



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:20 pm GMT

PDB ID : 1DWI  
Title : STUDY ON RADIATION DAMAGE ON A CRYOCOOLED CRYSTAL.  
PART 5: STRUCTURE AFTER IRRADIATION WITH 54.0\*10E15 PHO-  
TONS/MM2  
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	:	1.7.2 (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

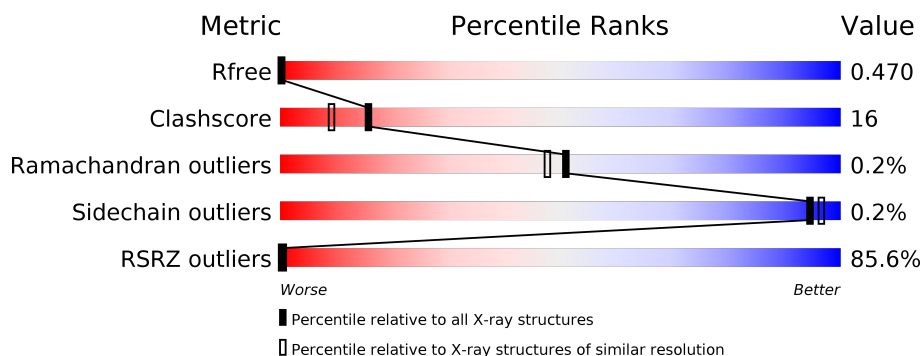
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	931	-	-	X	X
2	NAG	M	961	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	M	923	-	-	-	X
5	BMA	M	954	-	-	X	-
5	MAN	M	957	X	-	X	-
7	SO4	M	1002	-	-	-	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.

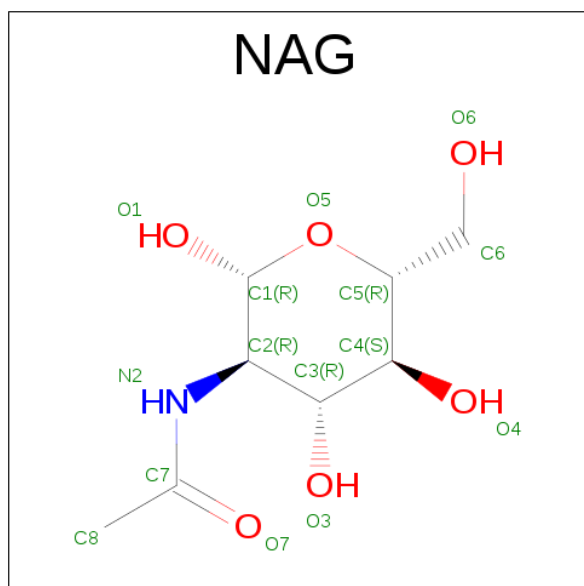
- Molecule 1 is a protein called MYROSINASE MA1.

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		

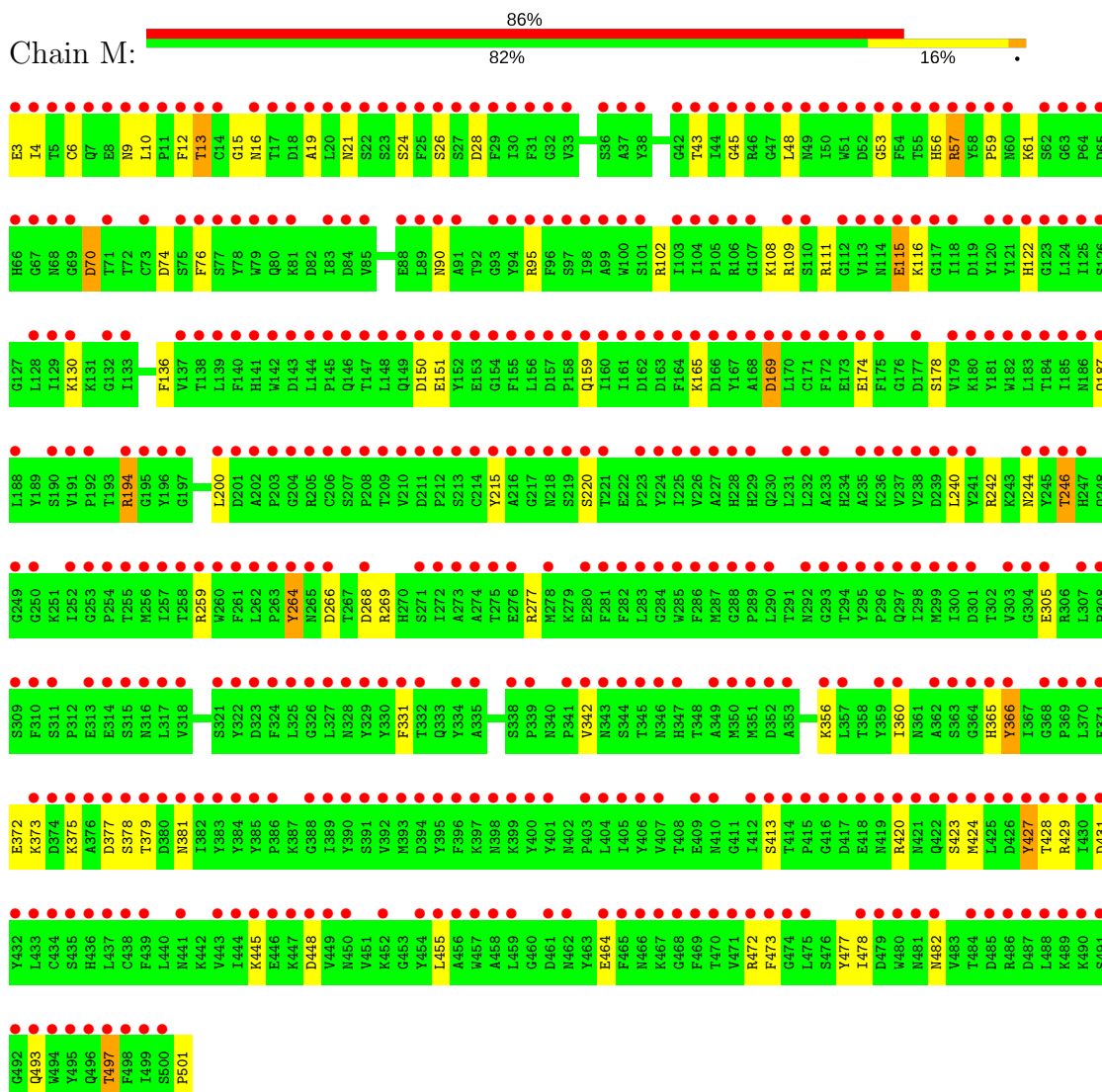
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	788	Total	O	0	0
			788	788		

### 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, $\alpha$ , $\beta$ , $\gamma$	134.30Å 136.40Å 80.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 9.94 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-2.00) 95.1 (9.94-1.99)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.93 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.280 , 0.285 0.447 , 0.470	Depositor DCC
$R_{free}$ test set	2433 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	5220	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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, 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	105	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	788	0	0	78	17
All	All	5220	0	4116	137	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 (137) 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:M:3089: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:M:3089: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:M:3089: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
1:M:130:LYS:HB3	9:M:2253:HOH:O	1.72	0.88
5:M:954:BMA:H61	5:M:957:MAN:H61	1.55	0.88
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:HH	1.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:21:ASN:HD21	2:M:901:NAG:C2	1.88	0.83
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:M:3087: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:116:LYS:HG2	9:M:2225:HOH:O	1.92	0.70
1:M:9:ASN:HB2	9:M:3077:HOH:O	1.91	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:45:GLY:HA2	9:M:2085:HOH:O	1.93	0.68
1:M:70:ASP:OD2	9:M:2125:HOH:O	2.11	0.68
7:M:1003:SO4:O2	9:M:3069:HOH:O	2.14	0.66
1:M:115:GLU:HG3	9:M:2223:HOH:O	1.95	0.66
5:M:954:BMA:H61	5:M:957:MAN:H62	1.76	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:M:3069: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:M:3089: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:159:GLN:NE2	9:M:2288:HOH:O	2.36	0.58
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
1:M:472:ARG:HG2	9:M:2658:HOH:O	2.11	0.51
3:M:921:NAG:O3	3:M:921:NAG:C2	2.56	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
1:M:59:PRO:HB3	9:M:2100:HOH:O	2.14	0.47
5:M:957:MAN:C5	9:M:3053:HOH:O	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:497:THR:HG23	9:M:2689:HOH:O	2.19	0.42
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:12:PHE:N	9:M:2023:HOH:O	2.26	0.42
1:M:4:ILE:CD1	1:M:445:LYS:HD2	2.49	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:M:3077:HOH:O	9:M:3077: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%)	51	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%)	94	96

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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	122	HIS
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	6.16	7 (50%)	15,19,21	3.51	8 (53%)
3	NAG	M	923	3	14,14,15	2.86	3 (21%)	15,19,21	3.90	7 (46%)
4	NAG	M	941	1,4	14,14,15	0.56	0	15,19,21	2.03	5 (33%)
4	FUC	M	942	4	9,10,11	1.65	2 (22%)	13,14,16	2.26	4 (30%)
4	NAG	M	943	4	14,14,15	1.03	1 (7%)	15,19,21	1.38	3 (20%)
4	BMA	M	944	4	11,11,12	1.92	2 (18%)	13,15,17	1.61	4 (30%)
4	XYP	M	945	4	9,9,10	1.37	2 (22%)	10,12,14	2.80	4 (40%)
5	NAG	M	951	1,5	14,14,15	1.91	3 (21%)	15,19,21	2.52	2 (13%)
5	FUC	M	952	5	9,10,11	3.07	5 (55%)	13,14,16	1.93	2 (15%)
5	NAG	M	953	5	14,14,15	1.47	3 (21%)	15,19,21	1.71	3 (20%)
5	BMA	M	954	5	11,11,12	2.64	3 (27%)	13,15,17	4.43	7 (53%)
5	XYP	M	955	5	9,9,10	1.95	3 (33%)	10,12,14	2.32	4 (40%)
5	MAN	M	956	5	11,11,12	1.90	2 (18%)	13,15,17	2.69	7 (53%)
5	MAN	M	957	5	11,11,12	3.06	7 (63%)	13,15,17	7.12	10 (76%)
3	NAG	M	981	1,3	14,14,15	2.34	4 (28%)	15,19,21	2.51	3 (20%)
3	NAG	M	983	3	14,14,15	1.42	2 (14%)	15,19,21	2.67	9 (60%)

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 (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	954	BMA	C2-C3	-7.27	1.42	1.52
3	M	981	NAG	O7-C7	-6.30	1.08	1.23
3	M	923	NAG	C6-C5	-6.06	1.31	1.51
5	M	951	NAG	C1-C2	-5.26	1.45	1.52
3	M	923	NAG	C4-C5	-4.53	1.43	1.53
3	M	921	NAG	C7-N2	-4.50	1.17	1.34
4	M	944	BMA	C2-C3	-4.37	1.46	1.52
5	M	953	NAG	C3-C2	-3.31	1.45	1.52
5	M	951	NAG	O5-C1	-2.50	1.39	1.43
5	M	951	NAG	C2-N2	-2.38	1.42	1.46
5	M	957	MAN	C6-C5	-2.31	1.44	1.51
3	M	981	NAG	O5-C1	-2.26	1.40	1.43
5	M	952	FUC	C4-C3	-2.07	1.47	1.52
3	M	981	NAG	O4-C4	2.03	1.47	1.43
5	M	957	MAN	C4-C3	2.06	1.57	1.52
4	M	945	XYP	O3B-C3B	2.12	1.47	1.43
5	M	954	BMA	O3-C3	2.14	1.47	1.43
5	M	957	MAN	O5-C1	2.15	1.47	1.43
4	M	942	FUC	O2-C2	2.16	1.48	1.43
5	M	953	NAG	C1-C2	2.19	1.55	1.52
5	M	953	NAG	O7-C7	2.25	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	983	NAG	C4-C5	2.26	1.57	1.53
4	M	943	NAG	C1-C2	2.33	1.55	1.52
5	M	952	FUC	C1-C2	2.38	1.57	1.52
4	M	945	XYP	C4B-C3B	2.42	1.55	1.52
5	M	955	XYP	O5B-C5B	2.50	1.47	1.42
5	M	957	MAN	C1-C2	2.60	1.58	1.52
4	M	944	BMA	O5-C5	2.70	1.49	1.43
3	M	921	NAG	O5-C5	2.82	1.49	1.43
3	M	921	NAG	O4-C4	2.86	1.49	1.43
5	M	955	XYP	O3B-C3B	2.95	1.49	1.43
4	M	942	FUC	C2-C3	2.97	1.56	1.52
3	M	983	NAG	C1-C2	3.05	1.56	1.52
3	M	921	NAG	C4-C5	3.09	1.59	1.53
5	M	956	MAN	C4-C5	3.22	1.59	1.53
5	M	957	MAN	O4-C4	3.23	1.50	1.43
5	M	955	XYP	C2B-C3B	3.34	1.57	1.52
5	M	954	BMA	C4-C5	3.46	1.60	1.53
5	M	952	FUC	O4-C4	3.58	1.51	1.43
5	M	957	MAN	C2-C3	3.73	1.57	1.52
3	M	921	NAG	C3-C2	3.80	1.60	1.52
3	M	981	NAG	C8-C7	4.31	1.59	1.50
5	M	956	MAN	O5-C5	4.47	1.52	1.43
5	M	952	FUC	C2-C3	5.23	1.59	1.52
5	M	952	FUC	C4-C5	5.42	1.63	1.53
3	M	923	NAG	O5-C5	6.82	1.57	1.43
3	M	921	NAG	O7-C7	7.23	1.40	1.23
5	M	957	MAN	O5-C5	7.54	1.59	1.43
3	M	921	NAG	O3-C3	20.29	1.89	1.43

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	957	MAN	C1-O5-C5	-15.59	90.67	112.17
3	M	923	NAG	C1-O5-C5	-7.55	101.75	112.17
3	M	921	NAG	O3-C3-C2	-7.34	93.66	109.39
5	M	957	MAN	O4-C4-C3	-6.77	95.62	110.36
5	M	954	BMA	O4-C4-C3	-6.33	96.58	110.36
3	M	921	NAG	C1-O5-C5	-6.17	103.67	112.17
5	M	957	MAN	C2-C3-C4	-6.12	100.20	110.88
3	M	981	NAG	C8-C7-N2	-5.85	105.54	116.11
5	M	951	NAG	C1-O5-C5	-5.56	104.50	112.17
5	M	952	FUC	C1-C2-C3	-5.47	102.72	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	945	XYP	C5B-C4B-C3B	-5.40	102.81	109.65
4	M	942	FUC	O3-C3-C2	-5.24	100.48	110.02
3	M	921	NAG	O4-C4-C5	-5.14	96.32	109.28
5	M	954	BMA	C1-C2-C3	-5.12	103.16	109.65
5	M	954	BMA	O2-C2-C3	-5.07	100.22	110.17
3	M	983	NAG	O5-C1-C2	-4.85	104.72	111.47
5	M	957	MAN	O5-C1-C2	-4.65	103.51	110.79
5	M	955	XYP	C5B-C4B-C3B	-4.59	103.83	109.65
4	M	941	NAG	C1-O5-C5	-4.35	106.17	112.17
3	M	983	NAG	C1-C2-N2	-4.21	103.29	110.49
3	M	921	NAG	C4-C3-C2	-4.20	104.86	111.02
4	M	945	XYP	O2B-C2B-C3B	-4.15	102.03	110.17
4	M	945	XYP	O3B-C3B-C2B	-3.91	102.91	110.02
3	M	921	NAG	O7-C7-C8	-3.88	114.99	122.06
4	M	942	FUC	C1-C2-C3	-3.87	104.74	109.65
5	M	956	MAN	C3-C4-C5	-3.85	103.44	110.22
3	M	923	NAG	C4-C3-C2	-3.70	105.59	111.02
4	M	941	NAG	C2-N2-C7	-3.59	117.70	122.94
5	M	956	MAN	O2-C2-C3	-3.57	103.16	110.17
5	M	956	MAN	C2-C3-C4	-3.50	104.77	110.88
3	M	983	NAG	C2-N2-C7	-3.47	117.89	122.94
5	M	955	XYP	C4B-C3B-C2B	-3.44	106.86	110.86
4	M	942	FUC	O2-C2-C3	-3.44	103.43	110.17
3	M	921	NAG	O4-C4-C3	-3.42	102.91	110.36
3	M	923	NAG	O6-C6-C5	-3.42	99.85	111.34
5	M	957	MAN	C3-C4-C5	-3.38	104.27	110.22
3	M	921	NAG	O3-C3-C4	-3.37	103.03	110.36
3	M	983	NAG	C1-O5-C5	-3.16	107.81	112.17
3	M	983	NAG	O4-C4-C3	-3.07	103.67	110.36
3	M	983	NAG	C6-C5-C4	-3.07	105.83	113.00
3	M	981	NAG	C2-N2-C7	-3.00	118.56	122.94
3	M	983	NAG	C3-C4-C5	-2.96	105.00	110.22
4	M	943	NAG	C2-N2-C7	-2.86	118.77	122.94
5	M	953	NAG	O5-C1-C2	-2.80	107.58	111.47
5	M	955	XYP	O4B-C4B-C3B	-2.79	104.70	110.17
5	M	953	NAG	O4-C4-C3	-2.76	104.34	110.36
4	M	941	NAG	O5-C1-C2	-2.63	107.82	111.47
5	M	954	BMA	C1-O5-C5	-2.57	108.62	112.17
5	M	957	MAN	O2-C2-C1	-2.56	103.96	109.18
5	M	956	MAN	C6-C5-C4	-2.47	107.22	113.00
4	M	941	NAG	C1-C2-N2	-2.45	106.30	110.49
5	M	955	XYP	O2B-C2B-C3B	-2.43	105.41	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	943	NAG	O4-C4-C3	-2.39	105.15	110.36
5	M	953	NAG	C2-N2-C7	-2.38	119.47	122.94
4	M	942	FUC	O3-C3-C4	-2.35	105.25	110.36
4	M	941	NAG	C8-C7-N2	-2.35	111.87	116.11
4	M	943	NAG	O5-C1-C2	-2.22	108.38	111.47
5	M	952	FUC	C6-C5-C4	-2.22	109.13	113.07
3	M	983	NAG	C4-C3-C2	-2.10	107.94	111.02
3	M	923	NAG	C8-C7-N2	-2.04	112.43	116.11
4	M	944	BMA	O4-C4-C5	2.00	114.33	109.28
3	M	983	NAG	O3-C3-C2	2.09	113.86	109.39
4	M	944	BMA	C3-C4-C5	2.09	113.89	110.22
5	M	956	MAN	C1-O5-C5	2.10	115.06	112.17
3	M	921	NAG	C8-C7-N2	2.46	120.56	116.11
4	M	944	BMA	O3-C3-C4	2.58	115.98	110.36
5	M	956	MAN	O2-C2-C1	2.89	115.06	109.18
4	M	944	BMA	C2-C3-C4	3.04	116.17	110.88
4	M	945	XYP	C1B-C2B-C3B	3.26	113.78	109.65
5	M	954	BMA	C3-C4-C5	3.66	116.67	110.22
5	M	957	MAN	O6-C6-C5	4.36	126.02	111.34
3	M	923	NAG	O3-C3-C4	4.40	119.92	110.36
3	M	923	NAG	O5-C1-C2	5.21	118.72	111.47
5	M	956	MAN	C1-C2-C3	5.26	116.31	109.65
5	M	957	MAN	C1-C2-C3	5.43	116.53	109.65
5	M	954	BMA	C6-C5-C4	6.00	127.05	113.00
3	M	981	NAG	O7-C7-N2	6.33	134.11	121.92
5	M	951	NAG	O5-C1-C2	6.54	120.57	111.47
5	M	957	MAN	O4-C4-C5	8.61	130.98	109.28
3	M	923	NAG	C3-C4-C5	9.13	126.30	110.22
5	M	954	BMA	O4-C4-C5	9.87	134.15	109.28
5	M	957	MAN	C6-C5-C4	12.88	143.14	113.00

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	0.82	0	6,6,6	1.34	1 (16%)
7	SO4	M	1003	-	4,4,4	0.57	0	6,6,6	0.50	0
7	SO4	M	1004	-	4,4,4	1.44	1 (25%)	6,6,6	1.46	1 (16%)
7	SO4	M	1005	-	4,4,4	0.20	0	6,6,6	0.35	0
7	SO4	M	1006	-	4,4,4	1.97	1 (25%)	6,6,6	2.43	3 (50%)
7	SO4	M	1007	-	4,4,4	1.14	0	6,6,6	1.34	1 (16%)
7	SO4	M	1008	-	4,4,4	0.83	0	6,6,6	0.34	0
7	SO4	M	1009	-	4,4,4	1.55	1 (25%)	6,6,6	2.88	5 (83%)
8	GOL	M	1010	-	5,5,5	0.69	0	5,5,5	1.11	1 (20%)
8	GOL	M	1020	-	5,5,5	1.29	1 (20%)	5,5,5	1.00	0
8	GOL	M	1021	-	5,5,5	0.93	0	5,5,5	1.07	0
8	GOL	M	1023	-	5,5,5	0.64	0	5,5,5	1.05	0
8	GOL	M	1024	-	5,5,5	0.82	0	5,5,5	1.20	1 (20%)
2	NAG	M	901	1	14,14,15	1.18	1 (7%)	15,19,21	1.97	3 (20%)
2	NAG	M	911	1	14,14,15	1.63	2 (14%)	15,19,21	2.08	2 (13%)
2	NAG	M	931	1	14,14,15	1.98	5 (35%)	15,19,21	8.50	11 (73%)
2	NAG	M	961	1	14,14,15	1.34	2 (14%)	15,19,21	2.91	4 (26%)
2	NAG	M	971	1	14,14,15	1.30	1 (7%)	15,19,21	2.49	6 (40%)
2	NAG	M	991	1	14,14,15	1.22	1 (7%)	15,19,21	1.99	4 (26%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	971	NAG	O7-C7	-4.01	1.13	1.23
2	M	931	NAG	O7-C7	-3.81	1.14	1.23
2	M	991	NAG	O7-C7	-3.67	1.14	1.23
2	M	931	NAG	C1-C2	-3.44	1.47	1.52
2	M	911	NAG	O7-C7	-3.33	1.15	1.23
2	M	961	NAG	O7-C7	-3.26	1.15	1.23
2	M	901	NAG	O7-C7	-2.73	1.16	1.23
2	M	931	NAG	C2-N2	-2.56	1.41	1.46
2	M	931	NAG	O5-C1	-2.13	1.40	1.43
2	M	961	NAG	C2-N2	2.09	1.50	1.46
8	M	1020	GOL	O1-C1	2.17	1.51	1.42
7	M	1009	SO4	O1-S	2.57	1.59	1.45
7	M	1004	SO4	O1-S	2.70	1.60	1.45
2	M	931	NAG	O4-C4	3.10	1.50	1.43
7	M	1006	SO4	O2-S	3.75	1.66	1.45
2	M	911	NAG	O5-C5	4.03	1.51	1.43

All (43) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	931	NAG	O7-C7-N2	-7.97	106.58	121.92
2	M	971	NAG	O5-C1-C2	-6.84	101.95	111.47
2	M	931	NAG	C1-O5-C5	-6.53	103.16	112.17
2	M	911	NAG	C1-O5-C5	-6.11	103.74	112.17
2	M	901	NAG	C1-O5-C5	-5.99	103.90	112.17
2	M	931	NAG	O7-C7-C8	-5.10	112.77	122.06
2	M	991	NAG	C4-C3-C2	-4.60	104.28	111.02
2	M	961	NAG	C1-C2-N2	-4.41	102.95	110.49
2	M	961	NAG	O3-C3-C2	-4.15	100.50	109.39
2	M	911	NAG	C4-C3-C2	-3.71	105.59	111.02
2	M	991	NAG	O3-C3-C2	-3.62	101.62	109.39
2	M	931	NAG	O4-C4-C5	-3.37	100.79	109.28
7	M	1006	SO4	O3-S-O2	-3.30	91.08	109.26
7	M	1009	SO4	O3-S-O1	-3.27	91.24	109.26
7	M	1006	SO4	O2-S-O1	-3.18	87.42	109.64
2	M	961	NAG	O4-C4-C5	-3.14	101.36	109.28
7	M	1009	SO4	O2-S-O1	-3.10	88.00	109.64
2	M	931	NAG	O4-C4-C3	-2.74	104.40	110.36
2	M	971	NAG	O3-C3-C2	-2.73	103.55	109.39
2	M	991	NAG	C1-C2-N2	-2.62	106.02	110.49
2	M	931	NAG	C4-C3-C2	-2.48	107.39	111.02
8	M	1024	GOL	C3-C2-C1	-2.48	101.68	111.52
7	M	1009	SO4	O4-S-O1	-2.28	96.69	109.26
2	M	901	NAG	C4-C3-C2	-2.14	107.88	111.02
7	M	1009	SO4	O3-S-O2	2.02	120.41	109.26
8	M	1010	GOL	O2-C2-C1	2.12	118.87	108.84
2	M	971	NAG	O7-C7-C8	2.25	126.15	122.06
7	M	1007	SO4	O4-S-O1	2.28	121.83	109.26
2	M	931	NAG	C1-C2-N2	2.28	114.39	110.49
7	M	1002	SO4	O3-S-O2	2.29	121.88	109.26
2	M	971	NAG	C2-N2-C7	2.30	126.30	122.94
7	M	1006	SO4	O4-S-O1	2.41	122.53	109.26
2	M	971	NAG	C1-O5-C5	2.61	115.77	112.17
2	M	901	NAG	O5-C1-C2	2.85	115.44	111.47
7	M	1004	SO4	O4-S-O3	2.93	122.18	108.96
2	M	991	NAG	O5-C1-C2	3.11	115.80	111.47
2	M	971	NAG	O4-C4-C3	3.43	117.82	110.36
2	M	931	NAG	C3-C4-C5	3.92	117.13	110.22
7	M	1009	SO4	O4-S-O3	4.51	129.27	108.96
2	M	961	NAG	C1-O5-C5	8.30	123.61	112.17
2	M	931	NAG	C8-C7-N2	13.51	140.50	116.11
2	M	931	NAG	O5-C1-C2	16.62	134.59	111.47
2	M	931	NAG	C2-N2-C7	21.07	153.68	122.94

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%)	3.31	427 (85%) <b>0</b> <b>0</b>	30, 34, 47, 75	37 (7%)

All (427) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	212	PRO	9.1
1	M	376	ALA	8.1
1	M	23	SER	7.5
1	M	345	THR	7.2
1	M	390	TYR	7.1
1	M	378	SER	7.0
1	M	143	ASP	6.8
1	M	326	GLY	6.6
1	M	18	ASP	6.6
1	M	482	ASN	6.4
1	M	417	ASP	6.2
1	M	374	ASP	6.2
1	M	283	LEU	6.2
1	M	313	GLU	6.2
1	M	12	PHE	6.1
1	M	138	THR	6.1
1	M	10	LEU	6.1
1	M	380	ASP	6.1
1	M	206	CYS	6.0
1	M	203	PRO	5.9
1	M	255	THR	5.9
1	M	150	ASP	5.7
1	M	497	THR	5.6
1	M	167	TYR	5.5
1	M	3	GLU	5.5
1	M	99	ALA	5.5
1	M	13	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	M	404	LEU	5.5
1	M	9	ASN	5.5
1	M	443	VAL	5.5
1	M	377	ASP	5.5
1	M	419	ASN	5.4
1	M	97	SER	5.4
1	M	79	TRP	5.4
1	M	140	PHE	5.4
1	M	30[A]	ILE	5.3
1	M	305[A]	GLU	5.3
1	M	5	THR	5.3
1	M	142	TRP	5.3
1	M	7	GLN	5.3
1	M	17	THR	5.3
1	M	154	GLY	5.2
1	M	480	TRP	5.2
1	M	341	PRO	5.2
1	M	317	LEU	5.2
1	M	45	GLY	5.2
1	M	364	GLY	5.2
1	M	20[A]	LEU	5.1
1	M	434	CYS	5.1
1	M	209	THR	5.1
1	M	73	CYS	5.1
1	M	342[A]	VAL	5.1
1	M	183	LEU	5.1
1	M	366[A]	TYR	5.0
1	M	400	TYR	5.0
1	M	401	TYR	5.0
1	M	144	LEU	5.0
1	M	481	ASN	5.0
1	M	152	TYR	5.0
1	M	298	ILE	5.0
1	M	257	ILE	5.0
1	M	245	TYR	5.0
1	M	71	THR	4.9
1	M	223	PRO	4.9
1	M	330	TYR	4.9
1	M	433	LEU	4.9
1	M	25	PHE	4.8
1	M	55	THR	4.8
1	M	365	HIS	4.8

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Mol	Chain	Res	Type	RSRZ
1	M	363[A]	SER	4.8
1	M	213[A]	SER	4.8
1	M	396	PHE	4.7
1	M	280	GLU	4.7
1	M	449[A]	VAL	4.7
1	M	112	GLY	4.7
1	M	196	TYR	4.7
1	M	253	GLY	4.7
1	M	301	ASP	4.7
1	M	347	HIS	4.7
1	M	50	ILE	4.6
1	M	186	ASN	4.6
1	M	318	VAL	4.6
1	M	492	GLY	4.6
1	M	432	TYR	4.6
1	M	177	ASP	4.5
1	M	52	ASP	4.5
1	M	444	ILE	4.5
1	M	490	LYS	4.5
1	M	300	ILE	4.4
1	M	370	LEU	4.4
1	M	27	SER	4.4
1	M	77	SER	4.4
1	M	430	ILE	4.4
1	M	425	LEU	4.4
1	M	224	TYR	4.4
1	M	89	LEU	4.3
1	M	375	LYS	4.3
1	M	36	SER	4.3
1	M	272	ILE	4.3
1	M	360[A]	ILE	4.3
1	M	457	TRP	4.3
1	M	405	ILE	4.3
1	M	339	PRO	4.3
1	M	185	ILE	4.2
1	M	16	ASN	4.2
1	M	184	THR	4.2
1	M	164	PHE	4.2
1	M	399	LYS	4.2
1	M	153	GLU	4.2
1	M	478	ILE	4.1
1	M	197	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	M	149	GLN	4.1
1	M	471	VAL	4.1
1	M	452	LYS	4.1
1	M	420	ARG	4.1
1	M	258	THR	4.1
1	M	335	ALA	4.1
1	M	139	LEU	4.1
1	M	256	MET	4.1
1	M	467	LYS	4.0
1	M	469	PHE	4.0
1	M	290	LEU	4.0
1	M	157	ASP	4.0
1	M	458	ALA	4.0
1	M	491	SER	4.0
1	M	11	PRO	4.0
1	M	329	TYR	4.0
1	M	171	CYS	4.0
1	M	474	GLY	4.0
1	M	147	THR	4.0
1	M	204	GLY	4.0
1	M	240	LEU	4.0
1	M	132	GLY	4.0
1	M	24	SER	3.9
1	M	252	ILE	3.9
1	M	210	VAL	3.9
1	M	485	ASP	3.9
1	M	494	TRP	3.9
1	M	274	ALA	3.9
1	M	344[A]	SER	3.9
1	M	53	GLY	3.9
1	M	160	ILE	3.9
1	M	389	ILE	3.9
1	M	350	MET	3.9
1	M	6	CYS	3.9
1	M	43	THR	3.8
1	M	191	VAL	3.8
1	M	359	TYR	3.8
1	M	166	ASP	3.8
1	M	76	PHE	3.8
1	M	90	ASN	3.8
1	M	226	VAL	3.8
1	M	172	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	M	260	TRP	3.8
1	M	145	PRO	3.8
1	M	200	LEU	3.8
1	M	195	GLY	3.8
1	M	238	VAL	3.8
1	M	285	TRP	3.7
1	M	63	GLY	3.7
1	M	113	VAL	3.7
1	M	182	TRP	3.7
1	M	403	PRO	3.7
1	M	93	GLY	3.7
1	M	398	ASN	3.7
1	M	48	LEU	3.7
1	M	221	THR	3.7
1	M	122	HIS	3.7
1	M	381	ASN	3.7
1	M	349	ALA	3.6
1	M	33	VAL	3.6
1	M	268	ASP	3.6
1	M	310	PHE	3.6
1	M	57	ARG	3.6
1	M	101[A]	SER	3.6
1	M	194	ARG	3.6
1	M	409	GLU	3.6
1	M	324	PHE	3.6
1	M	383	TYR	3.6
1	M	406	TYR	3.6
1	M	88[A]	GLU	3.6
1	M	418	GLU	3.6
1	M	296	PRO	3.6
1	M	128	LEU	3.6
1	M	49	ASN	3.6
1	M	304	GLY	3.6
1	M	321	SER	3.6
1	M	286	PHE	3.6
1	M	465	PHE	3.6
1	M	151	GLU	3.6
1	M	287	MET	3.6
1	M	51	TRP	3.5
1	M	162	ASP	3.5
1	M	208	PRO	3.5
1	M	421	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	M	115	GLU	3.5
1	M	254	PRO	3.5
1	M	211	ASP	3.5
1	M	118[A]	ILE	3.5
1	M	295	TYR	3.5
1	M	427	TYR	3.5
1	M	426	ASP	3.5
1	M	54	PHE	3.5
1	M	428	THR	3.5
1	M	338[A]	SER	3.5
1	M	31	PHE	3.5
1	M	441	ASN	3.5
1	M	493	GLN	3.4
1	M	215	TYR	3.4
1	M	293	GLY	3.4
1	M	488	LEU	3.4
1	M	307	LEU	3.4
1	M	388	GLY	3.4
1	M	85	VAL	3.4
1	M	26	SER	3.3
1	M	21	ASN	3.3
1	M	316	ASN	3.3
1	M	395	TYR	3.3
1	M	294	THR	3.3
1	M	455	LEU	3.3
1	M	19	ALA	3.3
1	M	362	ALA	3.3
1	M	78	TYR	3.3
1	M	499	ILE	3.3
1	M	38	TYR	3.3
1	M	181	TYR	3.3
1	M	29	PHE	3.3
1	M	371	PHE	3.3
1	M	129	ILE	3.3
1	M	116	LYS	3.3
1	M	174	GLU	3.3
1	M	141	HIS	3.3
1	M	282	PHE	3.3
1	M	161	ILE	3.3
1	M	315	SER	3.2
1	M	308	PRO	3.2
1	M	459	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	M	247	HIS	3.2
1	M	120	TYR	3.2
1	M	353	ALA	3.2
1	M	126[A]	SER	3.2
1	M	468	GLY	3.2
1	M	56	HIS	3.2
1	M	146	GLN	3.2
1	M	66	HIS	3.2
1	M	487	ASP	3.2
1	M	327	LEU	3.2
1	M	4	ILE	3.2
1	M	225	ILE	3.2
1	M	386	PRO	3.1
1	M	423	SER	3.1
1	M	334	TYR	3.1
1	M	439	PHE	3.1
1	M	137	VAL	3.1
1	M	249	GLY	3.1
1	M	169[A]	ASP	3.1
1	M	22	SER	3.1
1	M	382	ILE	3.1
1	M	219	SER	3.1
1	M	42	GLY	3.1
1	M	373	LYS	3.1
1	M	218	ASN	3.1
1	M	44	ILE	3.1
1	M	98	ILE	3.1
1	M	424	MET	3.1
1	M	229	HIS	3.1
1	M	96	PHE	3.1
1	M	275	THR	3.1
1	M	311	SER	3.1
1	M	322	TYR	3.1
1	M	448	ASP	3.0
1	M	170	LEU	3.0
1	M	415	PRO	3.0
1	M	62[A]	SER	3.0
1	M	220[A]	SER	3.0
1	M	397	LYS	3.0
1	M	241	TYR	2.9
1	M	384	TYR	2.9
1	M	410	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	37	ALA	2.9
1	M	65	ASP	2.9
1	M	107	GLY	2.9
1	M	416	GLY	2.9
1	M	103	ILE	2.9
1	M	91	ALA	2.9
1	M	190	SER	2.9
1	M	28	ASP	2.9
1	M	104	ILE	2.9
1	M	47	GLY	2.9
1	M	188	LEU	2.9
1	M	187	GLN	2.8
1	M	450	ASN	2.8
1	M	83	ILE	2.8
1	M	233	ALA	2.8
1	M	94	TYR	2.8
1	M	264	TYR	2.8
1	M	325	LEU	2.8
1	M	32	GLY	2.8
1	M	81	LYS	2.8
1	M	479	ASP	2.8
1	M	498	PHE	2.8
1	M	121	TYR	2.8
1	M	117	GLY	2.8
1	M	346	ASN	2.8
1	M	368	GLY	2.8
1	M	278	MET	2.8
1	M	436	HIS	2.8
1	M	80	GLN	2.8
1	M	148	LEU	2.8
1	M	231	LEU	2.8
1	M	303	VAL	2.8
1	M	95	ARG	2.8
1	M	500	SER	2.8
1	M	484	THR	2.7
1	M	391	SER	2.7
1	M	266	ASP	2.7
1	M	431	ASP	2.7
1	M	263	PRO	2.7
1	M	464	GLU	2.7
1	M	84	ASP	2.7
1	M	271[A]	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	235	ALA	2.7
1	M	262	LEU	2.7
1	M	357	LEU	2.7
1	M	414	THR	2.7
1	M	351	MET	2.7
1	M	486	ARG	2.7
1	M	456	ALA	2.7
1	M	130	LYS	2.7
1	M	114	ASN	2.7
1	M	259	ARG	2.7
1	M	466	ASN	2.7
1	M	217	GLY	2.7
1	M	281	PHE	2.7
1	M	356	LYS	2.7
1	M	473	PHE	2.7
1	M	58	TYR	2.6
1	M	8	GLU	2.6
1	M	407	VAL	2.6
1	M	214	CYS	2.6
1	M	106	ARG	2.6
1	M	173	GLU	2.6
1	M	201	ASP	2.6
1	M	109	ARG	2.6
1	M	59	PRO	2.6
1	M	179	VAL	2.6
1	M	60	ASN	2.6
1	M	489	LYS	2.6
1	M	454	TYR	2.6
1	M	309[A]	SER	2.6
1	M	461	ASP	2.6
1	M	250	GLY	2.6
1	M	192	PRO	2.6
1	M	265	ASN	2.6
1	M	385	TYR	2.6
1	M	75	SER	2.6
1	M	246	THR	2.6
1	M	175	PHE	2.6
1	M	64	PRO	2.6
1	M	124	LEU	2.6
1	M	297	GLN	2.6
1	M	392	VAL	2.5
1	M	393	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	232	LEU	2.5
1	M	273	ALA	2.5
1	M	446	GLU	2.5
1	M	413	SER	2.5
1	M	299	MET	2.5
1	M	125	ILE	2.5
1	M	435	SER	2.5
1	M	156	LEU	2.5
1	M	438	CYS	2.5
1	M	155	PHE	2.5
1	M	236	LYS	2.5
1	M	447	LYS	2.5
1	M	412	ILE	2.4
1	M	284	GLY	2.4
1	M	276	GLU	2.4
1	M	429	ARG	2.4
1	M	68	ASN	2.4
1	M	394	ASP	2.4
1	M	202	ALA	2.4
1	M	470	THR	2.4
1	M	165	LYS	2.4
1	M	237	VAL	2.4
1	M	343	ASN	2.4
1	M	67	GLY	2.4
1	M	105	PRO	2.4
1	M	422	GLN	2.4
1	M	239	ASP	2.4
1	M	228	HIS	2.3
1	M	314	GLU	2.3
1	M	472	ARG	2.3
1	M	158	PRO	2.3
1	M	261	PHE	2.3
1	M	462[A]	ASN	2.3
1	M	180	LYS	2.3
1	M	159	GLN	2.3
1	M	14	CYS	2.3
1	M	289	PRO	2.3
1	M	69	GLY	2.3
1	M	495	TYR	2.3
1	M	496	GLN	2.3
1	M	323	ASP	2.2
1	M	100	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	123	GLY	2.2
1	M	244	ASN	2.2
1	M	379	THR	2.2
1	M	288	GLY	2.2
1	M	352	ASP	2.2
1	M	207	SER	2.2
1	M	445	LYS	2.2
1	M	475	LEU	2.2
1	M	168	ALA	2.2
1	M	292	ASN	2.2
1	M	216	ALA	2.2
1	M	369	PRO	2.2
1	M	205	ARG	2.1
1	M	227	ALA	2.1
1	M	133	ILE	2.1
1	M	46	ARG	2.1
1	M	437	LEU	2.1
1	M	332	THR	2.1
1	M	328	ASN	2.1
1	M	331	PHE	2.1
1	M	163	ASP	2.0
1	M	110	SER	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	0.54	0.43	-0.33	56,64,76,78	0
3	NAG	M	981	14/15	0.63	0.29	-0.41	28,35,39,42	0
4	NAG	M	941	14/15	0.66	0.31	-0.42	33,41,45,46	0
3	NAG	M	921	14/15	0.70	0.25	-1.01	37,42,50,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FUC	M	942	10/11	0.54	0.37	-	43,51,58,66	0
5	XYP	M	955	9/10	0.43	0.44	-	51,56,62,82	0
4	XYP	M	945	9/10	0.63	0.30	-	60,66,70,72	0
5	NAG	M	953	14/15	0.75	0.24	-	39,42,47,51	0
5	FUC	M	952	10/11	0.72	0.28	-	37,40,52,52	0
4	BMA	M	944	11/12	0.45	0.48	-	57,62,67,71	0
5	BMA	M	954	11/12	0.55	0.24	-	44,49,54,66	0
5	NAG	M	951	14/15	0.73	0.27	-	36,39,45,47	0
3	NAG	M	983	14/15	0.71	0.34	-	45,50,68,75	0
5	MAN	M	956	11/12	0.48	0.47	-	44,58,70,75	0
4	NAG	M	943	14/15	0.69	0.26	-	39,46,51,57	0
5	MAN	M	957	11/12	0.56	0.55	-	52,61,73,74	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	0.49	0.68	5.17	62,69,81,86	0
8	GOL	M	1010	6/6	0.40	0.58	5.01	54,60,62,70	6
7	SO4	M	1009	5/5	0.47	0.54	3.80	57,58,65,78	1
2	NAG	M	931	14/15	0.60	0.41	3.76	54,60,67,68	0
7	SO4	M	1002	5/5	0.75	0.41	1.26	45,48,50,55	5
8	GOL	M	1020	6/6	0.42	0.42	0.91	24,32,37,37	1
7	SO4	M	1004	5/5	0.86	0.31	0.43	32,46,48,53	5
2	NAG	M	901	14/15	0.53	0.32	-0.64	44,53,65,67	0
8	GOL	M	1021	6/6	0.66	0.27	-0.75	30,40,45,49	6
8	GOL	M	1024	6/6	0.69	0.27	-1.01	34,35,40,41	0
2	NAG	M	971	14/15	0.39	0.41	-	74,82,88,88	0
7	SO4	M	1003	5/5	0.62	0.53	-	44,46,54,55	5
7	SO4	M	1008	5/5	0.79	0.26	-	51,54,57,57	5
7	SO4	M	1005	5/5	0.75	0.30	-	36,40,45,47	0
8	GOL	M	1023	6/6	0.33	0.91	-	49,50,61,63	6
7	SO4	M	1007	5/5	0.77	0.45	-	32,52,53,56	5
2	NAG	M	911	14/15	0.68	0.25	-	43,46,55,63	0
7	SO4	M	1006	5/5	0.78	0.55	-	44,49,53,53	5
2	NAG	M	991	14/15	0.35	0.60	-	53,58,72,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ZN	M	1001	1/1	0.86	0.12	-	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.