



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 20, 2017 – 10:29 PM EST

PDB ID : 1LED
Title : STRUCTURES OF THE LECTIN IV OF GRIFFONIA SIMPLICIFOLIA AND ITS COMPLEX WITH THE LEWIS B HUMAN BLOOD GROUP DETERMINANT AT 2.0 ANGSTROMS RESOLUTION
Authors : Delbaere, L.; Vandonselaar, M.; Quail, J.
Deposited on : unknown
Resolution : 2.00 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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtrriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

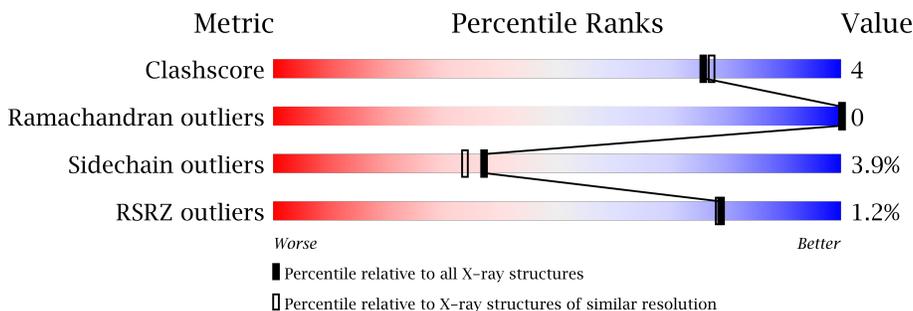
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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. 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	243	

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
8	SO4	A	500	-	-	-	X

2 Entry composition [i](#)

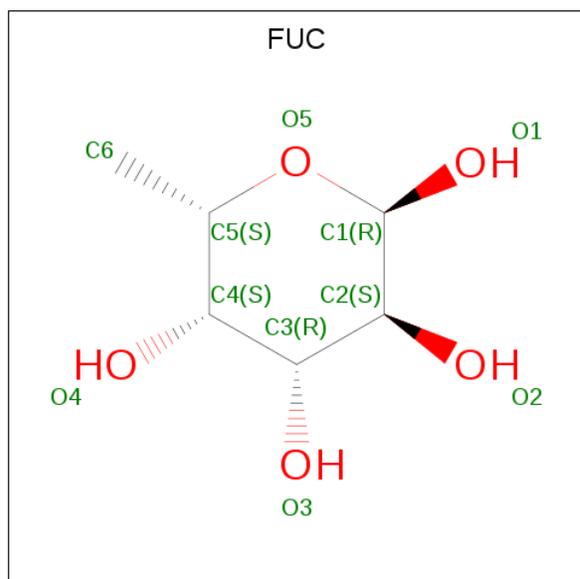
There are 9 unique types of molecules in this entry. The entry contains 2140 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 WEST-CENTRAL AFRICAN LEGUME LECTIN IV.

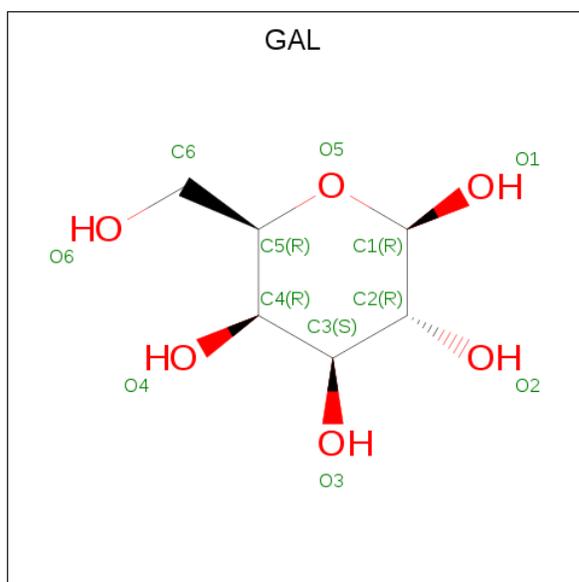
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
1	A	243	1904	1226	309	369	0	0	0

- Molecule 2 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



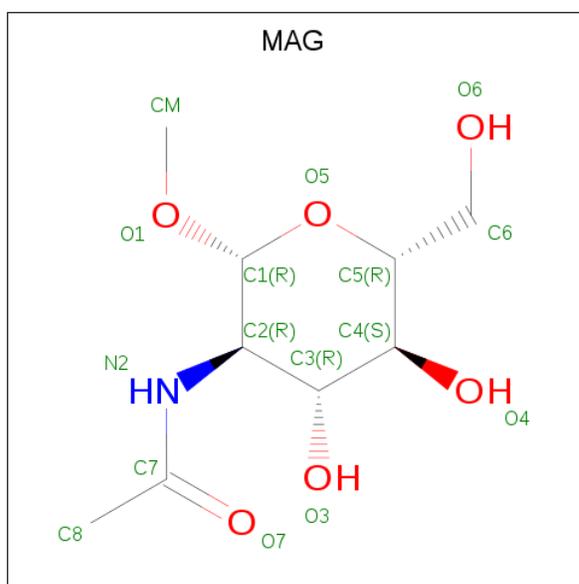
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	10	6	4	0	0
2	A	1	10	6	4	0	0
2	A	1	10	6	4	0	0

- Molecule 3 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C₆H₁₂O₆).



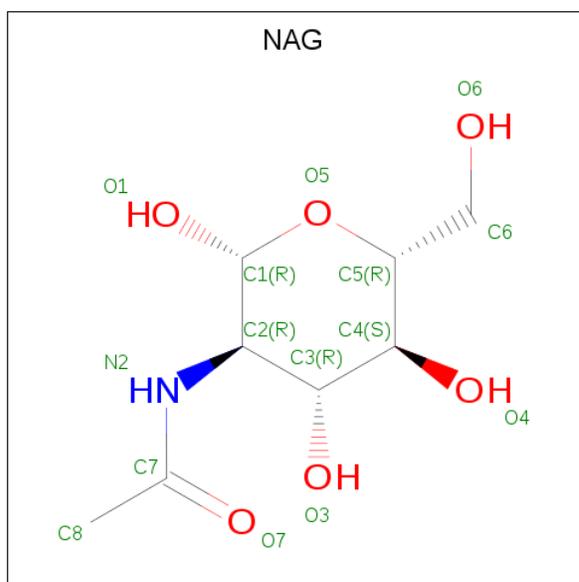
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is BETA-METHYL-N-ACETYL-D-GLUCOSAMINE (three-letter code: MAG) (formula: $C_9H_{17}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	9	1	6		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (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		

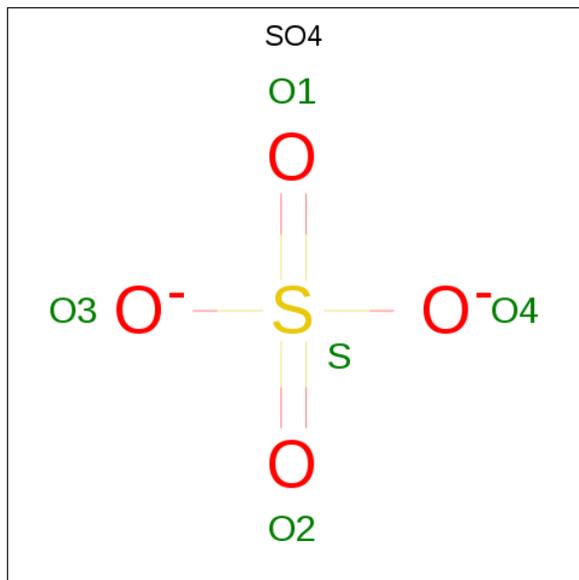
- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mn	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		

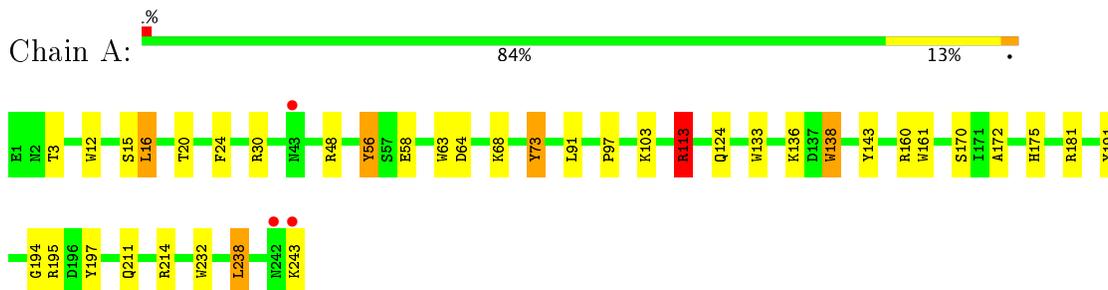
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	144	Total	O	0	0
			144	144		

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: WEST-CENTRAL AFRICAN LEGUME LECTIN IV



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.90Å 78.90Å 89.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00 39.45 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 99.8 (39.45-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.00Å)	Xtrriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.181 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	27.1	Xtrriage
Anisotropy	0.056	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2140	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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: NAG, CA, MN, GAL, FUC, MAG, PCA, SO4

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	0.86	1/1953 (0.1%)	1.64	26/2670 (1.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	TYR	CE2-CZ	-5.04	1.31	1.38

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	A	214	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	A	133	TRP	CD1-CG-CD2	9.39	113.81	106.30
1	A	73	TYR	CB-CG-CD2	-8.97	115.62	121.00
1	A	195	ARG	NE-CZ-NH1	8.08	124.34	120.30

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	1904	0	1811	14	0
2	A	30	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	11	0	9	0	0
4	A	16	0	15	0	0
5	A	28	0	24	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	5	0	0	0	0
9	A	144	0	0	3	0
All	All	2140	0	1889	14	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 4.

The worst 5 of 14 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:103:LYS:HD3	1:A:113:ARG:HG2	1.85	0.56
1:A:138:TRP:HE1	2:A:252:FUC:HO2	1.53	0.56
1:A:238:LEU:HD23	1:A:243:LYS:HD2	1.91	0.53
1:A:175:HIS:HD2	9:A:351:HOH:O	1.93	0.51
1:A:56:TYR:CE2	1:A:58:GLU:HB2	2.47	0.49

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	241/243 (99%)	229 (95%)	12 (5%)	0	100 100

There are no Ramachandran outliers to report.

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	203/203 (100%)	195 (96%)	8 (4%)	37 34

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	LEU
1	A	238	LEU
1	A	160	ARG
1	A	68	LYS
1	A	113	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	163	ASN
1	A	211	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	PCA	A	1	1	8,8,9	1.45	1 (12%)	9,10,12	2.63	4 (44%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CA-C	3.53	1.54	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	OE-CD-CG	-3.75	119.95	126.86
1	A	1	PCA	CG-CD-N	-2.32	101.73	108.33
1	A	1	PCA	CB-CG-CD	2.78	109.03	104.30
1	A	1	PCA	OE-CD-N	5.35	138.32	124.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are 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	FUC	A	252	3	9,10,11	1.81	3 (33%)	13,14,16	1.28	1 (7%)
3	GAL	A	253	2,4	11,11,12	1.16	1 (9%)	13,15,17	1.29	1 (7%)
2	FUC	A	254	4	9,10,11	0.86	0	13,14,16	0.55	0
4	MAG	A	255	3,2	16,16,16	2.03	6 (37%)	21,22,22	2.87	7 (33%)
5	NAG	A	256	5	14,14,15	0.94	0	15,19,21	0.95	1 (6%)
5	NAG	A	257	1,2,5	14,14,15	1.11	2 (14%)	15,19,21	1.20	2 (13%)
2	FUC	A	262	5	9,10,11	0.80	0	13,14,16	0.94	0
8	SO4	A	500	-	4,4,4	0.33	0	6,6,6	0.23	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	FUC	A	252	3	-	0/0/17/20	0/1/1/1
3	GAL	A	253	2,4	-	0/2/19/22	0/1/1/1
2	FUC	A	254	4	-	0/0/17/20	0/1/1/1
4	MAG	A	255	3,2	-	0/8/28/28	0/1/1/1
5	NAG	A	256	5	-	0/6/23/26	0/1/1/1
5	NAG	A	257	1,2,5	-	0/6/23/26	0/1/1/1
2	FUC	A	262	5	-	0/0/17/20	0/1/1/1
8	SO4	A	500	-	-	0/0/0/0	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	257	NAG	C1-C2	-2.24	1.49	1.52
5	A	257	NAG	C4-C3	-2.10	1.47	1.52
4	A	255	MAG	C2-N2	2.03	1.49	1.45
4	A	255	MAG	C1-C2	2.31	1.57	1.53
4	A	255	MAG	C4-C3	2.32	1.58	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	255	MAG	O1-C1-C2	-10.68	91.77	108.02
4	A	255	MAG	O5-C1-O1	-3.28	103.22	110.92
4	A	255	MAG	O4-C4-C3	-2.93	103.99	110.36
4	A	255	MAG	O7-C7-C8	-2.26	117.94	122.06
5	A	257	NAG	C1-O5-C5	2.13	115.10	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	252	FUC	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	242/243 (99%)	-0.39	3 (1%) 79 78	12, 23, 48, 89	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	LYS	5.1
1	A	242	ASN	4.3
1	A	43	ASN	2.5

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	PCA	A	1	8/9	0.69	0.34	-	71,79,83,84	0

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. 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(Å ²)	Q<0.9
8	SO4	A	500	5/5	0.48	0.48	10.09	58,60,61,63	5
2	FUC	A	254	10/11	0.92	0.16	1.58	27,32,36,39	0
5	NAG	A	257	14/15	0.93	0.11	0.96	30,35,40,52	0
3	GAL	A	253	11/12	0.94	0.10	0.66	26,30,32,34	0
2	FUC	A	252	10/11	0.93	0.13	-0.00	27,29,31,33	0
7	CA	A	251	1/1	0.99	0.04	-2.67	20,20,20,20	0
6	MN	A	250	1/1	0.99	0.06	-2.76	21,21,21,21	0
2	FUC	A	262	10/11	0.95	0.14	-	33,35,36,41	0
5	NAG	A	256	14/15	0.91	0.13	-	29,43,49,53	0
4	MAG	A	255	16/16	0.81	0.21	-	35,40,50,54	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.