



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:03 PM GMT

PDB ID : 1DWA  
Title : STUDY ON RADIATION DAMAGE ON A CRYOCOOLED CRYSTAL.  
PART 1: STRUCTURE PRIOR TO IRRADIATION  
Authors : Burmeister, W.P.  
Deposited on : 1999-12-05  
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](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 (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

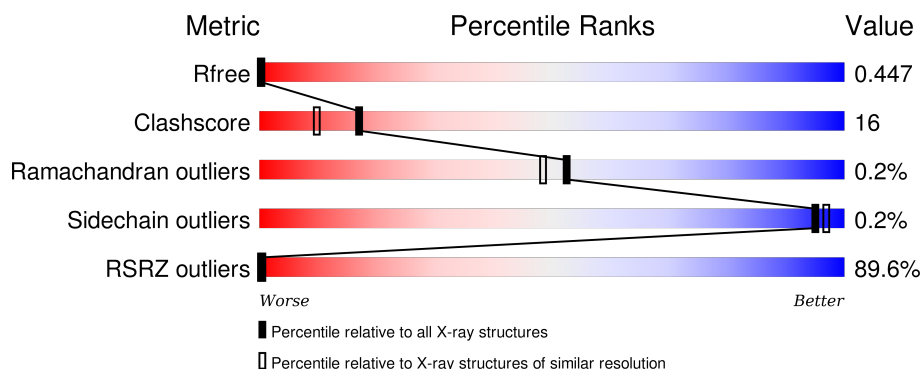
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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  $\geq 3$ , 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	499	<div> <div>90%</div> <div>82%16%.</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	901	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	M	931	-	-	X	X
2	NAG	M	961	X	-	-	X
3	NAG	M	923	-	-	-	X
5	BMA	M	954	-	-	X	-
5	MAN	M	957	X	-	X	-
7	SO4	M	1003	-	-	X	-
7	SO4	M	1004	-	-	X	-
7	SO4	M	1006	-	X	-	-
7	SO4	M	1009	-	X	X	X
8	GOL	M	1010	-	-	X	X
8	GOL	M	1020	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5220 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
			Total	C	N	O	S			
1	M	499	4083	2619	660	788	16	0	21	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	497	THR	SER	SEE REMARK 999	UNP P29736

- Molecule 2 is SUGAR (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	M	1	14	8	1	5	0	0
2	M	1	14	8	1	5	0	0

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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		

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

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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

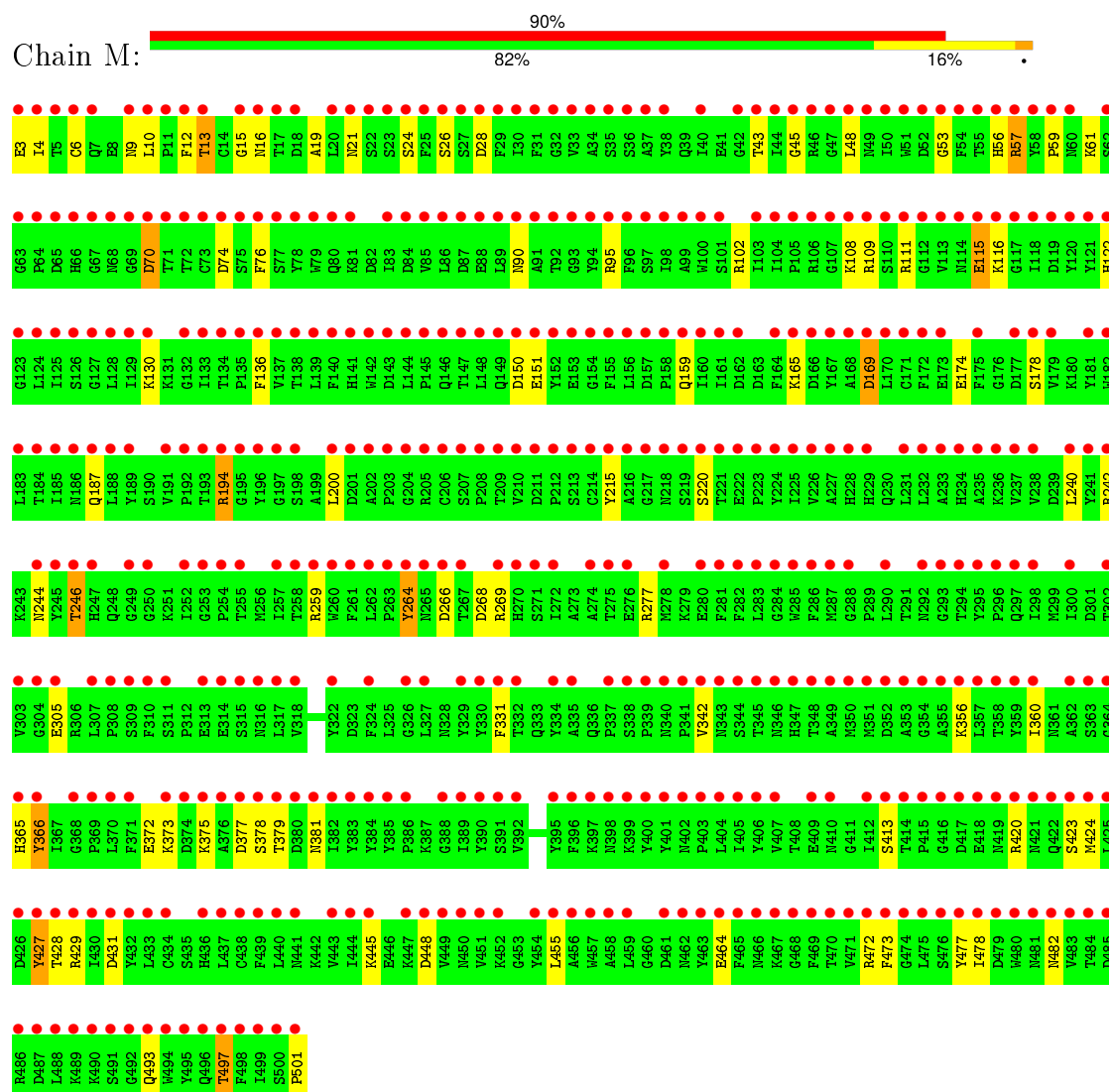
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	752	Total	O	0	0
			752	752		
9	W	36	Total	O	0	0
			36	36		

### 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 errors 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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	134.30Å 136.40Å 80.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.40 – 2.00 9.94 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (17.40-2.00) 98.8 (9.94-1.99)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.10 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.165 , 0.179 0.436 , 0.447	Depositor DCC
$R_{free}$ test set	2459 reflections (4.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.2	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 64.2	EDS
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 50123 reflections	Xtriage
$F_o, F_c$ correlation	0.64	EDS
Total number of atoms	5220	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	1.15	18/4291 (0.4%)	1.32	41/5835 (0.7%)

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

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	264	TYR	CE1-CZ	-21.78	1.10	1.38
1	M	264	TYR	CZ-OH	20.20	1.72	1.37
1	M	16	ASN	CG-ND2	12.66	1.64	1.32
1	M	356	LYS	CE-NZ	-11.08	1.21	1.49
1	M	423	SER	CB-OG	9.83	1.55	1.42

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	448	ASP	CB-CG-OD2	-18.65	101.51	118.30
1	M	115	GLU	OE1-CD-OE2	-15.25	105.00	123.30
1	M	264	TYR	CZ-CE2-CD2	-12.25	108.77	119.80
1	M	264	TYR	CE1-CZ-CE2	11.60	138.36	119.80
1	M	109	ARG	NE-CZ-NH1	-11.36	114.62	120.30

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	13	THR	Mainchain

## 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	M	4083	0	3835	104	4
2	M	84	0	77	18	0
3	M	56	0	49	4	0
4	M	58	0	50	0	0
5	M	80	0	66	10	0
6	M	1	0	0	0	1
7	M	40	0	0	10	0
8	M	30	0	39	4	0
9	M	752	0	0	70	16
9	W	36	0	0	8	1
All	All	5220	0	4116	136	21

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 16.

The worst 5 of 136 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:244:ASN:HD21	2:M:931:NAG:C1	0.96	1.56
1:M:21:ASN:HD21	2:M:901:NAG:C1	0.90	1.52
1:M:264:TYR:OH	1:M:264:TYR:CZ	1.72	1.42
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CZ	1.57	1.37
8:M:1010:GOL:C1	9:W:2026:HOH:O	1.71	1.34

The worst 5 of 21 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:1001:ZN:ZN	6:M:1001:ZN:ZN[3_656]	1.10	1.10
9:M:2279:HOH:O	9:M:2279:HOH:O[3_656]	1.10	1.10
9:M:2009:HOH:O	9:M:2520:HOH:O[4_576]	1.36	0.84
9:M:2248:HOH:O	9:M:2534:HOH:O[4_576]	1.37	0.83
9:M:2247:HOH:O	9:M:2247:HOH:O[4_576]	1.42	0.78

## 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	518/499 (104%)	504 (97%)	13 (2%)	1 (0%)	52 48

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	456/435 (105%)	455 (100%)	1 (0%)	95 97

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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	244	ASN
1	M	365	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](#)

16 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	5.95	7 (50%)	15,19,21	3.61	8 (53%)
3	NAG	M	923	3	14,14,15	2.78	3 (21%)	15,19,21	3.87	7 (46%)
4	NAG	M	941	1,4	14,14,15	0.55	0	15,19,21	1.98	4 (26%)
4	FUC	M	942	4	10,10,11	1.57	2 (20%)	14,14,16	2.20	4 (28%)
4	NAG	M	943	4	14,14,15	1.01	1 (7%)	15,19,21	1.33	2 (13%)
4	BMA	M	944	4	11,11,12	1.87	2 (18%)	14,15,17	1.70	4 (28%)
4	XYP	M	945	4	9,9,10	1.35	2 (22%)	12,12,14	2.70	4 (33%)
5	NAG	M	951	1,5	14,14,15	1.89	3 (21%)	15,19,21	2.16	3 (20%)
5	FUC	M	952	5	10,10,11	2.82	5 (50%)	14,14,16	1.90	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	M	953	5	14,14,15	1.43	3 (21%)	15,19,21	1.66	4 (26%)
5	BMA	M	954	5	11,11,12	2.58	3 (27%)	14,15,17	4.51	8 (57%)
5	XYP	M	955	5	9,9,10	1.93	3 (33%)	12,12,14	2.70	5 (41%)
5	MAN	M	956	5	11,11,12	1.84	2 (18%)	14,15,17	2.80	8 (57%)
5	MAN	M	957	5	11,11,12	2.95	6 (54%)	14,15,17	7.39	11 (78%)
3	NAG	M	981	1,3	14,14,15	2.38	3 (21%)	15,19,21	2.45	3 (20%)
3	NAG	M	983	3	14,14,15	1.40	3 (21%)	15,19,21	2.22	7 (46%)

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	NAG	M	941	1,4	-	0/6/23/26	0/1/1/1
4	FUC	M	942	4	-	0/0/17/20	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
3	NAG	M	981	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	983	3	-	0/6/23/26	0/1/1/1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	954	BMA	C2-C3	-7.12	1.42	1.52
3	M	981	NAG	O7-C7	-6.36	1.08	1.23
3	M	923	NAG	C6-C5	-5.84	1.31	1.51
5	M	951	NAG	C1-C2	-5.26	1.45	1.52
3	M	923	NAG	C4-C5	-4.54	1.43	1.53

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	957	MAN	C1-O5-C5	-17.00	90.67	112.25
5	M	957	MAN	O5-C5-C6	-8.83	88.23	107.35
3	M	923	NAG	C1-O5-C5	-8.27	101.75	112.25
3	M	921	NAG	O3-C3-C2	-7.80	93.66	109.11
3	M	921	NAG	C1-O5-C5	-6.76	103.67	112.25

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.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	921	NAG	3	0
5	M	954	BMA	7	0
5	M	957	MAN	9	0
3	M	983	NAG	1	0

## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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
7	SO4	M	1002	-	4,4,4	1.88	1 (25%)	6,6,6	1.04	0
7	SO4	M	1003	-	4,4,4	0.83	0	6,6,6	0.72	0
7	SO4	M	1004	-	4,4,4	2.13	1 (25%)	6,6,6	1.94	2 (33%)
7	SO4	M	1005	-	4,4,4	0.48	0	6,6,6	0.32	0
7	SO4	M	1006	-	4,4,4	2.85	1 (25%)	6,6,6	3.18	3 (50%)
7	SO4	M	1007	-	4,4,4	1.67	1 (25%)	6,6,6	1.32	1 (16%)
7	SO4	M	1008	-	4,4,4	1.13	0	6,6,6	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SO4	M	1009	-	4,4,4	2.25	2 (50%)	6,6,6	3.61	3 (50%)
8	GOL	M	1010	-	5,5,5	0.67	0	5,5,5	1.16	1 (20%)
8	GOL	M	1020	-	5,5,5	1.26	1 (20%)	5,5,5	1.05	0
8	GOL	M	1021	-	5,5,5	0.91	0	5,5,5	1.13	0
8	GOL	M	1023	-	5,5,5	0.62	0	5,5,5	1.03	0
8	GOL	M	1024	-	5,5,5	0.80	0	5,5,5	1.17	1 (20%)
2	NAG	M	901	1	14,14,15	1.16	1 (7%)	15,19,21	1.98	2 (13%)
2	NAG	M	911	1	14,14,15	1.59	2 (14%)	15,19,21	2.25	4 (26%)
2	NAG	M	931	1	14,14,15	1.97	5 (35%)	15,19,21	7.88	11 (73%)
2	NAG	M	961	1	14,14,15	1.33	2 (14%)	15,19,21	2.84	3 (20%)
2	NAG	M	971	1	14,14,15	1.30	1 (7%)	15,19,21	1.90	6 (40%)
2	NAG	M	991	1	14,14,15	1.22	1 (7%)	15,19,21	1.69	2 (13%)

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
7	SO4	M	1002	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1003	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1004	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1005	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1006	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1007	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1008	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1009	-	-	0/0/0/0	0/0/0/0
8	GOL	M	1010	-	-	0/4/4/4	0/0/0/0
8	GOL	M	1020	-	-	0/4/4/4	0/0/0/0
8	GOL	M	1021	-	-	0/4/4/4	0/0/0/0
8	GOL	M	1023	-	-	0/4/4/4	0/0/0/0
8	GOL	M	1024	-	-	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	-	0/6/23/26	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

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



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	971	NAG	O7-C7	-4.04	1.13	1.23
2	M	931	NAG	O7-C7	-3.83	1.14	1.23
2	M	991	NAG	O7-C7	-3.69	1.14	1.23
2	M	931	NAG	C1-C2	-3.45	1.47	1.52
2	M	911	NAG	O7-C7	-3.35	1.15	1.23

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	931	NAG	O7-C7-N2	-7.50	106.58	121.86
2	M	931	NAG	C1-O5-C5	-7.16	103.16	112.25
7	M	1006	SO4	O2-S-O1	-6.97	87.42	109.50
7	M	1009	SO4	O2-S-O1	-6.78	88.00	109.50
2	M	911	NAG	C1-O5-C5	-6.70	103.74	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	M	961	NAG	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	1003	SO4	2	0
7	M	1004	SO4	6	0
7	M	1009	SO4	8	0
8	M	1010	GOL	4	0
2	M	901	NAG	5	0
2	M	911	NAG	3	0
2	M	931	NAG	8	0
2	M	961	NAG	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, 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	499/499 (100%)	3.30	447 (89%) <b>0</b> <b>0</b>	7, 11, 25, 52	2 (0%)

The worst 5 of 447 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	212	PRO	8.3
1	M	376	ALA	7.5
1	M	23	SER	7.0
1	M	469	PHE	6.9
1	M	378	SER	6.8

### 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
3	NAG	M	923	14/15	0.50	0.44	0.16	33,41,53,55	0
4	NAG	M	941	14/15	0.66	0.33	0.06	10,18,22,23	0
3	NAG	M	921	14/15	0.63	0.32	-0.17	15,19,28,33	0
3	NAG	M	981	14/15	0.68	0.30	-0.39	5,12,17,19	0
5	XYP	M	955	9/10	0.49	0.41	-	28,34,39,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MAN	M	956	11/12	0.43	0.48	-	21,35,47,52	0
4	FUC	M	942	10/11	0.59	0.37	-	20,28,35,43	0
5	NAG	M	953	14/15	0.74	0.25	-	16,19,24,28	0
4	NAG	M	943	14/15	0.69	0.30	-	17,23,29,34	0
4	XYP	M	945	9/10	0.51	0.37	-	37,43,48,49	0
5	FUC	M	952	10/11	0.64	0.29	-	15,17,29,29	0
5	MAN	M	957	11/12	0.50	0.58	-	29,39,50,51	0
4	BMA	M	944	11/12	0.35	0.48	-	34,39,44,49	0
5	BMA	M	954	11/12	0.55	0.27	-	21,26,31,43	0
5	NAG	M	951	14/15	0.74	0.27	-	13,16,22,24	0
3	NAG	M	983	14/15	0.53	0.36	-	22,27,45,52	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
8	GOL	M	1010	6/6	0.46	0.52	12.33	31,38,40,47	6
7	SO4	M	1009	5/5	0.57	0.56	8.92	34,35,42,55	1
2	NAG	M	931	14/15	0.63	0.42	4.98	31,38,44,45	0
2	NAG	M	961	14/15	0.55	0.63	3.20	39,46,58,64	0
8	GOL	M	1020	6/6	0.58	0.37	2.06	1,10,14,14	1
7	SO4	M	1002	5/5	0.82	0.36	0.60	22,25,28,33	5
7	SO4	M	1004	5/5	0.73	0.30	0.59	10,23,26,30	5
2	NAG	M	901	14/15	0.49	0.40	0.57	21,30,42,44	0
8	GOL	M	1021	6/6	0.69	0.26	-0.45	7,17,22,27	6
8	GOL	M	1024	6/6	0.67	0.27	-0.77	11,12,18,18	0
7	SO4	M	1005	5/5	0.73	0.31	-	13,17,22,24	0
8	GOL	M	1023	6/6	0.56	0.54	-	27,27,38,41	6
6	ZN	M	1001	1/1	0.83	0.20	-	32,32,32,32	0
2	NAG	M	911	14/15	0.63	0.32	-	20,23,32,41	0
7	SO4	M	1003	5/5	0.58	0.55	-	21,24,31,32	5
7	SO4	M	1008	5/5	0.74	0.37	-	29,31,34,34	5
7	SO4	M	1006	5/5	0.80	0.46	-	21,26,30,31	5
7	SO4	M	1007	5/5	0.74	0.32	-	9,29,30,33	5
2	NAG	M	971	14/15	0.53	0.41	-	52,60,66,66	0
2	NAG	M	991	14/15	0.37	0.64	-	30,36,49,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.