



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:25 AM GMT

PDB ID : 2AEP
Title : An epidemiologically significant epitope of a 1998 influenza virus neuraminidase forms a highly hydrated interface in the NA-antibody complex.
Authors : Venkatramani, L.; Bochkareva, E.; Lee, J.T.; Gulati, U.; Laver, W.G.; Bochkarev, A.; Air, G.M.
Deposited on : 2005-07-23
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/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 (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

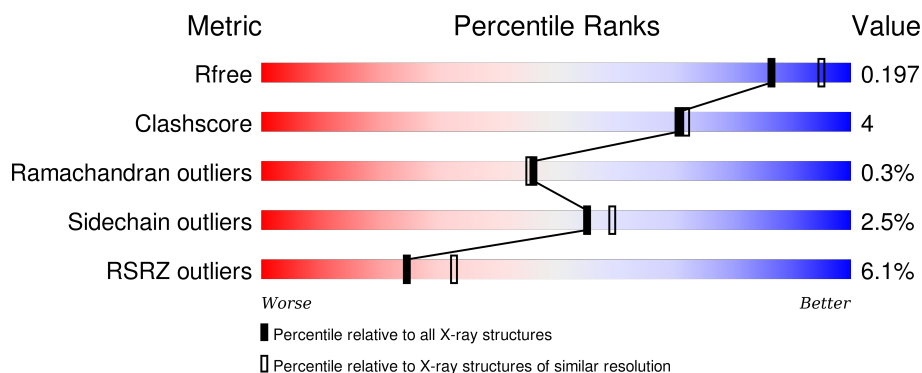
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	395	<div> <div>92%</div> <div>6% ..</div> </div>
2	H	217	<div> <div>12%</div> <div>56%</div> <div>10%</div> <div>34%</div> </div>
3	L	214	<div> <div>5%</div> <div>52%</div> <div>7% .</div> <div>40%</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
4	GLC	A	702	X	-	-	-
4	GLC	H	701	X	-	-	-
5	NAG	A	686	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5812 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
			Total	C	N	O	S			
1	A	388	3019	1876	537	584	22	0	1	0

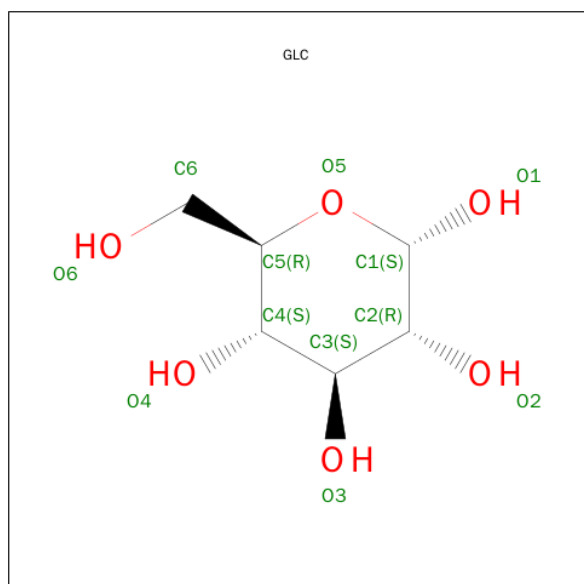
- Molecule 2 is a protein called FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	143	1102	701	179	217	5	0	0	0

- Molecule 3 is a protein called FAB light chain.

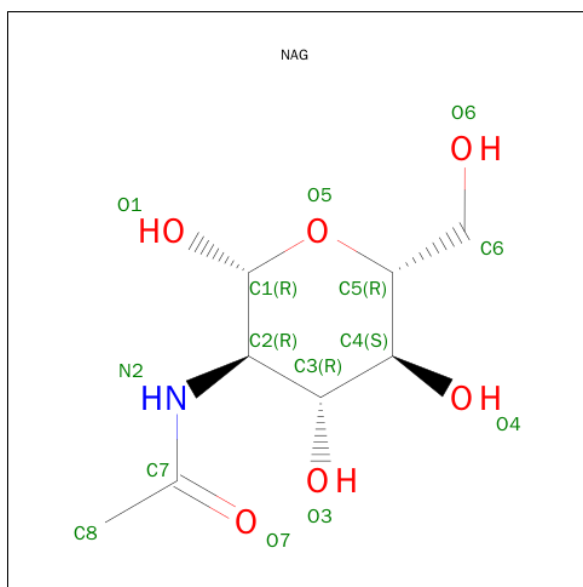
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	129	1005	628	169	204	4	0	0	0

- Molecule 4 is SUGAR (GLUCOSE) (three-letter code: GLC) (formula: C₆H₁₂O₆).



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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

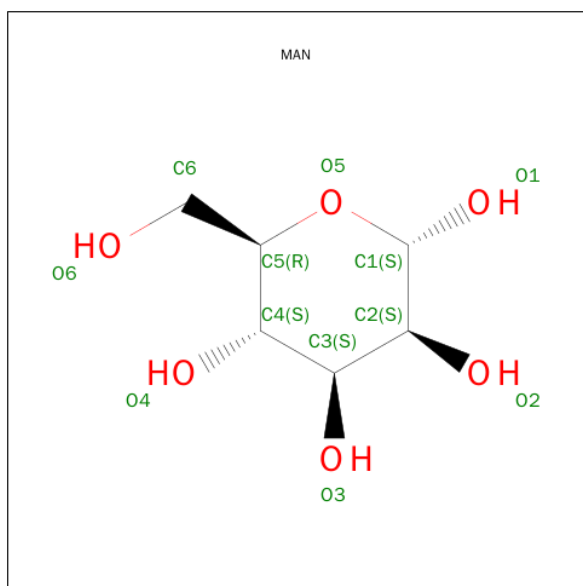
- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	5	Total	C	N	O	0	0
			61	34	2	25		

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	2	Total	C	O	0	0
			22	12	10		

- Molecule 8 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		

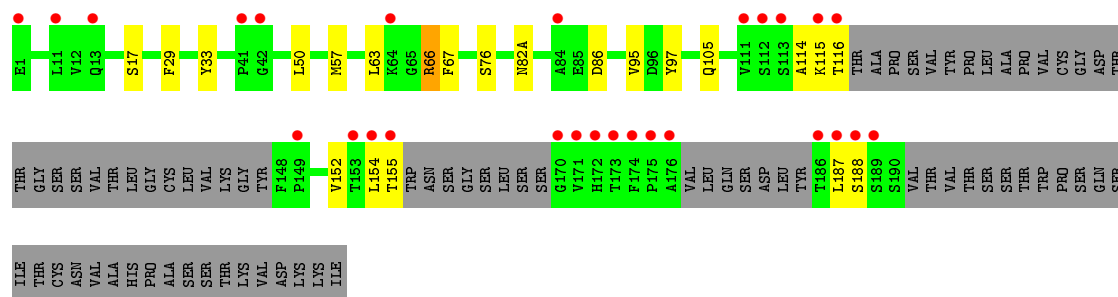
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	347	Total	O	0	0
			347	347		
11	H	75	Total	O	0	0
			75	75		
11	L	84	Total	O	0	0
			84	84		

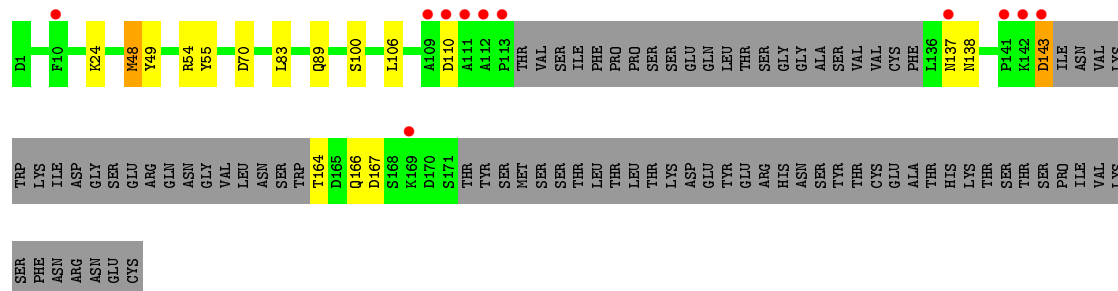
- Molecule 1: neuraminidase



- Chain H: 



- Chain L:  5% 52% 7% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.06Å 155.06Å 102.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.10) 92.2 (19.97-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.188 , 0.224 0.196 , 0.197	Depositor DCC
R_{free} test set	7413 reflections (12.22%)	DCC
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 73146 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5812	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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, 0.375 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: BMA, NAG, CA, GLC, SO4, 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	1.16	5/3099 (0.2%)	1.01	6/4197 (0.1%)
2	H	1.07	0/1128	0.98	1/1530 (0.1%)
3	L	1.11	2/1025 (0.2%)	1.06	6/1384 (0.4%)
All	All	1.13	7/5252 (0.1%)	1.01	13/7111 (0.2%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	48	MET	SD-CE	-7.82	1.34	1.77
1	A	412	VAL	CB-CG1	-6.75	1.38	1.52
1	A	174	VAL	CB-CG2	-6.54	1.39	1.52
1	A	352	TRP	CB-CG	-6.35	1.38	1.50
3	L	100	SER	CB-OG	6.32	1.50	1.42

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	A	85	ARG	NE-CZ-NH2	-8.74	115.93	120.30
3	L	110	ASP	CB-CG-OD2	7.77	125.29	118.30
3	L	54	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	A	309	ASP	CB-CG-OD1	6.97	124.57	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3019	0	2854	20	0
2	H	1102	0	1053	11	0
3	L	1005	0	962	6	0
4	A	12	0	12	2	0
4	H	12	0	12	0	0
5	A	56	0	52	7	0
6	A	61	0	52	6	0
7	L	22	0	19	5	0
8	L	11	0	10	3	0
9	A	1	0	0	0	0
10	A	5	0	0	0	0
11	A	347	0	0	6	0
11	H	75	0	0	1	0
11	L	84	0	0	3	0
All	All	5812	0	5026	44	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 44 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:306:ASN:HD21	1:A:308:LYS:HE2	1.40	0.86
5:A:686:NAG:H81	5:A:634:NAG:H5	1.57	0.85
1:A:200:ASN:HD22	6:A:703(A):NAG:H83	1.48	0.79
1:A:306:ASN:OD1	1:A:308:LYS:HG2	1.83	0.78
1:A:264:HIS:HD2	11:A:995:HOH:O	1.75	0.69

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	386/395 (98%)	369 (96%)	16 (4%)	1 (0%)	46	45
2	H	135/217 (62%)	127 (94%)	7 (5%)	1 (1%)	26	21
3	L	123/214 (58%)	117 (95%)	6 (5%)	0	100	100
All	All	644/826 (78%)	613 (95%)	29 (4%)	2 (0%)	46	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	114	ALA
1	A	200	ASN

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	338/344 (98%)	336 (99%)	2 (1%)	90	94
2	H	120/185 (65%)	112 (93%)	8 (7%)	20	16
3	L	113/192 (59%)	109 (96%)	4 (4%)	43	44
All	All	571/721 (79%)	557 (98%)	14 (2%)	55	59

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	115	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	152	VAL
3	L	89	GLN
2	H	105	GLN
3	L	83	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	GLN
3	L	138	ASN
3	L	89	GLN
1	A	358	ASN
3	L	137	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

7 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$
6	NAG	A	703(A)	1,6	14,14,15	1.80	3 (21%)	15,19,21	2.54	5 (33%)
6	NAG	A	704(B)	6	14,14,15	1.48	1 (7%)	15,19,21	1.52	3 (20%)
6	BMA	A	705(C)	7,6	11,11,12	0.89	1 (9%)	14,15,17	1.75	3 (21%)
6	MAN	A	706(D)	6	11,11,12	1.21	2 (18%)	14,15,17	1.82	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	A	707(E)	6	11,11,12	0.68	0	14,15,17	1.84	5 (35%)
7	MAN	L	215(F)	7,6	11,11,12	0.89	0	14,15,17	2.94	6 (42%)
7	MAN	L	216(G)	7	11,11,12	0.54	0	14,15,17	1.30	2 (14%)

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
6	NAG	A	703(A)	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	704(B)	6	-	0/6/23/26	0/1/1/1
6	BMA	A	705(C)	7,6	-	0/2/19/22	0/1/1/1
6	MAN	A	706(D)	6	-	0/2/19/22	0/1/1/1
6	MAN	A	707(E)	6	-	0/2/19/22	0/1/1/1
7	MAN	L	215(F)	7,6	-	0/2/19/22	0/1/1/1
7	MAN	L	216(G)	7	-	0/2/19/22	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703(A)	NAG	C8-C7	-4.45	1.41	1.50
6	A	704(B)	NAG	C8-C7	-4.15	1.42	1.50
6	A	706(D)	MAN	O5-C1	-2.54	1.39	1.43
6	A	705(C)	BMA	O5-C1	-2.13	1.40	1.43
6	A	703(A)	NAG	C4-C5	2.04	1.57	1.53

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	215(F)	MAN	O2-C2-C1	-4.35	100.49	109.21
6	A	705(C)	BMA	C1-O5-C5	-4.24	106.86	112.25
6	A	703(A)	NAG	C4-C3-C2	-3.88	105.19	111.23
6	A	703(A)	NAG	O7-C7-C8	-3.35	115.92	122.06
6	A	705(C)	BMA	C6-C5-C4	-2.75	106.22	113.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	703(A)	NAG	4	0
6	A	705(C)	BMA	2	0
7	L	215(F)	MAN	5	0

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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$
10	SO4	A	602	-	4,4,4	0.96	0	6,6,6	0.29	0
5	NAG	A	629	1	14,14,15	0.76	0	15,19,21	1.76	6 (40%)
5	NAG	A	634	1	14,14,15	1.63	3 (21%)	15,19,21	1.99	7 (46%)
5	NAG	A	646	1	14,14,15	1.10	1 (7%)	15,19,21	1.64	4 (26%)
5	NAG	A	686	1	14,14,15	1.00	0	15,19,21	2.10	2 (13%)
4	GLC	A	702	-	12,12,12	0.78	0	17,17,17	1.42	3 (17%)
4	GLC	H	701	-	12,12,12	0.97	0	17,17,17	1.24	2 (11%)
8	MAN	L	217(H)	-	11,11,12	0.51	0	14,15,17	2.58	4 (28%)

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
10	SO4	A	602	-	-	0/0/0/0	0/0/0/0
5	NAG	A	629	1	-	0/6/23/26	0/1/1/1
5	NAG	A	634	1	-	0/6/23/26	0/1/1/1
5	NAG	A	646	1	-	0/6/23/26	0/1/1/1
5	NAG	A	686	1	-	0/6/23/26	0/1/1/1
4	GLC	A	702	-	1/1/5/5	0/2/22/22	0/1/1/1
4	GLC	H	701	-	1/1/5/5	0/2/22/22	0/1/1/1
8	MAN	L	217(H)	-	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	646	NAG	C8-C7	-2.56	1.45	1.50
5	A	634	NAG	O4-C4	2.12	1.48	1.43
5	A	634	NAG	C1-C2	2.30	1.55	1.52
5	A	634	NAG	O7-C7	3.92	1.32	1.23

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	646	NAG	O6-C6-C5	-2.95	101.57	111.33
4	A	702	GLC	O5-C1-C2	-2.85	105.25	109.80
8	L	217(H)	MAN	O2-C2-C1	-2.83	103.53	109.21
5	A	646	NAG	C3-C4-C5	-2.70	105.50	110.20
5	A	634	NAG	C8-C7-N2	-2.57	111.19	116.11

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	701	GLC	C1
4	A	702	GLC	C1

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	634	NAG	4	0
5	A	646	NAG	3	0
5	A	686	NAG	1	0
4	A	702	GLC	2	0
8	L	217(H)	MAN	3	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	388/395 (98%)	-0.24	2 (0%) 91 93	23, 29, 40, 52	0
2	H	143/217 (65%)	0.92	27 (18%) 2 2	26, 44, 90, 94	0
3	L	129/214 (60%)	0.41	11 (8%) 13 18	26, 37, 71, 80	0
All	All	660/826 (79%)	0.14	40 (6%) 25 33	23, 32, 69, 94	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	155	THR	7.6
2	H	187	LEU	7.2
3	L	112	ALA	7.1
2	H	112	SER	6.5
2	H	116	THR	5.2

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, 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
6	NAG	A	703(A)	14/15	0.97	0.08	-0.79	20,29,31,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	A	704(B)	14/15	0.97	0.08	-	27,31,37,45	0
6	MAN	A	707(E)	11/12	0.92	0.27	-	50,55,57,58	0
6	BMA	A	705(C)	11/12	0.97	0.07	-	29,33,35,36	0
7	MAN	L	215(F)	11/12	0.94	0.15	-	38,46,53,61	0
6	MAN	A	706(D)	11/12	0.95	0.14	-	34,37,42,46	0
7	MAN	L	216(G)	11/12	0.92	0.28	-	67,71,73,75	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, 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(\AA^2)	Q<0.9
5	NAG	A	686	14/15	0.87	0.28	4.44	53,59,67,68	0
4	GLC	A	702	12/12	0.83	0.27	1.84	46,58,61,63	0
4	GLC	H	701	12/12	0.94	0.14	1.74	32,41,51,52	0
5	NAG	A	646	14/15	0.90	0.15	1.05	40,48,53,57	0
5	NAG	A	634	14/15	0.81	0.23	1.01	44,52,57,62	0
10	SO4	A	602	5/5	1.00	0.07	-1.47	26,31,34,35	0
9	CA	A	601	1/1	1.00	0.04	-2.46	35,35,35,35	0
5	NAG	A	629	14/15	0.78	0.40	-	64,72,75,76	0
8	MAN	L	217(H)	11/12	0.86	0.27	-	75,79,80,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.