



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:03 PM 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 X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

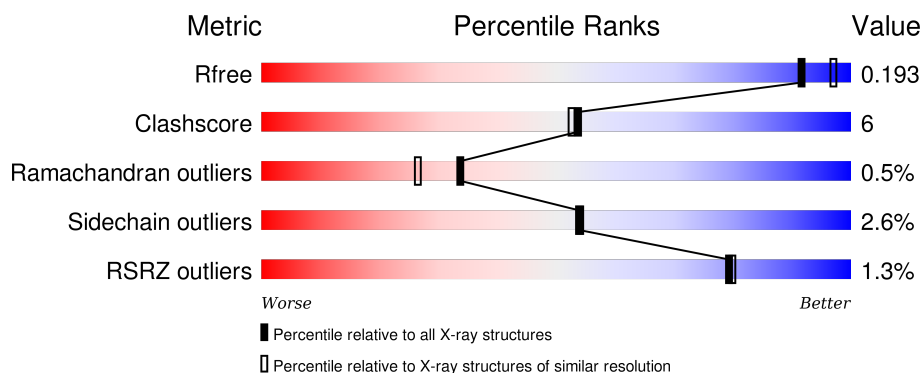
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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  $\geq 3$ , 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	<div> <div></div> <div>87%</div> <div>10%</div> <div>.</div> </div>

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
5	GOL	A	516	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	518	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3719 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	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: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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:  $C_3H_8O_3$ ).



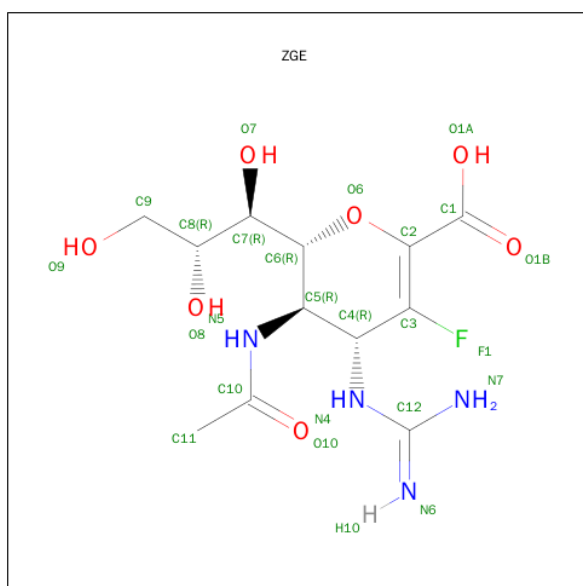
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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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: C<sub>12</sub>H<sub>19</sub>FN<sub>4</sub>O<sub>7</sub>).



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

- 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		

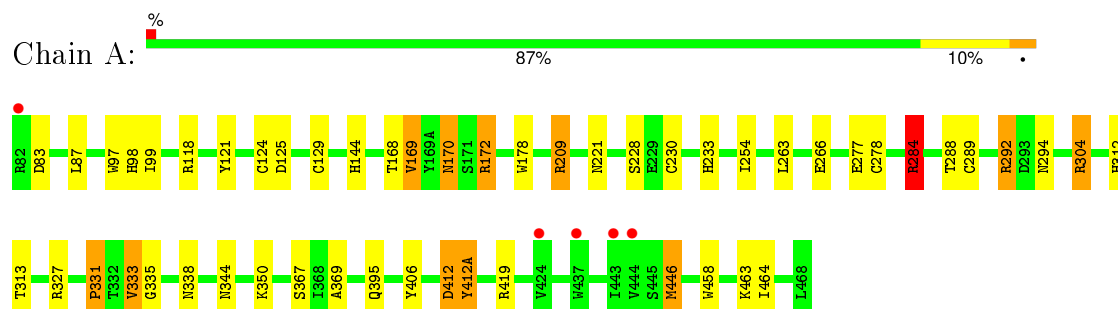
- Molecule 8 is water.

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





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	1734 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 65.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	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

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 6.

All (42) 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:344:ASN:HB2	8:A:623:HOH:O	1.42	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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 sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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 [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	400/388 (103%)	382 (96%)	16 (4%)	2 (0%)	34 26

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 [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	355/341 (104%)	343 (97%)	12 (3%)	44 41

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
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 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 ⓘ

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	14,14,15	1.17	0	15,19,21	2.13	6 (40%)
2	NAG	A	502	2	14,14,15	1.07	1 (7%)	15,19,21	1.89	6 (40%)
2	BMA	A	503	2	11,11,12	1.03	1 (9%)	14,15,17	1.75	6 (42%)
2	MAN	A	504	2	11,11,12	0.89	0	14,15,17	2.31	6 (42%)
2	MAN	A	505	2	11,11,12	0.98	0	14,15,17	1.76	3 (21%)
2	MAN	A	506	2	11,11,12	0.98	1 (9%)	14,15,17	1.07	1 (7%)
2	MAN	A	507	2	11,11,12	0.76	0	14,15,17	1.32	1 (7%)
2	MAN	A	508	2	11,11,12	0.89	0	14,15,17	1.65	2 (14%)
2	MAN	A	509	2	11,11,12	0.86	0	14,15,17	3.20	9 (64%)
3	NAG	A	510	1,3	14,14,15	0.77	0	15,19,21	1.76	4 (26%)
3	NAG	A	511	3	14,14,15	0.98	1 (7%)	15,19,21	1.60	3 (20%)

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	1/1/1/1
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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	NAG	O5-C1	-2.97	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	BMA	O4-C4	-2.34	1.37	1.43
2	A	506	MAN	C2-C3	2.22	1.55	1.52
3	A	511	NAG	C1-C2	2.74	1.56	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	509	MAN	C1-C2-C3	-6.71	101.60	109.54
2	A	501	NAG	O4-C4-C3	-3.76	101.87	110.34
2	A	502	NAG	C1-O5-C5	-3.37	107.97	112.25
2	A	502	NAG	C3-C2-N2	-3.32	102.61	110.56
2	A	504	MAN	O2-C2-C1	-3.26	102.67	109.21
2	A	504	MAN	C6-C5-C4	-3.18	105.18	113.02
2	A	501	NAG	C8-C7-N2	-3.10	110.18	116.11
2	A	501	NAG	C3-C4-C5	-2.93	105.09	110.20
2	A	505	MAN	O4-C4-C3	-2.84	103.94	110.34
2	A	504	MAN	O6-C6-C5	-2.80	102.10	111.33
2	A	506	MAN	O6-C6-C5	-2.74	102.29	111.33
3	A	510	NAG	C3-C4-C5	-2.70	105.48	110.20
2	A	504	MAN	O5-C1-C2	-2.68	106.51	110.86
3	A	510	NAG	O7-C7-C8	-2.68	117.15	122.06
2	A	503	BMA	O3-C3-C4	-2.65	104.37	110.34
2	A	505	MAN	C1-C2-C3	-2.54	106.54	109.54
2	A	501	NAG	C3-C2-N2	-2.51	104.54	110.56
2	A	503	BMA	O2-C2-C1	-2.51	104.18	109.21
2	A	509	MAN	O4-C4-C3	-2.47	104.78	110.34
3	A	510	NAG	O6-C6-C5	-2.37	103.49	111.33
2	A	503	BMA	C6-C5-C4	-2.36	107.19	113.02
2	A	504	MAN	C1-C2-C3	-2.32	106.80	109.54
2	A	503	BMA	C2-C3-C4	-2.26	107.19	111.04
2	A	507	MAN	O2-C2-C1	-2.11	104.98	109.21
2	A	502	NAG	C4-C3-C2	-2.08	108.00	111.23
2	A	509	MAN	O3-C3-C2	2.01	113.64	110.00
2	A	502	NAG	O3-C3-C2	2.10	113.28	109.11
2	A	502	NAG	C8-C7-N2	2.13	120.18	116.11
2	A	502	NAG	O3-C3-C4	2.13	115.13	110.34
2	A	503	BMA	O5-C5-C6	2.19	112.08	107.35
2	A	509	MAN	C6-C5-C4	2.21	118.46	113.02
2	A	509	MAN	O5-C1-C2	2.35	114.67	110.86
3	A	511	NAG	C4-C3-C2	2.44	115.02	111.23
2	A	501	NAG	O7-C7-C8	2.65	126.92	122.06
2	A	509	MAN	O3-C3-C4	2.69	116.38	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	511	NAG	C1-O5-C5	3.18	116.28	112.25
2	A	508	MAN	O5-C5-C6	3.20	114.27	107.35
3	A	511	NAG	O5-C5-C6	3.28	114.45	107.35
2	A	509	MAN	O2-C2-C3	3.30	116.75	110.12
2	A	503	BMA	C3-C4-C5	3.37	116.07	110.20
3	A	510	NAG	C8-C7-N2	3.45	122.71	116.11
2	A	508	MAN	C1-O5-C5	3.81	117.08	112.25
2	A	501	NAG	C1-O5-C5	3.96	117.28	112.25
2	A	509	MAN	O2-C2-C1	4.13	117.49	109.21
2	A	505	MAN	C1-O5-C5	4.18	117.55	112.25
2	A	504	MAN	C1-O5-C5	5.00	118.60	112.25
2	A	509	MAN	C1-O5-C5	5.81	119.62	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	509	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	509	MAN	1	0
3	A	510	NAG	1	0

## 5.6 Ligand geometry [i](#)

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	14,14,15	0.87	0	15,19,21	1.80	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	A	513	-	5,5,5	0.23	0	5,5,5	0.57	0
5	GOL	A	514	-	5,5,5	0.42	0	5,5,5	0.87	0
5	GOL	A	515	-	5,5,5	0.79	0	5,5,5	1.31	1 (20%)
5	GOL	A	516	-	5,5,5	0.34	0	5,5,5	0.26	0
5	GOL	A	517	-	5,5,5	0.45	0	5,5,5	0.58	0
5	GOL	A	518	-	5,5,5	0.35	0	5,5,5	1.11	0
5	GOL	A	519	-	5,5,5	0.70	0	5,5,5	0.79	0
6	ZGE	A	520[A]	1	17,24,24	4.87	6 (35%)	15,34,34	2.80	4 (26%)
6	ZGE	A	520[B]	-	17,24,24	1.63	3 (17%)	15,34,34	1.45	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
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
6	ZGE	A	520[A]	1	-	0/15/42/42	0/1/1/1
6	ZGE	A	520[B]	-	-	0/15/42/42	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	520[A]	ZGE	C11-C10	-8.83	1.32	1.50
6	A	520[A]	ZGE	C10-N5	-2.04	1.26	1.34
6	A	520[A]	ZGE	F1-C3	2.30	1.39	1.36
6	A	520[B]	ZGE	C5-N5	2.34	1.49	1.45
6	A	520[A]	ZGE	O6-C2	3.52	1.42	1.36
6	A	520[B]	ZGE	C2-C3	3.68	1.37	1.32
6	A	520[B]	ZGE	O6-C2	3.98	1.43	1.36
6	A	520[A]	ZGE	O10-C10	4.62	1.33	1.23
6	A	520[A]	ZGE	C2-C3	16.65	1.54	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	520[A]	ZGE	O6-C2-C3	-8.15	113.19	123.37
6	A	520[A]	ZGE	C6-C5-N5	-5.03	102.31	111.07
6	A	520[B]	ZGE	O6-C2-C3	-4.33	117.96	123.37
4	A	512	NAG	C2-N2-C7	-3.60	118.42	123.04
6	A	520[A]	ZGE	C7-C6-C5	-2.90	109.94	114.32
4	A	512	NAG	C3-C4-C5	-2.40	106.02	110.20
6	A	520[B]	ZGE	C6-C5-N5	-2.38	106.93	111.07
4	A	512	NAG	C1-O5-C5	-2.37	109.24	112.25
6	A	520[A]	ZGE	O9-C9-C8	-2.10	106.53	111.10
5	A	515	GOL	O2-C2-C1	2.54	120.28	108.65
4	A	512	NAG	C8-C7-N2	2.83	121.51	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	514	GOL	2	0
5	A	517	GOL	2	0
5	A	518	GOL	3	0
6	A	520[A]	ZGE	1	0
6	A	520[B]	ZGE	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	388/388 (100%)	-0.24	5 (1%) 79 80	24, 31, 43, 72	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	ARG	2.9
1	A	444	VAL	2.5
1	A	437	TRP	2.5
1	A	443	ILE	2.5
1	A	424	VAL	2.4

### 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. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	A	501	14/15	0.94	0.16	1.59	29,34,45,48	0
2	NAG	A	502	14/15	0.96	0.16	1.11	30,34,42,59	0
2	MAN	A	505	11/12	0.96	0.11	0.37	33,37,41,42	0
2	BMA	A	503	11/12	0.97	0.14	0.32	33,36,40,44	0
2	MAN	A	506	11/12	0.95	0.08	-0.09	31,34,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	A	508	11/12	0.78	0.55	-	72,82,90,91	0
3	NAG	A	511	14/15	0.65	0.46	-	70,82,89,95	0
2	MAN	A	504	11/12	0.98	0.10	-	32,35,43,54	0
2	MAN	A	509	11/12	0.70	0.57	-	74,86,106,107	0
3	NAG	A	510	14/15	0.94	0.28	-	41,45,54,60	0
2	MAN	A	507	11/12	0.96	0.29	-	45,50,60,69	0

## 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. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	GOL	A	516	6/6	0.89	0.36	6.40	55,72,77,80	0
5	GOL	A	518	6/6	0.91	0.27	3.96	53,56,72,73	0
5	GOL	A	514	6/6	0.96	0.17	0.95	37,55,64,79	0
5	GOL	A	513	6/6	0.95	0.11	0.48	42,57,62,67	0
5	GOL	A	517	6/6	0.91	0.10	0.26	63,65,72,72	0
6	ZGE	A	520[B]	24/24	0.97	0.10	-0.33	23,29,33,40	24
6	ZGE	A	520[A]	24/24	0.97	0.10	-0.33	28,31,33,35	24
5	GOL	A	515	6/6	0.97	0.11	-0.89	35,40,43,45	0
7	CA	A	521	1/1	0.99	0.05	-1.25	35,35,35,35	0
5	GOL	A	519	6/6	0.84	0.15	-	45,64,68,69	0
4	NAG	A	512	14/15	0.94	0.30	-	49,57,69,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.