Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2021 – 10:42 am BST

PDB ID	:	7O9S
Title	:	Hantaan virus Gn in complex with Fab nnHTN-Gn2
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Deposited on	:	2021-04-16
Resolution	:	2.70 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:

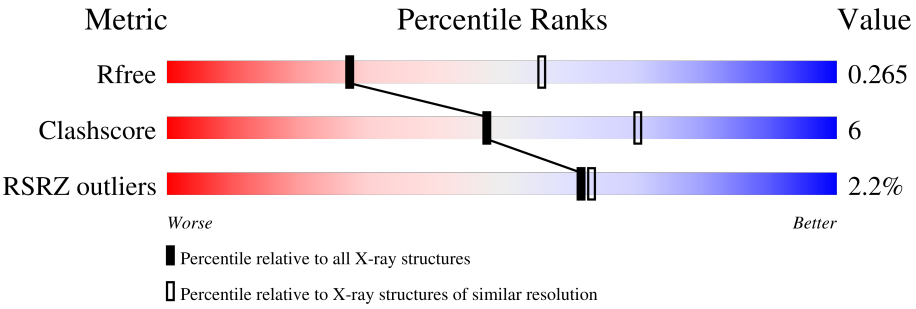
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	229	83% 11% 6%
2	L	215	87% 13%
3	A	365	4% 77% 16% 7%

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	GOL	H	302	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5854 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 Fab nnHTN-Gn2 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	216	Total	C	N	O	S	0	0	0
			1601	1010	268	316	7			

- Molecule 2 is a protein called Fab nnHTN-Gn2 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1578	981	259	331	7			

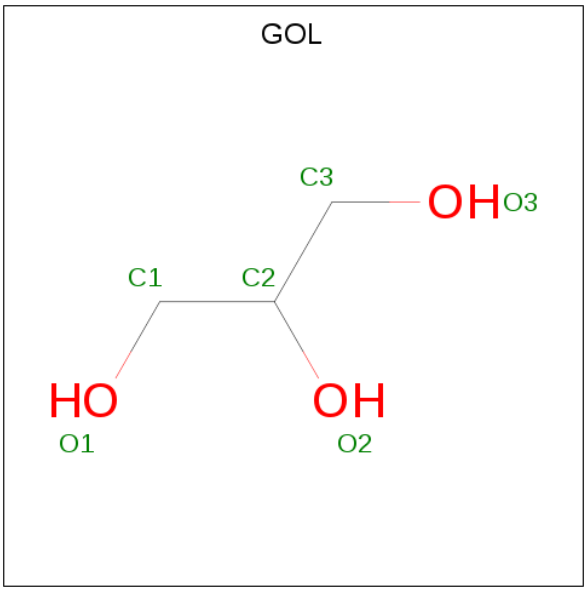
- Molecule 3 is a protein called Envelope polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	340	Total	C	N	O	S	0	0	0
			2629	1671	426	507	25			

There are 11 discrepancies between the modelled and reference sequences:

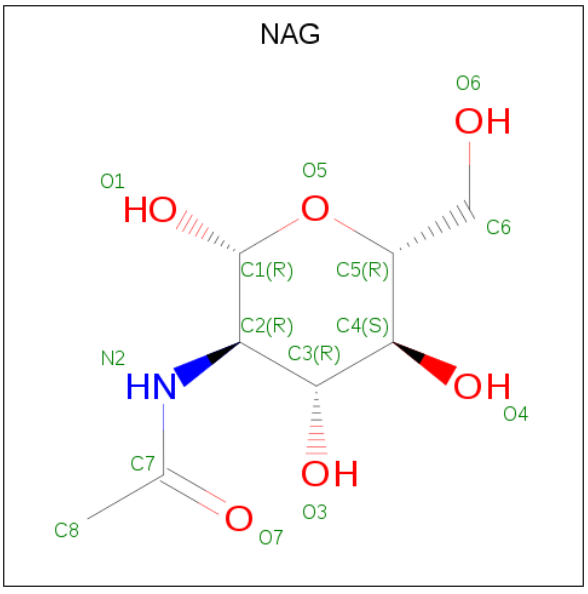
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	THR	-	cloning artifact	UNP A0A077D153
A	17	GLY	-	cloning artifact	UNP A0A077D153
A	372	GLY	-	expression tag	UNP A0A077D153
A	373	THR	-	expression tag	UNP A0A077D153
A	374	LYS	-	expression tag	UNP A0A077D153
A	375	HIS	-	expression tag	UNP A0A077D153
A	376	HIS	-	expression tag	UNP A0A077D153
A	377	HIS	-	expression tag	UNP A0A077D153
A	378	HIS	-	expression tag	UNP A0A077D153
A	379	HIS	-	expression tag	UNP A0A077D153
A	380	HIS	-	expression tag	UNP A0A077D153

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



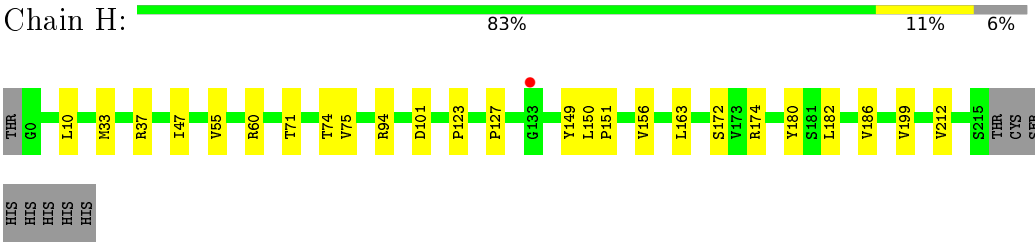
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

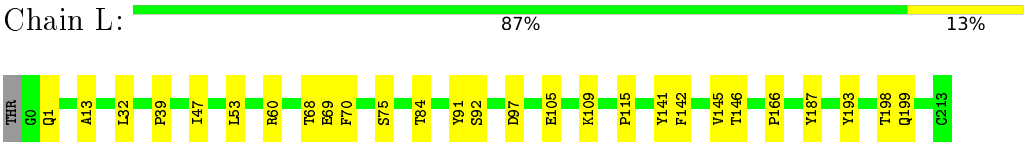
- Molecule 1: Fab nnHTN-Gn2 Heavy chain

Chain H:



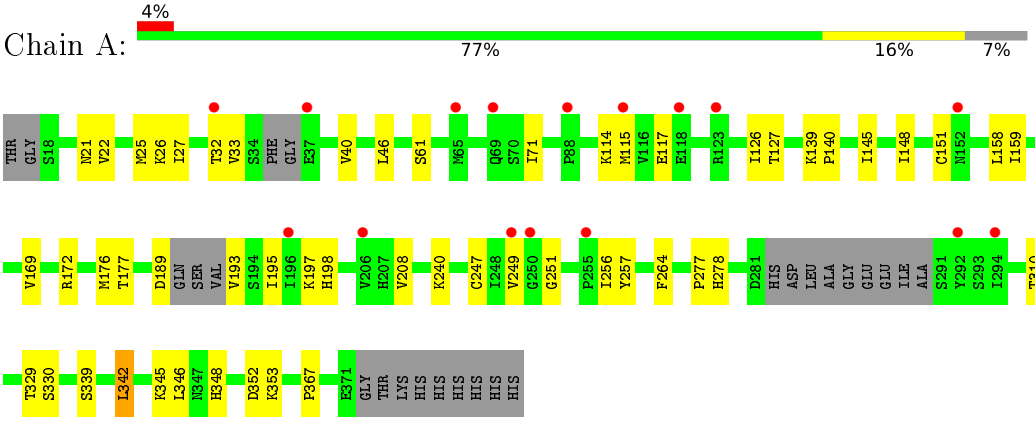
- Molecule 2: Fab nnHTN-Gn2 Light chain

Chain L:



- Molecule 3: Envelope polyprotein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.13Å 76.90Å 174.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.67 – 2.70 70.36 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (51.67-2.70) 99.5 (70.36-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.56 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.211 , 0.267 0.209 , 0.265	Depositor DCC
R_{free} test set	1409 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	61.4	Xtriage
Anisotropy	1.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5854	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG

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	H	0.26	0/1643	0.52	0/2258
2	L	0.26	0/1608	0.48	0/2201
3	A	0.26	0/2690	0.54	1/3651 (0.0%)
All	All	0.26	0/5941	0.52	1/8110 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	342	LEU	CA-CB-CG	5.52	127.99	115.30

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	H	1601	0	1577	18	0
2	L	1578	0	1525	17	0
3	A	2629	0	2570	40	0
4	H	12	0	16	1	0
4	L	6	0	8	1	0
5	A	28	0	26	1	0
All	All	5854	0	5722	70	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 6.

All (70) 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)
3:A:22:VAL:HG22	3:A:165:ARG:HB2	1.69	0.73
1:H:163:LEU:HD21	1:H:186:VAL:HG21	1.70	0.72
3:A:195:ILE:O	3:A:198:HIS:ND1	2.23	0.69
1:H:156:VAL:H	4:H:302:GOL:H12	1.58	0.66
3:A:159:ILE:HB	3:A:166:VAL:HG12	1.78	0.66
3:A:151:CYS:O	3:A:172:ARG:NH2	2.27	0.66
1:H:33:MET:HE1	1:H:94:ARG:HG3	1.80	0.64
3:A:46:LEU:HB2	3:A:140:PRO:HG2	1.80	0.63
3:A:32:THR:HG23	3:A:177:THR:HG23	1.81	0.63
1:H:123:PRO:HB3	1:H:149:TYR:HB3	1.80	0.63
1:H:150:LEU:HD22	1:H:151:PRO:HA	1.81	0.62
2:L:146:THR:HG23	2:L:198:THR:HB	1.82	0.61
3:A:240:LYS:HD2	3:A:329:THR:HG22	1.83	0.61
1:H:10:LEU:HB2	1:H:151:PRO:HG3	1.84	0.60
2:L:115:PRO:HB3	2:L:141:TYR:HB3	1.86	0.58
3:A:208:VAL:HG12	3:A:249:VAL:HG12	1.89	0.55
2:L:39:PRO:HG2	2:L:166:PRO:HB3	1.89	0.54
1:H:71:THR:HG1	1:H:74:THR:HG1	1.46	0.54
3:A:33:VAL:HG13	3:A:148:ILE:HG13	1.90	0.53
3:A:176:MET:O	3:A:177:THR:OG1	2.25	0.53
3:A:61:SER:HA	3:A:159:ILE:HA	1.91	0.53
1:H:33:MET:HG3	1:H:75:VAL:HG21	1.90	0.52
3:A:26:LYS:HA	3:A:169:VAL:HG13	1.91	0.52
3:A:139:LYS:HE2	3:A:320:PRO:HB2	1.91	0.52
3:A:126:ILE:HB	3:A:145:ILE:HB	1.91	0.51
1:H:71:THR:OG1	1:H:74:THR:OG1	2.24	0.51
3:A:345:LYS:NZ	3:A:352:ASP:O	2.31	0.51
2:L:47:ILE:HG12	2:L:53:LEU:HD23	1.94	0.50
3:A:71:ILE:HD11	3:A:115:MET:HE1	1.93	0.50
1:H:127:PRO:HB3	1:H:212:VAL:HG12	1.94	0.50
3:A:278:HIS:HB3	3:A:322:TYR:CD1	2.47	0.49
3:A:40:VAL:HG13	3:A:251:GLY:O	2.12	0.49
3:A:176:MET:N	3:A:176:MET:SD	2.87	0.48
3:A:240:LYS:HD3	3:A:330:SER:HA	1.96	0.48
3:A:264:PHE:HZ	3:A:367:PRO:HG3	1.79	0.48
3:A:114:LYS:HA	3:A:117:GLU:OE1	2.14	0.47
3:A:189:ASP:OD2	3:A:193:VAL:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:127:THR:HG21	3:A:159:ILE:HD13	1.96	0.47
1:H:55:VAL:HG21	3:A:158:LEU:HB2	1.96	0.47
1:H:101:ASP:OD1	3:A:21:ASN:ND2	2.30	0.47
1:H:156:VAL:HG22	1:H:199:VAL:HG22	1.97	0.46
1:H:172:SER:HA	1:H:182:LEU:HB3	1.97	0.46
2:L:68:THR:HG23	2:L:69:GLU:HG2	1.97	0.45
2:L:39:PRO:HA	4:L:301:GOL:H32	1.98	0.45
3:A:117:GLU:OE2	3:A:257:TYR:OH	2.30	0.45
2:L:92:SER:HA	3:A:165:ARG:NH2	2.31	0.45
3:A:348:HIS:HB2	5:A:402:NAG:H82	1.97	0.45
3:A:25:MET:HE3	3:A:27:ILE:HD11	1.98	0.45
2:L:13:ALA:HA	2:L:109:LYS:HB2	1.99	0.45
2:L:32:LEU:HD22	2:L:70:PHE:CG	2.53	0.44
2:L:60:ARG:HB2	2:L:75:SER:O	2.16	0.44
2:L:145:VAL:HG12	2:L:199:GLN:HB2	1.98	0.44
3:A:197:LYS:HD2	3:A:197:LYS:HA	1.66	0.44
3:A:247:CYS:HB2	3:A:256:ILE:CG1	2.47	0.44
2:L:84:THR:HA	2:L:105:GLU:HA	1.99	0.43
3:A:114:LYS:HE3	3:A:114:LYS:HB3	1.74	0.43
2:L:1:GLN:N	2:L:1:GLN:OE1	2.51	0.43
1:H:37:ARG:HB3	1:H:47:ILE:HD11	2.01	0.43
1:H:174:ARG:HD2	1:H:180:TYR:CZ	2.54	0.42
1:H:150:LEU:HA	1:H:151:PRO:HA	1.87	0.42
2:L:109:LYS:HA	2:L:142:PHE:CZ	2.55	0.42
3:A:247:CYS:HB2	3:A:256:ILE:HG13	2.02	0.42
3:A:277:PRO:HB2	3:A:346:LEU:HD13	2.02	0.42
2:L:187:TYR:O	2:L:193:TYR:OH	2.37	0.42
3:A:339:SER:HB2	3:A:342:LEU:HB2	2.02	0.42
2:L:91:TYR:CE1	3:A:163:PRO:HB3	2.55	0.41
3:A:310:THR:O	3:A:353:LYS:HA	2.20	0.41
1:H:60:ARG:NH2	2:L:97:ASP:OD2	2.54	0.41
3:A:159:ILE:HB	3:A:166:VAL:CG1	2.48	0.41
3:A:32:THR:HG22	3:A:176:MET:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry

5 ligands 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	$\#\|Z\| > 2$
5	NAG	A	401	3	14,14,15	0.26	0	17,19,21	0.59	1 (5%)
4	GOL	L	301	-	5,5,5	0.89	0	5,5,5	0.97	0
5	NAG	A	402	3	14,14,15	0.30	0	17,19,21	0.47	0
4	GOL	H	302	-	5,5,5	0.92	0	5,5,5	0.95	0
4	GOL	H	301	-	5,5,5	0.91	0	5,5,5	0.99	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	401	3	-	2/6/23/26	0/1/1/1
4	GOL	L	301	-	-	2/4/4/4	-
5	NAG	A	402	3	-	3/6/23/26	0/1/1/1
4	GOL	H	302	-	-	0/4/4/4	-
4	GOL	H	301	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	401	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	301	GOL	C1-C2-C3-O3
5	A	401	NAG	C4-C5-C6-O6
5	A	402	NAG	O5-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
5	A	402	NAG	C4-C5-C6-O6
4	L	301	GOL	O2-C2-C3-O3
5	A	402	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	GOL	1	0
5	A	402	NAG	1	0
4	H	302	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	H	216/229 (94%)	0.23	1 (0%) 91 92	53, 71, 114, 175	0
2	L	214/215 (99%)	0.05	0 100 100	55, 75, 110, 133	0
3	A	340/365 (93%)	0.53	16 (4%) 31 30	54, 83, 147, 186	0
All	All	770/809 (95%)	0.31	17 (2%) 62 63	53, 77, 133, 186	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	255	PRO	3.2
3	A	292	TYR	2.9
3	A	118	GLU	2.8
3	A	123	ARG	2.8
3	A	249	VAL	2.7
3	A	88	PRO	2.6
3	A	65	MET	2.6
3	A	152	ASN	2.4
3	A	250	GLY	2.3
3	A	294	ILE	2.3
3	A	69	GLN	2.3
3	A	37	GLU	2.3
3	A	206	VAL	2.3
3	A	115	MET	2.2
3	A	196	ILE	2.1
3	A	32	THR	2.1
1	H	133	GLY	2.0

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 (i)

There are no monosaccharides 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, 95^{th} 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
4	GOL	H	302	6/6	0.79	0.46	72,90,99,99	0
5	NAG	A	402	14/15	0.80	0.29	91,136,149,156	0
4	GOL	L	301	6/6	0.83	0.22	73,78,82,87	0
4	GOL	H	301	6/6	0.86	0.37	73,82,92,95	0
5	NAG	A	401	14/15	0.91	0.18	74,92,97,99	0

6.5 Other polymers (i)

There are no such residues in this entry.