



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:36 PM GMT

PDB ID : 1PUM  
Title : Mistletoe lectin I in complex with galactose  
Authors : Krauspenhaar, R.; Voelter, W.; Stoeva, S.; Mikhailov, A.; Konareva, N.; Betzel, C.  
Deposited on : 2003-06-25  
Resolution : 2.30 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

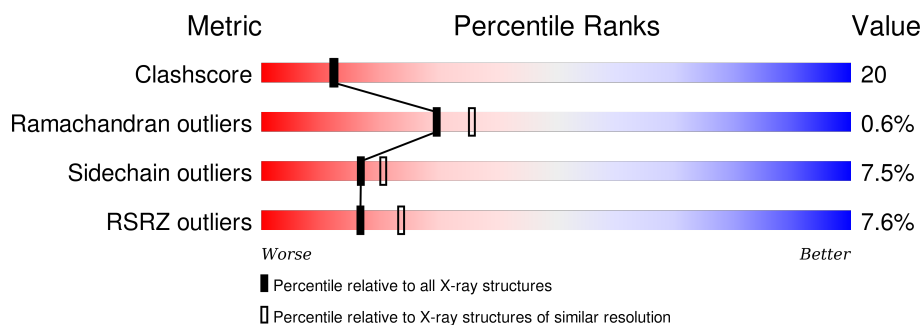
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	A	249	<div> <div>7%</div> <div>63%</div> <div>31%</div> <div>6%</div> </div>
2	B	263	<div> <div>8%</div> <div>77%</div> <div>19%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	A	1010	-	X	-	-
10	GOL	A	1011	-	X	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	A	1012	-	X	-	X
10	GOL	A	1014	-	X	-	X
10	GOL	A	1017	-	X	-	-
10	GOL	A	1024	-	X	-	X
10	GOL	A	1025	-	X	-	-
10	GOL	B	1013	-	X	-	X
10	GOL	B	1015	-	X	-	-
10	GOL	B	1016	-	X	-	X
10	GOL	B	1018	-	X	-	-
10	GOL	B	1019	-	X	-	X
10	GOL	B	1020	-	X	-	X
10	GOL	B	1021	-	X	-	-
10	GOL	B	1022	-	X	-	X
10	GOL	B	1023	-	X	-	-
7	GAL	B	1008	-	-	-	X
7	GAL	B	1009	-	-	-	X
9	SO4	A	1029	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 4505 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 lectin I A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1922	1217	329	372	4			

- Molecule 2 is a protein called lectin I B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	263	Total	C	N	O	S	0	0	0
			1996	1238	353	393	12			

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

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

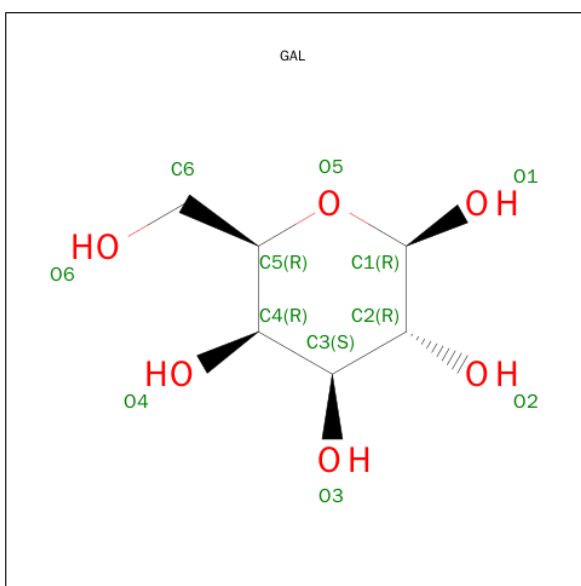


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 7 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).

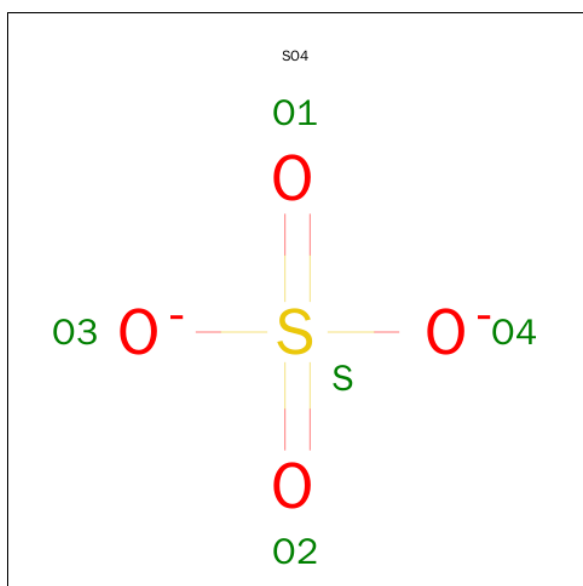


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			12	6	6		
7	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Cl	0	0
			2	2		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 10 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
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 11 is water.

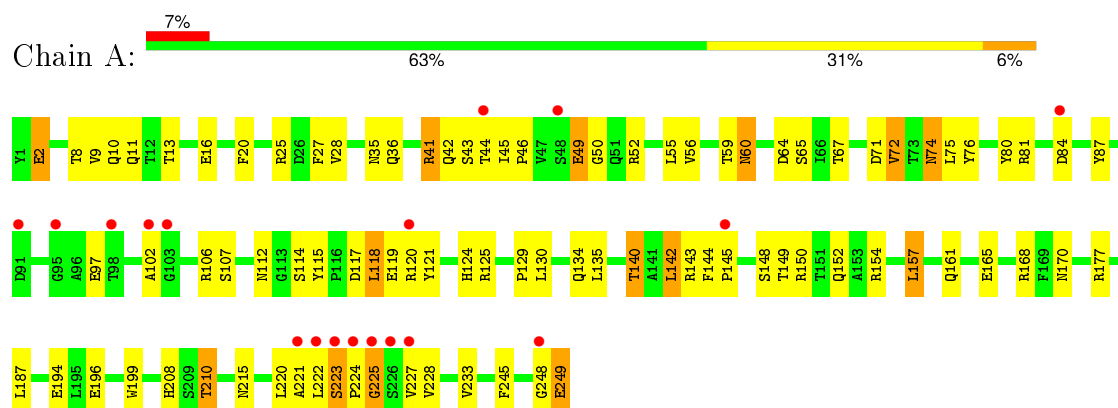
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	142	Total	O	0	0
			142	142		
11	B	219	Total	O	0	0
			219	219		



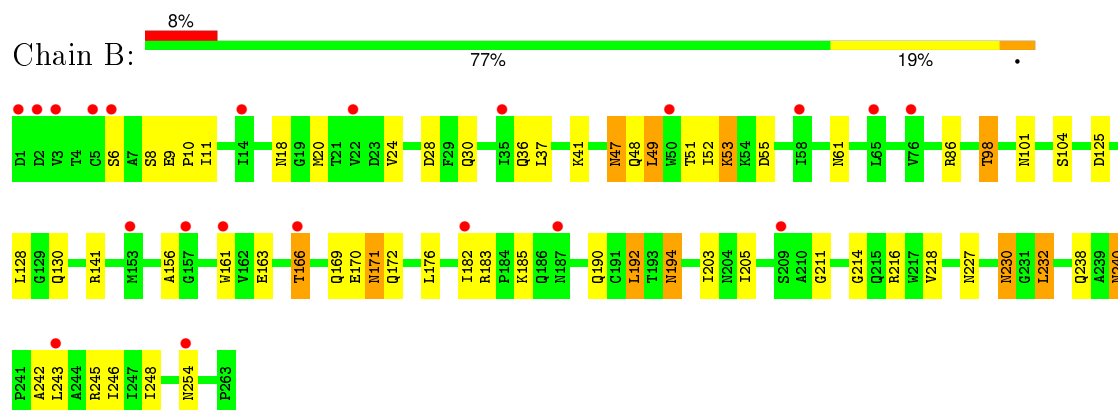
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $RSRZ > 2$ ). 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: lectin I A chain



#### • Molecule 2: lectin I B chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.83Å 106.83Å 310.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30 25.66 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (10.00-2.30) 96.5 (25.66-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.209 , 0.246 0.203 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 45932 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4505	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 2.95% 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: GOL, NAG, CL, NDG, GAL, SO4, FUL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.42	0/1960	0.70	0/2668
2	B	0.43	0/2035	0.75	0/2777
All	All	0.43	0/3995	0.73	0/5445

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	A	1922	0	1900	80	0
2	B	1996	0	1932	77	0
3	B	28	0	25	5	0
4	B	28	0	25	1	0
5	A	14	0	13	0	0
6	B	24	0	22	3	0
7	B	24	0	24	2	0
8	A	2	0	0	0	0
9	A	10	0	0	0	0
10	A	42	0	28	5	0
10	B	54	0	37	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	142	0	0	4	0
11	B	219	0	0	3	0
All	All	4505	0	4006	161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:HG23	1:A:11:GLN:H	1.16	1.04
2:B:194:ASN:H	2:B:194:ASN:HD22	1.01	1.00
1:A:148:SER:HB2	10:A:1012:GOL:H11	1.45	0.97
2:B:156:ALA:HB2	11:B:1242:HOH:O	1.68	0.92
2:B:41:LYS:H	2:B:48:GLN:HE22	1.19	0.91
1:A:149:THR:HA	1:A:152:GLN:HE21	1.40	0.86
2:B:194:ASN:N	2:B:194:ASN:HD22	1.72	0.86
2:B:230:ASN:HD22	2:B:232:LEU:H	1.19	0.84
2:B:18:ASN:HD22	2:B:183:ARG:HH22	1.22	0.83
1:A:102:ALA:HA	1:A:106:ARG:HH21	1.43	0.83
1:A:71:ASP:HB3	1:A:74:ASN:HD21	1.42	0.83
2:B:230:ASN:ND2	2:B:232:LEU:H	1.78	0.81
2:B:194:ASN:H	2:B:194:ASN:ND2	1.80	0.80
4:B:266:NAG:H61	4:B:267:NAG:C1	2.13	0.79
2:B:125:ASP:H	2:B:130:GLN:HE22	1.32	0.78
2:B:240:ASN:HD21	2:B:242:ALA:HB3	1.49	0.76
1:A:41:ARG:NH1	1:A:45:ILE:HD11	2.02	0.74
1:A:25:ARG:HH12	1:A:170:ASN:HD21	1.34	0.74
2:B:194:ASN:HD21	2:B:214:GLY:HA2	1.53	0.74
2:B:166:THR:H	2:B:172:GLN:HE22	1.33	0.74
2:B:55:ASP:HB2	2:B:86:ARG:HH22	1.53	0.73
2:B:194:ASN:HD21	2:B:214:GLY:CA	2.00	0.73
2:B:227:ASN:HD22	2:B:230:ASN:H	1.34	0.73
2:B:128:LEU:HD22	2:B:211:GLY:HA2	1.70	0.73
1:A:9:VAL:HG23	1:A:11:GLN:N	1.98	0.72
2:B:98:THR:HG22	2:B:216:ARG:HH22	1.54	0.72
6:B:268:NAG:H3	6:B:269:FUL:O2	1.91	0.70
1:A:13:THR:OG1	1:A:16:GLU:HG3	1.92	0.69
1:A:60:ASN:HD21	1:A:64:ASP:H	1.41	0.69
2:B:169:GLN:HE21	2:B:171:ASN:HD21	1.39	0.68
2:B:41:LYS:H	2:B:48:GLN:NE2	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:ASN:ND2	2:B:242:ALA:H	1.94	0.66
10:A:1024:GOL:H12	2:B:141:ARG:HG2	1.76	0.66
1:A:52:ARG:HH12	1:A:71:ASP:CG	2.00	0.65
2:B:169:GLN:HG2	2:B:171:ASN:ND2	2.13	0.64
2:B:125:ASP:H	2:B:130:GLN:NE2	1.95	0.64
2:B:11:ILE:HG13	2:B:51:THR:OG1	1.97	0.64
1:A:60:ASN:ND2	1:A:64:ASP:H	1.95	0.64
1:A:115:TYR:CE1	1:A:125:ARG:HD3	2.33	0.63
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.64	0.63
2:B:41:LYS:HZ1	2:B:47:ASN:HD21	1.45	0.63
2:B:36:GLN:HE22	7:B:1008:GAL:H62	1.63	0.63
1:A:97:GLU:HG2	1:A:106:ARG:HD3	1.80	0.63
1:A:112:ASN:HB2	11:A:7805:HOH:O	1.96	0.63
2:B:41:LYS:NZ	2:B:47:ASN:HD21	1.96	0.62
1:A:2:GLU:HG3	1:A:27:PHE:CD2	2.35	0.62
1:A:215:ASN:ND2	2:B:8:SER:HB3	2.15	0.62
1:A:49:GLU:OE1	1:A:50:GLY:N	2.33	0.61
1:A:41:ARG:HH11	1:A:45:ILE:HD11	1.63	0.61
2:B:240:ASN:HD21	2:B:242:ALA:CB	2.14	0.61
2:B:194:ASN:ND2	2:B:214:GLY:CA	2.63	0.61
2:B:238:GLN:NE2	2:B:243:LEU:HD21	2.16	0.61
2:B:194:ASN:ND2	2:B:214:GLY:O	2.34	0.60
1:A:71:ASP:HB3	1:A:74:ASN:ND2	2.16	0.59
2:B:230:ASN:HD22	2:B:230:ASN:C	2.06	0.59
2:B:36:GLN:HE22	7:B:1008:GAL:C6	2.15	0.59
1:A:227:VAL:HG12	1:A:228:VAL:N	2.18	0.59
1:A:41:ARG:HD2	11:A:7895:HOH:O	2.04	0.58
1:A:60:ASN:HD22	1:A:60:ASN:C	2.06	0.58
2:B:240:ASN:C	2:B:240:ASN:HD22	2.07	0.58
2:B:41:LYS:N	2:B:48:GLN:HE22	1.94	0.58
1:A:120:ARG:HD3	1:A:121:TYR:CE1	2.39	0.58
1:A:120:ARG:HG2	1:A:120:ARG:HH11	1.68	0.57
1:A:245:PHE:HE1	1:A:248:GLY:H	1.52	0.57
1:A:125:ARG:NH1	1:A:196:GLU:OE2	2.38	0.57
1:A:60:ASN:OD1	1:A:140:THR:HG22	2.06	0.56
2:B:11:ILE:N	2:B:11:ILE:HD12	2.20	0.56
1:A:223:SER:HB2	1:A:224:PRO:CD	2.36	0.56
2:B:190:GLN:HE21	2:B:205:ILE:HG22	1.71	0.55
2:B:170:GLU:OE2	2:B:185:LYS:NZ	2.38	0.55
2:B:254:ASN:HD22	2:B:254:ASN:N	2.05	0.55
1:A:121:TYR:O	1:A:150:ARG:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:ASP:OD1	2:B:30:GLN:HG2	2.07	0.55
2:B:171:ASN:HD22	2:B:171:ASN:C	2.09	0.54
2:B:55:ASP:HB2	2:B:86:ARG:NH2	2.21	0.54
1:A:52:ARG:NH1	1:A:71:ASP:OD1	2.37	0.54
1:A:115:TYR:O	1:A:119:GLU:HG3	2.07	0.53
2:B:240:ASN:HD22	2:B:242:ALA:H	1.56	0.53
1:A:74:ASN:ND2	1:A:76:TYR:H	2.07	0.53
1:A:221:ALA:C	1:A:222:LEU:HD22	2.29	0.53
2:B:18:ASN:ND2	2:B:183:ARG:HH22	1.99	0.52
1:A:74:ASN:HD22	1:A:75:LEU:N	2.07	0.52
2:B:240:ASN:ND2	2:B:242:ALA:HB3	2.20	0.52
1:A:118:LEU:HG	1:A:157:LEU:HD13	1.90	0.52
2:B:230:ASN:ND2	2:B:232:LEU:HB2	2.24	0.52
1:A:25:ARG:HH22	1:A:170:ASN:ND2	2.08	0.52
2:B:203:ILE:HD12	2:B:246:ILE:HG22	1.91	0.52
1:A:102:ALA:HA	1:A:106:ARG:NH2	2.20	0.51
1:A:222:LEU:N	1:A:222:LEU:HD22	2.24	0.51
1:A:129:PRO:O	1:A:134:GLN:HG2	2.10	0.51
1:A:59:THR:HA	1:A:64:ASP:O	2.10	0.51
1:A:249:GLU:OE1	1:A:249:GLU:HA	2.11	0.51
2:B:227:ASN:ND2	2:B:230:ASN:H	2.07	0.50
1:A:35:ASN:O	1:A:36:GLN:HB2	2.11	0.50
1:A:52:ARG:NH1	1:A:52:ARG:HG3	2.26	0.49
2:B:9:GLU:CD	2:B:53:LYS:HE3	2.32	0.49
1:A:245:PHE:HE1	1:A:248:GLY:N	2.10	0.49
3:B:264:NDG:H3	3:B:264:NDG:O7	2.11	0.49
2:B:24:VAL:HB	2:B:47:ASN:HB2	1.95	0.48
2:B:240:ASN:C	2:B:240:ASN:ND2	2.66	0.48
1:A:215:ASN:HD21	2:B:10:PRO:HD3	1.77	0.48
1:A:210:THR:HG21	2:B:8:SER:O	2.14	0.48
1:A:84:ASP:H	10:A:1017:GOL:H11	1.79	0.48
1:A:45:ILE:HG23	1:A:49:GLU:HG3	1.95	0.48
2:B:166:THR:H	2:B:172:GLN:NE2	2.07	0.48
6:B:268:NAG:H3	6:B:269:FUL:HO2	1.78	0.47
1:A:20:PHE:HZ	1:A:56:VAL:HG13	1.78	0.47
1:A:8:THR:O	1:A:8:THR:HG23	2.13	0.47
3:B:264:NDG:O7	3:B:264:NDG:C3	2.63	0.47
1:A:144:PHE:HA	1:A:145:PRO:HD3	1.82	0.47
2:B:52:ILE:HD12	2:B:52:ILE:N	2.30	0.46
1:A:80:TYR:CE2	1:A:142:LEU:HG	2.49	0.46
2:B:9:GLU:OE1	2:B:53:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:ASN:HB3	2:B:230:ASN:ND2	2.31	0.46
1:A:194:GLU:HB3	1:A:220:LEU:HD22	1.98	0.46
1:A:117:ASP:O	1:A:120:ARG:HB3	2.17	0.45
2:B:245:ARG:HD3	11:B:1212:HOH:O	2.16	0.45
1:A:150:ARG:NE	1:A:154:ARG:HH22	2.13	0.45
2:B:61:ASN:N	10:B:1016:GOL:O1	2.48	0.45
1:A:118:LEU:CG	1:A:157:LEU:HD13	2.46	0.45
1:A:42:GLN:C	1:A:44:THR:H	2.20	0.44
1:A:106:ARG:HD2	11:A:7896:HOH:O	2.16	0.44
1:A:46:PRO:O	1:A:49:GLU:HB2	2.18	0.44
1:A:223:SER:O	1:A:225:GLY:N	2.50	0.44
2:B:101:ASN:ND2	2:B:104:SER:H	2.14	0.44
1:A:168:ARG:HD3	1:A:199:TRP:CD2	2.53	0.44
2:B:171:ASN:C	2:B:171:ASN:ND2	2.70	0.44
2:B:161:TRP:CD1	2:B:163:GLU:HG3	2.53	0.44
2:B:52:ILE:N	2:B:52:ILE:CD1	2.80	0.43
1:A:223:SER:CB	1:A:224:PRO:CD	2.96	0.43
1:A:161:GLN:HA	1:A:165:GLU:CG	2.48	0.43
1:A:74:ASN:HD22	1:A:74:ASN:C	2.21	0.43
2:B:171:ASN:HD22	2:B:172:GLN:N	2.16	0.43
1:A:41:ARG:HD3	1:A:45:ILE:HD11	1.99	0.43
3:B:264:NDG:H5	3:B:265:NAG:O6	2.18	0.43
1:A:143:ARG:HE	10:A:1014:GOL:C3	2.32	0.43
2:B:232:LEU:HB3	2:B:248:ILE:HB	2.01	0.42
1:A:67:THR:O	1:A:80:TYR:HA	2.20	0.42
2:B:49:LEU:HB3	10:B:1016:GOL:H12	2.01	0.42
1:A:120:ARG:HG2	1:A:120:ARG:NH1	2.32	0.42
1:A:65:SER:O	1:A:143:ARG:HD3	2.19	0.42
2:B:125:ASP:N	2:B:130:GLN:HE22	2.10	0.42
2:B:20:MET:HB2	2:B:37:LEU:HG	2.01	0.42
1:A:87:TYR:CD1	1:A:87:TYR:N	2.86	0.42
2:B:98:THR:CG2	11:B:1162:HOH:O	2.68	0.42
2:B:10:PRO:C	2:B:11:ILE:HD12	2.39	0.42
2:B:11:ILE:HG21	3:B:264:NDG:C8	2.50	0.42
1:A:148:SER:HB2	10:A:1012:GOL:C1	2.33	0.41
1:A:74:ASN:O	1:A:75:LEU:HB2	2.21	0.41
2:B:182:ILE:CG2	2:B:192:LEU:HD22	2.50	0.41
6:B:268:NAG:C3	6:B:269:FUL:O2	2.64	0.41
2:B:230:ASN:ND2	2:B:230:ASN:C	2.73	0.41
3:B:264:NDG:H5	3:B:265:NAG:H4	2.03	0.41
1:A:220:LEU:HB2	1:A:228:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:HG12	1:A:72:VAL:HG23	2.03	0.41
1:A:135:LEU:HA	1:A:135:LEU:HD12	1.84	0.41
1:A:177:ARG:NH1	11:A:7827:HOH:O	2.54	0.40
2:B:169:GLN:HG2	2:B:171:ASN:HD21	1.86	0.40
2:B:141:ARG:HB2	2:B:176:LEU:HB2	2.04	0.40
1:A:114:SER:O	1:A:118:LEU:HB2	2.22	0.40
1:A:208:HIS:O	2:B:6:SER:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	247/249 (99%)	236 (96%)	8 (3%)	3 (1%)	16	16
2	B	261/263 (99%)	249 (95%)	12 (5%)	0	100	100
All	All	508/512 (99%)	485 (96%)	20 (4%)	3 (1%)	30	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	A	223	SER
1	A	225	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was



analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	189 (90%)	20 (10%)	10	12
2	B	217/217 (100%)	205 (94%)	12 (6%)	27	36
All	All	426/426 (100%)	394 (92%)	32 (8%)	17	21

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	10	GLN
1	A	41	ARG
1	A	49	GLU
1	A	55	LEU
1	A	60	ASN
1	A	72	VAL
1	A	74	ASN
1	A	81	ARG
1	A	107	SER
1	A	118	LEU
1	A	124	HIS
1	A	130	LEU
1	A	140	THR
1	A	142	LEU
1	A	157	LEU
1	A	187	LEU
1	A	210	THR
1	A	233	VAL
1	A	249	GLU
2	B	47	ASN
2	B	49	LEU
2	B	53	LYS
2	B	98	THR
2	B	166	THR
2	B	171	ASN
2	B	192	LEU
2	B	194	ASN
2	B	218	VAL
2	B	230	ASN
2	B	232	LEU
2	B	240	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	36	GLN
1	A	60	ASN
1	A	74	ASN
1	A	152	GLN
1	A	161	GLN
1	A	170	ASN
1	A	215	ASN
2	B	18	ASN
2	B	36	GLN
2	B	44	ASN
2	B	47	ASN
2	B	48	GLN
2	B	82	ASN
2	B	101	ASN
2	B	130	GLN
2	B	171	ASN
2	B	172	GLN
2	B	190	GLN
2	B	194	ASN
2	B	215	GLN
2	B	227	ASN
2	B	230	ASN
2	B	238	GLN
2	B	240	ASN
2	B	254	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

6 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	NDG	B	264	3	14,14,15	0.41	0	15,19,21	0.67	0
3	NAG	B	265	3,2	14,14,15	0.63	0	15,19,21	0.72	1 (6%)
4	NAG	B	266	2,4	14,14,15	0.55	0	15,19,21	1.24	2 (13%)
4	NAG	B	267	4	14,14,15	0.55	0	15,19,21	1.09	2 (13%)
6	NAG	B	268	2,6	14,14,15	0.55	0	15,19,21	0.75	1 (6%)
6	FUL	B	269	6	10,10,11	0.44	0	14,14,16	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDG	B	264	3	-	0/6/23/26	0/1/1/1
3	NAG	B	265	3,2	-	0/6/23/26	0/1/1/1
4	NAG	B	266	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	267	4	-	0/6/23/26	0/1/1/1
6	NAG	B	268	2,6	-	0/6/23/26	0/1/1/1
6	FUL	B	269	6	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	266	NAG	C2-N2-C7	-3.34	118.75	123.04
4	B	267	NAG	C2-N2-C7	-3.01	119.18	123.04
6	B	268	NAG	C2-N2-C7	-2.16	120.26	123.04
3	B	265	NAG	C2-N2-C7	-2.12	120.31	123.04
4	B	267	NAG	C4-C3-C2	-2.11	107.94	111.23
4	B	266	NAG	C4-C3-C2	2.29	114.79	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	264	NDG	5	0
3	B	265	NAG	2	0
4	B	266	NAG	1	0
4	B	267	NAG	1	0
6	B	268	NAG	3	0
6	B	269	FUL	3	0

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	1004	1	14,14,15	0.69	0	15,19,21	0.94	0
10	GOL	A	1010	-	5,5,5	4.86	5 (100%)	5,5,5	5.72	3 (60%)
10	GOL	A	1011	-	5,5,5	4.89	5 (100%)	5,5,5	5.73	3 (60%)
10	GOL	A	1012	-	5,5,5	4.93	5 (100%)	5,5,5	5.71	3 (60%)
10	GOL	A	1014	-	5,5,5	4.86	5 (100%)	5,5,5	5.71	3 (60%)
10	GOL	A	1017	-	5,5,5	4.86	5 (100%)	5,5,5	5.70	3 (60%)
10	GOL	A	1024	-	5,5,5	4.77	5 (100%)	5,5,5	5.67	3 (60%)
10	GOL	A	1025	-	5,5,5	4.72	5 (100%)	5,5,5	5.71	3 (60%)
9	SO4	A	1028	-	4,4,4	0.22	0	6,6,6	0.08	0
9	SO4	A	1029	-	4,4,4	2.38	2 (50%)	6,6,6	0.44	0
7	GAL	B	1008	-	12,12,12	2.16	5 (41%)	17,17,17	1.54	4 (23%)
7	GAL	B	1009	-	12,12,12	2.04	4 (33%)	17,17,17	1.42	3 (17%)
10	GOL	B	1013	-	5,5,5	4.61	5 (100%)	5,5,5	5.61	3 (60%)
10	GOL	B	1015	-	5,5,5	4.82	5 (100%)	5,5,5	5.72	3 (60%)
10	GOL	B	1016	-	5,5,5	4.75	5 (100%)	5,5,5	5.64	3 (60%)
10	GOL	B	1018	-	5,5,5	4.93	5 (100%)	5,5,5	5.68	3 (60%)
10	GOL	B	1019	-	5,5,5	4.77	5 (100%)	5,5,5	5.68	3 (60%)
10	GOL	B	1020	-	5,5,5	4.83	5 (100%)	5,5,5	5.68	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	GOL	B	1021	-	5,5,5	4.78	5 (100%)	5,5,5	5.69	3 (60%)
10	GOL	B	1022	-	5,5,5	4.77	5 (100%)	5,5,5	5.70	3 (60%)
10	GOL	B	1023	-	5,5,5	4.83	5 (100%)	5,5,5	5.68	3 (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
5	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
10	GOL	A	1010	-	-	0/4/4/4	0/0/0/0
10	GOL	A	1011	-	-	0/4/4/4	0/0/0/0
10	GOL	A	1012	-	-	0/4/4/4	0/0/0/0
10	GOL	A	1014	-	-	0/4/4/4	0/0/0/0
10	GOL	A	1017	-	-	0/4/4/4	0/0/0/0
10	GOL	A	1024	-	-	0/4/4/4	0/0/0/0
10	GOL	A	1025	-	-	0/4/4/4	0/0/0/0
9	SO4	A	1028	-	-	0/0/0/0	0/0/0/0
9	SO4	A	1029	-	-	0/0/0/0	0/0/0/0
7	GAL	B	1008	-	-	0/2/22/22	0/1/1/1
7	GAL	B	1009	-	-	0/2/22/22	0/1/1/1
10	GOL	B	1013	-	-	0/4/4/4	0/0/0/0
10	GOL	B	1015	-	-	0/4/4/4	0/0/0/0
10	GOL	B	1016	-	-	0/4/4/4	0/0/0/0
10	GOL	B	1018	-	-	0/4/4/4	0/0/0/0
10	GOL	B	1019	-	-	0/4/4/4	0/0/0/0
10	GOL	B	1020	-	-	0/4/4/4	0/0/0/0
10	GOL	B	1021	-	-	0/4/4/4	0/0/0/0
10	GOL	B	1022	-	-	0/4/4/4	0/0/0/0
10	GOL	B	1023	-	-	0/4/4/4	0/0/0/0

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1018	GOL	C3-C2	-8.44	1.20	1.52
10	A	1011	GOL	C3-C2	-8.39	1.20	1.52
10	B	1023	GOL	C3-C2	-8.37	1.20	1.52
10	A	1017	GOL	C3-C2	-8.25	1.20	1.52
10	A	1014	GOL	C3-C2	-8.24	1.20	1.52
10	B	1020	GOL	C3-C2	-8.22	1.20	1.52
10	A	1010	GOL	C3-C2	-8.20	1.21	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1024	GOL	C3-C2	-8.19	1.21	1.52
10	B	1015	GOL	C3-C2	-8.18	1.21	1.52
10	B	1019	GOL	C3-C2	-8.17	1.21	1.52
10	A	1012	GOL	C3-C2	-8.16	1.21	1.52
10	B	1021	GOL	C3-C2	-8.15	1.21	1.52
10	B	1016	GOL	C3-C2	-8.09	1.21	1.52
10	B	1022	GOL	C3-C2	-7.99	1.21	1.52
10	A	1025	GOL	C3-C2	-7.92	1.22	1.52
10	B	1013	GOL	C3-C2	-7.79	1.22	1.52
7	B	1009	GAL	C3-C2	-4.57	1.40	1.52
7	B	1008	GAL	C3-C2	-4.05	1.41	1.52
10	B	1016	GOL	C1-C2	-3.86	1.37	1.52
10	A	1011	GOL	C1-C2	-3.61	1.38	1.52
10	A	1012	GOL	C1-C2	-3.58	1.38	1.52
10	B	1023	GOL	C1-C2	-3.41	1.39	1.52
10	A	1017	GOL	C1-C2	-3.38	1.39	1.52
10	A	1024	GOL	C1-C2	-3.35	1.39	1.52
10	A	1014	GOL	C1-C2	-3.35	1.39	1.52
10	A	1010	GOL	C1-C2	-3.29	1.39	1.52
10	B	1020	GOL	C1-C2	-3.28	1.39	1.52
10	A	1025	GOL	C1-C2	-3.28	1.39	1.52
10	B	1018	GOL	C1-C2	-3.27	1.39	1.52
10	B	1022	GOL	C1-C2	-3.26	1.39	1.52
10	B	1019	GOL	C1-C2	-3.22	1.40	1.52
10	B	1021	GOL	C1-C2	-3.22	1.40	1.52
10	A	1012	GOL	O2-C2	-3.18	1.34	1.43
10	B	1015	GOL	C1-C2	-3.12	1.40	1.52
10	B	1013	GOL	C1-C2	-3.09	1.40	1.52
10	B	1018	GOL	O2-C2	-3.03	1.34	1.43
10	B	1020	GOL	O2-C2	-3.00	1.34	1.43
10	B	1023	GOL	O2-C2	-2.96	1.34	1.43
10	B	1015	GOL	O2-C2	-2.92	1.34	1.43
10	A	1011	GOL	O2-C2	-2.92	1.34	1.43
10	A	1014	GOL	O2-C2	-2.89	1.34	1.43
10	A	1010	GOL	O2-C2	-2.86	1.34	1.43
10	A	1017	GOL	O2-C2	-2.80	1.35	1.43
10	A	1024	GOL	O2-C2	-2.76	1.35	1.43
10	B	1022	GOL	O2-C2	-2.72	1.35	1.43
10	B	1016	GOL	O2-C2	-2.68	1.35	1.43
10	B	1021	GOL	O2-C2	-2.68	1.35	1.43
10	A	1025	GOL	O2-C2	-2.57	1.35	1.43
10	B	1019	GOL	O2-C2	-2.56	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1013	GOL	O2-C2	-2.14	1.37	1.43
7	B	1009	GAL	O5-C1	2.27	1.47	1.43
7	B	1008	GAL	O5-C1	2.50	1.47	1.43
7	B	1009	GAL	O3-C3	2.79	1.49	1.43
10	A	1011	GOL	O3-C3	2.90	1.54	1.42
10	B	1023	GOL	O3-C3	2.92	1.54	1.42
7	B	1008	GAL	C1-C2	2.98	1.58	1.52
7	B	1009	GAL	C4-C3	2.98	1.60	1.52
7	B	1008	GAL	O3-C3	3.01	1.50	1.43
9	A	1029	SO4	O4-S	3.11	1.58	1.47
10	B	1020	GOL	O3-C3	3.12	1.55	1.42
10	A	1024	GOL	O3-C3	3.16	1.56	1.42
10	B	1018	GOL	O3-C3	3.23	1.56	1.42
10	B	1019	GOL	O3-C3	3.29	1.56	1.42
10	B	1015	GOL	O3-C3	3.31	1.56	1.42
10	B	1021	GOL	O3-C3	3.31	1.56	1.42
10	A	1014	GOL	O3-C3	3.32	1.56	1.42
10	B	1016	GOL	O3-C3	3.32	1.56	1.42
9	A	1029	SO4	O3-S	3.34	1.59	1.47
10	A	1017	GOL	O3-C3	3.35	1.56	1.42
7	B	1008	GAL	C4-C3	3.37	1.61	1.52
10	A	1012	GOL	O3-C3	3.40	1.57	1.42
10	A	1010	GOL	O3-C3	3.45	1.57	1.42
10	B	1022	GOL	O3-C3	3.50	1.57	1.42
10	A	1025	GOL	O3-C3	3.59	1.57	1.42
10	B	1016	GOL	O1-C1	3.77	1.58	1.42
10	B	1013	GOL	O3-C3	3.94	1.59	1.42
10	B	1013	GOL	O1-C1	4.02	1.59	1.42
10	B	1023	GOL	O1-C1	4.23	1.60	1.42
10	A	1024	GOL	O1-C1	4.25	1.60	1.42
10	A	1025	GOL	O1-C1	4.32	1.61	1.42
10	B	1019	GOL	O1-C1	4.38	1.61	1.42
10	A	1011	GOL	O1-C1	4.40	1.61	1.42
10	B	1021	GOL	O1-C1	4.40	1.61	1.42
10	B	1020	GOL	O1-C1	4.41	1.61	1.42
10	B	1022	GOL	O1-C1	4.43	1.61	1.42
10	A	1010	GOL	O1-C1	4.43	1.61	1.42
10	A	1017	GOL	O1-C1	4.43	1.61	1.42
10	A	1014	GOL	O1-C1	4.44	1.61	1.42
10	B	1018	GOL	O1-C1	4.48	1.61	1.42
10	B	1015	GOL	O1-C1	4.50	1.61	1.42
10	A	1012	GOL	O1-C1	4.53	1.61	1.42

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1008	GAL	O3-C3-C4	-3.40	102.69	110.34
7	B	1009	GAL	O3-C3-C4	-3.25	103.03	110.34
7	B	1008	GAL	C1-C2-C3	-3.00	105.97	110.43
7	B	1009	GAL	C1-C2-C3	-2.60	106.56	110.43
7	B	1009	GAL	O3-C3-C2	2.11	115.09	110.34
7	B	1008	GAL	C4-C3-C2	2.12	114.74	110.79
7	B	1008	GAL	O3-C3-C2	2.53	116.03	110.34
10	A	1011	GOL	O1-C1-C2	2.93	124.37	110.18
10	A	1012	GOL	O1-C1-C2	3.01	124.78	110.18
10	B	1016	GOL	O1-C1-C2	3.02	124.81	110.18
10	A	1024	GOL	O1-C1-C2	3.05	124.99	110.18
10	A	1014	GOL	O1-C1-C2	3.17	125.55	110.18
10	B	1022	GOL	O1-C1-C2	3.17	125.57	110.18
10	B	1015	GOL	O1-C1-C2	3.19	125.64	110.18
10	B	1021	GOL	O1-C1-C2	3.19	125.66	110.18
10	A	1025	GOL	O1-C1-C2	3.19	125.66	110.18
10	B	1023	GOL	O1-C1-C2	3.19	125.67	110.18
10	B	1018	GOL	O1-C1-C2	3.20	125.71	110.18
10	A	1010	GOL	O1-C1-C2	3.22	125.80	110.18
10	B	1019	GOL	O1-C1-C2	3.23	125.84	110.18
10	B	1020	GOL	O1-C1-C2	3.23	125.85	110.18
10	A	1017	GOL	O1-C1-C2	3.24	125.90	110.18
10	B	1013	GOL	O1-C1-C2	3.38	126.59	110.18
10	A	1011	GOL	O2-C2-C3	6.50	138.45	108.65
10	B	1015	GOL	O2-C2-C3	6.51	138.49	108.65
10	A	1012	GOL	O2-C2-C3	6.55	138.68	108.65
10	B	1023	GOL	O2-C2-C3	6.59	138.88	108.65
10	B	1020	GOL	O2-C2-C3	6.60	138.90	108.65
10	B	1018	GOL	O2-C2-C3	6.60	138.92	108.65
10	A	1024	GOL	O2-C2-C3	6.61	138.97	108.65
10	B	1021	GOL	O2-C2-C3	6.61	138.97	108.65
10	B	1019	GOL	O2-C2-C3	6.62	139.00	108.65
10	A	1017	GOL	O2-C2-C3	6.62	139.00	108.65
10	A	1010	GOL	O2-C2-C3	6.62	139.02	108.65
10	A	1014	GOL	O2-C2-C3	6.63	139.03	108.65
10	B	1022	GOL	O2-C2-C3	6.66	139.18	108.65
10	A	1025	GOL	O2-C2-C3	6.70	139.35	108.65
10	B	1016	GOL	O2-C2-C3	6.90	140.31	108.65
10	B	1013	GOL	O2-C2-C3	7.09	141.15	108.65
10	B	1013	GOL	O3-C3-C2	9.72	157.31	110.18
10	B	1016	GOL	O3-C3-C2	10.09	159.12	110.18
10	B	1018	GOL	O3-C3-C2	10.33	160.28	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	1019	GOL	O3-C3-C2	10.33	160.29	110.18
10	B	1023	GOL	O3-C3-C2	10.34	160.32	110.18
10	B	1020	GOL	O3-C3-C2	10.34	160.32	110.18
10	B	1021	GOL	O3-C3-C2	10.36	160.40	110.18
10	A	1024	GOL	O3-C3-C2	10.37	160.47	110.18
10	A	1025	GOL	O3-C3-C2	10.37	160.49	110.18
10	B	1022	GOL	O3-C3-C2	10.37	160.49	110.18
10	A	1017	GOL	O3-C3-C2	10.38	160.52	110.18
10	A	1014	GOL	O3-C3-C2	10.41	160.69	110.18
10	A	1010	GOL	O3-C3-C2	10.42	160.73	110.18
10	B	1015	GOL	O3-C3-C2	10.51	161.14	110.18
10	A	1012	GOL	O3-C3-C2	10.53	161.25	110.18
10	A	1011	GOL	O3-C3-C2	10.64	161.80	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1012	GOL	2	0
10	A	1014	GOL	1	0
10	A	1017	GOL	1	0
10	A	1024	GOL	1	0
7	B	1008	GAL	2	0
10	B	1016	GOL	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	A	249/249 (100%)	0.45	18 (7%)	18 26	28, 40, 62, 76	4 (1%)
2	B	263/263 (100%)	0.21	21 (7%)	15 21	21, 32, 52, 70	0
All	All	512/512 (100%)	0.32	39 (7%)	17 24	21, 36, 59, 76	4 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	GLY	6.6
1	A	224	PRO	6.3
1	A	248	GLY	4.6
1	A	223	SER	4.3
1	A	226	SER	4.3
1	A	98	THR	4.2
2	B	1	ASP	4.0
1	A	44	THR	3.9
1	A	95	GLY	3.6
1	A	221	ALA	3.5
1	A	222	LEU	3.4
2	B	3	VAL	3.4
2	B	182	ILE	3.3
1	A	91	ASP	3.1
2	B	14	ILE	2.8
2	B	166	THR	2.8
1	A	227	VAL	2.7
2	B	209	SER	2.5
2	B	2	ASP	2.5
2	B	76	VAL	2.5
2	B	22	VAL	2.4
1	A	48	SER	2.4
2	B	6	SER	2.4
2	B	35	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	65	LEU	2.4
1	A	145	PRO	2.3
2	B	5	CYS	2.3
1	A	84	ASP	2.3
2	B	157	GLY	2.3
2	B	161	TRP	2.2
1	A	103	GLY	2.2
1	A	120	ARG	2.2
2	B	254	ASN	2.2
2	B	58	ILE	2.1
2	B	187	ASN	2.1
2	B	50	TRP	2.1
2	B	153	MET	2.1
1	A	102	ALA	2.0
2	B	243	LEU	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	B	265	14/15	0.96	0.11	-0.82	31,39,42,50	0
6	FUL	B	269	10/11	0.75	0.33	-	55,56,57,58	10
4	NAG	B	267	14/15	0.73	0.41	-	79,84,86,87	0
6	NAG	B	268	14/15	0.84	0.20	-	45,49,52,54	14
4	NAG	B	266	14/15	0.84	0.25	-	57,64,67,74	0
3	NDG	B	264	14/15	0.78	0.37	-	55,62,67,70	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
10	GOL	A	1024	6/6	0.82	0.40	6.46	76,77,78,79	0
10	GOL	B	1019	6/6	0.80	0.25	4.57	70,72,73,74	0
10	GOL	B	1020	6/6	0.76	0.30	4.46	56,62,64,64	0
10	GOL	B	1013	6/6	0.73	0.32	3.97	40,46,47,49	0
10	GOL	A	1011	6/6	0.83	0.27	3.89	49,50,51,52	0
7	GAL	B	1008	12/12	0.88	0.22	3.52	36,45,49,51	0
10	GOL	B	1016	6/6	0.81	0.26	2.91	65,67,68,68	0
10	GOL	A	1014	6/6	0.86	0.22	2.77	81,82,82,84	0
9	SO4	A	1029	5/5	0.85	0.32	2.68	89,90,91,91	0
7	GAL	B	1009	12/12	0.85	0.31	2.34	52,57,58,60	0
10	GOL	B	1022	6/6	0.65	0.23	2.10	80,81,81,81	0
10	GOL	A	1012	6/6	0.83	0.23	2.08	67,68,69,70	0
10	GOL	A	1025	6/6	0.80	0.26	1.51	64,69,70,70	0
10	GOL	B	1023	6/6	0.92	0.16	1.05	38,48,49,51	0
9	SO4	A	1028	5/5	0.91	0.20	-0.48	64,64,65,65	5
10	GOL	A	1010	6/6	0.91	0.13	-1.11	73,74,74,75	0
10	GOL	B	1015	6/6	0.62	0.33	-	86,89,89,90	0
8	CL	A	1027	1/1	0.93	0.15	-	68,68,68,68	0
5	NAG	A	1004	14/15	0.82	0.44	-	66,69,74,74	0
8	CL	A	1026	1/1	0.73	0.11	-	68,68,68,68	1
10	GOL	B	1018	6/6	0.81	0.37	-	74,76,77,79	0
10	GOL	A	1017	6/6	0.77	0.21	-	96,97,97,98	0
10	GOL	B	1021	6/6	0.70	0.58	-	89,90,91,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.