



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:03 AM GMT

PDB ID : 3NW8
Title : Glycoprotein B from Herpes simplex virus type 1, Y179S mutant, high-pH
Authors : Stampfer, S.D.; Lou, H.; Cohen, G.H.; Eisenberg, R.J.; Heldwein, E.E.
Deposited on : 2010-07-09
Resolution : 2.76 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

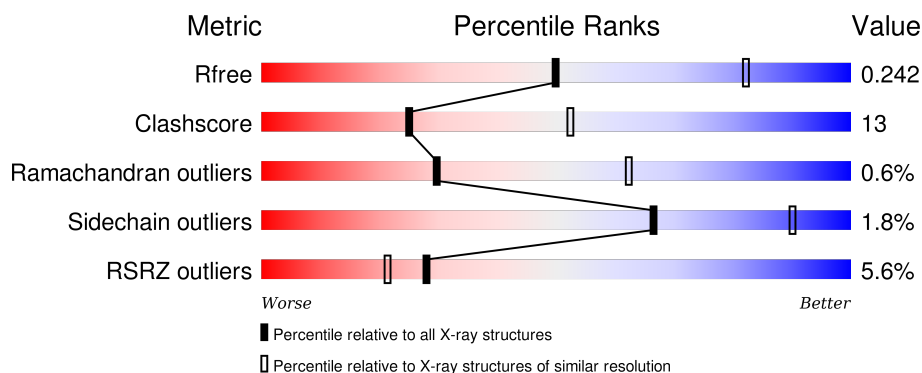
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	703	<div> <div>4%</div> <div>62% 23% • 14%</div> </div>
1	B	703	<div> <div>6%</div> <div>63% 22% • 14%</div> </div>
1	C	703	<div> <div>6%</div> <div>59% 27% 14%</div> </div>
1	D	703	<div> <div>4%</div> <div>64% 21% • 13%</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
2	NAG	B	1674	X	-	-	-
3	MRY	A	2000	-	-	-	X
3	MRY	A	2001	-	-	-	X
3	MRY	A	2002	-	-	-	X
3	MRY	B	2000	-	-	-	X
3	MRY	B	2001	-	-	-	X
3	MRY	C	2000	-	-	-	X
3	MRY	D	2000	-	-	-	X
4	NA	C	1	-	-	-	X
4	NA	D	3	-	-	-	X
6	NAG	C	1398	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 19958 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	B	606	Total	C	N	O	S	0	0	0
			4857	3062	852	921	22			
1	A	607	Total	C	N	O	S	0	0	0
			4863	3062	856	923	22			
1	C	605	Total	C	N	O	S	0	0	0
			4853	3059	856	916	22			
1	D	609	Total	C	N	O	S	0	0	0
			4881	3077	861	921	22			

There are 24 discrepancies between the modelled and reference sequences:

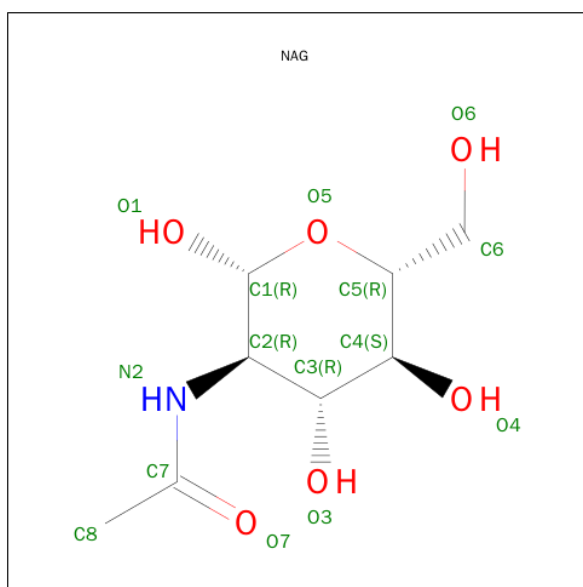
Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ASP	-	EXPRESSION TAG	UNP P06437
B	29	PRO	-	EXPRESSION TAG	UNP P06437
B	58	ALA	PRO	SEE REMARK 999	UNP P06437
B	179	SER	TYR	ENGINEERED MUTATION	UNP P06437
B	313	SER	THR	SEE REMARK 999	UNP P06437
B	443	LEU	GLN	SEE REMARK 999	UNP P06437
A	28	ASP	-	EXPRESSION TAG	UNP P06437
A	29	PRO	-	EXPRESSION TAG	UNP P06437
A	58	ALA	PRO	SEE REMARK 999	UNP P06437
A	179	SER	TYR	ENGINEERED MUTATION	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	179	SER	TYR	ENGINEERED MUTATION	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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	179	SER	TYR	ENGINEERED MUTATION	UNP P06437
D	313	SER	THR	SEE REMARK 999	UNP P06437
D	443	LEU	GLN	SEE REMARK 999	UNP P06437

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



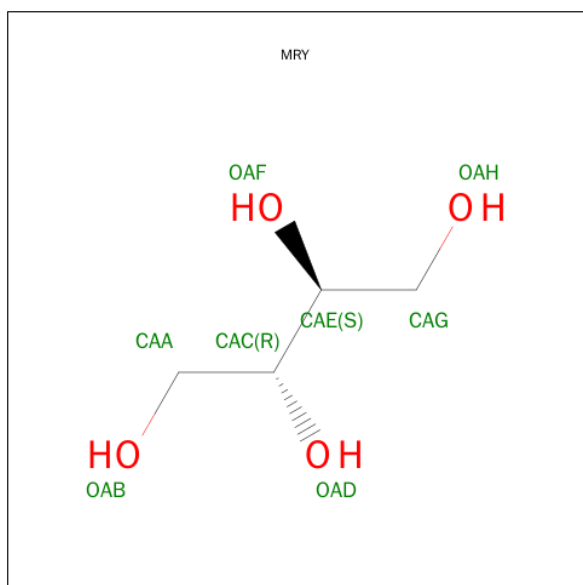
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	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	B	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		
4	C	2	Total	Na	0	0
			2	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

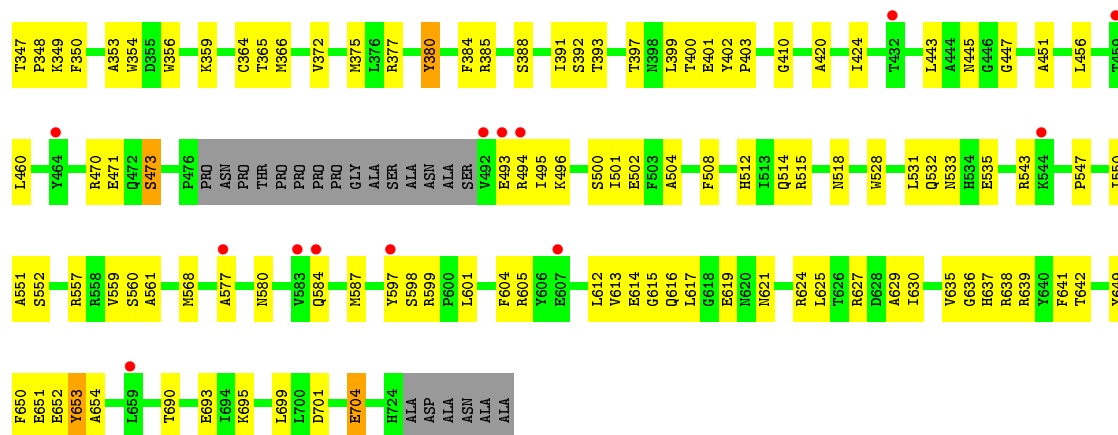
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

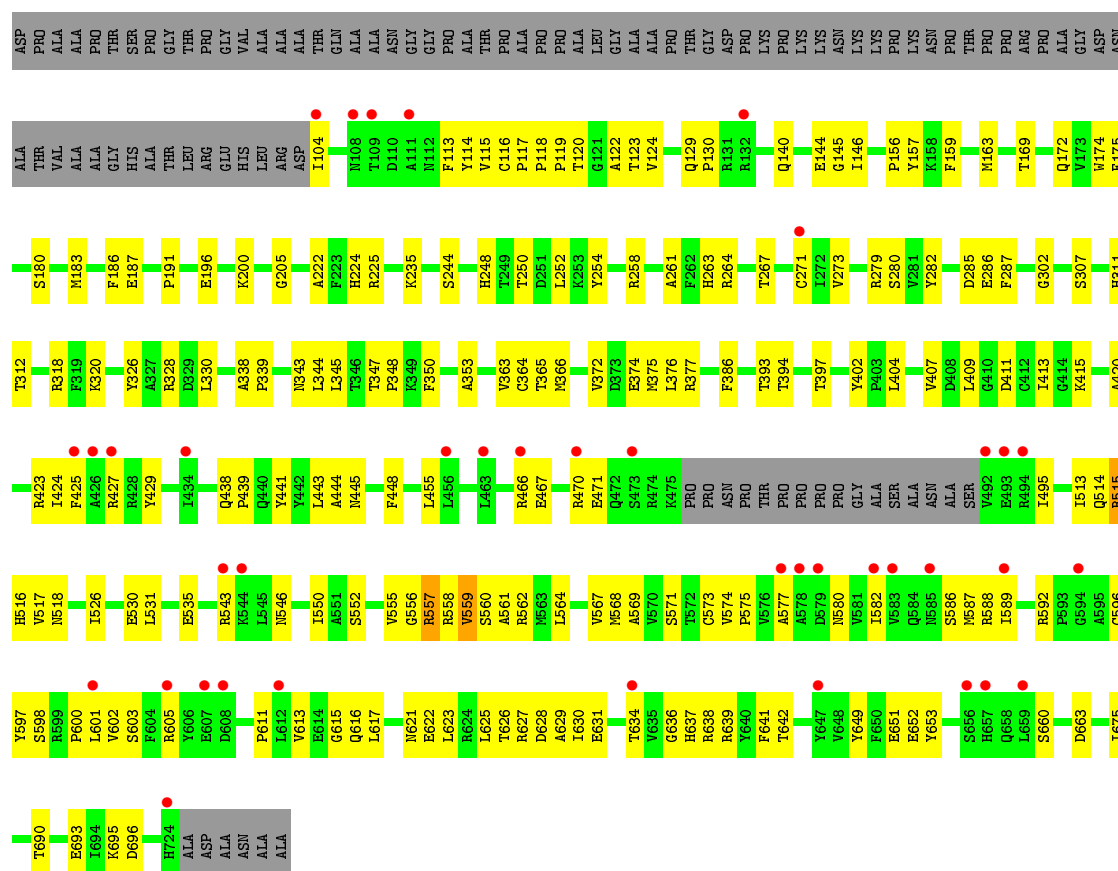
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	2	Total	C	N	O	0	0
			28	16	2	10		
6	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is water.

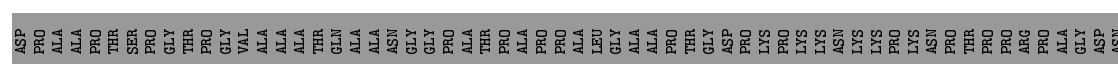
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	61	Total	O	0	0
			61	61		
7	A	53	Total	O	0	0
			53	53		
7	C	44	Total	O	0	0
			44	44		
7	D	51	Total	O	0	0
			51	51		

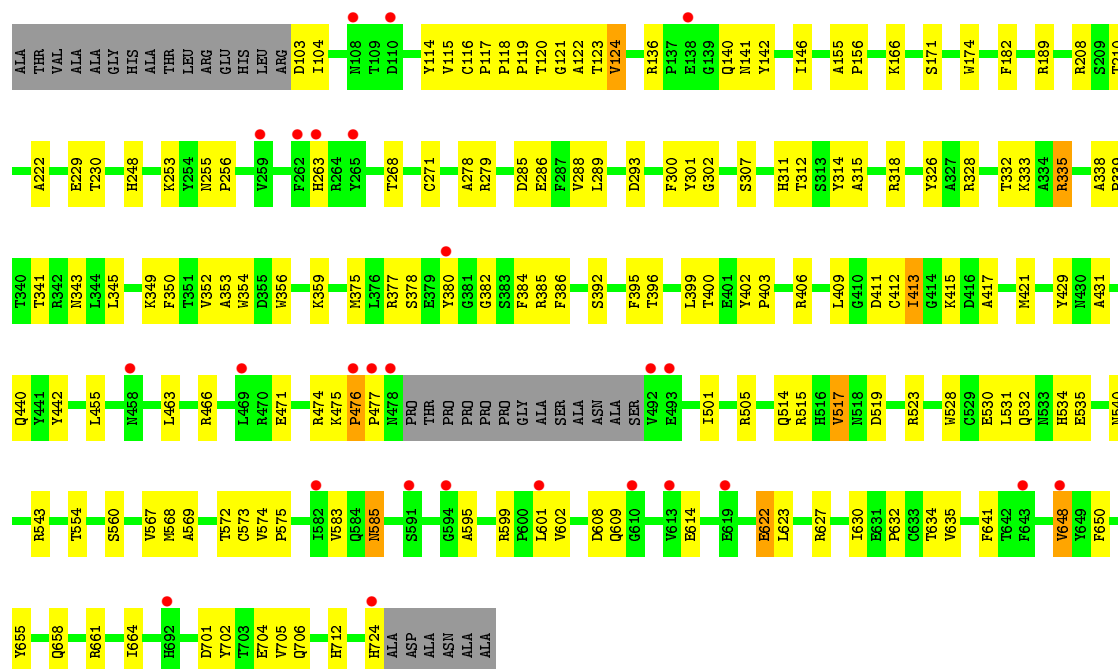


• Molecule 1: Envelope glycoprotein B



• 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	117.98Å 117.98Å 321.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.69 – 2.76 48.69 – 2.76	Depositor EDS
% Data completeness (in resolution range)	84.4 (48.69-2.76) 84.4 (48.69-2.76)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.202 , 0.242 0.198 , 0.242	Depositor DCC
R_{free} test set	5311 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.3	EDS
Estimated twinning fraction	0.019 for -h,-k,l 0.477 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 118749 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	19958	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 60.86 % 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 1.4278e-05. 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CL, MRY, 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	0.23	0/4981	0.40	0/6771
1	B	0.23	0/4976	0.40	0/6764
1	C	0.23	0/4972	0.40	0/6757
1	D	0.23	0/5001	0.41	0/6800
All	All	0.23	0/19930	0.40	0/27092

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	4863	0	4644	118	0
1	B	4857	0	4637	124	0
1	C	4853	0	4637	130	0
1	D	4881	0	4668	116	0
2	A	56	0	52	1	0
2	B	42	0	39	0	0
2	C	28	0	26	1	0
2	D	28	0	26	0	0
3	A	32	0	40	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	20	3	0
3	C	24	0	30	2	0
3	D	8	0	10	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
6	C	28	0	25	2	0
6	D	28	0	25	1	0
7	A	53	0	0	0	0
7	B	61	0	0	3	0
7	C	44	0	0	1	0
7	D	51	0	0	0	0
All	All	19958	0	18879	490	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 13.

The worst 5 of 490 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:HB3	1.37	1.03
1:A:116:CYS:HB3	1:A:560:SER:HB3	1.53	0.89
1:C:119:PRO:HD2	1:C:562:ARG:HG3	1.54	0.89
1:D:400:THR:HB	1:D:476:PRO:HG3	1.57	0.87
1:C:466:ARG:HH11	1:C:470:ARG:HH22	1.20	0.86

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	603/703 (86%)	556 (92%)	43 (7%)	4 (1%)	26	59
1	B	602/703 (86%)	543 (90%)	56 (9%)	3 (0%)	34	67
1	C	601/703 (86%)	551 (92%)	47 (8%)	3 (0%)	34	67
1	D	605/703 (86%)	545 (90%)	56 (9%)	4 (1%)	26	59
All	All	2411/2812 (86%)	2195 (91%)	202 (8%)	14 (1%)	30	62

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	476	PRO
1	B	401	GLU
1	A	653	TYR
1	A	699	LEU
1	B	642	THR

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	520/593 (88%)	514 (99%)	6 (1%)	78	94
1	B	520/593 (88%)	511 (98%)	9 (2%)	68	90
1	C	518/593 (87%)	511 (99%)	7 (1%)	74	92
1	D	522/593 (88%)	507 (97%)	15 (3%)	50	81
All	All	2080/2372 (88%)	2043 (98%)	37 (2%)	66	90

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	140	GLN
1	C	559	VAL
1	D	648	VAL
1	C	187	GLU
1	C	235	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	321	GLN
1	C	580	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 ⓘ

4 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	C	1398	1,6	14,14,15	0.57	0	15,19,21	0.91	1 (6%)
6	NAG	C	1399	6	14,14,15	0.48	0	15,19,21	0.85	0
6	NAG	D	1398	1,6	14,14,15	0.55	0	15,19,21	0.68	0
6	NAG	D	1399	6	14,14,15	0.44	0	15,19,21	0.82	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
6	NAG	C	1398	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	1399	6	-	0/6/23/26	0/1/1/1
6	NAG	D	1398	1,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	1399	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1398	NAG	C1-O5-C5	2.18	115.01	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1398	NAG	2	0
6	D	1398	NAG	1	0
6	D	1399	NAG	1	0

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 5 are monoatomic - leaving 21 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	A	1141	1	14,14,15	0.50	0	15,19,21	0.67	0
2	NAG	A	1398	1	14,14,15	0.44	0	15,19,21	0.82	0
2	NAG	A	1430	-	14,14,15	0.54	0	15,19,21	0.80	0
2	NAG	A	1674	1	14,14,15	0.51	0	15,19,21	0.59	0
3	MRY	A	2000	-	7,7,7	0.37	0	6,8,8	0.44	0
3	MRY	A	2001	-	7,7,7	0.26	0	6,8,8	0.47	0
3	MRY	A	2002	-	7,7,7	0.30	0	6,8,8	0.47	0
3	MRY	A	731	-	7,7,7	0.29	0	6,8,8	0.50	0
2	NAG	B	1141	1	14,14,15	0.55	0	15,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1398	1	14,14,15	0.49	0	15,19,21	0.81	1 (6%)
2	NAG	B	1674	1	14,14,15	0.51	0	15,19,21	0.63	0
3	MRY	B	2000	-	7,7,7	0.26	0	6,8,8	0.39	0
3	MRY	B	2001	-	7,7,7	0.33	0	6,8,8	0.26	0
2	NAG	C	1430	1	14,14,15	0.43	0	15,19,21	1.38	1 (6%)
2	NAG	C	1674	1	14,14,15	0.53	0	15,19,21	0.67	0
3	MRY	C	2000	-	7,7,7	0.28	0	6,8,8	0.42	0
3	MRY	C	2001	-	7,7,7	0.50	0	6,8,8	0.34	0
3	MRY	C	2002	-	7,7,7	0.27	0	6,8,8	0.50	0
2	NAG	D	1141	1	14,14,15	0.50	0	15,19,21	0.76	0
2	NAG	D	1430	1	14,14,15	0.46	0	15,19,21	1.25	2 (13%)
3	MRY	D	2000	-	7,7,7	0.28	0	6,8,8	0.39	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	1141	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1398	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1430	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1674	1	-	0/6/23/26	0/1/1/1
3	MRY	A	2000	-	-	0/8/8/8	0/0/0/0
3	MRY	A	2001	-	-	0/8/8/8	0/0/0/0
3	MRY	A	2002	-	-	0/8/8/8	0/0/0/0
3	MRY	A	731	-	-	0/8/8/8	0/0/0/0
2	NAG	B	1141	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1398	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1674	1	1/1/5/7	0/6/23/26	0/1/1/1
3	MRY	B	2000	-	-	0/8/8/8	0/0/0/0
3	MRY	B	2001	-	-	0/8/8/8	0/0/0/0
2	NAG	C	1430	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1674	1	-	0/6/23/26	0/1/1/1
3	MRY	C	2000	-	-	0/8/8/8	0/0/0/0
3	MRY	C	2001	-	-	0/8/8/8	0/0/0/0
3	MRY	C	2002	-	-	0/8/8/8	0/0/0/0
2	NAG	D	1141	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1430	1	-	0/6/23/26	0/1/1/1
3	MRY	D	2000	-	-	0/8/8/8	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1430	NAG	C2-N2-C7	-2.08	120.36	123.04
2	B	1398	NAG	C1-O5-C5	2.18	115.02	112.25
2	D	1430	NAG	C1-O5-C5	2.84	115.85	112.25
2	C	1430	NAG	C1-O5-C5	4.32	117.73	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1674	NAG	C1

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1398	NAG	1	0
3	A	2002	MRY	1	0
3	B	2000	MRY	3	0
2	C	1430	NAG	1	0
3	C	2000	MRY	1	0
3	C	2001	MRY	1	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	607/703 (86%)	0.47	28 (4%)	36	29	20, 49, 110, 233	0
1	B	606/703 (86%)	0.58	42 (6%)	20	14	21, 55, 118, 212	0
1	C	605/703 (86%)	0.51	39 (6%)	23	17	21, 52, 114, 207	0
1	D	609/703 (86%)	0.48	26 (4%)	39	32	18, 51, 107, 175	0
All	All	2427/2812 (86%)	0.51	135 (5%)	28	21	18, 52, 113, 233	0

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	THR	5.4
1	D	469	LEU	5.3
1	A	459	THR	5.3
1	D	478	ASN	4.8
1	A	112	ASN	4.6

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(\AA^2)	Q<0.9
6	NAG	C	1398	14/15	0.83	0.31	6.52	100,100,100,100	0
6	NAG	D	1398	14/15	0.86	0.23	0.02	101,101,101,101	0
6	NAG	C	1399	14/15	0.76	0.41	-	105,105,105,105	0
6	NAG	D	1399	14/15	0.67	0.42	-	123,123,123,123	0

6.4 Ligands ⓘ

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
4	NA	D	3	1/1	0.89	0.73	19.84	38,38,38,38	0
3	MRY	A	2001	8/8	0.89	0.28	7.32	77,77,77,77	0
3	MRY	B	2001	8/8	0.84	0.29	5.34	75,75,75,75	0
3	MRY	C	2000	8/8	0.82	0.25	5.26	72,72,72,72	0
3	MRY	D	2000	8/8	0.79	0.28	4.41	80,80,80,80	0
3	MRY	A	2002	8/8	0.79	0.33	3.53	74,74,74,74	0
3	MRY	A	2000	8/8	0.82	0.26	3.07	42,42,42,42	0
4	NA	C	1	1/1	0.85	0.25	2.96	50,50,50,50	0
3	MRY	B	2000	8/8	0.90	0.27	2.15	53,53,53,53	0
3	MRY	A	731	8/8	0.82	0.28	1.48	65,65,65,65	0
2	NAG	B	1398	14/15	0.71	0.32	1.47	114,114,114,114	0
2	NAG	A	1398	14/15	0.89	0.18	-0.85	79,79,79,79	0
2	NAG	D	1430	14/15	0.81	0.63	-	119,119,119,119	0
2	NAG	B	1141	14/15	0.61	0.32	-	134,134,134,134	0
2	NAG	A	1674	14/15	0.71	0.35	-	70,70,70,70	0
5	CL	A	5	1/1	0.93	0.26	-	71,71,71,71	0
2	NAG	A	1430	14/15	0.71	0.35	-	96,96,96,96	0
4	NA	B	2	1/1	0.82	0.22	-	60,60,60,60	0
2	NAG	C	1430	14/15	0.86	0.40	-	91,91,91,91	0
2	NAG	B	1674	14/15	0.52	0.60	-	120,120,120,120	0
3	MRY	C	2001	8/8	0.69	0.58	-	72,72,72,72	0
4	NA	C	4	1/1	0.94	0.36	-	87,87,87,87	0
2	NAG	A	1141	14/15	0.44	0.58	-	147,147,147,147	0
2	NAG	C	1674	14/15	0.75	0.30	-	78,78,78,78	0
2	NAG	D	1141	14/15	0.64	0.31	-	63,131,131,131	0
3	MRY	C	2002	8/8	0.83	0.33	-	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.