



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2018 – 11:49 PM EDT

PDB ID : 6HG0
Title : Influenza A Virus N9 Neuraminidase complex with NANA (Tern/Australia).
Authors : Salinger, M.T.; Hobbs, J.R.; Murray, J.W.; Laver, W.G.; Kuhn, P.; Garman, E.F.
Deposited on : 2018-08-22
Resolution : 1.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031172
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

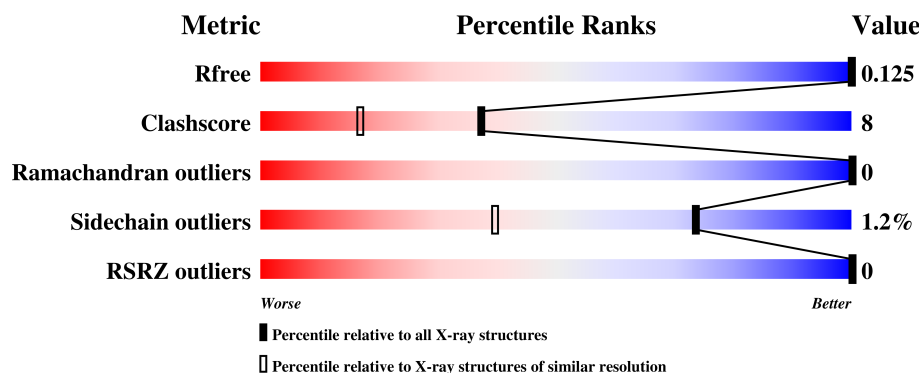
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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}	111664	1286 (1.32-1.28)
Clashscore	122126	1332 (1.32-1.28)
Ramachandran outliers	120053	1282 (1.32-1.28)
Sidechain outliers	120020	1282 (1.32-1.28)
RSRZ outliers	108989	1250 (1.32-1.28)

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 $\leq 5\%$. 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	 89% 9% ..

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
6	GOL	A	518	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	519	-	-	X	-
7	PO4	A	521	-	-	X	-

2 Entry composition [i](#)

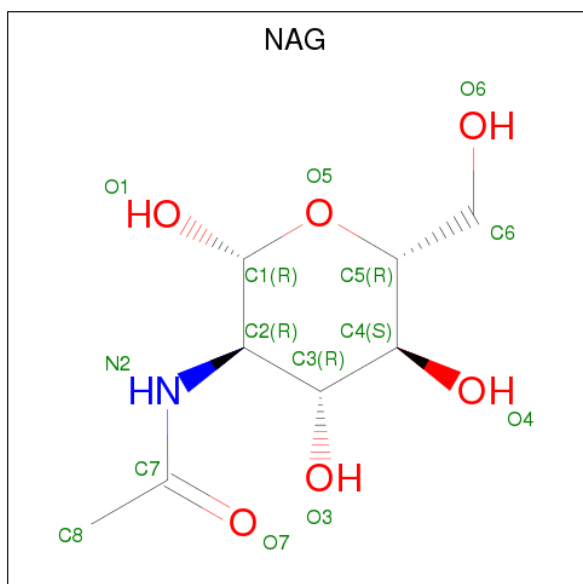
There are 10 unique types of molecules in this entry. The entry contains 4347 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	36	0
			3366	2085	599	652	30			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



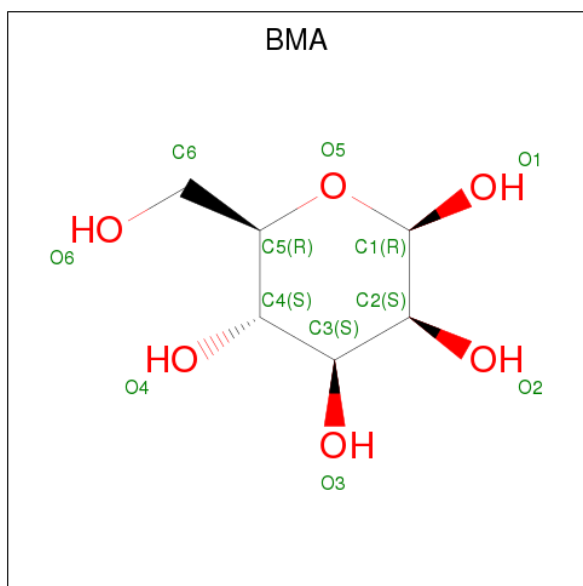
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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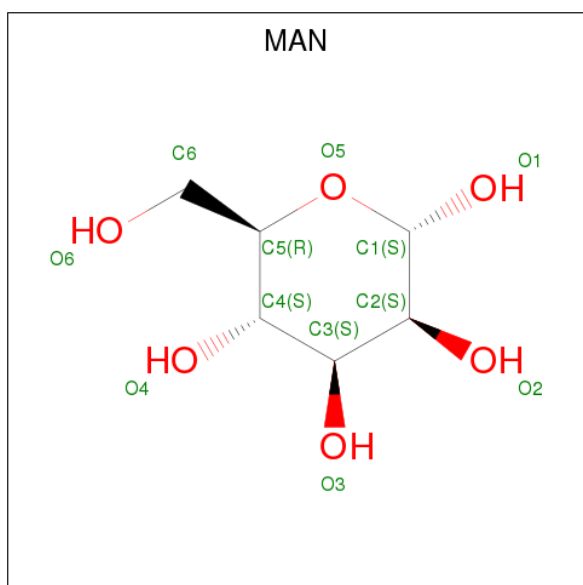
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			11	6	5			

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

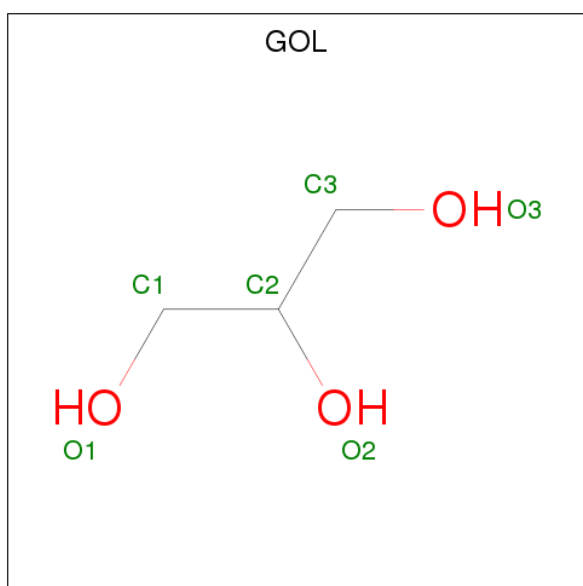


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



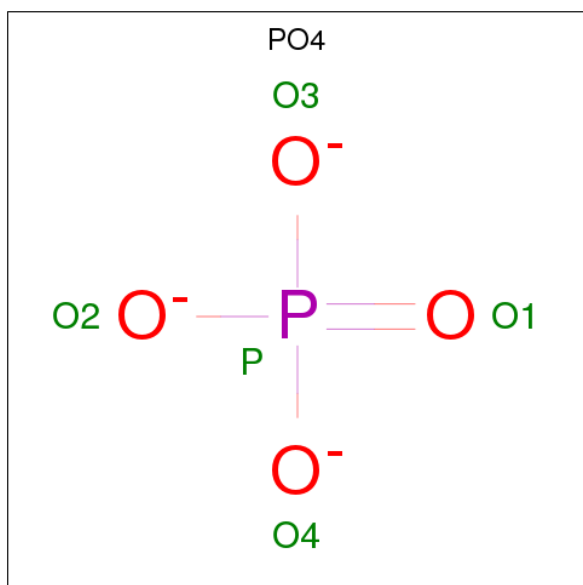
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 12 6 6	0	1
6	A	1	Total C O 6 3 3	0	0

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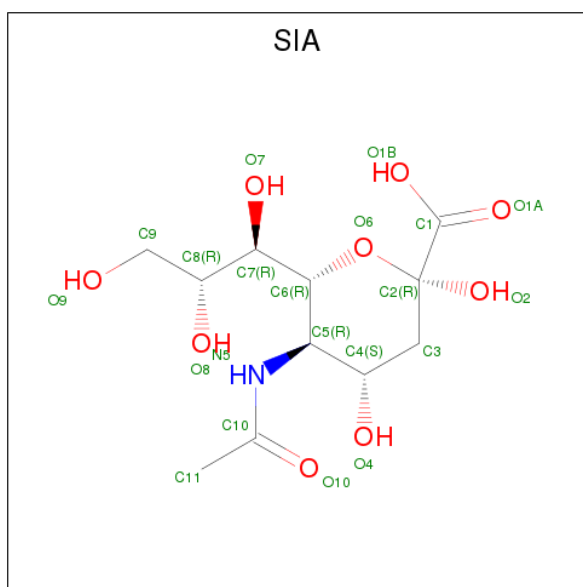
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is O-SIALIC ACID (three-letter code: SIA) (formula: C₁₁H₁₉NO₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			21	11	1	9		
8	A	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	K	0	0
			1	1		

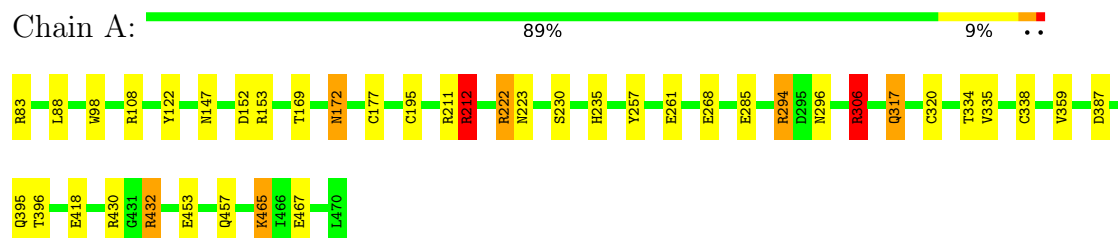
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	727	Total	O	0	2
			729	729		

3 Residue-property plots [i](#)

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

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	181.20Å 181.20Å 181.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 1.30 48.43 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.47-1.30) 99.7 (48.43-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.51 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.091 , 0.120 0.098 , 0.125	Depositor DCC
R_{free} test set	6197 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4347	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 2.90% 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: GOL, BMA, NAG, PO4, SIA, K, CA, 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	0.92	7/3449 (0.2%)	0.98	6/4691 (0.1%)

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	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	GLU	CD-OE1	16.73	1.44	1.25
1	A	261	GLU	CD-OE2	-10.28	1.14	1.25
1	A	285	GLU	CD-OE2	7.82	1.34	1.25
1	A	453	GLU	CD-OE1	-7.42	1.17	1.25
1	A	268[A]	GLU	CD-OE1	7.15	1.33	1.25
1	A	268[B]	GLU	CD-OE1	7.15	1.33	1.25
1	A	261	GLU	CD-OE1	-7.01	1.18	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	ARG	NE-CZ-NH1	-7.42	116.59	120.30
1	A	430	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	212[A]	ARG	NH1-CZ-NH2	-5.35	113.51	119.40
1	A	212[B]	ARG	NH1-CZ-NH2	-5.35	113.51	119.40
1	A	294	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	257	TYR	CB-CG-CD1	5.08	124.05	121.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	ARG	Sidechain
1	A	212[A]	ARG	Sidechain
1	A	222[A]	ARG	Sidechain
1	A	306[A]	ARG	Sidechain
1	A	317[B]	GLN	Mainchain
1	A	432	ARG	Sidechain
1	A	83	ARG	Sidechain

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	3366	0	3166	50	0
2	A	84	0	73	5	0
3	A	11	0	8	0	0
4	A	77	0	65	0	0
5	A	2	0	0	0	0
6	A	30	0	37	16	0
7	A	5	0	0	4	0
8	A	42	0	36	0	0
9	A	1	0	0	0	0
10	A	729	0	0	14	0
All	All	4347	0	3385	59	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 8.

All (59) 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)
6:A:519:GOL:O3	7:A:521:PO4:O2	1.52	1.26
1:A:147:ASN:HD22	2:A:511:NAG:H83	1.00	1.09
1:A:396[B]:THR:HG22	1:A:457[B]:GLN:HE22	1.17	1.08
1:A:396[B]:THR:HG22	1:A:457[B]:GLN:NE2	1.73	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:HH12	6:A:518:GOL:H31	1.26	0.96
1:A:306[B]:ARG:HH21	1:A:317[B]:GLN:HE22	1.10	0.94
1:A:147:ASN:HD22	2:A:511:NAG:C8	1.82	0.93
1:A:147:ASN:ND2	2:A:511:NAG:H83	1.83	0.92
1:A:169:THR:H	1:A:172:ASN:HD21	1.18	0.91
1:A:88:LEU:H	1:A:235:HIS:HD2	1.20	0.89
1:A:465[A]:LYS:HB3	1:A:465[A]:LYS:HZ3	1.37	0.89
1:A:172:ASN:HB3	10:A:1126:HOH:O	1.74	0.86
1:A:320[B]:CYS:CB	1:A:338:CYS:SG	2.64	0.85
1:A:334[B]:THR:HG22	10:A:623:HOH:O	1.75	0.85
1:A:465[A]:LYS:HB3	1:A:465[A]:LYS:NZ	1.91	0.84
1:A:306[B]:ARG:NH2	1:A:317[B]:GLN:HE22	1.76	0.82
1:A:88:LEU:H	1:A:235:HIS:CD2	2.01	0.78
1:A:396[B]:THR:CG2	1:A:457[B]:GLN:NE2	2.46	0.77
1:A:320[B]:CYS:HB3	1:A:338:CYS:SG	2.26	0.75
6:A:519:GOL:H32	10:A:931:HOH:O	1.85	0.75
1:A:177:CYS:SG	1:A:195[B]:CYS:HB2	2.28	0.74
1:A:359[B]:VAL:CG1	10:A:759:HOH:O	2.36	0.73
1:A:359[B]:VAL:HG12	10:A:759:HOH:O	1.88	0.73
1:A:212[A]:ARG:NH2	10:A:601:HOH:O	2.21	0.73
2:A:511:NAG:H81	10:A:895:HOH:O	1.91	0.70
1:A:98:TRP:H	1:A:395:GLN:HE22	1.37	0.70
1:A:169:THR:H	1:A:172:ASN:ND2	1.92	0.68
1:A:108:ARG:HH12	6:A:518:GOL:C3	2.03	0.67
1:A:467[A]:GLU:HG3	10:A:892:HOH:O	1.95	0.67
1:A:396[B]:THR:HG23	10:A:742:HOH:O	1.95	0.65
1:A:465[A]:LYS:NZ	1:A:465[A]:LYS:CB	2.56	0.65
1:A:172:ASN:HB3	10:A:728:HOH:O	1.96	0.64
6:A:519:GOL:H2	7:A:521:PO4:P	2.39	0.62
1:A:222[A]:ARG:HD3	10:A:614:HOH:O	2.00	0.62
1:A:294:ARG:HE	1:A:296:ASN:HD22	1.49	0.59
1:A:320[B]:CYS:HB2	1:A:338:CYS:SG	2.39	0.58
1:A:152:ASP:H	6:A:519:GOL:C3	2.16	0.58
6:A:519:GOL:H2	7:A:521:PO4:O2	2.01	0.58
1:A:306[B]:ARG:HH21	1:A:317[B]:GLN:NE2	1.93	0.55
6:A:518:GOL:O3	6:A:518:GOL:O1	2.27	0.53
1:A:396[B]:THR:H	1:A:457[B]:GLN:HE22	1.57	0.51
6:A:518:GOL:H11	10:A:607:HOH:O	2.10	0.51
6:A:518:GOL:C1	10:A:607:HOH:O	2.59	0.50
1:A:153:ARG:HH22	6:A:519:GOL:C1	2.25	0.49
1:A:147:ASN:ND2	2:A:511:NAG:C8	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:NH1	6:A:518:GOL:H31	2.10	0.48
1:A:122:TYR:CG	1:A:230:SER:HA	2.49	0.47
1:A:294:ARG:HH11	1:A:296:ASN:ND2	2.13	0.47
1:A:465[A]:LYS:HZ2	1:A:465[A]:LYS:CB	2.27	0.47
1:A:152:ASP:H	6:A:519:GOL:H31	1.79	0.46
1:A:396[B]:THR:H	1:A:457[B]:GLN:NE2	2.13	0.45
1:A:222[A]:ARG:NH2	10:A:614:HOH:O	2.48	0.44
6:A:519:GOL:H2	7:A:521:PO4:O1	2.19	0.43
1:A:335[A]:VAL:HA	1:A:387:ASP:O	2.19	0.43
1:A:320[B]:CYS:HB3	1:A:338:CYS:HA	2.01	0.42
1:A:294:ARG:HH11	1:A:296:ASN:HD21	1.68	0.42
1:A:153:ARG:HH12	6:A:519:GOL:H12	1.85	0.41
1:A:396[B]:THR:CG2	1:A:457[B]:GLN:HE21	2.29	0.41
1:A:153:ARG:HH22	6:A:519:GOL:H12	1.85	0.41

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	424/388 (109%)	408 (96%)	16 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	379/341 (111%)	371 (98%)	8 (2%)	56 16

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	223[A]	ASN
1	A	223[B]	ASN
1	A	306[A]	ARG
1	A	306[B]	ARG
1	A	306[C]	ARG
1	A	465[A]	LYS
1	A	465[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	235	HIS
1	A	296	ASN
1	A	347	ASN
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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 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$
2	NAG	A	501	1,9,2	14,14,15	0.64	0	17,19,21	1.23	1 (5%)
2	NAG	A	502	9,3,2	14,14,15	0.99	1 (7%)	17,19,21	1.16	1 (5%)
3	BMA	A	503	2,4	11,11,12	0.60	0	15,15,17	0.66	0
4	MAN	A	504	3,4	11,11,12	0.93	1 (9%)	15,15,17	1.88	3 (20%)
4	MAN	A	505	4	11,11,12	1.11	1 (9%)	15,15,17	0.81	0
4	MAN	A	506	4	11,11,12	1.00	1 (9%)	15,15,17	1.10	1 (6%)
4	MAN	A	507	3,4	11,11,12	1.10	2 (18%)	15,15,17	1.12	1 (6%)
4	MAN	A	508	9,4	11,11,12	1.35	2 (18%)	15,15,17	1.16	1 (6%)
4	MAN	A	509	4	11,11,12	1.51	2 (18%)	15,15,17	2.79	3 (20%)
4	MAN	A	510	4	11,11,12	1.33	1 (9%)	15,15,17	1.76	4 (26%)
2	NAG	A	511	1,2	14,14,15	2.04	5 (35%)	17,19,21	2.37	9 (52%)
2	NAG	A	512	2	14,14,15	0.94	1 (7%)	17,19,21	2.12	5 (29%)
2	NAG	A	513	1,2	14,14,15	0.99	0	17,19,21	1.53	3 (17%)
2	NAG	A	514	2	14,14,15	1.52	3 (21%)	17,19,21	2.79	8 (47%)
6	GOL	A	517[A]	-	5,5,5	1.24	1 (20%)	5,5,5	1.35	1 (20%)
6	GOL	A	517[B]	-	5,5,5	0.59	0	5,5,5	0.52	0
6	GOL	A	518	-	5,5,5	1.14	0	5,5,5	1.93	2 (40%)
6	GOL	A	519	-	5,5,5	1.15	0	5,5,5	1.68	1 (20%)
6	GOL	A	520	-	5,5,5	0.53	0	5,5,5	0.99	0
7	PO4	A	521	-	4,4,4	1.27	1 (25%)	6,6,6	0.77	0
8	SIA	A	522	-	18,21,21	3.80	5 (27%)	19,31,31	1.33	2 (10%)
8	SIA	A	523	-	18,21,21	1.32	1 (5%)	19,31,31	1.24	1 (5%)

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	501	1,9,2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	9,3,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	A	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	504	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	505	4	-	0/2/19/22	0/1/1/1
4	MAN	A	506	4	-	0/2/19/22	0/1/1/1
4	MAN	A	507	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	508	9,4	-	0/2/19/22	0/1/1/1
4	MAN	A	509	4	-	0/2/19/22	0/1/1/1
4	MAN	A	510	4	-	0/2/19/22	0/1/1/1
2	NAG	A	511	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	512	2	-	0/6/23/26	0/1/1/1
2	NAG	A	513	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	514	2	-	0/6/23/26	0/1/1/1
6	GOL	A	517[A]	-	-	0/4/4/4	0/0/0/0
6	GOL	A	517[B]	-	-	0/4/4/4	0/0/0/0
6	GOL	A	518	-	-	0/4/4/4	0/0/0/0
6	GOL	A	519	-	-	0/4/4/4	0/0/0/0
6	GOL	A	520	-	-	0/4/4/4	0/0/0/0
7	PO4	A	521	-	-	0/0/0/0	0/0/0/0
8	SIA	A	522	-	-	0/14/38/38	0/1/1/1
8	SIA	A	523	-	-	0/14/38/38	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	522	SIA	O6-C2	-9.75	1.32	1.43
8	A	523	SIA	C4-C5	-4.02	1.49	1.53
8	A	522	SIA	C4-C5	-4.00	1.49	1.53
4	A	508	MAN	O5-C1	-2.77	1.39	1.43
2	A	511	NAG	C4-C3	-2.51	1.45	1.52
2	A	511	NAG	C1-C2	-2.44	1.49	1.52
4	A	504	MAN	C2-C3	-2.43	1.48	1.52
4	A	507	MAN	O5-C1	-2.38	1.39	1.43
4	A	507	MAN	O5-C5	-2.36	1.38	1.43
4	A	505	MAN	O5-C1	-2.14	1.40	1.43
2	A	511	NAG	O5-C1	-2.08	1.40	1.43
7	A	521	PO4	P-O3	-2.07	1.47	1.54
8	A	522	SIA	O6-C6	2.08	1.47	1.44
4	A	508	MAN	O6-C6	2.12	1.51	1.42
2	A	502	NAG	C1-C2	2.25	1.55	1.52
2	A	511	NAG	O4-C4	2.42	1.48	1.43
4	A	506	MAN	C2-C3	2.45	1.56	1.52
2	A	514	NAG	O4-C4	2.46	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	517[A]	GOL	O2-C2	2.54	1.50	1.43
4	A	509	MAN	C4-C3	2.54	1.58	1.52
2	A	514	NAG	O5-C5	2.63	1.48	1.43
2	A	512	NAG	C8-C7	2.66	1.56	1.50
8	A	522	SIA	C6-C5	2.78	1.57	1.53
4	A	509	MAN	O6-C6	3.18	1.55	1.42
2	A	514	NAG	O7-C7	3.30	1.31	1.23
4	A	510	MAN	O6-C6	3.39	1.56	1.42
2	A	511	NAG	C8-C7	5.08	1.61	1.50
8	A	522	SIA	O2-C2	11.40	1.52	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	514	NAG	O5-C5-C6	-6.02	97.62	107.15
4	A	509	MAN	C1-C2-C3	-5.97	102.11	109.66
4	A	504	MAN	O2-C2-C1	-5.06	98.97	109.17
2	A	512	NAG	C2-N2-C7	-4.42	116.50	122.94
8	A	522	SIA	O2-C2-O6	-4.38	99.69	109.69
2	A	514	NAG	O6-C6-C5	-4.38	96.01	111.29
2	A	512	NAG	O3-C3-C2	-4.16	100.48	109.39
2	A	512	NAG	O5-C5-C6	-4.09	100.68	107.15
2	A	502	NAG	O5-C1-C2	-3.94	106.08	111.52
2	A	513	NAG	O5-C1-C2	-3.82	106.25	111.52
2	A	511	NAG	O7-C7-N2	-3.82	114.74	121.94
2	A	514	NAG	C3-C4-C5	-3.77	103.50	110.24
6	A	519	GOL	O3-C3-C2	-3.62	92.56	110.11
2	A	514	NAG	C1-O5-C5	-3.47	107.41	112.19
4	A	509	MAN	O5-C5-C4	-3.34	102.69	110.83
4	A	510	MAN	C1-C2-C3	-3.06	105.79	109.66
2	A	511	NAG	C2-N2-C7	-2.98	118.60	122.94
2	A	511	NAG	O3-C3-C4	-2.89	103.60	110.34
2	A	511	NAG	O5-C5-C6	-2.83	102.66	107.15
6	A	518	GOL	O3-C3-C2	-2.79	96.58	110.11
6	A	518	GOL	O2-C2-C1	-2.75	96.42	109.00
2	A	514	NAG	C8-C7-N2	-2.71	111.35	116.10
8	A	523	SIA	O6-C6-C7	-2.65	103.21	107.33
2	A	513	NAG	O4-C4-C5	-2.64	102.69	109.31
2	A	512	NAG	O5-C1-C2	-2.54	108.01	111.52
2	A	511	NAG	O6-C6-C5	-2.46	102.70	111.29
6	A	517[A]	GOL	O2-C2-C3	-2.44	97.85	109.00
2	A	511	NAG	O4-C4-C3	-2.40	104.73	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	512	NAG	O7-C7-C8	-2.35	117.83	122.07
8	A	522	SIA	C6-C5-N5	-2.11	107.29	110.94
2	A	501	NAG	O5-C5-C4	-2.03	105.89	110.83
4	A	510	MAN	O3-C3-C2	2.01	113.77	110.04
2	A	513	NAG	C6-C5-C4	2.14	118.04	112.99
2	A	511	NAG	C3-C4-C5	2.16	114.10	110.24
2	A	514	NAG	O7-C7-N2	2.34	126.36	121.94
4	A	504	MAN	C1-O5-C5	2.51	115.64	112.19
4	A	510	MAN	C1-O5-C5	2.68	115.87	112.19
4	A	507	MAN	C1-O5-C5	2.73	115.94	112.19
4	A	508	MAN	C1-O5-C5	2.77	116.00	112.19
4	A	506	MAN	C1-O5-C5	2.95	116.24	112.19
4	A	504	MAN	O2-C2-C3	2.98	116.00	110.19
2	A	511	NAG	O7-C7-C8	3.19	127.83	122.07
4	A	510	MAN	O2-C2-C3	3.22	116.46	110.19
2	A	514	NAG	O4-C4-C5	3.43	117.89	109.31
2	A	514	NAG	C6-C5-C4	3.88	122.17	112.99
2	A	511	NAG	C6-C5-C4	4.78	124.28	112.99
4	A	509	MAN	C1-O5-C5	7.38	122.34	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	511	NAG	5	0
6	A	518	GOL	6	0
6	A	519	GOL	10	0
7	A	521	PO4	4	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 [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	0 100 100	7, 10, 17, 43	0

There are no RSRZ outliers to report.

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](#)

There are no carbohydrates in this entry.

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	GOL	A	518	6/6	0.68	0.18	47,53,71,72	0
4	MAN	A	510	11/12	0.71	0.18	63,79,88,122	0
4	MAN	A	509	11/12	0.88	0.16	37,44,51,87	0
2	NAG	A	512	14/15	0.90	0.23	43,60,81,102	0
2	NAG	A	511	14/15	0.93	0.12	20,31,45,46	0
2	NAG	A	514	14/15	0.93	0.24	29,42,54,56	0
6	GOL	A	517[A]	6/6	0.94	0.10	15,23,28,32	0
6	GOL	A	519	6/6	0.94	0.18	12,25,42,53	6
6	GOL	A	517[B]	6/6	0.94	0.10	1,1,1,2	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	A	508	11/12	0.95	0.09	24,28,41,43	0
5	CA	A	515	1/1	0.95	0.06	29,29,29,29	1
7	PO4	A	521	5/5	0.96	0.12	19,20,28,29	5
8	SIA	A	522	21/21	0.97	0.05	9,11,12,20	0
2	NAG	A	513	14/15	0.97	0.11	12,19,28,30	0
8	SIA	A	523	21/21	0.97	0.12	13,16,19,23	0
4	MAN	A	507	11/12	0.97	0.07	15,18,22,29	0
6	GOL	A	520	6/6	0.97	0.12	22,29,39,43	0
4	MAN	A	505	11/12	0.98	0.05	12,13,17,18	0
4	MAN	A	504	11/12	0.98	0.06	11,13,20,28	0
2	NAG	A	501	14/15	0.98	0.06	9,11,22,23	0
4	MAN	A	506	11/12	0.98	0.05	11,11,13,14	0
2	NAG	A	502	14/15	0.98	0.05	9,11,15,21	0
3	BMA	A	503	11/12	0.98	0.05	10,11,13,16	0
5	CA	A	516	1/1	1.00	0.02	11,11,11,11	0
9	K	A	524	1/1	1.00	0.03	23,23,23,23	1

6.5 Other polymers

There are no such residues in this entry.