WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:10 am GMT

PDB ID	:	1F8D
Title	:	Native Influenza Neuraminidase in Complex with 9-amino-2-deoxy-2,3-dehydro-N-neuraminic Acid
Authors	:	Smith, B.J.; Colman, P.M.; Von Itzstein, M.; Danylec, B.; Varghese, J.N.
Deposited on	:	2000-06-30
Resolution	:	1.40 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 1.40 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.
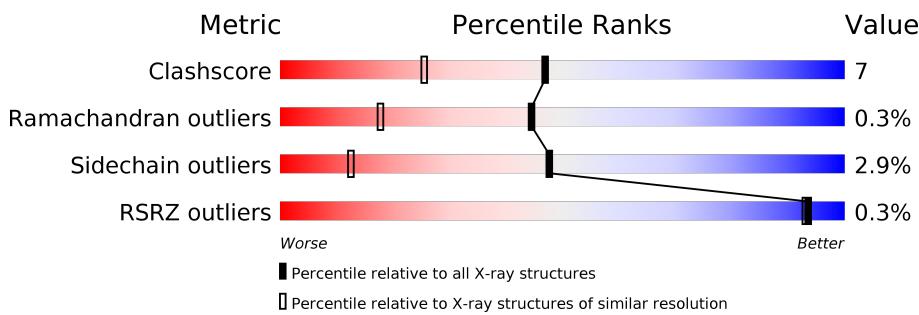
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1411 (1.40-1.40)
Ramachandran outliers	110173	1373 (1.40-1.40)
Sidechain outliers	110143	1372 (1.40-1.40)
RSRZ outliers	101464	1315 (1.40-1.40)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	388	88% 12% •
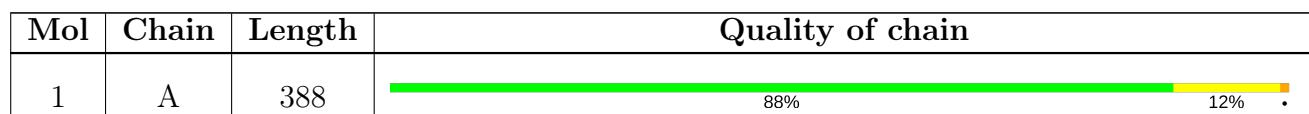
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	A	471	X	-	-	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 3579 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 3069	C 1915	N 538	O 593	S 23	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	376	MET	ILE	CONFLICT	GB 324880
A	386	ASP	GLU	CONFLICT	GB 324880
A	387	LYS	ARG	CONFLICT	GB 324880

- Molecule 2 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	7	Total 83	C 46	N 2	O 35	0	0

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
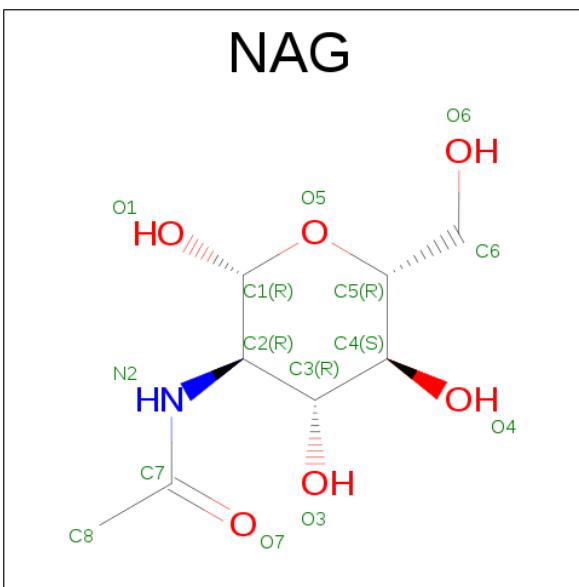
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Ca 2	0	0

- Molecule 5 is 9-AMINO-2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID (three-letter code: 9AM) (formula: $C_{11}H_{18}N_2O_7$).
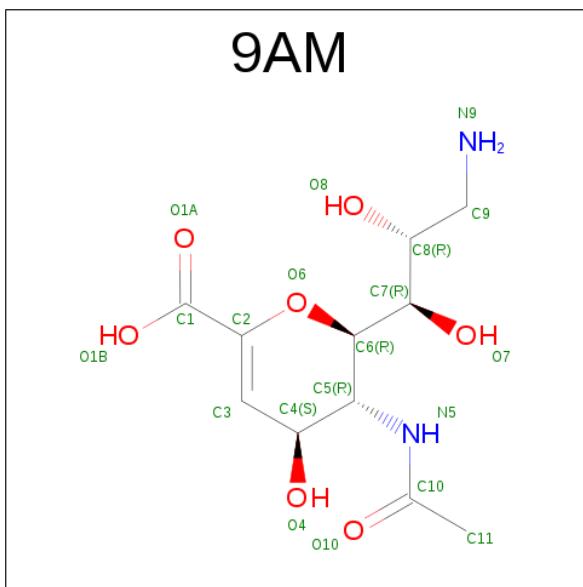
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	20	11	2	7	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	363	363	363	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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
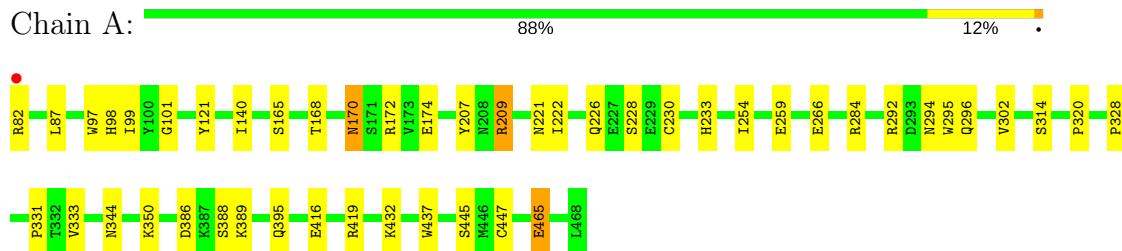
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, α, β, γ	180.74Å 180.74Å 180.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.40 48.30 – 1.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.40) 74.5 (48.30-1.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 1.40Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.201 , 0.231 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	14.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.52, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3579	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \|L\| >$, $< L^2 >$ 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: 9AM, CA, NAG, MAN

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	0.52	0/3156	0.78	1/4298 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	1	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	226	GLN	N-CA-C	5.20	125.05	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	471	MAN	C1

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3069	0	2894	41	0
2	A	83	0	70	0	0
3	A	42	0	39	3	0
4	A	2	0	0	0	0
5	A	20	0	17	0	0
6	A	363	0	0	4	0
All	All	3579	0	3020	43	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 7.

All (43) 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:172:ARG:HD3	1:A:209:ARG:NH1	1.68	1.07
1:A:168:THR:H	1:A:170:ASN:HD21	1.11	0.92
1:A:87:LEU:H	1:A:233:HIS:HD2	1.14	0.92
1:A:172:ARG:HD3	1:A:209:ARG:HH12	1.42	0.82
1:A:87:LEU:H	1:A:233:HIS:CD2	2.01	0.77
1:A:168:THR:H	1:A:170:ASN:ND2	1.86	0.72
1:A:97:TRP:H	1:A:395:GLN:HE22	1.38	0.71
1:A:172:ARG:CD	1:A:209:ARG:NH1	2.54	0.66
1:A:284:ARG:HH21	1:A:284:ARG:HG2	1.59	0.66
1:A:98:HIS:HE1	1:A:419:ARG:HH21	1.41	0.64
1:A:98:HIS:CE1	1:A:419:ARG:HH21	2.16	0.63
1:A:292:ARG:HE	1:A:294:ASN:HD22	1.46	0.63
1:A:465:GLU:CD	1:A:465:GLU:H	2.03	0.61
1:A:170:ASN:HB3	6:A:1438:HOH:O	2.05	0.57
1:A:320:PRO:HG2	1:A:389:LYS:HE2	1.87	0.56
1:A:292:ARG:HH11	1:A:294:ASN:ND2	2.05	0.55
1:A:174:GLU:OE2	1:A:209:ARG:NH1	2.42	0.53
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.92	0.51
1:A:320:PRO:HD2	1:A:388:SER:O	2.10	0.51
1:A:121:TYR:CG	1:A:228:SER:HA	2.47	0.50
1:A:98:HIS:HD2	1:A:99:ILE:O	1.95	0.49
1:A:168:THR:N	1:A:170:ASN:HD21	1.94	0.48
1:A:328:PRO:HD3	1:A:344:ASN:HD22	1.79	0.47
1:A:320:PRO:O	1:A:331:PRO:HD2	2.14	0.47
3:A:1086:NAG:O4	3:A:1087:NAG:N2	2.47	0.47
1:A:432:LYS:HD3	1:A:432:LYS:HA	1.73	0.47
1:A:344:ASN:HB3	6:A:1348:HOH:O	2.15	0.46
1:A:172:ARG:CD	1:A:209:ARG:HH12	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1086:NAG:O4	3:A:1087:NAG:C2	2.63	0.45
1:A:292:ARG:HH11	1:A:294:ASN:HD21	1.65	0.44
1:A:98:HIS:CE1	1:A:447:CYS:HB2	2.52	0.44
1:A:333:VAL:HA	1:A:386:ASP:O	2.18	0.43
1:A:295:TRP:CG	1:A:296:GLN:HG3	2.53	0.43
1:A:320:PRO:CG	1:A:389:LYS:HE2	2.48	0.43
1:A:170:ASN:H	1:A:170:ASN:HD22	1.67	0.42
1:A:284:ARG:HG2	1:A:284:ARG:NH2	2.32	0.42
1:A:207:TYR:CZ	1:A:259:GLU:HA	2.56	0.41
1:A:432:LYS:HE3	6:A:1418:HOH:O	2.19	0.41
1:A:140:ILE:HD11	6:A:1484:HOH:O	2.20	0.41
1:A:437:TRP:CD1	3:A:1146:NAG:H82	2.55	0.41
1:A:168:THR:OG1	1:A:170:ASN:ND2	2.54	0.41
1:A:101:GLY:N	1:A:445[B]:SER:OG	2.54	0.40
1:A:302:VAL:O	1:A:314:SER:HA	2.20	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	387/388 (100%)	369 (95%)	17 (4%)	1 (0%)	44	18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	ILE

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	342/341 (100%)	332 (97%)	10 (3%)	48	12

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	165	SER
1	A	170	ASN
1	A	209	ARG
1	A	221	ASN
1	A	230	CYS
1	A	254	ILE
1	A	266	GLU
1	A	416	GLU
1	A	465	GLU

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

Mol	Chain	Res	Type
1	A	95	ASN
1	A	98	HIS
1	A	144	HIS
1	A	170	ASN
1	A	221	ASN
1	A	233	HIS
1	A	294	ASN
1	A	344	ASN
1	A	346	ASN
1	A	392	GLN
1	A	395	GLN
1	A	400	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

7 carbohydrates 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	A	469	1,2	14,14,15	1.15	1 (7%)	15,19,21	1.92	5 (33%)
2	NAG	A	470	2	14,14,15	1.63	1 (7%)	15,19,21	1.55	3 (20%)
2	MAN	A	471	2	11,11,12	0.88	1 (9%)	13,15,17	1.31	2 (15%)
2	MAN	A	472	2	11,11,12	1.95	2 (18%)	13,15,17	2.28	3 (23%)
2	MAN	A	473	2	11,11,12	1.23	1 (9%)	13,15,17	1.26	1 (7%)
2	MAN	A	474	2	11,11,12	1.61	2 (18%)	13,15,17	1.01	1 (7%)
2	MAN	A	475	2	11,11,12	1.19	2 (18%)	13,15,17	1.61	2 (15%)

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	A	469	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	470	2	-	0/6/23/26	0/1/1/1
2	MAN	A	471	2	1/1/4/5	0/2/19/22	0/1/1/1
2	MAN	A	472	2	-	0/2/19/22	0/1/1/1
2	MAN	A	473	2	-	0/2/19/22	0/1/1/1
2	MAN	A	474	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	A	475	2	-	0/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	472	MAN	C4-C3	2.00	1.57	1.52
2	A	474	MAN	C4-C3	2.10	1.57	1.52
2	A	471	MAN	C2-C3	2.34	1.55	1.52
2	A	475	MAN	O5-C1	2.36	1.47	1.43
2	A	473	MAN	C4-C3	2.59	1.59	1.52
2	A	475	MAN	C2-C3	2.62	1.56	1.52
2	A	469	NAG	C1-C2	3.00	1.56	1.52
2	A	474	MAN	C2-C3	3.29	1.57	1.52
2	A	470	NAG	C1-C2	5.21	1.59	1.52
2	A	472	MAN	C2-C3	5.47	1.59	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	469	NAG	C8-C7-N2	-3.86	109.14	116.11
2	A	469	NAG	C1-C2-N2	-3.45	104.59	110.49
2	A	472	MAN	O2-C2-C1	-3.29	102.48	109.18
2	A	470	NAG	C2-N2-C7	-2.47	119.35	122.94
2	A	469	NAG	O5-C1-C2	-2.39	108.15	111.47
2	A	470	NAG	C4-C3-C2	-2.25	107.73	111.02
2	A	471	MAN	C6-C5-C4	-2.11	108.06	113.00
2	A	472	MAN	O6-C6-C5	-2.05	104.45	111.34
2	A	471	MAN	C1-O5-C5	2.16	115.14	112.17
2	A	470	NAG	C1-C2-N2	2.34	114.48	110.49
2	A	469	NAG	C1-O5-C5	2.60	115.75	112.17
2	A	469	NAG	O7-C7-C8	2.65	126.89	122.06
2	A	474	MAN	C1-O5-C5	2.78	116.00	112.17
2	A	475	MAN	O6-C6-C5	2.97	121.35	111.34
2	A	473	MAN	C1-O5-C5	3.44	116.91	112.17
2	A	475	MAN	C1-O5-C5	4.33	118.13	112.17
2	A	472	MAN	C1-O5-C5	5.90	120.29	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	471	MAN	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	9AM	A	0	-	17,20,20	1.91	5 (29%)	17,28,28	1.46	2 (11%)
3	NAG	A	1086	1,3	14,14,15	0.75	0	15,19,21	1.82	5 (33%)
3	NAG	A	1087	3	14,14,15	2.30	4 (28%)	15,19,21	3.50	8 (53%)
3	NAG	A	1146	1	14,14,15	1.18	1 (7%)	15,19,21	2.53	5 (33%)

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	9AM	A	0	-	-	0/14/34/34	0/1/1/1
3	NAG	A	1086	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1087	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1146	1	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	0	9AM	O8-C8	-2.44	1.38	1.43
5	A	0	9AM	O4-C4	-2.33	1.38	1.43
3	A	1146	NAG	C4-C5	2.65	1.58	1.53
3	A	1087	NAG	C3-C2	2.87	1.58	1.52
3	A	1087	NAG	O5-C5	3.02	1.49	1.43
5	A	0	9AM	C3-C2	3.13	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	0	9AM	C4-C3	3.88	1.55	1.50
5	A	0	9AM	C7-C6	4.11	1.58	1.52
3	A	1087	NAG	C4-C3	4.76	1.64	1.52
3	A	1087	NAG	C4-C5	5.38	1.64	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1087	NAG	O5-C1-C2	-8.15	100.13	111.47
3	A	1146	NAG	C2-N2-C7	-7.02	112.70	122.94
3	A	1087	NAG	C4-C3-C2	-4.87	103.88	111.02
5	A	0	9AM	O6-C2-C3	-4.18	118.46	124.31
3	A	1086	NAG	O6-C6-C5	-3.93	98.13	111.34
3	A	1146	NAG	C8-C7-N2	-3.69	109.44	116.11
3	A	1086	NAG	C6-C5-C4	-2.92	106.16	113.00
3	A	1087	NAG	C8-C7-N2	-2.80	111.05	116.11
5	A	0	9AM	C8-C7-C6	-2.64	107.91	113.04
3	A	1086	NAG	O5-C1-C2	-2.33	108.23	111.47
3	A	1146	NAG	C3-C4-C5	-2.15	106.43	110.22
3	A	1086	NAG	C3-C4-C5	2.08	113.89	110.22
3	A	1087	NAG	O3-C3-C4	2.22	115.18	110.36
3	A	1087	NAG	C1-O5-C5	2.26	115.28	112.17
3	A	1087	NAG	O4-C4-C3	2.36	115.50	110.36
3	A	1146	NAG	C1-O5-C5	2.39	115.45	112.17
3	A	1086	NAG	C1-O5-C5	2.85	116.09	112.17
3	A	1146	NAG	O7-C7-C8	3.13	127.75	122.06
3	A	1087	NAG	C1-C2-N2	3.52	116.50	110.49
3	A	1087	NAG	C2-N2-C7	7.05	133.23	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1086	NAG	2	0
3	A	1087	NAG	2	0
3	A	1146	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	388/388 (100%)	-0.56	1 (0%)	93	93	10, 13, 21, 50	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	ARG	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å²)	Q<0.9
2	MAN	A	474	11/12	0.97	0.07	0.22	13,14,16,16	0
2	MAN	A	471	11/12	0.96	0.06	0.02	15,16,19,20	0
2	MAN	A	473	11/12	0.96	0.06	-0.10	16,17,18,19	0
2	NAG	A	469	14/15	0.95	0.07	-0.14	13,16,22,22	0
2	MAN	A	472	11/12	0.96	0.08	-	17,18,22,27	0
2	MAN	A	475	11/12	0.89	0.09	-	23,25,28,30	0
2	NAG	A	470	14/15	0.95	0.07	-	14,16,19,23	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
5	9AM	A	0	20/20	0.97	0.05	-0.64	13,14,15,16	0
4	CA	A	999	1/1	1.00	0.02	-2.67	14,14,14,14	0
3	NAG	A	1086	14/15	0.87	0.15	-	21,24,28,30	0
3	NAG	A	1146	14/15	0.83	0.17	-	31,35,38,39	0
4	CA	A	998	1/1	0.76	0.18	-	30,30,30,30	1
3	NAG	A	1087	14/15	0.64	0.30	-	58,64,67,67	0

6.5 Other polymers ⓘ

There are no such residues in this entry.