



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2019 – 04:18 PM EDT

PDB ID : 5VC1
Title : Crystal structure of L-selectin lectin/EGF domains
Authors : Wedepohl, S.; Dervede, J.; Vahedi-Faridi, A.; Tauber, R.; Saenger, W.; Bulut, H.
Deposited on : 2017-03-30
Resolution : 1.94 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 : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

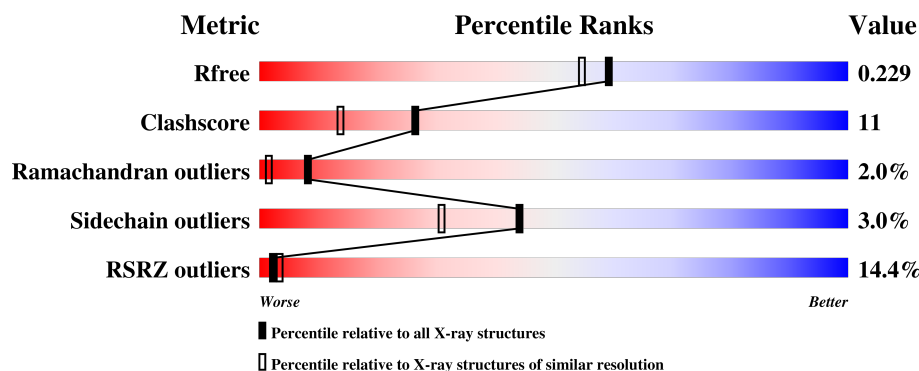
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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}	111664	3622 (1.96-1.92)
Clashscore	122126	3795 (1.96-1.92)
Ramachandran outliers	120053	3757 (1.96-1.92)
Sidechain outliers	120020	3757 (1.96-1.92)
RSRZ outliers	108989	3554 (1.96-1.92)

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	157	<div> <div>14%</div> <div>83%</div> <div>10%</div> <div>...</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
3	MAN	A	203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BMA	A	204	X	-	-	-
4	BMA	A	205	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 1431 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.

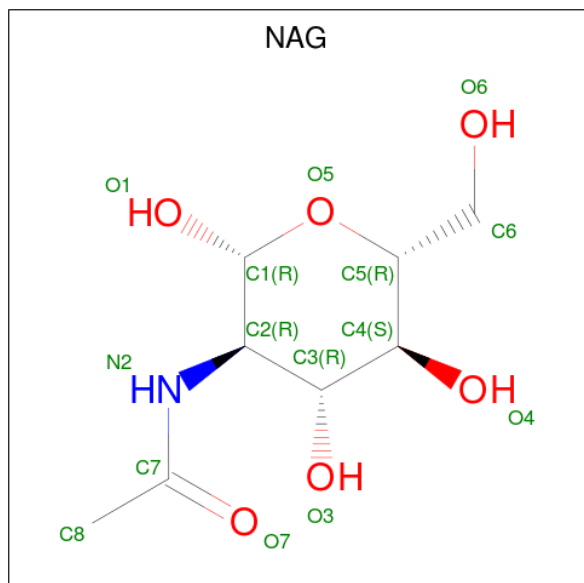
- Molecule 1 is a protein called L-selectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1266	797	219	239	11	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

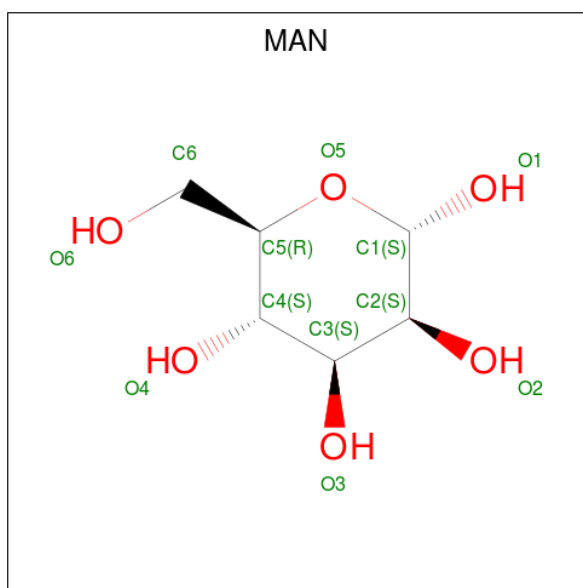
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLN	ASN	engineered mutation	UNP P14151
A	139	GLN	ASN	engineered mutation	UNP P14151

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



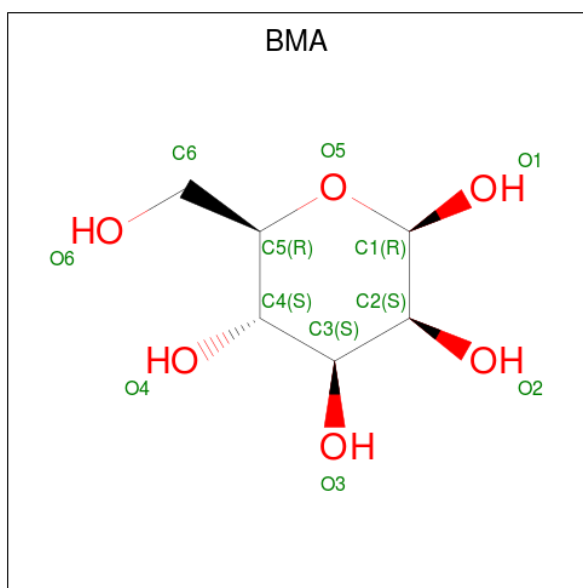
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

- Molecule 3 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



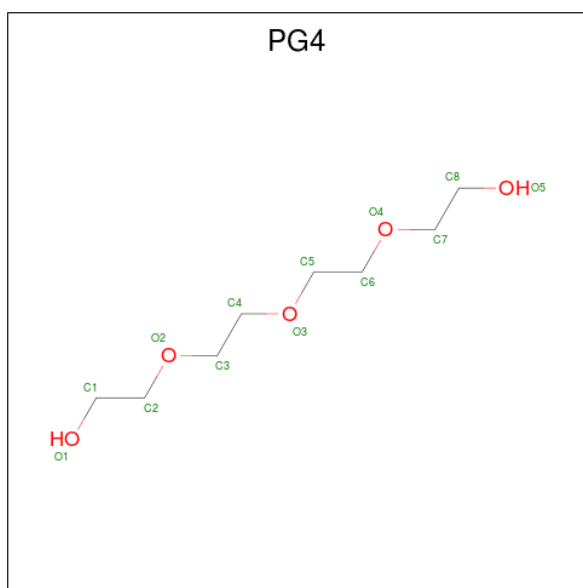
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



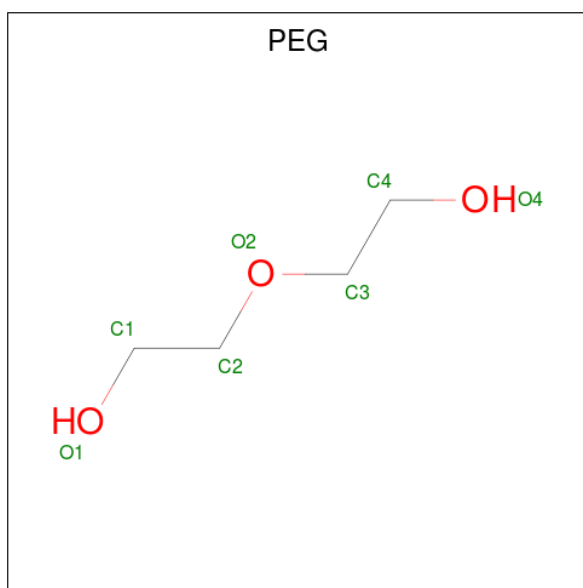
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



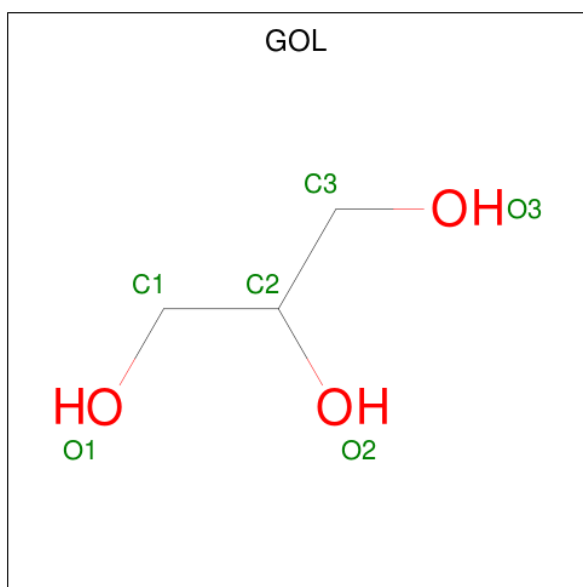
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

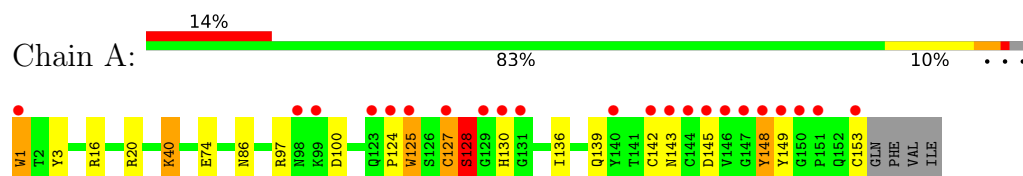
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	77	Total	O	0	0
			77	77		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: L-selectin



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	118.60Å 118.60Å 118.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.70 – 1.94 31.70 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.70-1.94) 99.9 (31.70-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.202 , 0.231 0.202 , 0.229	Depositor DCC
R_{free} test set	1034 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1431	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, CA, PG4, PEG, 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	0.45	0/1302	0.65	3/1764 (0.2%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	CYS	N-CA-C	-9.37	85.71	111.00
1	A	128	SER	N-CA-C	6.78	129.29	111.00
1	A	127	CYS	CB-CA-C	5.01	120.42	110.40

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	1266	0	1178	28	0
2	A	28	0	24	0	0
3	A	11	0	8	0	0
4	A	22	0	20	0	0
5	A	13	0	18	5	0
6	A	7	0	10	2	0
7	A	6	0	8	2	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	77	0	0	0	0
All	All	1431	0	1266	29	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 11.

All (29) 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:127:CYS:CB	1:A:142:CYS:SG	2.17	1.32
1:A:127:CYS:SG	1:A:142:CYS:CB	2.19	1.29
1:A:127:CYS:SG	1:A:142:CYS:SG	1.30	1.27
1:A:20:ARG:HH12	5:A:206:PG4:H71	1.43	0.83
1:A:127:CYS:SG	1:A:142:CYS:HB2	2.19	0.80
1:A:16:ARG:HH12	5:A:206:PG4:H42	1.57	0.69
1:A:127:CYS:HG	1:A:142:CYS:CB	1.89	0.66
1:A:128:SER:C	1:A:130:HIS:H	1.99	0.64
1:A:124:PRO:O	1:A:125:TRP:HB2	1.96	0.64
1:A:74:GLU:HG3	6:A:207:PEG:H11	1.82	0.62
1:A:127:CYS:HB3	1:A:142:CYS:SG	2.36	0.59
1:A:127:CYS:HB2	1:A:142:CYS:SG	2.34	0.58
1:A:148:TYR:HD1	1:A:149:TYR:H	1.53	0.56
1:A:136:ILE:HD11	1:A:139:GLN:HG3	1.91	0.53
1:A:130:HIS:O	1:A:153:CYS:HB3	2.09	0.52
1:A:97:ARG:HH21	1:A:100:ASP:HB3	1.74	0.52
1:A:124:PRO:O	1:A:125:TRP:CB	2.57	0.52
1:A:128:SER:C	1:A:130:HIS:N	2.64	0.50
1:A:128:SER:O	1:A:130:HIS:N	2.47	0.47
1:A:74:GLU:HG3	6:A:207:PEG:C1	2.45	0.47
1:A:1:TRP:NE1	1:A:3:TYR:CZ	2.83	0.46
1:A:97:ARG:NH2	1:A:100:ASP:HB3	2.31	0.45
1:A:16:ARG:HH12	5:A:206:PG4:H51	1.82	0.45
7:A:208:GOL:HO2	7:A:208:GOL:HO3	1.59	0.43
1:A:125:TRP:HE3	1:A:128:SER:HG	1.66	0.43
1:A:40:LYS:HD3	1:A:40:LYS:N	2.34	0.43
1:A:16:ARG:NH1	5:A:206:PG4:H42	2.31	0.41
1:A:86:ASN:O	7:A:208:GOL:H11	2.21	0.40
1:A:20:ARG:NH1	5:A:206:PG4:H71	2.24	0.40

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	152/157 (97%)	141 (93%)	8 (5%)	3 (2%)	8 1

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	TRP
1	A	145	ASP
1	A	128	SER

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	134/137 (98%)	130 (97%)	4 (3%)	44 31

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	TRP
1	A	40	LYS
1	A	143	ASN
1	A	148	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

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	$\# Z > 2$
2	NAG	A	201	1,2	14,14,15	0.26	0	17,19,21	0.42	0
2	NAG	A	202	3,2	14,14,15	0.40	0	17,19,21	0.46	0
3	MAN	A	203	2,4	11,11,12	1.14	1 (9%)	15,15,17	0.93	1 (6%)
4	BMA	A	204	8,3	11,11,12	0.98	0	15,15,17	1.15	1 (6%)
4	BMA	A	205	3	11,11,12	0.95	0	15,15,17	0.92	1 (6%)
5	PG4	A	206	-	12,12,12	0.52	0	11,11,11	0.28	0
6	PEG	A	207	-	6,6,6	0.49	0	5,5,5	0.25	0
7	GOL	A	208	-	5,5,5	0.22	0	5,5,5	0.84	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	201	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	202	3,2	-	0/6/23/26	0/1/1/1
3	MAN	A	203	2,4	1/1/4/5	0/2/19/22	0/1/1/1
4	BMA	A	204	8,3	1/1/4/5	0/2/19/22	0/1/1/1
4	BMA	A	205	3	1/1/4/5	0/2/19/22	0/1/1/1
5	PG4	A	206	-	-	5/10/10/10	-
6	PEG	A	207	-	-	3/4/4/4	-
7	GOL	A	208	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	203	MAN	O5-C1	-3.29	1.38	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	203	MAN	O2-C2-C3	-3.13	104.04	110.16
4	A	204	BMA	C1-O5-C5	2.91	116.15	112.20
4	A	205	BMA	O2-C2-C3	-2.36	105.55	110.16

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	205	BMA	C1
3	A	203	MAN	C1
4	A	204	BMA	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	208	GOL	C1-C2-C3-O3
5	A	206	PG4	O3-C5-C6-O4
5	A	206	PG4	O1-C1-C2-O2
5	A	206	PG4	O2-C3-C4-O3
6	A	207	PEG	O1-C1-C2-O2
5	A	206	PG4	O4-C7-C8-O5
7	A	208	GOL	O2-C2-C3-O3
5	A	206	PG4	C4-C3-O2-C2
6	A	207	PEG	C1-C2-O2-C3
6	A	207	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	206	PG4	5	0
6	A	207	PEG	2	0
7	A	208	GOL	2	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	153/157 (97%)	0.70	22 (14%) 2 3	16, 25, 85, 96	2 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	VAL	11.7
1	A	149	TYR	8.3
1	A	125	TRP	7.9
1	A	124	PRO	6.3
1	A	148	TYR	6.0
1	A	150	GLY	5.9
1	A	144	CYS	4.9
1	A	151	PRO	4.4
1	A	147	GLY	3.5
1	A	131	GLY	3.4
1	A	130	HIS	3.3
1	A	153	CYS	3.2
1	A	145	ASP	3.2
1	A	123	GLN	3.1
1	A	1	TRP	3.0
1	A	98	ASN	3.0
1	A	127	CYS	2.9
1	A	99	LYS	2.6
1	A	129	GLY	2.6
1	A	142	CYS	2.4
1	A	140	TYR	2.3
1	A	143	ASN	2.2

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 carbohydrates 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
7	GOL	A	208	6/6	0.73	0.34	38,42,47,53	0
5	PG4	A	206	13/13	0.83	0.24	33,42,51,52	0
4	BMA	A	205	11/12	0.84	0.20	36,41,43,44	0
6	PEG	A	207	7/7	0.89	0.15	33,38,50,50	0
2	NAG	A	201	14/15	0.91	0.13	23,32,44,46	0
2	NAG	A	202	14/15	0.94	0.14	27,30,34,35	0
3	MAN	A	203	11/12	0.94	0.12	23,27,35,35	0
4	BMA	A	204	11/12	0.96	0.10	18,20,23,25	0
8	CA	A	209	1/1	0.99	0.10	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.