



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 01:27 pm GMT

PDB ID : 1E73  
Title : 2-F-GLUCOSYLATED MYROSINASE FROM SINAPIS ALBA WITH  
BOUND L-ASCORBATE  
Authors : Burmeister, W.P.  
Deposited on : 2000-08-23  
Resolution : 1.50 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](mailto: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.

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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)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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) : recalc28949

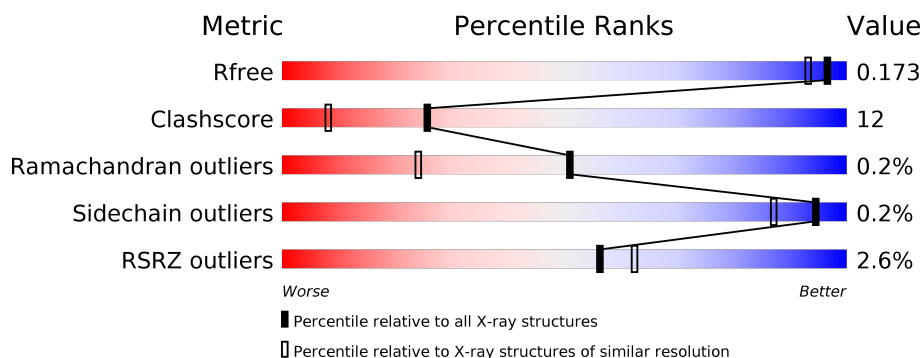
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	100719	2279 (1.50-1.50)
Clashscore	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)
RSRZ outliers	101464	2305 (1.50-1.50)

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  $\geq 3$ , 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	M	501	<div> <div>3%</div> <div>84%</div> <div>14%</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	M	931	-	-	-	X
2	NAG	M	961	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BMA	M	954	-	-	X	-
5	MAN	M	957	X	-	X	-
8	SO4	M	1502	-	-	-	X
8	SO4	M	1504	-	-	X	-
8	SO4	M	1509	-	-	X	-
9	GOL	M	1510	-	-	-	X
9	GOL	M	1511[A]	-	-	-	X
9	GOL	M	1511[B]	-	-	-	X
9	GOL	M	1512	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5216 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 MYROSINASE MA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	499	Total	C	N	O	S	0	21	0
			4082	2618	660	788	16			

- 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	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	M	2	Total	C	N	O	0	0
			28	16	2	10		

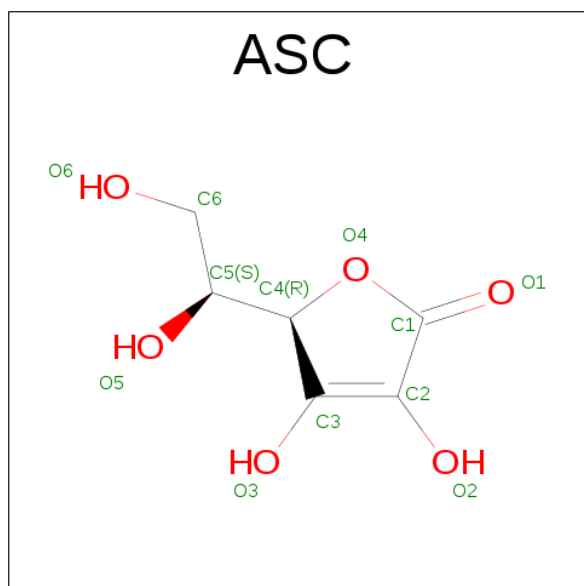
- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	M	5	Total	C	N	O	0	0
			58	33	2	23		

- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

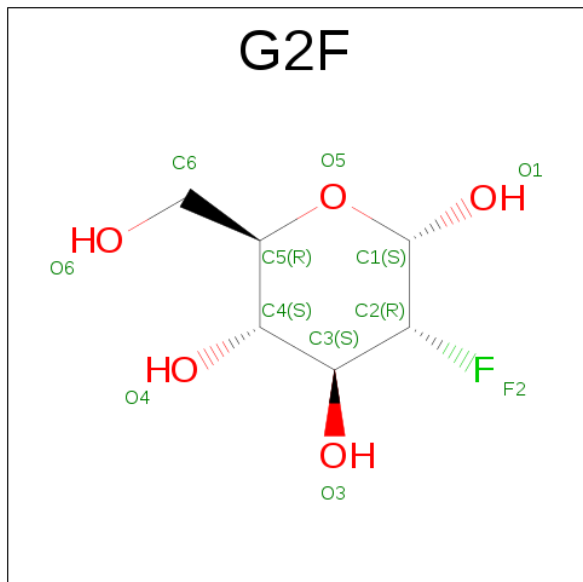
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	7	Total	C	N	O	0	0
			80	45	2	33		

- Molecule 6 is ASCORBIC ACID (three-letter code: ASC) (formula:  $C_6H_8O_6$ ).



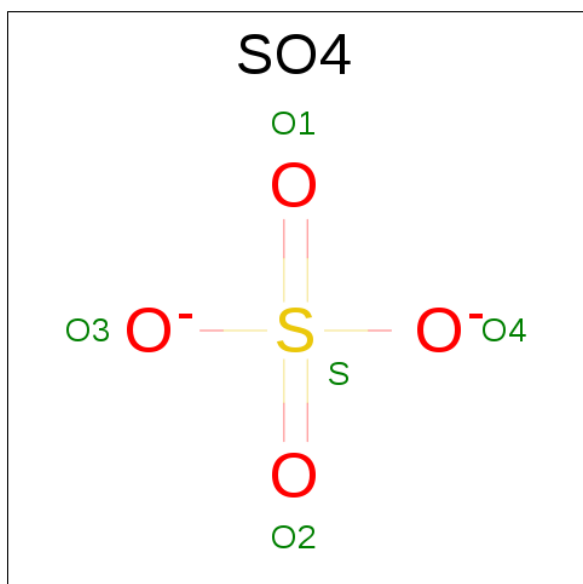
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 is SUGAR (2-DEOXY-2-FLUORO-ALPHA-D-GLUCOPYRANOSE) (three-letter code: G2F) (formula:  $C_6H_{11}FO_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	F	O	0	0
			11	6	1	4		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total 1	Zn 1	0	0

- Molecule 11 is water.

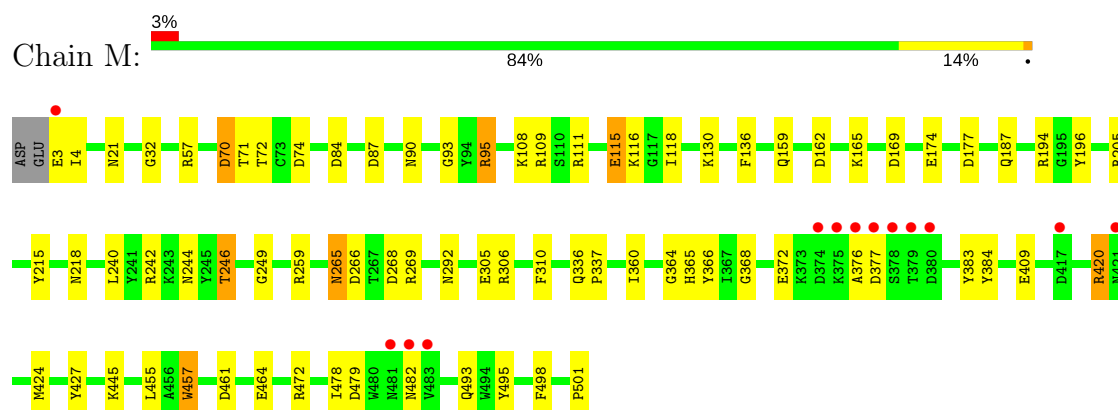
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	795	Total 795	O 795	0	0



### 3 Residue-property plots

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: MYROSINASE MA1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.30Å 137.20Å 80.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.50 9.99 – 1.50	Depositor EDS
% Data completeness (in resolution range)	79.8 (10.00-1.50) 79.8 (9.99-1.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.134 , 0.167 0.146 , 0.173	Depositor DCC
$R_{free}$ test set	4838 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.50 , 66.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XYP, GOL, ZN, BMA, NAG, ASC, G2F, SO4, MAN, FUC

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	M	0.72	3/4290 (0.1%)	1.35	37/5833 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1
5	M	1	0
All	All	1	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	409	GLU	CD-OE1	6.98	1.33	1.25
1	M	501	PRO	N-CD	6.39	1.56	1.47
1	M	464	GLU	CD-OE1	5.25	1.31	1.25

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	109	ARG	NE-CZ-NH2	-17.81	111.40	120.30
1	M	242	ARG	NE-CZ-NH2	-13.79	113.41	120.30
1	M	70	ASP	CB-CG-OD2	-11.61	107.85	118.30
1	M	95	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	M	109	ARG	NH1-CZ-NH2	8.88	129.17	119.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	957	MAN	C5

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	457	TRP	Mainchain

## 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	M	4082	0	3835	74	0
2	M	84	0	77	11	0
3	M	28	0	25	4	0
4	M	58	0	50	4	0
5	M	80	0	65	18	0
6	M	12	0	7	1	0
7	M	11	0	9	1	0
8	M	40	0	0	5	0
9	M	25	0	30	2	0
10	M	1	0	0	0	0
11	M	795	0	0	28	0
All	All	5216	0	4098	96	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 96 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:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CZ	1.30	1.60
1:M:90:ASN:HD21	2:M:911:NAG:C1	0.95	1.60
1:M:244:ASN:HD21	2:M:931:NAG:C1	0.96	1.60
1:M:292:ASN:HD21	5:M:951:NAG:C1	0.94	1.59
1:M:21:ASN:HD21	2:M:901:NAG:C1	0.95	1.57

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	M	518/501 (103%)	504 (97%)	13 (2%)	1 (0%)	51	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	187	GLN

### 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	M	456/437 (104%)	455 (100%)	1 (0%)	94	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	3	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	244	ASN
1	M	365	HIS
1	M	265	ASN
1	M	218	ASN

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Mol	Chain	Res	Type
1	M	292	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 ⓘ

14 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$
3	NAG	M	921	1,3	14,14,15	1.39	3 (21%)	15,19,21	3.11	8 (53%)
3	NAG	M	923	3	14,14,15	1.15	0	15,19,21	3.47	7 (46%)
4	FUC	M	941	4	9,10,11	1.39	1 (11%)	13,14,16	1.99	3 (23%)
4	NAG	M	942	1,4	14,14,15	0.88	1 (7%)	15,19,21	2.95	7 (46%)
4	NAG	M	943	4	14,14,15	1.10	1 (7%)	15,19,21	1.29	1 (6%)
4	BMA	M	944	4	11,11,12	2.27	3 (27%)	13,15,17	1.90	2 (15%)
4	XYP	M	945	4	9,9,10	0.91	0	10,12,14	2.26	3 (30%)
5	NAG	M	951	1,5	14,14,15	1.39	2 (14%)	15,19,21	3.21	8 (53%)
5	FUC	M	952	5	9,10,11	2.11	4 (44%)	13,14,16	2.90	7 (53%)
5	NAG	M	953	5	14,14,15	1.59	2 (14%)	15,19,21	2.60	5 (33%)
5	BMA	M	954	5	11,11,12	2.30	2 (18%)	13,15,17	5.84	10 (76%)
5	XYP	M	955	5	9,9,10	1.32	3 (33%)	10,12,14	2.60	4 (40%)
5	MAN	M	956	5	11,11,12	1.38	2 (18%)	13,15,17	2.21	4 (30%)
5	MAN	M	957	5	11,11,12	3.01	4 (36%)	13,15,17	6.09	10 (76%)

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
3	NAG	M	921	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	923	3	-	0/6/23/26	0/1/1/1
4	FUC	M	941	4	-	0/0/17/20	0/1/1/1
4	NAG	M	942	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	943	4	-	0/6/23/26	0/1/1/1
4	BMA	M	944	4	-	0/2/19/22	0/1/1/1
4	XYP	M	945	4	-	0/0/14/17	0/1/1/1
5	NAG	M	951	1,5	-	0/6/23/26	0/1/1/1
5	FUC	M	952	5	-	0/0/17/20	0/1/1/1
5	NAG	M	953	5	-	0/6/23/26	0/1/1/1
5	BMA	M	954	5	-	0/2/19/22	0/1/1/1
5	XYP	M	955	5	-	0/0/14/17	0/1/1/1
5	MAN	M	956	5	-	0/2/19/22	0/1/1/1
5	MAN	M	957	5	1/1/4/5	0/2/19/22	0/1/1/1

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	954	BMA	C2-C3	-6.01	1.44	1.52
4	M	944	BMA	C2-C3	-5.88	1.44	1.52
5	M	953	NAG	C3-C2	-2.65	1.46	1.52
5	M	952	FUC	C4-C5	2.01	1.56	1.53
5	M	955	XYP	C2B-C3B	2.01	1.55	1.52

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	957	MAN	C1-O5-C5	-11.67	96.08	112.17
3	M	923	NAG	C1-O5-C5	-10.03	98.34	112.17
3	M	921	NAG	C1-O5-C5	-7.89	101.29	112.17
5	M	951	NAG	C1-O5-C5	-7.89	101.30	112.17
5	M	954	BMA	O4-C4-C3	-7.46	94.13	110.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	957	MAN	C5

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	921	NAG	4	0
4	M	942	NAG	4	0
5	M	951	NAG	3	0
5	M	954	BMA	10	0
5	M	957	MAN	11	0

## 5.6 Ligand geometry

Of 22 ligands modelled in this entry, 1 is 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$
8	SO4	M	1502	-	4,4,4	0.60	0	6,6,6	0.82	0
8	SO4	M	1503	-	4,4,4	0.77	0	6,6,6	0.31	0
8	SO4	M	1504	-	4,4,4	0.98	0	6,6,6	0.83	0
8	SO4	M	1505	-	4,4,4	0.37	0	6,6,6	0.55	0
8	SO4	M	1506	-	4,4,4	0.99	0	6,6,6	1.05	0
8	SO4	M	1507	-	4,4,4	0.95	0	6,6,6	0.84	0
8	SO4	M	1508	-	4,4,4	0.71	0	6,6,6	0.35	0
8	SO4	M	1509	-	4,4,4	0.86	0	6,6,6	1.01	0
9	GOL	M	1510	-	5,5,5	0.41	0	5,5,5	0.51	0
9	GOL	M	1511[A]	-	5,5,5	0.88	0	5,5,5	1.52	1 (20%)
9	GOL	M	1511[B]	-	5,5,5	0.92	0	5,5,5	2.50	2 (40%)
9	GOL	M	1512	-	5,5,5	0.73	0	5,5,5	1.69	2 (40%)
9	GOL	M	1513	-	5,5,5	0.53	0	5,5,5	1.41	1 (20%)
2	NAG	M	901	1	14,14,15	1.16	1 (7%)	15,19,21	2.08	4 (26%)
2	NAG	M	911	1	14,14,15	1.27	1 (7%)	15,19,21	1.89	5 (33%)
2	NAG	M	931	1	14,14,15	1.77	3 (21%)	15,19,21	9.60	9 (60%)
2	NAG	M	961	1	14,14,15	1.40	2 (14%)	15,19,21	2.92	6 (40%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	M	971	1	14,14,15	1.33	1 (7%)	15,19,21	2.79	4 (26%)
2	NAG	M	991	1	14,14,15	1.31	1 (7%)	15,19,21	2.06	5 (33%)
6	ASC	M	995	-	12,12,12	4.54	8 (66%)	17,17,17	2.52	6 (35%)
7	G2F	M	999	1	11,11,12	1.54	2 (18%)	8,15,17	1.59	1 (12%)

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
8	SO4	M	1502	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1503	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1504	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1505	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1506	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1507	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1508	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1509	-	-	0/0/0/0	0/0/0/0
9	GOL	M	1510	-	-	0/4/4/4	0/0/0/0
9	GOL	M	1511[A]	-	-	0/4/4/4	0/0/0/0
9	GOL	M	1511[B]	-	-	0/4/4/4	0/0/0/0
9	GOL	M	1512	-	-	0/4/4/4	0/0/0/0
9	GOL	M	1513	-	-	0/4/4/4	0/0/0/0
2	NAG	M	901	1	-	0/6/23/26	0/1/1/1
2	NAG	M	911	1	-	0/6/23/26	0/1/1/1
2	NAG	M	931	1	-	2/6/23/26	0/1/1/1
2	NAG	M	961	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	M	971	1	-	0/6/23/26	0/1/1/1
2	NAG	M	991	1	-	0/6/23/26	0/1/1/1
6	ASC	M	995	-	-	0/6/22/22	0/1/1/1
7	G2F	M	999	1	-	0/2/19/22	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	995	ASC	O1-C1	-8.15	1.04	1.21
2	M	931	NAG	O7-C7	-4.23	1.13	1.23
2	M	971	NAG	O7-C7	-3.91	1.14	1.23
2	M	911	NAG	O7-C7	-3.71	1.14	1.23
2	M	931	NAG	C2-N2	-3.50	1.40	1.46

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	931	NAG	C1-O5-C5	-7.13	102.34	112.17
2	M	931	NAG	O7-C7-N2	-7.03	108.38	121.92
2	M	971	NAG	O5-C1-C2	-6.85	101.94	111.47
6	M	995	ASC	O4-C1-C2	-6.09	104.85	109.91
2	M	991	NAG	C4-C3-C2	-4.55	104.35	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	M	961	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	931	NAG	C8-C7-N2-C2
2	M	931	NAG	O7-C7-N2-C2

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	1504	SO4	4	0
8	M	1509	SO4	5	0
9	M	1510	GOL	1	0
9	M	1512	GOL	1	0
2	M	901	NAG	3	0
2	M	911	NAG	2	0
2	M	931	NAG	6	0
6	M	995	ASC	1	0
7	M	999	G2F	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	M	499/501 (99%)	-0.45	13 (2%) 56 62	10, 14, 28, 54	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	376	ALA	8.0
1	M	377	ASP	7.2
1	M	375	LYS	4.4
1	M	380	ASP	3.9
1	M	483	VAL	3.4

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	M	942	14/15	0.94	0.08	1.84	18,21,24,24	0
3	NAG	M	921	14/15	0.92	0.08	1.00	19,23,28,31	0
5	FUC	M	952	10/11	0.80	0.16	-	24,25,28,30	0
5	MAN	M	956	11/12	0.47	0.39	-	30,41,45,46	0
4	XYP	M	945	9/10	0.70	0.33	-	42,43,44,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	M	923	14/15	0.57	0.31	-	37,42,49,50	0
5	MAN	M	957	11/12	0.60	0.54	-	40,45,49,52	0
4	NAG	M	943	14/15	0.90	0.10	-	25,28,33,35	0
5	NAG	M	953	14/15	0.87	0.13	-	22,24,29,32	0
4	FUC	M	941	10/11	0.88	0.17	-	28,32,35,36	0
5	XYP	M	955	9/10	0.42	0.34	-	39,42,45,46	0
5	NAG	M	951	14/15	0.94	0.08	-	18,20,22,24	0
5	BMA	M	954	11/12	0.79	0.15	-	25,32,35,38	0
4	BMA	M	944	11/12	0.71	0.30	-	37,39,42,45	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	NAG	M	961	14/15	0.61	0.50	27.65	39,42,52,53	0
9	GOL	M	1511[A]	6/6	0.88	0.13	10.77	14,16,18,18	2
9	GOL	M	1511[B]	6/6	0.88	0.13	10.26	14,16,18,18	2
2	NAG	M	931	14/15	0.57	0.29	9.63	38,45,48,50	0
8	SO4	M	1502	5/5	0.98	0.16	9.63	23,23,27,29	5
9	GOL	M	1510	6/6	0.49	0.24	7.55	38,40,40,40	6
9	GOL	M	1512	6/6	0.92	0.11	3.99	17,23,26,31	6
2	NAG	M	901	14/15	0.74	0.17	1.46	32,35,37,39	0
7	G2F	M	999	11/12	0.91	0.10	1.29	18,26,31,33	0
6	ASC	M	995	12/12	0.96	0.07	0.18	16,17,19,19	0
9	GOL	M	1513	6/6	0.56	0.31	-	36,38,38,41	6
8	SO4	M	1505	5/5	0.99	0.04	-	18,19,22,25	0
2	NAG	M	971	14/15	0.53	0.52	-	57,62,65,66	0
8	SO4	M	1507	5/5	0.63	0.23	-	30,34,35,35	5
2	NAG	M	991	14/15	0.44	0.54	-	38,41,49,50	0
10	ZN	M	1515	1/1	1.00	0.03	-	11,11,11,11	1
2	NAG	M	911	14/15	0.82	0.17	-	24,27,31,32	0
8	SO4	M	1508	5/5	0.80	0.29	-	40,40,40,40	5
8	SO4	M	1503	5/5	0.95	0.12	-	22,25,28,29	5
8	SO4	M	1506	5/5	0.66	0.33	-	32,34,37,37	5
8	SO4	M	1509	5/5	0.90	0.35	-	42,43,45,45	1
8	SO4	M	1504	5/5	0.72	0.34	-	31,34,36,38	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.