



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:24 AM GMT

PDB ID : 3W09
Title : Influenza virus neuraminidase subtype N9 (TERN) complexed with 2,3-dif
guanidino-neu5ac2en inhibitor
Authors : Streltsov, V.A.
Deposited on : 2012-10-25
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

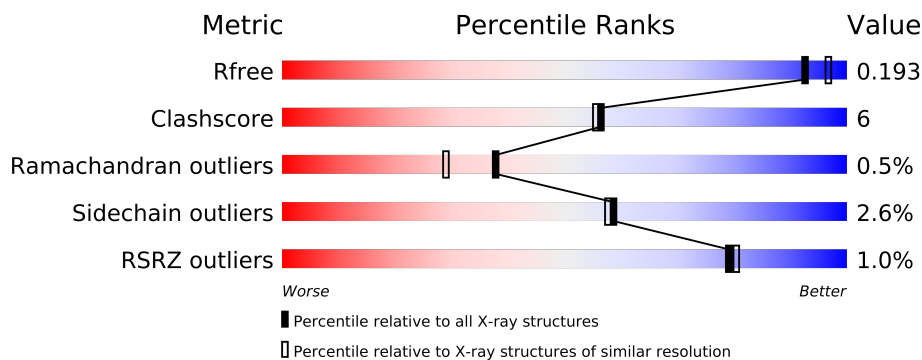
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	388	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3719 atoms, of which 0 are hydrogen and 0 are deuterium.

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	14	0
			3098	1925	545	603	25			

- Molecule 2 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



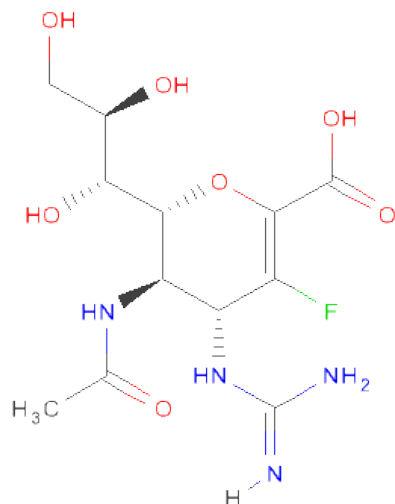
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 6 is (2R,3R,4R)-3-ACETAMIDO-4-CARBAMIMIDAMIDO-5-FLUORANYL-2-[(1R,2R)-1,2,3-TRIS(OXIDANYL)PROPYL]-3,4-DIHYDRO-2H-PYRAN-6-CARBOXYLIC ACID (three-letter code: ZGE) (formula: C₁₂H₁₉FN₄O₇).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	1
			48	24	2	8	14		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is water.

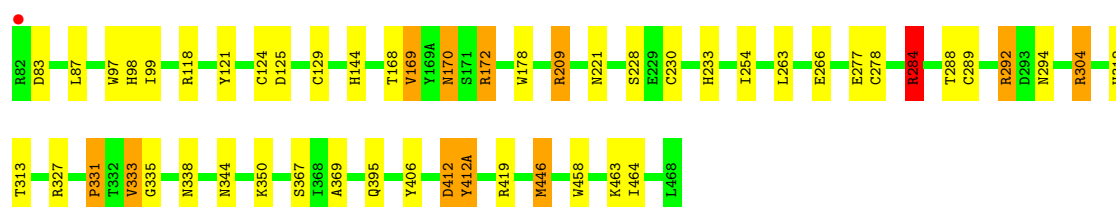
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	383	Total 383	O 383	0	0

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 errors 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

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	180.84Å 180.84Å 180.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.66 – 2.00 40.44 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.66-2.00) 99.6 (40.44-2.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.144 , 0.189 0.146 , 0.193	Depositor DCC
R_{free} test set	1728 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 61.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 34165 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3719	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, CA, ZGE, 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	1.09	5/3254 (0.2%)	1.02	15/4430 (0.3%)

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	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	TRP	CB-CG	5.67	1.60	1.50
1	A	169	VAL	C-N	5.53	1.46	1.34
1	A	335	GLY	C-O	5.19	1.31	1.23
1	A	458	TRP	CE3-CZ3	5.11	1.47	1.38
1	A	331	PRO	C-N	-5.04	1.22	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	ASP	O-C-N	-11.05	105.02	122.70
1	A	412(A)	TYR	O-C-N	-7.40	110.86	122.70
1	A	446[A]	MET	CG-SD-CE	7.39	112.03	100.20
1	A	446[B]	MET	CG-SD-CE	7.39	112.03	100.20
1	A	172	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	125	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	172	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	118	ARG	NE-CZ-NH1	6.05	123.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284[A]	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	284[B]	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	333	VAL	CA-CB-CG1	5.43	119.05	110.90
1	A	327	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	284[A]	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	284[B]	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	292	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	VAL	Mainchain
1	A	412	ASP	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3098	0	2910	39	0
2	A	105	0	88	1	0
3	A	28	0	25	1	0
4	A	14	0	13	0	0
5	A	42	0	56	7	0
6	A	48	0	35	3	0
7	A	1	0	0	0	0
8	A	383	0	0	8	3
All	All	3719	0	3127	42	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (42) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:344:ASN:HB2	8:A:623:HOH:O	1.42	1.19

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:168:THR:H	1:A:170[A]:ASN:HD21	1.09	1.00
1:A:87:LEU:H	1:A:233:HIS:HD2	1.03	0.98
1:A:338:ASN:H	5:A:518:GOL:H31	1.26	0.97
1:A:87:LEU:H	1:A:233:HIS:CD2	1.87	0.91
1:A:284[B]:ARG:NH2	8:A:650:HOH:O	2.14	0.81
1:A:172:ARG:HD3	1:A:209:ARG:NH1	1.98	0.78
1:A:97:TRP:H	1:A:395:GLN:HE22	1.34	0.75
1:A:463:LYS:HD2	8:A:718:HOH:O	1.86	0.75
1:A:406:TYR:OH	6:A:520[B]:ZGE:C2	2.33	0.74
1:A:367:SER:OG	5:A:517:GOL:H12	1.89	0.73
1:A:338:ASN:N	5:A:518:GOL:H31	2.05	0.72
1:A:168:THR:H	1:A:170[A]:ASN:ND2	1.89	0.66
1:A:168:THR:OG1	1:A:170[A]:ASN:ND2	2.30	0.64
1:A:98:HIS:HE1	1:A:419:ARG:HH11	1.44	0.62
1:A:98:HIS:CE1	1:A:419:ARG:HH11	2.19	0.61
1:A:98:HIS:HD2	1:A:99:ILE:O	1.84	0.61
2:A:509:MAN:H62	2:A:509:MAN:O2	2.01	0.61
5:A:514:GOL:H2	8:A:896:HOH:O	2.02	0.58
1:A:338:ASN:H	5:A:518:GOL:C3	2.09	0.58
1:A:369:ALA:HB3	5:A:517:GOL:H32	1.85	0.57
1:A:172:ARG:HD3	1:A:209:ARG:HH11	1.67	0.55
1:A:209:ARG:NH2	8:A:709:HOH:O	2.38	0.55
5:A:514:GOL:H11	8:A:896:HOH:O	2.07	0.54
1:A:168:THR:N	1:A:170[A]:ASN:HD21	1.92	0.51
1:A:406:TYR:OH	6:A:520[B]:ZGE:C3	2.57	0.50
1:A:292:ARG:HH21	1:A:294:ASN:ND2	2.10	0.49
1:A:292:ARG:HE	1:A:294:ASN:HD22	1.61	0.48
1:A:266[B]:GLU:CD	1:A:312:HIS:HD1	2.17	0.48
1:A:121:TYR:CG	1:A:228:SER:HA	2.49	0.47
1:A:209:ARG:HB3	1:A:209:ARG:HH21	1.79	0.47
1:A:278:CYS:HB3	1:A:289:CYS:HB3	1.96	0.47
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.96	0.46
1:A:288:THR:OG1	1:A:304:ARG:NH1	2.45	0.44
1:A:83:ASP:HB2	3:A:510:NAG:H83	2.00	0.44
1:A:230:CYS:HA	8:A:806:HOH:O	2.16	0.44
1:A:144:HIS:HD2	8:A:787:HOH:O	2.01	0.43
1:A:254[A]:ILE:HD12	1:A:312:HIS:CG	2.53	0.42
1:A:263:LEU:HD23	1:A:263:LEU:HA	1.77	0.42
1:A:124:CYS:HA	1:A:129:CYS:HA	2.02	0.41
1:A:277:GLU:OE2	6:A:520[A]:ZGE:H11	2.21	0.41

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:A:890:HOH:O	8:A:937:HOH:O[15_555]	1.87	0.33
8:A:644:HOH:O	8:A:708:HOH:O[5_555]	1.96	0.24
8:A:602:HOH:O	8:A:898:HOH:O[48_555]	2.03	0.17

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	400/388 (103%)	382 (96%)	16 (4%)	2 (0%)	38 29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412(A)	TYR
1	A	331	PRO

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	355/341 (104%)	343 (97%)	12 (3%)	49 45

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170[A]	ASN
1	A	170[B]	ASN
1	A	209	ARG
1	A	221	ASN
1	A	284[A]	ARG
1	A	284[B]	ARG

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Mol	Chain	Res	Type
1	A	304	ARG
1	A	313	THR
1	A	333	VAL
1	A	446[A]	MET
1	A	446[B]	MET
1	A	464	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

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

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

11 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	501	1,2	12,14,15	1.40	2 (16%)	15,19,21	2.29	7 (46%)
2	NAG	A	502	2	12,14,15	0.98	1 (8%)	15,19,21	2.15	4 (26%)
2	BMA	A	503	2	10,11,12	1.26	2 (20%)	11,15,17	3.31	6 (54%)
2	MAN	A	504	2	10,11,12	0.79	0	11,15,17	1.71	3 (27%)
2	MAN	A	505	2	10,11,12	1.02	1 (10%)	11,15,17	2.13	3 (27%)
2	MAN	A	506	2	10,11,12	0.72	0	11,15,17	1.03	1 (9%)
2	MAN	A	507	2	10,11,12	1.01	1 (10%)	11,15,17	1.57	1 (9%)
2	MAN	A	508	2	10,11,12	0.66	0	11,15,17	2.32	1 (9%)
2	MAN	A	509	2	10,11,12	0.81	0	11,15,17	2.24	8 (72%)
3	NAG	A	510	1,3	12,14,15	0.73	0	15,19,21	1.84	5 (33%)
3	NAG	A	511	3	12,14,15	0.87	0	15,19,21	2.16	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
2	BMA	A	503	2	-	0/2/19/22	0/1/1/1
2	MAN	A	504	2	-	0/2/19/22	0/1/1/1
2	MAN	A	505	2	-	0/2/19/22	0/1/1/1
2	MAN	A	506	2	-	0/2/19/22	0/1/1/1
2	MAN	A	507	2	-	0/2/19/22	0/1/1/1
2	MAN	A	508	2	-	0/2/19/22	0/1/1/1
2	MAN	A	509	2	-	0/2/19/22	0/1/1/1
3	NAG	A	510	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	511	3	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	NAG	C2-N2	-2.57	1.43	1.46
2	A	501	NAG	C2-N2	-2.54	1.43	1.46
2	A	503	BMA	O5-C5	-2.45	1.40	1.45
2	A	505	MAN	O5-C5	-2.33	1.41	1.45
2	A	503	BMA	O4-C4	-2.32	1.37	1.43
2	A	507	MAN	O5-C5	-2.31	1.41	1.45
2	A	501	NAG	O5-C5	-2.28	1.41	1.45

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	BMA	O5-C5-C4	-8.03	100.47	110.65
3	A	511	NAG	O5-C5-C6	7.11	114.45	106.98
2	A	508	MAN	O5-C5-C6	6.94	114.27	106.98
2	A	502	NAG	C3-C2-N2	-6.01	102.61	111.76
2	A	503	BMA	O5-C5-C6	4.86	112.08	106.98
2	A	501	NAG	C3-C2-N2	-4.74	104.54	111.76
2	A	505	MAN	O5-C5-C4	-4.27	105.23	110.65
2	A	505	MAN	O5-C5-C6	4.26	111.45	106.98
2	A	507	MAN	O5-C5-C6	3.86	111.04	106.98
2	A	501	NAG	O4-C4-C3	-3.78	101.87	110.35
3	A	510	NAG	C8-C7-N2	3.38	122.71	116.11
2	A	503	BMA	C3-C4-C5	3.28	116.07	110.20
2	A	504	MAN	C6-C5-C4	-3.24	105.18	113.00
3	A	510	NAG	C3-C2-N2	-3.06	107.09	111.76
2	A	509	MAN	O2-C2-C3	3.05	116.75	110.18
2	A	501	NAG	C8-C7-N2	-3.03	110.18	116.11
2	A	501	NAG	O5-C5-C4	-2.92	106.95	110.65
2	A	501	NAG	C3-C4-C5	-2.86	105.09	110.20
2	A	505	MAN	O4-C4-C3	-2.86	103.94	110.35
2	A	509	MAN	O5-C5-C6	2.76	109.88	106.98
2	A	504	MAN	O6-C6-C5	-2.69	102.10	111.36
2	A	509	MAN	O3-C3-C4	2.69	116.38	110.35
2	A	503	BMA	O3-C3-C4	-2.67	104.37	110.35
3	A	510	NAG	C3-C4-C5	-2.64	105.48	110.20
2	A	506	MAN	O6-C6-C5	-2.64	102.29	111.36
2	A	509	MAN	C4-C3-C2	2.55	113.92	110.50
2	A	502	NAG	O5-C5-C6	2.52	109.62	106.98
3	A	510	NAG	O7-C7-C8	-2.51	117.15	122.04
2	A	501	NAG	O7-C7-C8	2.50	126.92	122.04
2	A	509	MAN	O4-C4-C3	-2.49	104.78	110.35
2	A	501	NAG	O5-C5-C6	2.47	109.58	106.98
2	A	503	BMA	C4-C3-C2	-2.47	107.19	110.50
2	A	503	BMA	C6-C5-C4	-2.41	107.19	113.00
3	A	510	NAG	O6-C6-C5	-2.29	103.49	111.36
3	A	511	NAG	O5-C5-C4	-2.28	107.77	110.65
2	A	509	MAN	C6-C5-C4	2.26	118.46	113.00
2	A	504	MAN	O5-C5-C6	2.14	109.23	106.98
2	A	502	NAG	O3-C3-C4	2.13	115.13	110.35
2	A	509	MAN	O5-C5-C4	-2.12	107.96	110.65
2	A	502	NAG	C8-C7-N2	2.08	120.18	116.11
2	A	509	MAN	O3-C3-C2	2.02	113.64	109.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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$
4	NAG	A	512	1	12,14,15	1.08	1 (8%)	15,19,21	2.31	5 (33%)
5	GOL	A	513	-	5,5,5	0.23	0	5,5,5	0.51	0
5	GOL	A	514	-	5,5,5	0.42	0	5,5,5	0.82	0
5	GOL	A	515	-	5,5,5	0.74	0	5,5,5	1.34	1 (20%)
5	GOL	A	516	-	5,5,5	0.32	0	5,5,5	0.24	0
5	GOL	A	517	-	5,5,5	0.44	0	5,5,5	0.51	0
5	GOL	A	518	-	5,5,5	0.34	0	5,5,5	1.05	0
5	GOL	A	519	-	5,5,5	0.67	0	5,5,5	0.83	0
6	ZGE	A	520[A]	1	24,24,24	3.65	5 (20%)	33,34,34	2.96	13 (39%)
6	ZGE	A	520[B]	-	24,24,24	1.37	4 (16%)	33,34,34	1.70	5 (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
4	NAG	A	512	1	-	0/6/23/26	0/1/1/1
5	GOL	A	513	-	-	0/4/4/4	0/0/0/0
5	GOL	A	514	-	-	0/4/4/4	0/0/0/0
5	GOL	A	515	-	-	0/4/4/4	0/0/0/0
5	GOL	A	516	-	-	0/4/4/4	0/0/0/0
5	GOL	A	517	-	-	0/4/4/4	0/0/0/0
5	GOL	A	518	-	-	0/4/4/4	0/0/0/0
5	GOL	A	519	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ZGE	A	520[A]	1	-	0/22/42/42	0/1/1/1
6	ZGE	A	520[B]	-	-	0/22/42/42	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	520[A]	ZGE	C2-C3	13.89	1.54	1.32
6	A	520[A]	ZGE	C11-C10	-8.44	1.32	1.50
6	A	520[A]	ZGE	O10-C10	4.91	1.33	1.23
6	A	520[B]	ZGE	C2-C3	2.99	1.37	1.32
6	A	520[A]	ZGE	F1-C3	2.84	1.39	1.36
6	A	520[B]	ZGE	O6-C2	2.74	1.43	1.37
6	A	520[B]	ZGE	C12-N4	2.57	1.37	1.33
4	A	512	NAG	O5-C5	-2.51	1.40	1.45
6	A	520[A]	ZGE	O6-C2	2.38	1.42	1.37
6	A	520[B]	ZGE	C5-N5	2.24	1.49	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	520[A]	ZGE	O6-C2-C3	-8.19	113.19	123.66
6	A	520[A]	ZGE	O6-C2-C1	-7.72	97.97	111.83
6	A	520[A]	ZGE	F1-C3-C4	-6.41	110.59	115.15
4	A	512	NAG	O5-C5-C4	-6.06	102.96	110.65
6	A	520[B]	ZGE	F1-C3-C4	5.04	118.73	115.15
6	A	520[A]	ZGE	C6-C5-N5	-4.97	102.31	110.99
6	A	520[B]	ZGE	O6-C2-C3	-4.46	117.96	123.66
6	A	520[A]	ZGE	F1-C3-C2	-4.12	110.06	124.27
6	A	520[A]	ZGE	O6-C6-C5	3.49	114.66	110.29
4	A	512	NAG	O5-C5-C6	3.17	110.31	106.98
6	A	520[A]	ZGE	O1A-C1-C2	3.07	120.98	114.62
6	A	520[A]	ZGE	C6-O6-C2	3.02	124.81	113.40
6	A	520[A]	ZGE	C7-C6-C5	-2.92	109.94	114.24
4	A	512	NAG	C2-N2-C7	-2.78	118.42	123.09
4	A	512	NAG	C8-C7-N2	2.77	121.51	116.11
5	A	515	GOL	O2-C2-C1	2.65	120.28	108.22
6	A	520[A]	ZGE	C4-C3-C2	-2.55	112.99	120.00
6	A	520[B]	ZGE	O6-C2-C1	2.42	116.18	111.83
6	A	520[A]	ZGE	C3-C4-N4	-2.38	106.12	111.54
4	A	512	NAG	C3-C4-C5	-2.34	106.02	110.20
6	A	520[B]	ZGE	C6-C5-N5	-2.33	106.93	110.99
6	A	520[B]	ZGE	C6-O6-C2	2.14	121.50	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	520[A]	ZGE	O1B-C1-C2	-2.06	116.92	121.09
6	A	520[A]	ZGE	O9-C9-C8	-2.02	106.53	111.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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(Å ²)	Q<0.9
1	A	388/388 (100%)	-0.33	1 (0%) 91 93	24, 31, 43, 72	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	ARG	2.6

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	510	14/15	0.23	-	41,45,54,60	0
2	MAN	A	508	11/12	0.47	-	72,82,90,91	0
2	MAN	A	504	11/12	0.08	-	32,35,43,54	0
2	MAN	A	509	11/12	0.48	-	74,86,106,107	0
2	NAG	A	501	14/15	0.17	-	29,34,45,48	0
2	MAN	A	505	11/12	0.09	-	33,37,41,42	0
3	NAG	A	511	14/15	0.43	-	70,82,89,95	0
2	NAG	A	502	14/15	0.13	-	30,34,42,59	0
2	MAN	A	506	11/12	0.07	-	31,34,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BMA	A	503	11/12	0.09	-	33,36,40,44	0
2	MAN	A	507	11/12	0.21	-	45,50,60,69	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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	A	513	6/6	0.15	-	42,57,62,67	0
7	CA	A	521	1/1	0.04	-	35,35,35,35	0
6	ZGE	A	520[A]	24/24	0.08	-	28,31,33,35	24
5	GOL	A	518	6/6	0.35	-	53,56,72,73	0
6	ZGE	A	520[B]	24/24	0.08	-	23,29,33,40	24
4	NAG	A	512	14/15	0.29	-	49,57,69,82	0
5	GOL	A	515	6/6	0.10	-	35,40,43,45	0
5	GOL	A	516	6/6	0.40	-	55,72,77,80	0
5	GOL	A	514	6/6	0.14	-	37,55,64,79	0
5	GOL	A	519	6/6	0.14	-	45,64,68,69	0
5	GOL	A	517	6/6	0.13	-	63,65,72,72	0

6.5 Other polymers

There are no such residues in this entry.