



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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

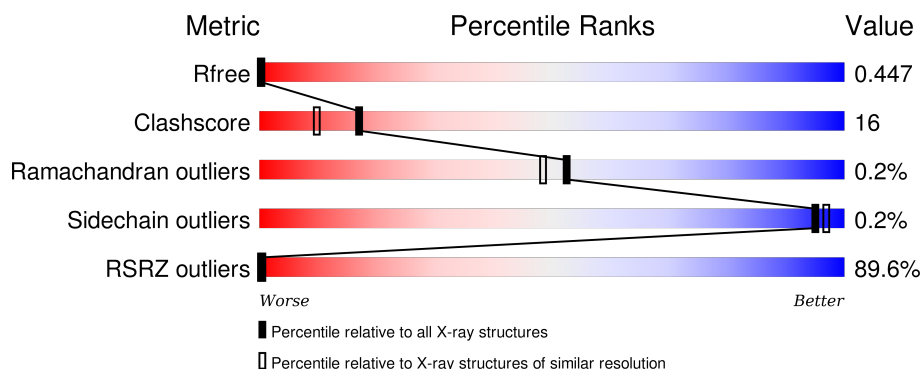
# 1 Overall quality at a glance

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	

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		

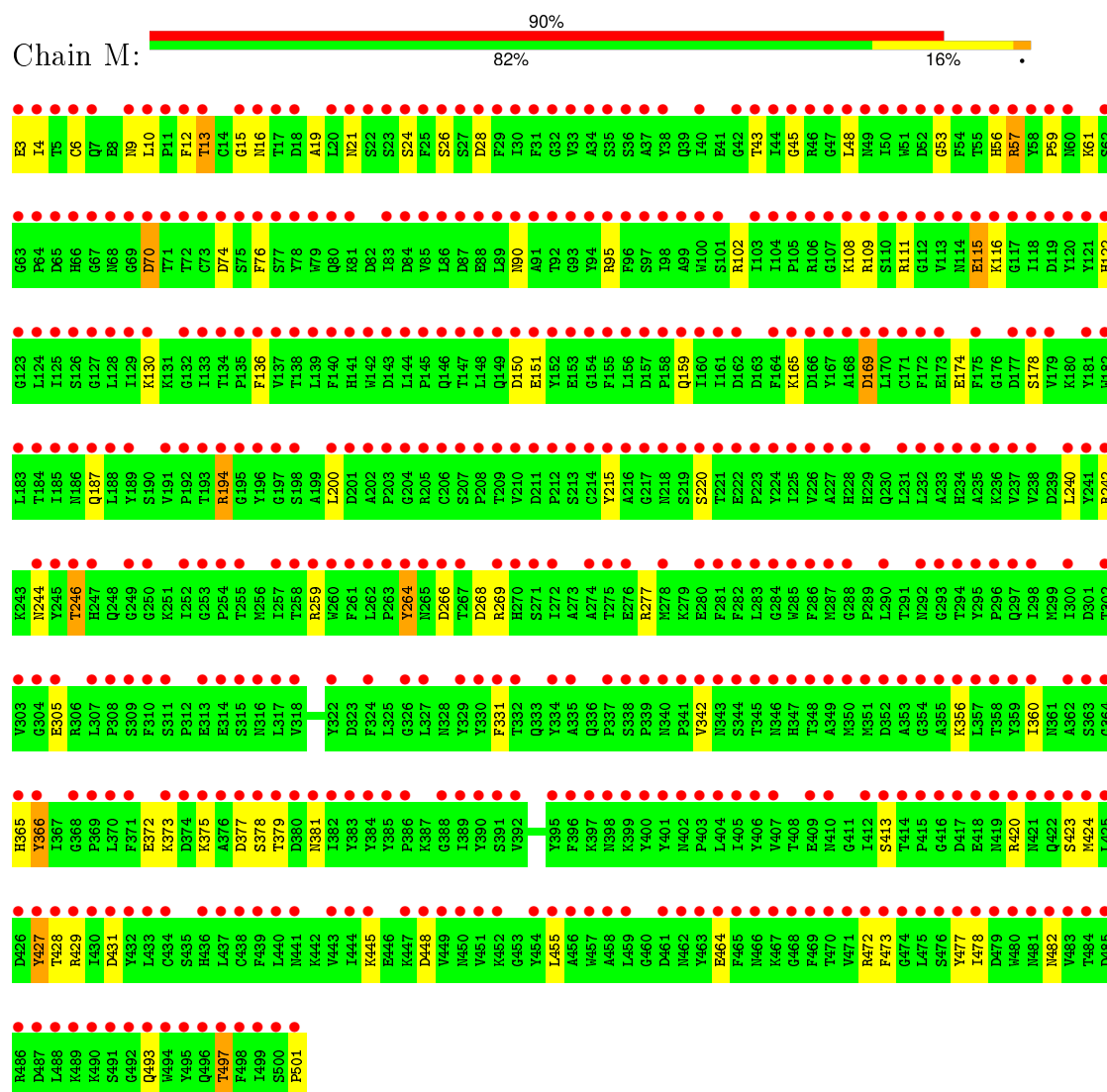
- Molecule 9 is water.

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

All (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
1	M	13	THR	C-O	-9.72	1.04	1.23
1	M	6	CYS	CB-SG	-9.15	1.66	1.82
1	M	178	SER	CB-OG	8.91	1.53	1.42
1	M	501	PRO	CA-C	7.25	1.67	1.52
1	M	24	SER	CB-OG	7.00	1.51	1.42
1	M	115	GLU	CD-OE2	6.86	1.33	1.25
1	M	26	SER	CB-OG	5.51	1.49	1.42
1	M	413	SER	CB-OG	-5.36	1.35	1.42
1	M	246	THR	CB-CG2	-5.35	1.34	1.52
1	M	61	LYS	CD-CE	-5.18	1.38	1.51
1	M	501	PRO	N-CD	5.17	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	242	ARG	NE-CZ	5.11	1.39	1.33
1	M	464	GLU	CG-CD	-5.06	1.44	1.51

All (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
1	M	269	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	M	372	GLU	OE1-CD-OE2	-10.19	111.07	123.30
1	M	169[A]	ASP	CB-CG-OD2	-9.73	109.55	118.30
1	M	169[B]	ASP	CB-CG-OD2	-9.73	109.55	118.30
1	M	194	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	M	242	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	M	268	ASP	CB-CG-OD1	8.74	126.17	118.30
1	M	269	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	M	266	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	M	74	ASP	CB-CG-OD1	7.91	125.42	118.30
1	M	427	TYR	CG-CD1-CE1	-7.74	115.11	121.30
1	M	448	ASP	OD1-CG-OD2	7.70	137.92	123.30
1	M	264	TYR	OH-CZ-CE2	-7.51	99.82	120.10
1	M	264	TYR	CD1-CE1-CZ	-6.94	113.55	119.80
1	M	372	GLU	CG-CD-OE2	6.55	131.39	118.30
1	M	109	ARG	NH1-CZ-NH2	6.45	126.50	119.40
1	M	246	THR	OG1-CB-CG2	-6.39	95.31	110.00
1	M	482	ASN	CB-CG-OD1	6.24	134.09	121.60
1	M	76	PHE	CB-CG-CD1	-6.10	116.53	120.80
1	M	482	ASN	CA-CB-CG	-6.03	100.13	113.40
1	M	194	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	M	70	ASP	CB-CG-OD1	5.82	123.54	118.30
1	M	377	ASP	O-C-N	-5.62	113.70	122.70
1	M	497	THR	OG1-CB-CG2	-5.55	97.24	110.00
1	M	102	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	M	420	ARG	CD-NE-CZ	5.51	131.31	123.60
1	M	429	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	M	420	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	M	277	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	M	427	TYR	CZ-CE2-CD2	-5.34	114.99	119.80
1	M	19	ALA	CB-CA-C	-5.24	102.24	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	366[A]	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	M	366[B]	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	M	57	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	M	473	PHE	CB-CG-CD2	5.14	124.40	120.80
1	M	478	ILE	CB-CG1-CD1	5.08	128.13	113.90

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.

All (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
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CZ	2.14	1.30
1:M:15:GLY:HA3	9:M:2032:HOH:O	1.25	1.28
1:M:427:TYR:HE2	9:M:2614:HOH:O	1.19	1.25
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:OH	1.33	1.24
1:M:428:THR:HG23	9:M:2617:HOH:O	1.27	1.24
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CE2	2.22	1.23
3:M:921:NAG:O3	3:M:921:NAG:C3	1.89	1.19
1:M:477:TYR:HE1	9:M:2659:HOH:O	1.21	1.18
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CE2	1.78	1.17
1:M:431:ASP:OD1	9:M:2620:HOH:O	1.66	1.10
1:M:477:TYR:CE1	9:M:2659:HOH:O	1.94	1.08
8:M:1010:GOL:H11	9:W:2026:HOH:O	1.27	1.08
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CE2	2.33	1.07
1:M:215:TYR:O	9:M:2355:HOH:O	1.69	1.07
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CD2	1.92	1.05
8:M:1010:GOL:C2	9:W:2026:HOH:O	1.91	1.04
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:OH	2.03	1.03
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CE2	1.91	1.02
1:M:427:TYR:CE2	9:M:2614:HOH:O	1.95	1.01
7:M:1004:SO4:O2	7:M:1009:SO4:S	2.19	1.00
1:M:165:LYS:NZ	2:M:931:NAG:H82	1.76	0.99
2:M:961:NAG:H61	9:M:3056:HOH:O	1.62	0.98
1:M:259:ARG:HG2	9:M:2483:HOH:O	1.64	0.96
1:M:472:ARG:CZ	9:M:2659:HOH:O	2.12	0.95
1:M:246:THR:HG22	9:M:2377:HOH:O	1.66	0.94
1:M:150:ASP:OD2	9:M:2277:HOH:O	1.88	0.91
1:M:379:THR:HG23	9:M:2548:HOH:O	1.71	0.90
1:M:53:GLY:O	9:M:2097:HOH:O	1.90	0.89
5:M:954:BMA:H61	5:M:957:MAN:C6	2.03	0.89
7:M:1004:SO4:O2	7:M:1009:SO4:O2	1.91	0.88
5:M:954:BMA:H61	5:M:957:MAN:H61	1.55	0.88
1:M:130:LYS:HB3	9:M:2253:HOH:O	1.72	0.88
1:M:215:TYR:HB2	9:M:2102:HOH:O	1.72	0.86
1:M:165:LYS:HZ1	2:M:931:NAG:H82	1.34	0.86
1:M:130:LYS:HG3	9:M:2243:HOH:O	1.76	0.84
1:M:15:GLY:CA	9:M:2032:HOH:O	1.93	0.84
1:M:21:ASN:HD21	2:M:901:NAG:C2	1.88	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:151:GLU:OE1	9:M:2279:HOH:O	1.97	0.82
5:M:954:BMA:C6	5:M:957:MAN:H61	2.11	0.81
1:M:381:ASN:ND2	9:M:2554:HOH:O	2.14	0.79
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CD2	2.61	0.78
7:M:1009:SO4:O1	9:W:2024:HOH:O	2.00	0.78
1:M:70:ASP:HB3	9:M:2078:HOH:O	1.83	0.76
3:M:983:NAG:H83	9:M:3062:HOH:O	1.86	0.76
5:M:954:BMA:C6	5:M:957:MAN:C6	2.65	0.74
1:M:373:LYS:NZ	9:M:2554:HOH:O	2.21	0.74
1:M:130:LYS:HB3	9:M:2091:HOH:O	1.87	0.74
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:CZ	2.22	0.74
1:M:90:ASN:ND2	2:M:911:NAG:C2	2.53	0.72
1:M:264:TYR:OH	1:M:264:TYR:CE2	2.42	0.71
1:M:360[B]:ILE:HG13	1:M:366[B]:TYR:CE2	2.24	0.71
1:M:9:ASN:HB2	9:W:2014:HOH:O	1.91	0.70
1:M:116:LYS:HG2	9:M:2225:HOH:O	1.92	0.70
3:M:921:NAG:O3	9:M:3019:HOH:O	2.10	0.70
1:M:472:ARG:NE	9:M:2659:HOH:O	2.20	0.70
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CZ	2.67	0.69
1:M:493:GLN:NE2	9:M:2681:HOH:O	2.24	0.69
7:M:1004:SO4:S	7:M:1009:SO4:O3	2.51	0.68
1:M:70:ASP:OD2	9:M:2125:HOH:O	2.11	0.68
1:M:45:GLY:HA2	9:M:2085:HOH:O	1.93	0.68
7:M:1003:SO4:O2	9:W:2006:HOH:O	2.14	0.66
5:M:954:BMA:H61	5:M:957:MAN:H62	1.76	0.66
1:M:115:GLU:HG3	9:M:2223:HOH:O	1.95	0.66
1:M:111:ARG:O	9:M:2213:HOH:O	2.14	0.66
1:M:169[B]:ASP:HB2	1:M:240:LEU:HD21	1.78	0.65
1:M:472:ARG:NH2	9:M:2659:HOH:O	2.26	0.65
1:M:220[A]:SER:OG	9:M:2359:HOH:O	2.15	0.64
1:M:4:ILE:HD11	1:M:445:LYS:HD2	1.80	0.64
7:M:1003:SO4:O4	9:W:2006:HOH:O	2.16	0.63
1:M:200:LEU:HB3	9:M:2336:HOH:O	1.98	0.63
7:M:1004:SO4:O2	7:M:1009:SO4:O3	2.15	0.63
8:M:1010:GOL:O2	9:W:2026:HOH:O	2.01	0.61
7:M:1004:SO4:O1	7:M:1009:SO4:O3	2.20	0.60
1:M:365:HIS:HE1	9:M:2532:HOH:O	1.83	0.60
1:M:342[A]:VAL:HG13	9:M:2359:HOH:O	2.02	0.60
7:M:1004:SO4:S	7:M:1009:SO4:S	3.00	0.59
1:M:45:GLY:HA2	9:M:2086:HOH:O	2.03	0.58
1:M:159:GLN:NE2	9:M:2288:HOH:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CZ	2.33	0.58
1:M:115:GLU:CD	9:M:2223:HOH:O	2.42	0.58
1:M:90:ASN:ND2	2:M:911:NAG:O5	2.36	0.58
1:M:115:GLU:OE2	9:M:2223:HOH:O	2.17	0.57
1:M:21:ASN:CG	2:M:901:NAG:C1	2.67	0.56
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CG	2.40	0.56
1:M:424:MET:HE3	9:M:2681:HOH:O	2.05	0.56
1:M:194:ARG:NH1	7:M:1009:SO4:O4	2.40	0.55
1:M:331:PHE:CD1	9:M:2483:HOH:O	2.53	0.55
1:M:165:LYS:HZ2	2:M:931:NAG:H82	1.67	0.55
5:M:954:BMA:C6	9:M:3055:HOH:O	2.47	0.55
1:M:21:ASN:ND2	2:M:901:NAG:C2	2.58	0.54
1:M:90:ASN:CG	2:M:911:NAG:C1	2.68	0.52
1:M:4:ILE:HD11	1:M:445:LYS:CD	2.39	0.52
1:M:244:ASN:HD21	2:M:931:NAG:C2	1.98	0.52
5:M:957:MAN:C4	9:M:3053:HOH:O	2.58	0.52
3:M:921:NAG:O3	3:M:921:NAG:C2	2.56	0.51
1:M:472:ARG:HG2	9:M:2658:HOH:O	2.11	0.51
1:M:21:ASN:ND2	2:M:901:NAG:O5	2.40	0.51
1:M:130:LYS:CB	9:M:2253:HOH:O	2.43	0.51
1:M:28:ASP:HA	9:M:2053:HOH:O	2.10	0.51
1:M:115:GLU:CG	9:M:2223:HOH:O	2.56	0.50
1:M:360[A]:ILE:HG23	9:M:2518:HOH:O	2.10	0.50
1:M:10:LEU:HD23	9:M:2023:HOH:O	2.12	0.49
1:M:108:LYS:HD2	9:M:2298:HOH:O	2.12	0.49
1:M:15:GLY:C	9:M:2032:HOH:O	2.34	0.48
1:M:70:ASP:CB	9:M:2078:HOH:O	2.51	0.48
1:M:360[A]:ILE:CG2	9:M:2518:HOH:O	2.61	0.48
1:M:95:ARG:HA	1:M:136:PHE:O	2.14	0.47
5:M:957:MAN:C5	9:M:3053:HOH:O	2.62	0.47
1:M:59:PRO:HB3	9:M:2100:HOH:O	2.14	0.47
5:M:954:BMA:O6	5:M:957:MAN:C6	2.49	0.46
1:M:12:PHE:HD2	9:M:2023:HOH:O	2.00	0.45
1:M:165:LYS:CE	2:M:931:NAG:H82	2.46	0.45
1:M:373:LYS:NZ	1:M:378:SER:OG	2.46	0.44
1:M:45:GLY:CA	9:M:2085:HOH:O	2.57	0.44
1:M:122:HIS:HE1	1:M:174:GLU:O	1.99	0.44
1:M:95:ARG:HB2	1:M:455:LEU:HD13	2.00	0.43
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:OH	2.05	0.43
5:M:957:MAN:C6	9:M:3053:HOH:O	2.67	0.43
1:M:497:THR:HG23	9:M:2689:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:59:PRO:HG3	9:M:2117:HOH:O	2.19	0.42
1:M:244:ASN:ND2	2:M:931:NAG:O5	2.42	0.42
1:M:4:ILE:CD1	1:M:445:LYS:HD2	2.49	0.42
1:M:12:PHE:N	9:M:2023:HOH:O	2.26	0.42
2:M:961:NAG:C6	9:M:3056:HOH:O	2.41	0.41
1:M:244:ASN:ND2	2:M:931:NAG:C2	2.68	0.41
1:M:48:LEU:N	9:M:2090:HOH:O	2.35	0.40
1:M:111:ARG:C	9:M:2213:HOH:O	2.58	0.40

All (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
9:M:2555:HOH:O	9:M:2555:HOH:O[4_576]	1.44	0.76
9:M:2018:HOH:O	9:M:2018:HOH:O[4_576]	1.63	0.57
9:M:2258:HOH:O	9:M:2258:HOH:O[4_576]	1.63	0.57
9:M:2385:HOH:O	9:M:2426:HOH:O[6_565]	1.71	0.49
9:M:2116:HOH:O	9:M:2132:HOH:O[3_656]	1.76	0.44
9:M:2245:HOH:O	9:M:2621:HOH:O[4_576]	1.90	0.30
1:M:45:GLY:N	1:M:57:ARG:O[3_656]	1.95	0.25
9:M:2523:HOH:O	9:M:2622:HOH:O[4_576]	2.01	0.19
1:M:375:LYS:O	1:M:375:LYS:CD[4_576]	2.04	0.16
9:M:2388:HOH:O	9:M:2441:HOH:O[6_565]	2.06	0.14
1:M:379:THR:CG2	9:M:2603:HOH:O[4_576]	2.07	0.13
9:M:2018:HOH:O	9:M:2019:HOH:O[4_576]	2.08	0.12
1:M:43:THR:OG1	1:M:56:HIS:O[3_656]	2.10	0.10
9:M:2047:HOH:O	9:M:2127:HOH:O[3_656]	2.10	0.10
9:M:3057:HOH:O	9:M:2085:HOH:O[3_656]	2.12	0.08
9:W:2014:HOH:O	9:W:2014:HOH:O[4_576]	2.12	0.08



## 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 ⓘ

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 ⓘ

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%)
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

All (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
3	M	921	NAG	C7-N2	-4.31	1.17	1.34
4	M	944	BMA	C2-C3	-4.28	1.46	1.52
5	M	953	NAG	C3-C2	-3.08	1.45	1.52
5	M	951	NAG	O5-C1	-2.45	1.39	1.43
5	M	951	NAG	C2-N2	-2.37	1.42	1.46
5	M	957	MAN	C6-C5	-2.23	1.44	1.51
3	M	981	NAG	O5-C1	-2.21	1.40	1.43
5	M	952	FUC	C4-C3	-2.02	1.47	1.52
4	M	945	XYP	O3B-C3B	2.03	1.47	1.43
5	M	954	BMA	O3-C3	2.05	1.47	1.43
3	M	983	NAG	C8-C7	2.08	1.54	1.50
5	M	957	MAN	O5-C1	2.10	1.47	1.43
4	M	942	FUC	O2-C2	2.11	1.48	1.43
5	M	953	NAG	C1-C2	2.17	1.55	1.52
3	M	983	NAG	C4-C5	2.25	1.57	1.53
5	M	953	NAG	O7-C7	2.30	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	943	NAG	C1-C2	2.31	1.55	1.52
5	M	952	FUC	C1-C2	2.36	1.57	1.52
4	M	945	XYP	C4B-C3B	2.39	1.55	1.52
5	M	955	XYP	O5B-C5B	2.55	1.47	1.42
5	M	957	MAN	C1-C2	2.57	1.58	1.52
4	M	944	BMA	O5-C5	2.58	1.49	1.43
3	M	921	NAG	O5-C5	2.70	1.49	1.43
3	M	921	NAG	O4-C4	2.74	1.49	1.43
5	M	955	XYP	O3B-C3B	2.83	1.49	1.43
4	M	942	FUC	C2-C3	2.93	1.56	1.52
3	M	983	NAG	C1-C2	3.03	1.56	1.52
3	M	921	NAG	C4-C5	3.07	1.59	1.53
5	M	957	MAN	O4-C4	3.10	1.50	1.43
5	M	956	MAN	C4-C5	3.20	1.59	1.53
5	M	955	XYP	C2B-C3B	3.29	1.57	1.52
5	M	952	FUC	O4-C4	3.44	1.51	1.43
5	M	954	BMA	C4-C5	3.44	1.60	1.53
3	M	921	NAG	C3-C2	3.62	1.60	1.52
5	M	957	MAN	C2-C3	3.68	1.57	1.52
5	M	956	MAN	O5-C5	4.28	1.52	1.43
3	M	981	NAG	C8-C7	4.65	1.59	1.50
5	M	952	FUC	C2-C3	5.15	1.59	1.52
5	M	952	FUC	C4-C5	5.16	1.63	1.52
3	M	923	NAG	O5-C5	6.52	1.57	1.43
5	M	957	MAN	O5-C5	7.21	1.59	1.43
3	M	921	NAG	O7-C7	7.34	1.40	1.23
3	M	921	NAG	O3-C3	19.50	1.89	1.43

All (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
5	M	957	MAN	O4-C4-C3	-6.54	95.62	110.34
5	M	954	BMA	O5-C5-C6	-6.47	93.34	107.35
5	M	957	MAN	C2-C3-C4	-6.38	100.20	111.04
5	M	954	BMA	O4-C4-C3	-6.11	96.58	110.34
5	M	951	NAG	C1-O5-C5	-6.11	104.50	112.25
5	M	952	FUC	C1-C2-C3	-5.77	102.72	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	945	XYP	C5B-C4B-C3B	-5.69	102.81	109.54
3	M	981	NAG	C8-C7-N2	-5.52	105.54	116.11
5	M	954	BMA	C1-C2-C3	-5.40	103.16	109.54
4	M	942	FUC	O3-C3-C2	-5.27	100.48	110.00
5	M	954	BMA	O2-C2-C3	-4.92	100.22	110.12
3	M	921	NAG	O4-C4-C5	-4.87	96.32	109.24
5	M	955	XYP	C5B-C4B-C3B	-4.83	103.83	109.54
5	M	955	XYP	O5B-C1B-C2B	-4.80	101.33	110.31
4	M	941	NAG	C1-O5-C5	-4.79	106.17	112.25
5	M	957	MAN	O5-C1-C2	-4.53	103.51	110.86
5	M	955	XYP	C4B-C3B-C2B	-4.43	106.86	111.24
4	M	941	NAG	C2-N2-C7	-4.15	117.70	123.04
3	M	921	NAG	C4-C3-C2	-4.10	104.86	111.23
4	M	942	FUC	C1-C2-C3	-4.06	104.74	109.54
4	M	945	XYP	O2B-C2B-C3B	-4.02	102.03	110.12
3	M	983	NAG	C2-N2-C7	-4.01	117.89	123.04
4	M	945	XYP	O3B-C3B-C2B	-3.92	102.91	110.00
5	M	956	MAN	C3-C4-C5	-3.88	103.44	110.20
3	M	921	NAG	O7-C7-C8	-3.85	114.99	122.06
5	M	956	MAN	C2-C3-C4	-3.69	104.77	111.04
3	M	923	NAG	C4-C3-C2	-3.63	105.59	111.23
3	M	983	NAG	C1-O5-C5	-3.49	107.81	112.25
3	M	981	NAG	C2-N2-C7	-3.48	118.56	123.04
3	M	923	NAG	O6-C6-C5	-3.48	99.85	111.33
5	M	956	MAN	O2-C2-C3	-3.46	103.16	110.12
5	M	957	MAN	C3-C4-C5	-3.40	104.27	110.20
4	M	942	FUC	O2-C2-C3	-3.33	103.43	110.12
4	M	943	NAG	C2-N2-C7	-3.32	118.77	123.04
3	M	921	NAG	O4-C4-C3	-3.30	102.91	110.34
3	M	921	NAG	O3-C3-C4	-3.24	103.03	110.34
5	M	956	MAN	O5-C5-C6	-3.20	100.42	107.35
3	M	983	NAG	C3-C4-C5	-2.98	105.00	110.20
3	M	983	NAG	O4-C4-C3	-2.96	103.67	110.34
3	M	983	NAG	C6-C5-C4	-2.91	105.83	113.02
5	M	954	BMA	C1-O5-C5	-2.86	108.62	112.25
5	M	953	NAG	C2-N2-C7	-2.78	119.47	123.04
5	M	951	NAG	O5-C5-C6	-2.76	101.37	107.35
5	M	955	XYP	O4B-C4B-C3B	-2.69	104.70	110.12
4	M	944	BMA	O5-C5-C6	-2.68	101.54	107.35
3	M	923	NAG	O5-C5-C6	-2.68	101.54	107.35
5	M	953	NAG	O4-C4-C3	-2.66	104.34	110.34
5	M	957	MAN	O2-C2-C1	-2.62	103.96	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	923	NAG	C3-C2-N2	-2.42	104.76	110.56
5	M	956	MAN	C6-C5-C4	-2.35	107.22	113.02
5	M	955	XYP	O2B-C2B-C3B	-2.34	105.41	110.12
4	M	943	NAG	O4-C4-C3	-2.30	105.15	110.34
4	M	942	FUC	O3-C3-C4	-2.26	105.25	110.34
5	M	953	NAG	C1-O5-C5	-2.23	109.42	112.25
4	M	941	NAG	C8-C7-N2	-2.21	111.87	116.11
3	M	983	NAG	C4-C3-C2	-2.12	107.94	111.23
5	M	953	NAG	O6-C6-C5	-2.01	104.69	111.33
4	M	941	NAG	C4-C3-C2	-2.01	108.11	111.23
5	M	952	FUC	C6-C5-C4	-2.01	109.13	113.08
4	M	944	BMA	C3-C4-C5	2.12	113.89	110.20
5	M	951	NAG	C2-N2-C7	2.19	125.86	123.04
5	M	956	MAN	C1-O5-C5	2.21	115.06	112.25
3	M	921	NAG	C8-C7-N2	2.32	120.56	116.11
3	M	983	NAG	O3-C3-C2	2.39	113.86	109.11
4	M	944	BMA	O3-C3-C4	2.50	115.98	110.34
5	M	956	MAN	O2-C2-C1	2.92	115.06	109.21
4	M	944	BMA	C2-C3-C4	3.02	116.17	111.04
4	M	945	XYP	C1B-C2B-C3B	3.59	113.78	109.54
5	M	954	BMA	C3-C4-C5	3.72	116.67	110.20
3	M	923	NAG	O3-C3-C4	4.26	119.92	110.34
5	M	957	MAN	O6-C6-C5	4.44	126.02	111.33
5	M	954	BMA	C6-C5-C4	5.69	127.05	113.02
5	M	956	MAN	C1-C2-C3	5.72	116.31	109.54
5	M	957	MAN	C1-C2-C3	5.91	116.53	109.54
3	M	981	NAG	O7-C7-N2	6.01	134.11	121.86
5	M	957	MAN	O4-C4-C5	8.20	130.98	109.24
3	M	923	NAG	C3-C4-C5	9.24	126.30	110.20
5	M	954	BMA	O4-C4-C5	9.40	134.15	109.24
5	M	957	MAN	C6-C5-C4	12.21	143.14	113.02

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
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

All (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
7	M	1002	SO4	O3-S	-3.28	1.35	1.47
2	M	961	NAG	O7-C7	-3.28	1.15	1.23
2	M	901	NAG	O7-C7	-2.74	1.16	1.23
2	M	931	NAG	C2-N2	-2.54	1.41	1.46
2	M	931	NAG	O5-C1	-2.09	1.40	1.43
7	M	1009	SO4	O2-S	2.08	1.54	1.47
2	M	961	NAG	C2-N2	2.08	1.50	1.46
8	M	1020	GOL	O1-C1	2.13	1.51	1.42
7	M	1007	SO4	O2-S	2.15	1.54	1.47
2	M	931	NAG	O4-C4	2.97	1.50	1.43
7	M	1009	SO4	O1-S	3.61	1.59	1.47
7	M	1004	SO4	O1-S	3.83	1.60	1.47
2	M	911	NAG	O5-C5	3.85	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1006	SO4	O2-S	5.52	1.66	1.47

All (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
2	M	901	NAG	C1-O5-C5	-6.58	103.90	112.25
2	M	931	NAG	O7-C7-C8	-5.06	112.77	122.06
2	M	991	NAG	C4-C3-C2	-4.47	104.28	111.23
2	M	961	NAG	O3-C3-C2	-4.35	100.50	109.11
2	M	991	NAG	O3-C3-C2	-3.78	101.62	109.11
2	M	911	NAG	C4-C3-C2	-3.63	105.59	111.23
7	M	1004	SO4	O2-S-O1	-3.36	98.86	109.50
2	M	931	NAG	O4-C4-C5	-3.19	100.79	109.24
2	M	961	NAG	O4-C4-C5	-2.97	101.36	109.24
2	M	971	NAG	O5-C5-C6	-2.82	101.24	107.35
2	M	971	NAG	O3-C3-C2	-2.81	103.55	109.11
2	M	931	NAG	O4-C4-C3	-2.64	104.40	110.34
2	M	931	NAG	O5-C5-C6	-2.63	101.66	107.35
2	M	931	NAG	C4-C3-C2	-2.47	107.39	111.23
8	M	1024	GOL	C3-C2-C1	-2.41	101.68	111.12
7	M	1007	SO4	O2-S-O1	-2.35	102.06	109.50
2	M	901	NAG	C4-C3-C2	-2.15	107.88	111.23
2	M	911	NAG	O5-C5-C6	-2.07	102.87	107.35
7	M	1006	SO4	O3-S-O2	-2.05	91.08	110.19
7	M	1009	SO4	O3-S-O1	-2.04	91.24	110.19
2	M	911	NAG	O3-C3-C2	-2.01	105.13	109.11
7	M	1006	SO4	O4-S-O3	2.06	117.36	108.98
8	M	1010	GOL	O2-C2-C1	2.23	118.87	108.65
2	M	971	NAG	O7-C7-C8	2.23	126.15	122.06
2	M	971	NAG	C2-N2-C7	2.54	126.30	123.04
2	M	971	NAG	C1-O5-C5	2.77	115.77	112.25
7	M	1004	SO4	O4-S-O3	3.25	122.18	108.98
2	M	971	NAG	O4-C4-C3	3.32	117.82	110.34
2	M	931	NAG	C3-C4-C5	3.98	117.13	110.20
2	M	931	NAG	C3-C2-N2	4.16	120.53	110.56
7	M	1009	SO4	O4-S-O3	4.99	129.27	108.98
2	M	961	NAG	C1-O5-C5	8.95	123.61	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	931	NAG	C8-C7-N2	12.74	140.50	116.11
2	M	931	NAG	C2-N2-C7	23.85	153.68	123.04

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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%) 0 0	7, 11, 25, 52	2 (0%)

All (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
1	M	345	THR	6.6
1	M	380	ASP	6.6
1	M	366[A]	TYR	6.3
1	M	375	LYS	6.3
1	M	419	ASN	6.2
1	M	417	ASP	6.2
1	M	481	ASN	6.1
1	M	78	TYR	6.1
1	M	420	ARG	5.8
1	M	360[A]	ILE	5.8
1	M	482	ASN	5.8
1	M	213[A]	SER	5.7
1	M	480	TRP	5.7
1	M	17	THR	5.6
1	M	83	ILE	5.5
1	M	390	TYR	5.5
1	M	112	GLY	5.5
1	M	471	VAL	5.5
1	M	364	GLY	5.4
1	M	4	ILE	5.3
1	M	79	TRP	5.3
1	M	457	TRP	5.3

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Mol	Chain	Res	Type	RSRZ
1	M	138	THR	5.3
1	M	434	CYS	5.2
1	M	3	GLU	5.2
1	M	209	THR	5.2
1	M	144	LEU	5.2
1	M	374	ASP	5.1
1	M	421	ASN	5.1
1	M	339	PRO	5.1
1	M	25	PHE	5.1
1	M	197	GLY	5.1
1	M	196	TYR	5.1
1	M	10	LEU	5.1
1	M	283	LEU	5.0
1	M	51	TRP	5.0
1	M	18	ASP	5.0
1	M	497	THR	4.9
1	M	80	GLN	4.9
1	M	55	THR	4.9
1	M	206	CYS	4.9
1	M	73	CYS	4.9
1	M	371	PHE	4.8
1	M	191	VAL	4.8
1	M	36	SER	4.8
1	M	305[A]	GLU	4.8
1	M	362	ALA	4.8
1	M	478	ILE	4.8
1	M	424	MET	4.8
1	M	142	TRP	4.7
1	M	245	TYR	4.7
1	M	415	PRO	4.7
1	M	465	PHE	4.7
1	M	27	SER	4.7
1	M	152	TYR	4.7
1	M	458	ALA	4.7
1	M	167	TYR	4.6
1	M	349	ALA	4.6
1	M	30[A]	ILE	4.6
1	M	334	TYR	4.6
1	M	50	ILE	4.6
1	M	444	ILE	4.6
1	M	449[A]	VAL	4.5
1	M	344[A]	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	M	215	TYR	4.5
1	M	208	PRO	4.5
1	M	183	LEU	4.5
1	M	210	VAL	4.5
1	M	363[A]	SER	4.5
1	M	89	LEU	4.4
1	M	12	PHE	4.4
1	M	470	THR	4.4
1	M	97	SER	4.4
1	M	93	GLY	4.4
1	M	43	THR	4.4
1	M	379	THR	4.4
1	M	377	ASP	4.4
1	M	101[A]	SER	4.4
1	M	359	TYR	4.4
1	M	300	ILE	4.4
1	M	59	PRO	4.3
1	M	488	LEU	4.3
1	M	54	PHE	4.3
1	M	24	SER	4.3
1	M	274	ALA	4.3
1	M	16	ASN	4.3
1	M	128	LEU	4.3
1	M	113	VAL	4.3
1	M	219	SER	4.3
1	M	388	GLY	4.2
1	M	433	LEU	4.2
1	M	404	LEU	4.2
1	M	430	ILE	4.2
1	M	129	ILE	4.2
1	M	160	ILE	4.2
1	M	132	GLY	4.1
1	M	330	TYR	4.1
1	M	214	CYS	4.1
1	M	203	PRO	4.1
1	M	9	ASN	4.1
1	M	499	ILE	4.1
1	M	281	PHE	4.1
1	M	338[A]	SER	4.1
1	M	20[A]	LEU	4.1
1	M	63	GLY	4.1
1	M	313	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	M	418	GLU	4.0
1	M	147	THR	4.0
1	M	29	PHE	4.0
1	M	396	PHE	4.0
1	M	164	PHE	4.0
1	M	500	SER	4.0
1	M	94	TYR	4.0
1	M	317	LEU	4.0
1	M	335	ALA	4.0
1	M	13	THR	4.0
1	M	71	THR	4.0
1	M	90	ASN	4.0
1	M	318	VAL	4.0
1	M	48	LEU	3.9
1	M	140	PHE	3.9
1	M	459	LEU	3.9
1	M	103	ILE	3.9
1	M	484	THR	3.9
1	M	38	TYR	3.9
1	M	154	GLY	3.9
1	M	124	LEU	3.9
1	M	139	LEU	3.9
1	M	223	PRO	3.9
1	M	260	TRP	3.9
1	M	342[A]	VAL	3.9
1	M	169[A]	ASP	3.9
1	M	68	ASN	3.9
1	M	192	PRO	3.9
1	M	249	GLY	3.9
1	M	485	ASP	3.9
1	M	298	ILE	3.8
1	M	432	TYR	3.8
1	M	99	ALA	3.8
1	M	264	TYR	3.8
1	M	308	PRO	3.8
1	M	368	GLY	3.8
1	M	81	LYS	3.8
1	M	490	LYS	3.8
1	M	326	GLY	3.8
1	M	257	ILE	3.8
1	M	285	TRP	3.8
1	M	200	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	M	115	GLU	3.8
1	M	69	GLY	3.8
1	M	118[A]	ILE	3.8
1	M	370	LEU	3.8
1	M	479	ASP	3.7
1	M	170	LEU	3.7
1	M	106	ARG	3.7
1	M	211	ASP	3.7
1	M	414	THR	3.7
1	M	11	PRO	3.7
1	M	45	GLY	3.7
1	M	53	GLY	3.7
1	M	474	GLY	3.7
1	M	498	PHE	3.7
1	M	104	ILE	3.7
1	M	310	PHE	3.7
1	M	493	GLN	3.7
1	M	422	GLN	3.6
1	M	401	TYR	3.6
1	M	278	MET	3.6
1	M	324	PHE	3.6
1	M	395	TYR	3.6
1	M	400	TYR	3.6
1	M	75	SER	3.6
1	M	220[A]	SER	3.6
1	M	357	LEU	3.6
1	M	66	HIS	3.6
1	M	60	ASN	3.6
1	M	58	TYR	3.6
1	M	275	THR	3.6
1	M	438	CYS	3.6
1	M	350	MET	3.6
1	M	52	ASP	3.5
1	M	491	SER	3.5
1	M	304	GLY	3.5
1	M	258	THR	3.5
1	M	425	LEU	3.5
1	M	62[A]	SER	3.5
1	M	332	THR	3.5
1	M	271[A]	SER	3.4
1	M	492	GLY	3.4
1	M	489	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	57	ARG	3.4
1	M	426	ASP	3.4
1	M	182	TRP	3.4
1	M	365	HIS	3.4
1	M	311	SER	3.4
1	M	315	SER	3.4
1	M	451	VAL	3.4
1	M	64	PRO	3.4
1	M	84	ASP	3.4
1	M	88[A]	GLU	3.4
1	M	56	HIS	3.4
1	M	77	SER	3.4
1	M	423	SER	3.4
1	M	120	TYR	3.4
1	M	76	PHE	3.3
1	M	110	SER	3.3
1	M	455	LEU	3.3
1	M	95	ARG	3.3
1	M	5	THR	3.3
1	M	157	ASP	3.3
1	M	439	PHE	3.3
1	M	240	LEU	3.3
1	M	141	HIS	3.3
1	M	382	ILE	3.3
1	M	121	TYR	3.3
1	M	443	VAL	3.3
1	M	49	ASN	3.3
1	M	441	ASN	3.2
1	M	384	TYR	3.2
1	M	151	GLU	3.2
1	M	226	VAL	3.2
1	M	126[A]	SER	3.2
1	M	26	SER	3.2
1	M	85	VAL	3.2
1	M	156	LEU	3.2
1	M	327	LEU	3.2
1	M	204	GLY	3.2
1	M	122	HIS	3.2
1	M	341	PRO	3.2
1	M	31	PHE	3.2
1	M	108	LYS	3.2
1	M	272	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	M	294	THR	3.2
1	M	172	PHE	3.2
1	M	473	PHE	3.2
1	M	105	PRO	3.2
1	M	501	PRO	3.2
1	M	329	TYR	3.2
1	M	428	THR	3.2
1	M	303	VAL	3.2
1	M	483	VAL	3.2
1	M	148	LEU	3.2
1	M	177	ASP	3.1
1	M	265	ASN	3.1
1	M	47	GLY	3.1
1	M	117	GLY	3.1
1	M	133	ILE	3.1
1	M	295	TYR	3.1
1	M	381	ASN	3.1
1	M	437	LEU	3.1
1	M	347	HIS	3.1
1	M	116	LYS	3.1
1	M	181	TYR	3.1
1	M	42	GLY	3.1
1	M	28	ASP	3.1
1	M	143	ASP	3.1
1	M	266	ASP	3.1
1	M	171	CYS	3.1
1	M	286	PHE	3.1
1	M	91	ALA	3.0
1	M	33	VAL	3.0
1	M	175	PHE	3.0
1	M	494	TRP	3.0
1	M	445	LYS	3.0
1	M	32	GLY	3.0
1	M	476	SER	3.0
1	M	67	GLY	3.0
1	M	218	ASN	3.0
1	M	161	ILE	3.0
1	M	216	ALA	3.0
1	M	353	ALA	3.0
1	M	237	VAL	3.0
1	M	149	GLN	3.0
1	M	448	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	125	ILE	3.0
1	M	383	TYR	3.0
1	M	399	LYS	3.0
1	M	145	PRO	3.0
1	M	233	ALA	3.0
1	M	235	ALA	3.0
1	M	221	THR	2.9
1	M	403	PRO	2.9
1	M	406	TYR	2.9
1	M	193	THR	2.9
1	M	409	GLU	2.9
1	M	22	SER	2.9
1	M	217	GLY	2.9
1	M	373	LYS	2.9
1	M	146	GLN	2.9
1	M	168	ALA	2.9
1	M	466	ASN	2.9
1	M	130	LYS	2.9
1	M	86	LEU	2.9
1	M	187	GLN	2.9
1	M	297	GLN	2.9
1	M	427	TYR	2.9
1	M	463	TYR	2.9
1	M	46	ARG	2.9
1	M	343	ASN	2.9
1	M	405	ILE	2.9
1	M	296	PRO	2.9
1	M	35	SER	2.8
1	M	413	SER	2.8
1	M	346	ASN	2.8
1	M	127	GLY	2.8
1	M	386	PRO	2.8
1	M	452	LYS	2.8
1	M	72	THR	2.8
1	M	450	ASN	2.8
1	M	229	HIS	2.8
1	M	255	THR	2.8
1	M	284	GLY	2.8
1	M	114	ASN	2.8
1	M	100	TRP	2.8
1	M	195	GLY	2.8
1	M	468	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	475	LEU	2.8
1	M	201	ASP	2.8
1	M	467	LYS	2.8
1	M	179	VAL	2.8
1	M	477	TYR	2.8
1	M	331	PHE	2.8
1	M	356	LYS	2.8
1	M	70	ASP	2.8
1	M	134	THR	2.8
1	M	407	VAL	2.8
1	M	178	SER	2.7
1	M	162	ASP	2.7
1	M	486	ARG	2.7
1	M	98	ILE	2.7
1	M	185	ILE	2.7
1	M	440	LEU	2.7
1	M	270	HIS	2.7
1	M	309[A]	SER	2.7
1	M	391	SER	2.7
1	M	487	ASP	2.7
1	M	322	TYR	2.7
1	M	290	LEU	2.7
1	M	392	VAL	2.7
1	M	462[A]	ASN	2.7
1	M	224	TYR	2.7
1	M	184	THR	2.7
1	M	412	ILE	2.7
1	M	123	GLY	2.7
1	M	96	PHE	2.7
1	M	21	ASN	2.7
1	M	351	MET	2.7
1	M	262	LEU	2.7
1	M	389	ILE	2.7
1	M	246	THR	2.7
1	M	436	HIS	2.7
1	M	456	ALA	2.7
1	M	232	LEU	2.6
1	M	119	ASP	2.6
1	M	158	PRO	2.6
1	M	207	SER	2.6
1	M	241	TYR	2.6
1	M	186	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	202	ALA	2.6
1	M	496	GLN	2.6
1	M	37	ALA	2.6
1	M	454	TYR	2.6
1	M	159	GLN	2.6
1	M	198	SER	2.6
1	M	263	PRO	2.6
1	M	252	ILE	2.6
1	M	385	TYR	2.6
1	M	92	THR	2.5
1	M	316	ASN	2.5
1	M	74	ASP	2.5
1	M	416	GLY	2.5
1	M	472	ARG	2.5
1	M	247	HIS	2.5
1	M	242	ARG	2.5
1	M	293	GLY	2.5
1	M	227	ALA	2.5
1	M	261	PHE	2.5
1	M	307	LEU	2.5
1	M	429	ARG	2.5
1	M	228	HIS	2.5
1	M	136	PHE	2.5
1	M	150	ASP	2.5
1	M	287	MET	2.5
1	M	153	GLU	2.5
1	M	495	TYR	2.5
1	M	431	ASP	2.5
1	M	194	ARG	2.5
1	M	107	GLY	2.4
1	M	188	LEU	2.4
1	M	238	VAL	2.4
1	M	34	ALA	2.4
1	M	410	ASN	2.4
1	M	44	ILE	2.4
1	M	15	GLY	2.4
1	M	398	ASN	2.4
1	M	65	ASP	2.4
1	M	340	ASN	2.4
1	M	40	ILE	2.3
1	M	225	ILE	2.3
1	M	231	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	250	GLY	2.3
1	M	267	THR	2.3
1	M	269	ARG	2.3
1	M	165	LYS	2.3
1	M	253	GLY	2.3
1	M	354	GLY	2.3
1	M	447	LYS	2.3
1	M	358	THR	2.3
1	M	205	ARG	2.3
1	M	109	ARG	2.2
1	M	314	GLU	2.2
1	M	236	LYS	2.2
1	M	254	PRO	2.2
1	M	234	HIS	2.2
1	M	461	ASP	2.2
1	M	111	ARG	2.2
1	M	369	PRO	2.2
1	M	464	GLU	2.2
1	M	7	GLN	2.2
1	M	352	ASP	2.2
1	M	259	ARG	2.1
1	M	222	GLU	2.1
1	M	302	THR	2.1
1	M	282	PHE	2.1
1	M	87	ASP	2.1
1	M	135	PRO	2.1
1	M	6	CYS	2.1
1	M	189	TYR	2.1
1	M	402	ASN	2.1
1	M	397	LYS	2.1
1	M	166	ASP	2.1
1	M	173	GLU	2.1
1	M	337	PRO	2.1
1	M	292	ASN	2.1
1	M	348	THR	2.0
1	M	276	GLU	2.0
1	M	355	ALA	2.0
1	M	280	GLU	2.0
1	M	155	PHE	2.0
1	M	137	VAL	2.0
1	M	244	ASN	2.0
1	M	288	GLY	2.0

## 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
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 [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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
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.