



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6ESC / pdb_00006esc
Title : Crystal structure of Pseudorabies virus glycoprotein B
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Deposited on : 2017-10-20
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

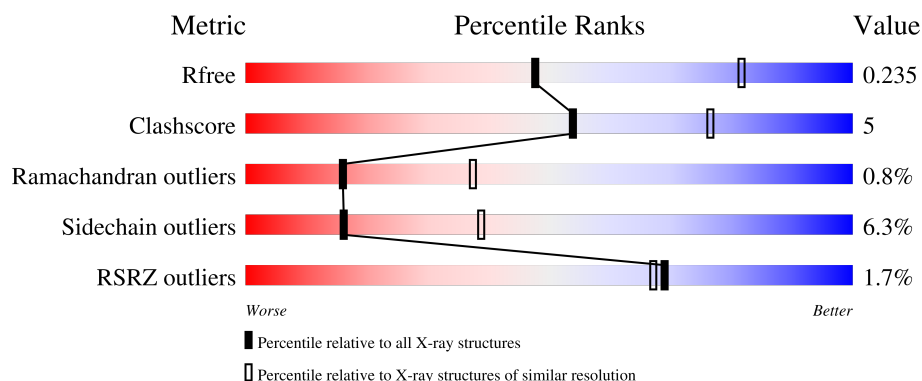
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	739	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4875 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
			Total	C	N	O	S			
1	A	594	4763	2987	865	893	18	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

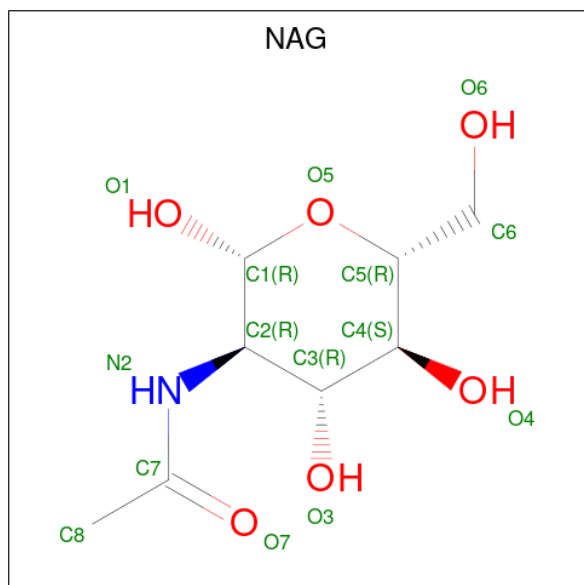
Chain	Residue	Modelled	Actual	Comment	Reference
A	757	SER	-	expression tag	UNP G3G8X1
A	758	ARG	-	expression tag	UNP G3G8X1
A	759	PHE	-	expression tag	UNP G3G8X1
A	760	GLU	-	expression tag	UNP G3G8X1
A	761	SER	-	expression tag	UNP G3G8X1
A	762	ASP	-	expression tag	UNP G3G8X1
A	763	ASP	-	expression tag	UNP G3G8X1
A	764	ASP	-	expression tag	UNP G3G8X1
A	765	ASP	-	expression tag	UNP G3G8X1
A	766	LYS	-	expression tag	UNP G3G8X1
A	767	ALA	-	expression tag	UNP G3G8X1
A	768	GLY	-	expression tag	UNP G3G8X1
A	769	TRP	-	expression tag	UNP G3G8X1
A	770	SER	-	expression tag	UNP G3G8X1
A	771	HIS	-	expression tag	UNP G3G8X1
A	772	PRO	-	expression tag	UNP G3G8X1
A	773	GLN	-	expression tag	UNP G3G8X1
A	774	PHE	-	expression tag	UNP G3G8X1
A	775	GLU	-	expression tag	UNP G3G8X1
A	776	LYS	-	expression tag	UNP G3G8X1
A	777	GLY	-	expression tag	UNP G3G8X1
A	778	GLY	-	expression tag	UNP G3G8X1
A	779	GLY	-	expression tag	UNP G3G8X1
A	780	SER	-	expression tag	UNP G3G8X1
A	781	GLY	-	expression tag	UNP G3G8X1
A	782	GLY	-	expression tag	UNP G3G8X1
A	783	GLY	-	expression tag	UNP G3G8X1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	784	SER	-	expression tag	UNP G3G8X1
A	785	GLY	-	expression tag	UNP G3G8X1
A	786	GLY	-	expression tag	UNP G3G8X1
A	787	GLY	-	expression tag	UNP G3G8X1
A	788	SER	-	expression tag	UNP G3G8X1
A	789	TRP	-	expression tag	UNP G3G8X1
A	790	SER	-	expression tag	UNP G3G8X1
A	791	HIS	-	expression tag	UNP G3G8X1
A	792	PRO	-	expression tag	UNP G3G8X1
A	793	GLN	-	expression tag	UNP G3G8X1
A	794	PHE	-	expression tag	UNP G3G8X1
A	795	GLU	-	expression tag	UNP G3G8X1
A	796	LYS	-	expression tag	UNP G3G8X1

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

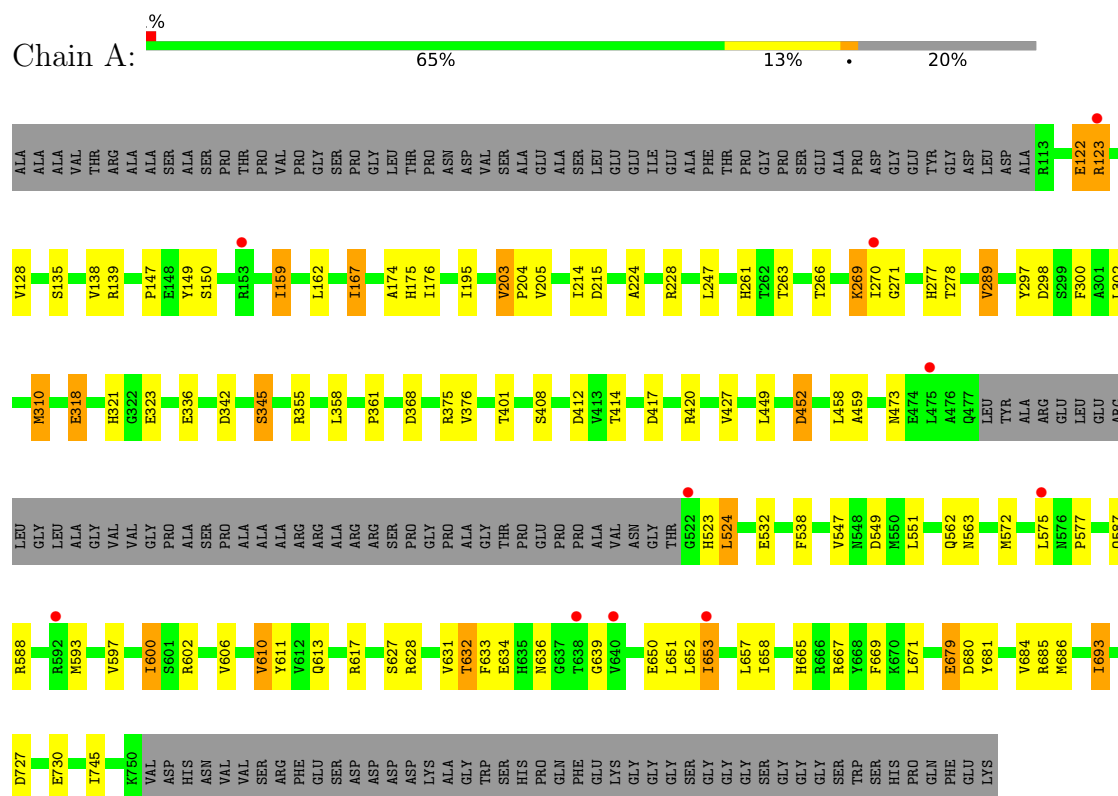
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	92	Total	O	0	0
			92	92		

3 Residue-property plots

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: Envelope glycoprotein B



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	99.89Å 99.89Å 272.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.15 – 2.70 46.15 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.15-2.70) 99.8 (46.15-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.193 , 0.236 0.191 , 0.235	Depositor DCC
R_{free} test set	1385 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.3	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4875	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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, 0.333 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	A	0.89	4/4869 (0.1%)	1.35	31/6608 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	310	MET	SD-CE	-7.91	1.59	1.79
1	A	572	MET	SD-CE	-6.97	1.62	1.79
1	A	653	ILE	CG1-CD1	5.93	1.74	1.51
1	A	205	VAL	CA-C	5.82	1.57	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	ASP	CA-CB-CG	7.46	120.06	112.60
1	A	345	SER	N-CA-C	-7.46	97.10	108.96
1	A	167	ILE	N-CA-CB	-7.19	102.43	112.35
1	A	693	ILE	CB-CA-C	6.68	120.52	110.63
1	A	215	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	563	ASN	CA-CB-CG	6.23	118.83	112.60
1	A	549	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	269	LYS	CA-C-N	5.97	130.35	122.95
1	A	269	LYS	C-N-CA	5.97	130.35	122.95
1	A	167	ILE	CB-CA-C	5.86	117.26	110.88
1	A	636	ASN	CA-CB-CG	5.80	118.40	112.60
1	A	652	LEU	CA-C-N	5.80	128.70	120.53
1	A	652	LEU	C-N-CA	5.80	128.70	120.53
1	A	562	GLN	CA-C-N	5.73	127.89	120.44
1	A	562	GLN	C-N-CA	5.73	127.89	120.44
1	A	300	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	368	ASP	CA-CB-CG	5.38	117.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	613	GLN	CA-C-N	5.36	128.20	120.38
1	A	613	GLN	C-N-CA	5.36	128.20	120.38
1	A	167	ILE	CA-CB-CG2	5.28	119.47	110.50
1	A	538	PHE	CA-C-N	5.21	128.03	120.79
1	A	538	PHE	C-N-CA	5.21	128.03	120.79
1	A	203	VAL	N-CA-CB	-5.15	104.00	111.21
1	A	375	ARG	N-CA-C	5.08	116.89	111.36
1	A	302	LEU	CA-C-N	5.04	128.74	120.63
1	A	302	LEU	C-N-CA	5.04	128.74	120.63
1	A	122	GLU	N-CA-C	-5.04	102.41	109.96
1	A	473	ASN	CA-C-N	5.01	127.00	120.28
1	A	473	ASN	C-N-CA	5.01	127.00	120.28
1	A	459	ALA	CA-C-N	5.01	127.88	120.82
1	A	459	ALA	C-N-CA	5.01	127.88	120.82

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	4763	0	4629	46	0
2	A	14	0	13	0	0
3	A	6	0	8	0	0
4	A	92	0	0	1	0
All	All	4875	0	4650	46	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 5.

All (46) 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:653:ILE:CD1	1:A:653:ILE:CG1	1.74	1.64
1:A:310:MET:CE	1:A:358:LEU:HD13	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:VAL:O	1:A:551:LEU:HG	1.95	0.66
1:A:128:VAL:HG23	1:A:606:VAL:HG22	1.84	0.59
1:A:587:GLN:NE2	1:A:602:ARG:HH11	2.00	0.58
1:A:310:MET:HE1	1:A:358:LEU:HD13	1.86	0.57
1:A:203:VAL:HG11	1:A:224:ALA:HB1	1.86	0.57
1:A:138:VAL:HG22	1:A:600:ILE:HD13	1.86	0.57
1:A:577:PRO:HG3	1:A:593:MET:HG2	1.87	0.56
1:A:606:VAL:HG21	1:A:651:LEU:HD12	1.89	0.55
1:A:587:GLN:HE21	1:A:602:ARG:HH11	1.55	0.55
1:A:128:VAL:CG2	1:A:606:VAL:HG22	2.36	0.54
1:A:634:GLU:HG3	1:A:639:GLY:O	2.07	0.54
1:A:417:ASP:H	1:A:420:ARG:HH21	1.56	0.53
1:A:269:LYS:HB3	1:A:277:HIS:HB3	1.89	0.53
1:A:128:VAL:HG23	1:A:606:VAL:CG2	2.38	0.53
1:A:297:TYR:CE2	1:A:376:VAL:HG11	2.44	0.53
1:A:611:TYR:HB2	1:A:632:THR:HG22	1.91	0.52
1:A:665:HIS:CD2	1:A:681:TYR:H	2.29	0.50
1:A:175:HIS:CD2	1:A:355:ARG:HH22	2.29	0.50
1:A:628:ARG:HD2	1:A:657:LEU:HD13	1.94	0.50
1:A:679:GLU:HB2	1:A:684:VAL:HG21	1.94	0.49
1:A:214:ILE:HG12	1:A:247:LEU:HD11	1.97	0.47
1:A:204:PRO:HD3	1:A:361:PRO:O	2.16	0.46
1:A:685:ARG:HE	1:A:685:ARG:HB2	1.61	0.46
1:A:610:VAL:HG13	1:A:633:PHE:HB3	1.98	0.46
1:A:159:ILE:HD12	1:A:449:LEU:HD21	1.97	0.46
1:A:138:VAL:HG22	1:A:600:ILE:CD1	2.46	0.46
1:A:175:HIS:HD2	1:A:355:ARG:HH22	1.62	0.45
1:A:261:HIS:HD2	1:A:263:THR:O	1.99	0.44
1:A:128:VAL:CG2	1:A:606:VAL:CG2	2.95	0.44
1:A:271:GLY:HA3	1:A:277:HIS:CE1	2.52	0.44
1:A:342:ASP:HB3	1:A:345:SER:O	2.17	0.43
1:A:631:VAL:HG21	1:A:651:LEU:HD22	2.00	0.43
1:A:122:GLU:O	1:A:123:ARG:HB2	2.18	0.43
1:A:665:HIS:HB3	1:A:680:ASP:HA	2.00	0.43
1:A:667:ARG:HB3	1:A:669:PHE:CE2	2.54	0.43
1:A:727:ASP:HB3	1:A:730:GLU:HB2	2.01	0.42
1:A:147:PRO:HB2	1:A:149:TYR:CE2	2.54	0.42
1:A:269:LYS:HE2	1:A:278:THR:O	2.21	0.41
1:A:318:GLU:HA	1:A:321:HIS:CE1	2.56	0.41
1:A:588:ARG:NH2	1:A:650:GLU:HB2	2.36	0.41
1:A:174:ALA:HB3	1:A:289:VAL:HG12	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:HD2	4:A:1110:HOH:O	2.21	0.40
1:A:420:ARG:HD2	1:A:524:LEU:HD12	2.02	0.40
1:A:671:LEU:HD23	1:A:686:MET:HE1	2.03	0.40

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	590/739 (80%)	554 (94%)	31 (5%)	5 (1%)	16 37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ARG
1	A	150	SER
1	A	427	VAL
1	A	318	GLU
1	A	452	ASP

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	509/612 (83%)	477 (94%)	32 (6%)	16 39

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	SER
1	A	159	ILE
1	A	162	LEU
1	A	167	ILE
1	A	176	ILE
1	A	195	ILE
1	A	228	ARG
1	A	266	THR
1	A	270	ILE
1	A	289	VAL
1	A	323	GLU
1	A	336	GLU
1	A	401	THR
1	A	408	SER
1	A	412	ASP
1	A	414	THR
1	A	452	ASP
1	A	458	LEU
1	A	523	HIS
1	A	524	LEU
1	A	532	GLU
1	A	575	LEU
1	A	597	VAL
1	A	600	ILE
1	A	610	VAL
1	A	617	ARG
1	A	627	SER
1	A	632	THR
1	A	658	ILE
1	A	679	GLU
1	A	693	ILE
1	A	745	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	175	HIS
1	A	197	ASN
1	A	208	GLN
1	A	241	ASN

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Mol	Chain	Res	Type
1	A	261	HIS
1	A	333	GLN
1	A	444	ASN
1	A	477	GLN
1	A	544	GLN
1	A	587	GLN
1	A	614	ASN
1	A	635	HIS
1	A	665	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	NAG	A	1001	1	14,14,15	0.36	0	17,19,21	1.13	1 (5%)
3	GOL	A	1002	-	5,5,5	0.24	0	5,5,5	0.50	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	A	1001	1	-	0/6/23/26	0/1/1/1
3	GOL	A	1002	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	NAG	C1-O5-C5	4.31	117.97	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	GOL	C1-C2-C3-O3
3	A	1002	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	594/739 (80%)	-0.10	10 (1%) 69 67	45, 69, 110, 147	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	ILE	4.0
1	A	475	LEU	2.9
1	A	653	ILE	2.8
1	A	522	GLY	2.4
1	A	638	THR	2.4
1	A	592	ARG	2.3
1	A	575	LEU	2.2
1	A	123	ARG	2.1
1	A	640	VAL	2.1
1	A	153	ARG	2.1

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	NAG	A	1001	14/15	0.90	0.09	76,83,90,92	0
3	GOL	A	1002	6/6	0.93	0.11	59,68,72,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.