



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 10:48 AM BST

PDB ID : 3NWF
Title : Glycoprotein B from Herpes simplex virus type 1, low-pH
Authors : Stampfer, S.D.; Lou, H.; Cohen, G.H.; Eisenberg, R.J.; Heldwein, E.E.
Deposited on : 2010-07-09
Resolution : 3.00 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

<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 : 2.13.1
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) : 2.13.1

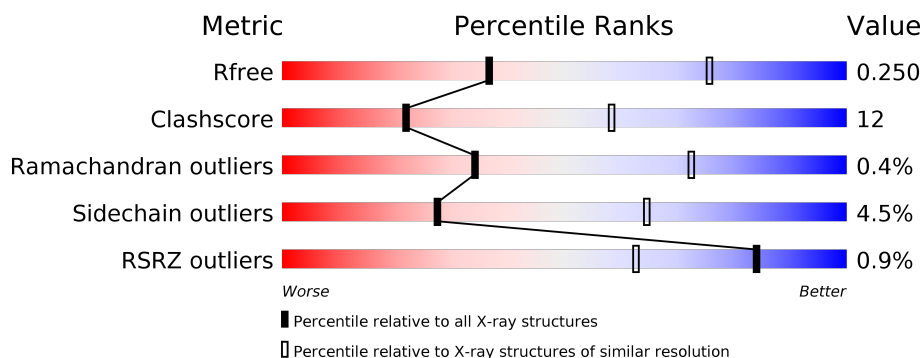
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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 $\leq 5\%$. 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	703	<div> <div></div> <div> <div></div> <div>64%</div> <div>22%</div> <div>14%</div> </div> </div>
1	B	703	<div> <div></div> <div> <div></div> <div>60%</div> <div>23%</div> <div>15%</div> </div> </div>
1	C	703	<div> <div></div> <div> <div></div> <div>60%</div> <div>24%</div> <div>14%</div> </div> </div>
1	D	703	<div> <div></div> <div> <div></div> <div>59%</div> <div>24%</div> <div>14%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19321 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.

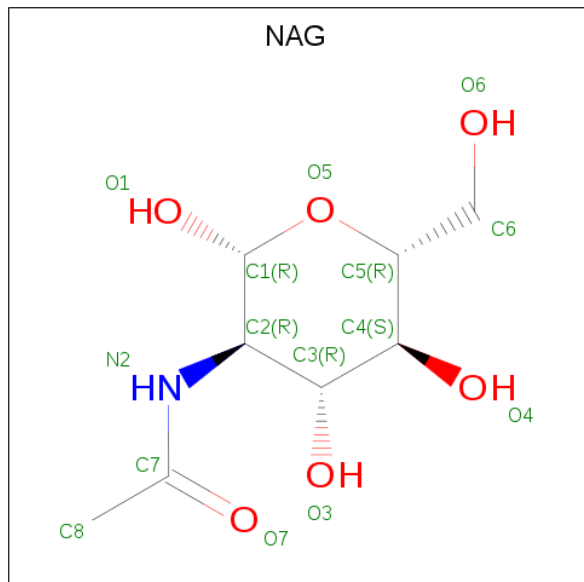
- Molecule 1 is a protein called Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	605	Total	C	N	O	S	0	0	0
			4814	3040	845	907	22			
1	B	596	Total	C	N	O	S	0	1	0
			4762	3012	837	891	22			
1	C	603	Total	C	N	O	S	0	0	0
			4727	2985	814	907	21			
1	D	605	Total	C	N	O	S	0	0	0
			4813	3036	841	914	22			

There are 20 discrepancies between the modelled and reference sequences:

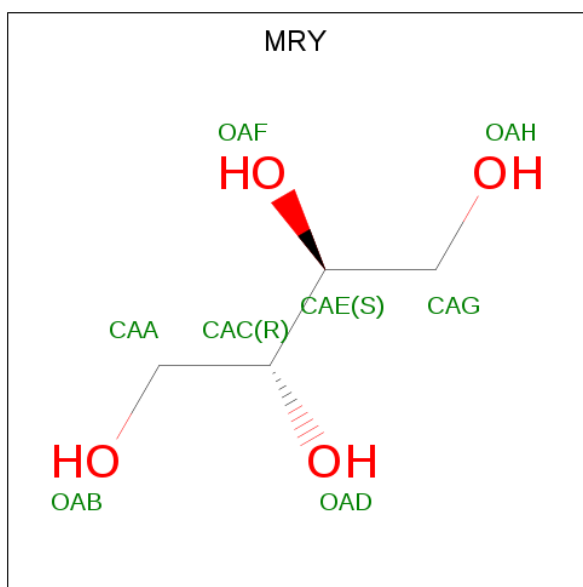
Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ASP	-	expression tag	UNP P06437
B	29	PRO	-	expression tag	UNP P06437
B	58	ALA	PRO	SEE REMARK 999	UNP P06437
B	313	SER	THR	SEE REMARK 999	UNP P06437
B	443	LEU	GLN	SEE REMARK 999	UNP P06437
A	28	ASP	-	expression tag	UNP P06437
A	29	PRO	-	expression tag	UNP P06437
A	58	ALA	PRO	SEE REMARK 999	UNP P06437
A	313	SER	THR	SEE REMARK 999	UNP P06437
A	443	LEU	GLN	SEE REMARK 999	UNP P06437
C	28	ASP	-	expression tag	UNP P06437
C	29	PRO	-	expression tag	UNP P06437
C	58	ALA	PRO	SEE REMARK 999	UNP P06437
C	313	SER	THR	SEE REMARK 999	UNP P06437
C	443	LEU	GLN	SEE REMARK 999	UNP P06437
D	28	ASP	-	expression tag	UNP P06437
D	29	PRO	-	expression tag	UNP P06437
D	58	ALA	PRO	SEE REMARK 999	UNP P06437
D	313	SER	THR	SEE REMARK 999	UNP P06437
D	443	LEU	GLN	SEE REMARK 999	UNP P06437

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



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

- Molecule 3 is MESO-ERYTHRITOL (three-letter code: MRY) (formula: $C_4H_{10}O_4$).



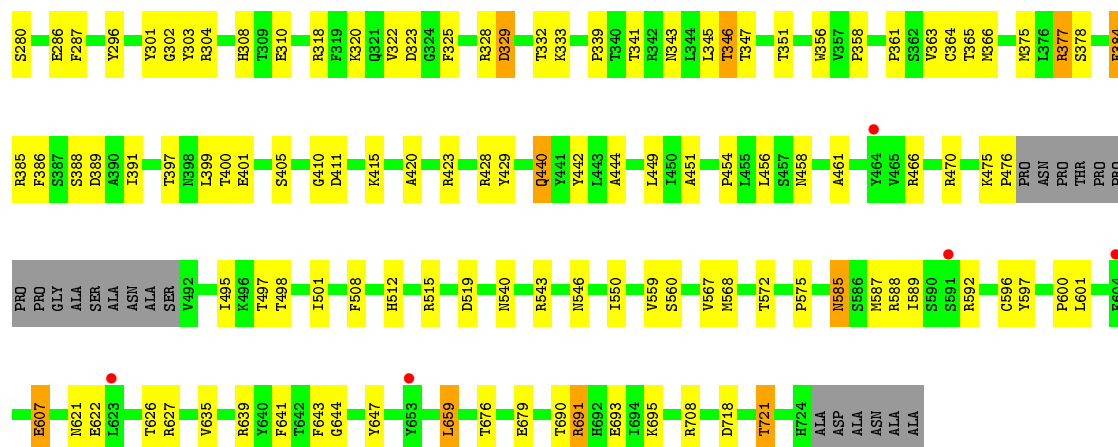
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		
3	B	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

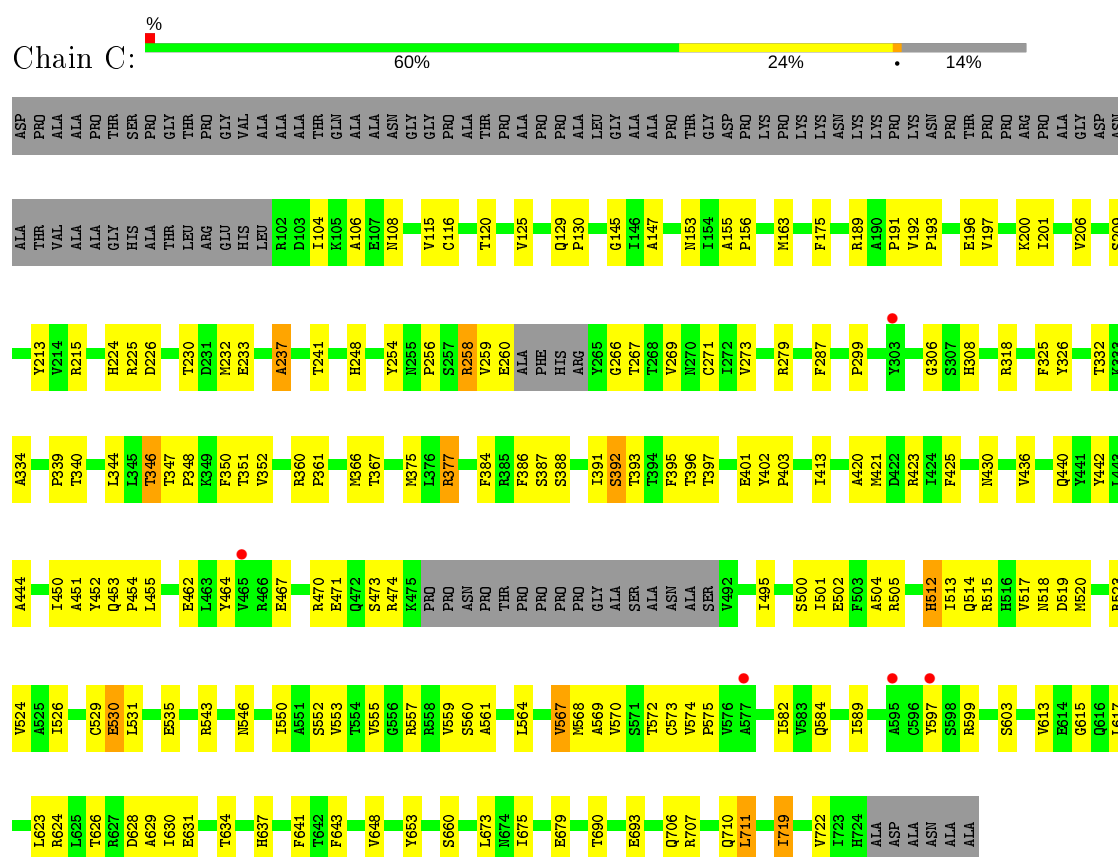
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

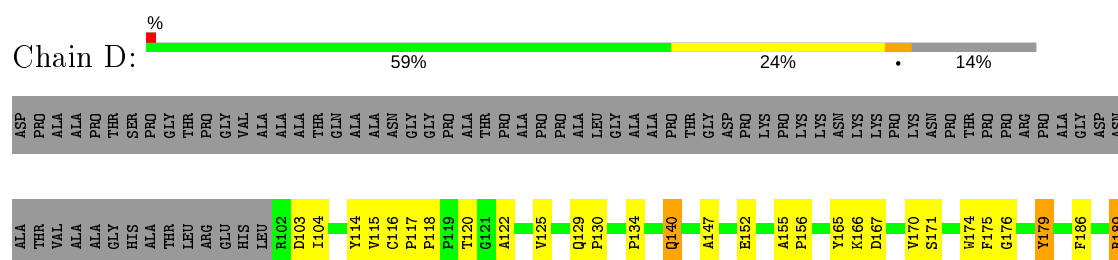
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total	O	0	0
			32	32		
5	B	17	Total	O	0	0
			17	17		
5	C	12	Total	O	0	0
			12	12		
5	D	15	Total	O	0	0
			15	15		

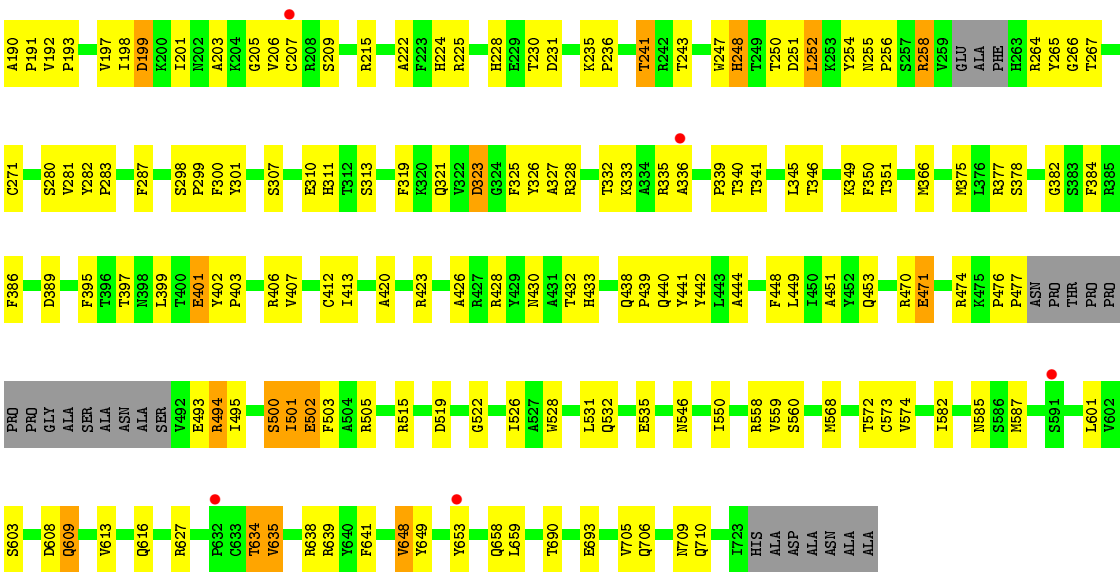


• Molecule 1: Envelope glycoprotein B



• Molecule 1: Envelope glycoprotein B





4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	117.80Å 117.80Å 318.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.54 – 3.00 50.37 – 2.82	Depositor EDS
% Data completeness (in resolution range)	93.3 (41.54-3.00) 86.6 (50.37-2.82)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.197 , 0.249 0.194 , 0.250	Depositor DCC
R_{free} test set	5715 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l 0.460 for h,-h-k,-l 0.039 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19321	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5300e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/4931	0.43	0/6708
1	B	0.24	0/4884	0.42	0/6644
1	C	0.23	0/4840	0.41	0/6599
1	D	0.24	0/4930	0.42	0/6713
All	All	0.24	0/19585	0.42	0/26664

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4814	0	4593	89	0
1	B	4762	0	4552	115	0
1	C	4727	0	4425	116	0
1	D	4813	0	4565	126	0
2	A	42	0	39	2	0
2	B	14	0	13	0	0
2	C	42	0	39	0	0
2	D	14	0	13	0	0
3	A	8	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	10	3	0
4	A	1	0	0	0	0
5	A	32	0	0	2	0
5	B	17	0	0	2	0
5	C	12	0	0	0	0
5	D	15	0	0	0	0
All	All	19321	0	18259	444	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 12.

The worst 5 of 444 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:C:116:CYS:HB3	1:C:560:SER:HB2	1.52	0.90
1:D:140:GLN:HE21	1:D:378:SER:HB2	1.37	0.90
1:A:116:CYS:HB3	1:A:560:SER:HB2	1.52	0.89
1:A:189:ARG:HB2	1:A:349:LYS:HE2	1.54	0.88
1:A:397:THR:HG21	1:A:442:TYR:HB3	1.58	0.83

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	599/703 (85%)	544 (91%)	51 (8%)	4 (1%)	22	60
1	B	591/703 (84%)	543 (92%)	47 (8%)	1 (0%)	47	82
1	C	597/703 (85%)	543 (91%)	52 (9%)	2 (0%)	41	76
1	D	599/703 (85%)	535 (89%)	61 (10%)	3 (0%)	29	68
All	All	2386/2812 (85%)	2165 (91%)	211 (9%)	10 (0%)	34	72

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	244	SER
1	C	237	ALA
1	D	199	ASP
1	A	413	ILE
1	A	688	VAL

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	512/593 (86%)	495 (97%)	17 (3%)	38	73
1	B	507/593 (86%)	482 (95%)	25 (5%)	25	61
1	C	494/593 (83%)	474 (96%)	20 (4%)	31	68
1	D	511/593 (86%)	482 (94%)	29 (6%)	20	56
All	All	2024/2372 (85%)	1933 (96%)	91 (4%)	27	64

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	721	THR
1	C	392	SER
1	D	558	ARG
1	C	108	ASN
1	C	258	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	453	GLN
1	C	709	ASN
1	D	181	GLN
1	B	468	HIS
1	D	140	GLN

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 ⓘ

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	$\# Z > 2$
2	NAG	C	1141	1	14,14,15	0.53	0	17,19,21	0.91	1 (5%)
2	NAG	A	1141	1	14,14,15	0.50	0	17,19,21	1.17	1 (5%)
2	NAG	A	1674	1	14,14,15	0.48	0	17,19,21	0.87	0
3	MRY	B	4000	-	7,7,7	0.61	0	8,8,8	0.87	0
2	NAG	B	1430	1	14,14,15	0.63	0	17,19,21	0.96	1 (5%)
2	NAG	C	1674	1	14,14,15	0.50	0	17,19,21	0.77	0
2	NAG	D	1141	1	14,14,15	0.52	0	17,19,21	0.76	0
3	MRY	A	4000	-	7,7,7	0.57	0	8,8,8	0.94	0
2	NAG	C	1398	1	14,14,15	0.49	0	17,19,21	0.83	1 (5%)
2	NAG	A	1398	1	14,14,15	0.58	0	17,19,21	0.76	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
2	NAG	C	1141	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1141	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1674	1	-	0/6/23/26	0/1/1/1
3	MRY	B	4000	-	-	1/8/8/8	-
2	NAG	B	1430	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1674	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1141	1	-	1/6/23/26	0/1/1/1
3	MRY	A	4000	-	-	0/8/8/8	-
2	NAG	C	1398	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1398	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1141	NAG	C1-O5-C5	3.01	116.27	112.19
2	B	1430	NAG	C1-O5-C5	2.36	115.39	112.19
2	C	1141	NAG	C1-O5-C5	2.35	115.38	112.19
2	C	1398	NAG	C1-O5-C5	2.10	115.03	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1398	NAG	C4-C5-C6-O6
2	A	1398	NAG	O5-C5-C6-O6
2	B	1430	NAG	C1-C2-N2-C7
2	C	1398	NAG	O5-C5-C6-O6
2	D	1141	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1141	NAG	1	0
3	B	4000	MRY	3	0
2	A	1398	NAG	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 [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	605/703 (86%)	-0.42	6 (0%) 82 59	5, 46, 115, 474	0
1	B	596/703 (84%)	-0.40	5 (0%) 86 65	9, 53, 129, 232	0
1	C	603/703 (85%)	-0.31	5 (0%) 86 65	19, 72, 139, 454	0
1	D	605/703 (86%)	-0.39	5 (0%) 86 65	17, 62, 124, 292	0
All	All	2409/2812 (85%)	-0.38	21 (0%) 84 63	5, 59, 129, 474	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	595	ALA	7.9
1	B	591	SER	5.2
1	C	577	ALA	4.9
1	D	336	ALA	4.3
1	A	650	PHE	4.2

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](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	D	1141	14/15	0.85	0.22	116,116,116,116	0
2	NAG	C	1141	14/15	0.89	0.13	113,113,113,113	0
4	NA	A	751	1/1	0.90	0.27	63,63,63,63	0
3	MRY	A	4000	8/8	0.91	0.26	54,54,54,54	0
2	NAG	C	1398	14/15	0.92	0.11	94,94,94,94	0
2	NAG	B	1430	14/15	0.93	0.13	85,85,85,85	0
2	NAG	C	1674	14/15	0.93	0.10	87,87,87,87	0
2	NAG	A	1141	14/15	0.93	0.10	81,81,81,81	0
3	MRY	B	4000	8/8	0.94	0.14	47,47,47,47	0
2	NAG	A	1674	14/15	0.95	0.10	73,73,73,73	0
2	NAG	A	1398	14/15	0.96	0.09	52,58,58,58	0

6.5 Other polymers

There are no such residues in this entry.