	105.47	110.05

There are no chirality outliers.

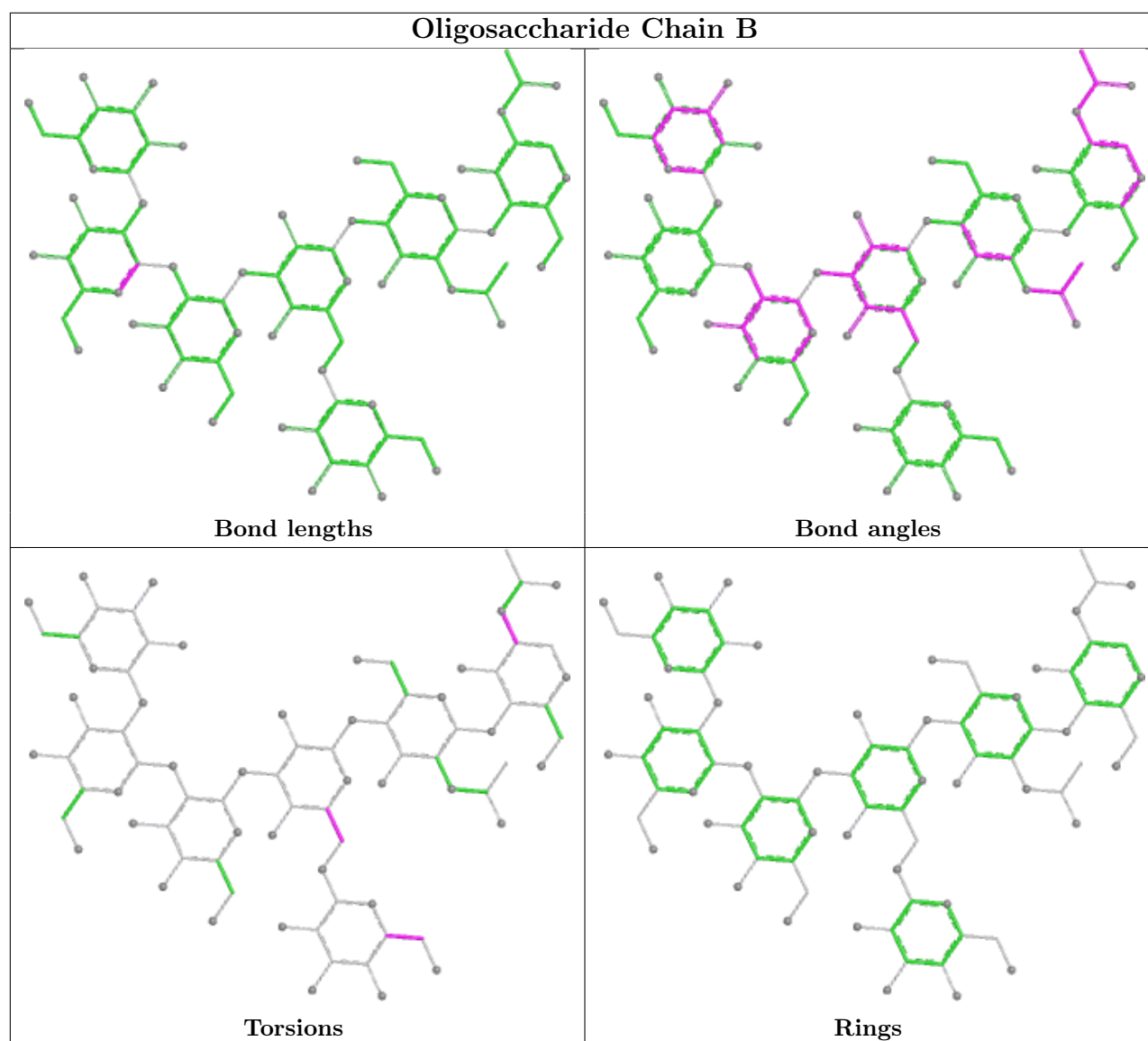
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C1-C2-N2-C7
2	B	3	BMA	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	7	MAN	O5-C5-C6-O6
2	B	7	MAN	C4-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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
3	NAG	A	476(A)	1	14,14,15	1.14	1 (7%)	17,19,21	1.49	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	477(A)	1	14,14,15	0.93	0	17,19,21	1.78	5 (29%)

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
3	NAG	A	476(A)	1	-	2/6/23/26	0/1/1/1
3	NAG	A	477(A)	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	476(A)	NAG	C4-C5	2.63	1.58	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	477(A)	NAG	C1-C2-N2	-3.49	104.94	110.43
3	A	477(A)	NAG	O3-C3-C2	2.79	115.19	109.40
3	A	477(A)	NAG	C4-C3-C2	-2.54	107.30	111.02
3	A	477(A)	NAG	C2-N2-C7	2.50	126.25	122.90
3	A	476(A)	NAG	O3-C3-C2	2.47	114.52	109.40
3	A	476(A)	NAG	C3-C4-C5	-2.37	105.94	110.23
3	A	476(A)	NAG	O4-C4-C5	2.36	115.13	109.32
3	A	476(A)	NAG	C6-C5-C4	2.26	118.58	113.02
3	A	476(A)	NAG	O4-C4-C3	-2.03	105.58	110.38
3	A	477(A)	NAG	C1-O5-C5	2.03	114.90	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	476(A)	NAG	O5-C5-C6-O6
3	A	476(A)	NAG	C4-C5-C6-O6

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	388/388 (100%)	-0.75	2 (0%) 87 87	3, 11, 23, 41	10 (2%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	GLU	3.7
1	A	344	ASN	2.7

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

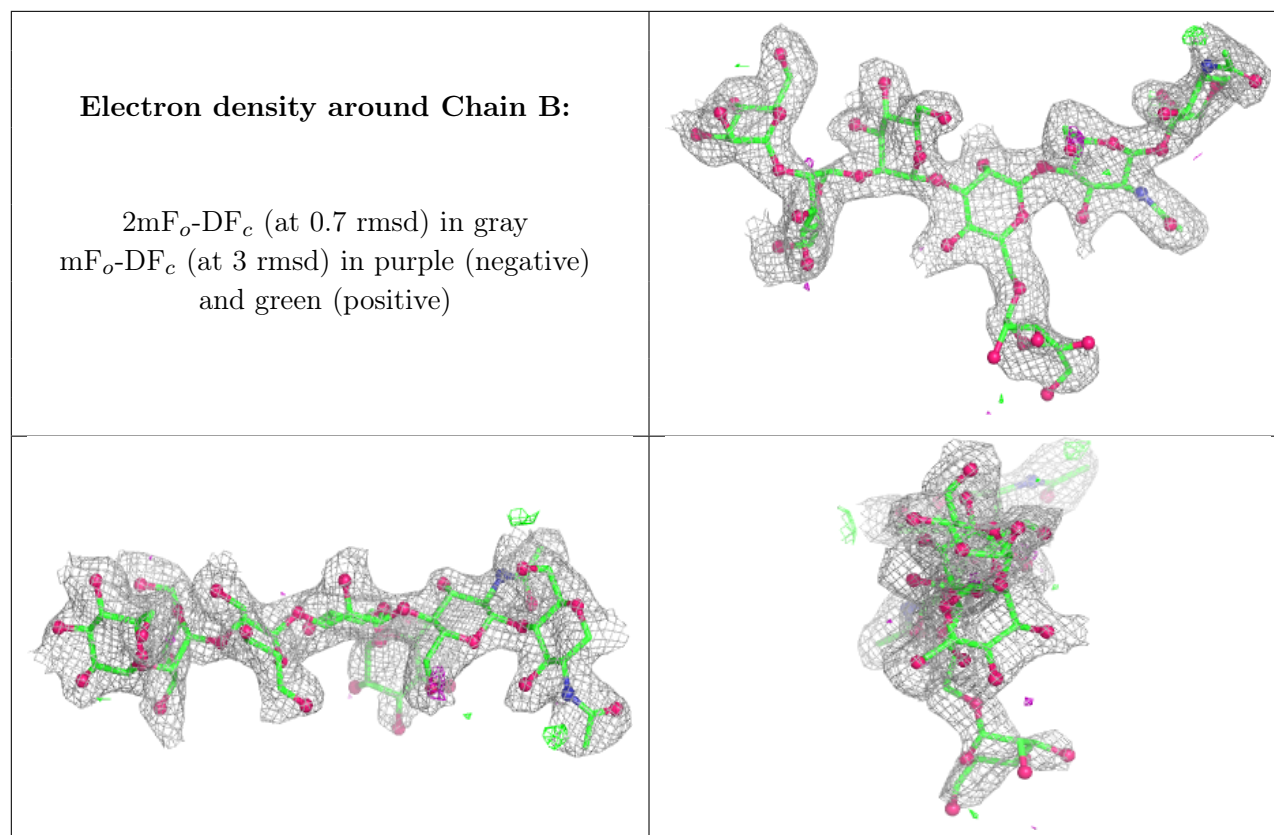
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
2	MAN	B	7	11/12	0.73	0.14	37,40,46,48	0
2	NAG	B	2	14/15	0.86	0.08	16,18,23,23	0
2	MAN	B	4	11/12	0.87	0.06	20,21,24,26	0
2	BMA	B	3	11/12	0.87	0.09	18,22,27,31	0
2	MAN	B	5	11/12	0.91	0.08	19,21,23,24	0
2	MAN	B	6	11/12	0.92	0.06	25,26,29,30	0
2	NAG	B	1	14/15	0.94	0.06	17,18,23,26	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($\text{\AA}^2$)	Q<0.9
3	NAG	A	476(A)	14/15	0.76	0.10	36,41,45,45	0
3	NAG	A	477(A)	14/15	0.85	0.11	29,34,36,36	0
4	CA	A	18	1/1	0.86	0.23	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.