Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 11:43 PM GMT

PDB ID	:	1YF8
Title	:	Crystal structure of Himalayan mistletoe RIP reveals the presence of a natural inhibitor and a new functionally active sugar-binding site
Authors	:	Mishra, V.; Bilgrami, S.; Sharma, R.S.; Kaur, P.; Yadav, S.; Betzel, C.; Babu, C.R.; Singh, T.P.
Deposited on	:	2004-12-31
Resolution	:	2.80 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

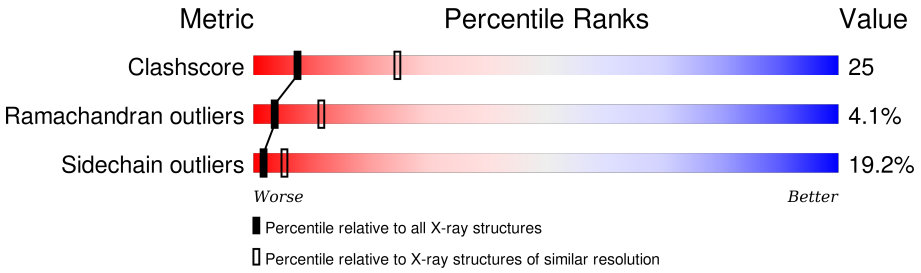
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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 >=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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	240	49% 37% 13%
2	B	255	56% 36% 7%

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
3	NAG	A	1003	X	-	-	-
6	MAN	B	260	X	-	-	-
7	MAN	B	264	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GAL	B	1015	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4125 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.

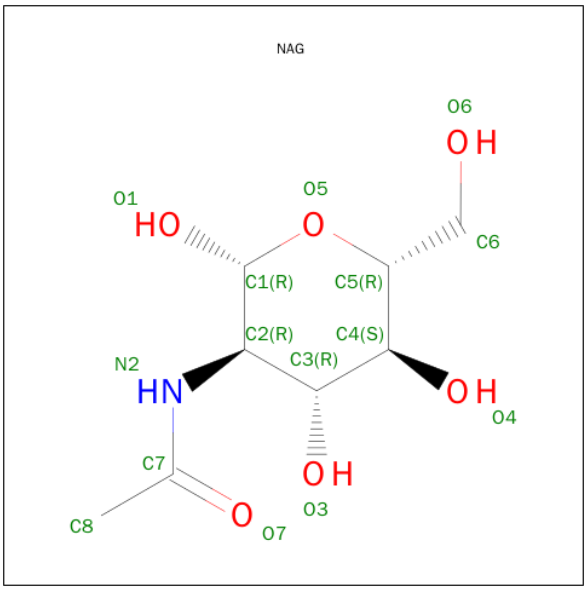
- Molecule 1 is a protein called Beta-galactoside-specific lectin 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1875	1191	319	361	4			

- Molecule 2 is a protein called Beta-galactoside-specific lectin 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	255	Total	C	N	O	S	0	0	0
			1938	1199	343	384	12			

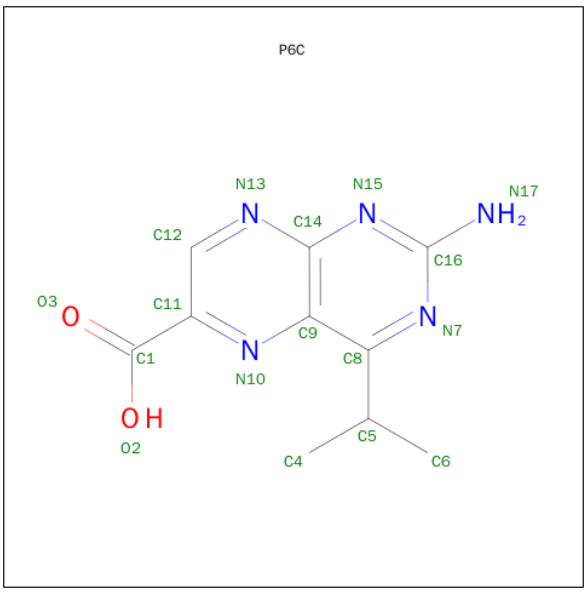
- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is 2-AMINO-4-ISOPROPYL-PTERIDINE-6-CARBOXYLIC ACID (three-letter

code: P6C) (formula: $C_{10}H_{11}N_5O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 17 10 5 2	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	4	Total C N O 50 28 2 20	0	0

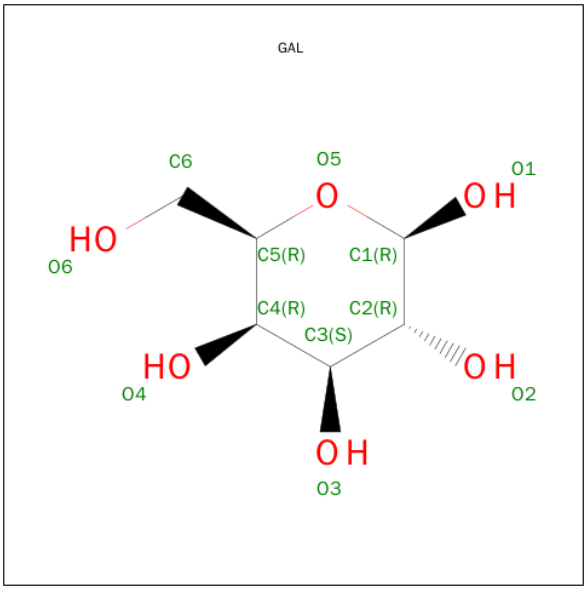
- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	3	Total C N O 39 22 2 15	0	0

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	2	Total C O 23 12 11	0	0
8	B	2	Total C O 23 12 11	0	0

- Molecule 9 is SUGAR (D-GALACTOSE) (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 11 6 5	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	55	Total O 55 55	0	0
10	B	52	Total O 52 52	0	0

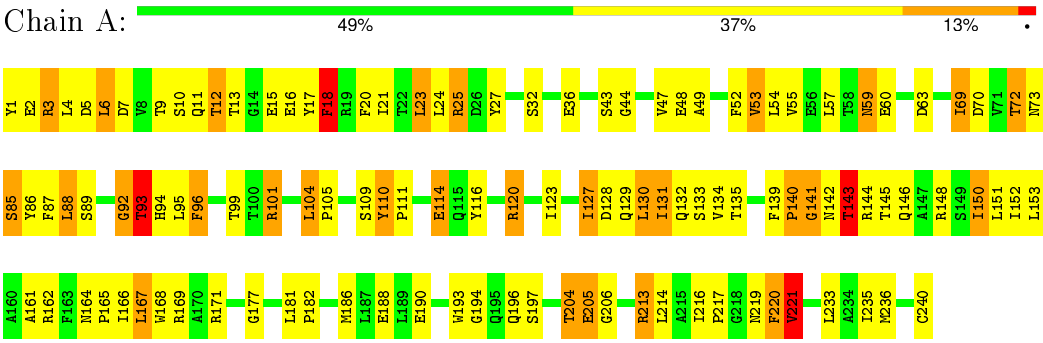
3 Residue-property plots (i)

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.

Note EDS was not executed.

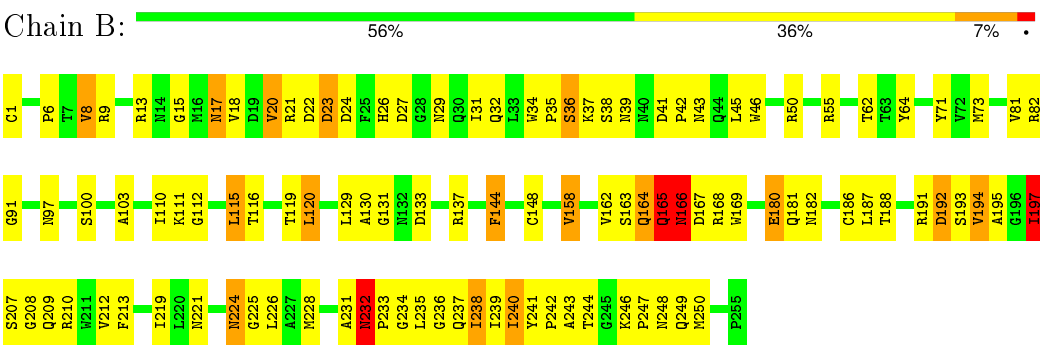
- Molecule 1: Beta-galactoside-specific lectin 4

Chain A:



- Molecule 2: Beta-galactoside-specific lectin 4

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	109.42Å 109.42Å 309.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.234 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4125	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, NAG, P6C, GAL, BMA, MAN

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	0.92	3/1913 (0.2%)	1.06	11/2602 (0.4%)
2	B	0.92	0/1978	1.04	5/2697 (0.2%)
All	All	0.92	3/3891 (0.1%)	1.05	16/5299 (0.3%)

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
6	B	2	0
7	B	1	0
All	All	3	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	SER	CB-OG	7.99	1.52	1.42
1	A	36	GLU	CG-CD	5.64	1.60	1.51
1	A	168	TRP	CB-CG	5.36	1.59	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	96	PHE	N-CA-CB	8.72	126.29	110.60
1	A	6	LEU	CA-CB-CG	8.39	134.59	115.30
1	A	88	LEU	CA-CB-CG	7.57	132.70	115.30
1	A	4	LEU	CA-CB-CG	6.77	130.87	115.30
2	B	236	GLY	N-CA-C	6.66	129.75	113.10
2	B	82	ARG	NE-CZ-NH1	6.40	123.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	165	GLN	C-N-CA	-6.27	106.02	121.70
1	A	142	ASN	CA-C-N	-6.02	103.95	117.20
2	B	166	ASN	C-N-CA	5.42	135.26	121.70
2	B	210	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	143	THR	O-C-N	-5.26	114.29	122.70
1	A	96	PHE	O-C-N	5.21	131.03	122.70
1	A	18	PHE	CB-CA-C	5.09	120.58	110.40
1	A	123	ILE	CG1-CB-CG2	-5.09	100.21	111.40
1	A	92	GLY	N-CA-C	5.06	125.76	113.10
1	A	93	THR	C-N-CA	5.02	134.25	121.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	260	MAN	C3,C1
7	B	264	MAN	C1

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1875	0	1849	103	0
2	B	1938	0	1851	93	0
3	A	14	0	13	0	0
4	A	17	0	9	2	0
5	B	28	0	25	2	0
6	B	50	0	43	5	0
7	B	39	0	34	1	0
8	B	46	0	42	8	0
9	B	11	0	10	5	0
10	A	55	0	0	4	0
10	B	52	0	0	3	0
All	All	4125	0	3876	201	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 25.

All (201) 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:18:PHE:HB2	1:A:167:LEU:HD21	1.27	1.16
5:B:256:NAG:H62	5:B:257:NAG:H2	1.17	1.10
6:B:259:NAG:H3	6:B:259:NAG:H83	1.39	1.02
1:A:139:PHE:HB3	1:A:140:PRO:HD2	1.45	0.96
1:A:101:ARG:HG2	1:A:101:ARG:HH11	1.32	0.94
2:B:32:GLN:HE22	9:B:1013:GAL:H4	1.34	0.92
2:B:224:ASN:ND2	2:B:226:LEU:H	1.72	0.86
2:B:244:THR:HG23	2:B:246:LYS:H	1.40	0.86
2:B:244:THR:HG22	2:B:249:GLN:CD	1.97	0.86
1:A:127:ILE:H	1:A:127:ILE:HD12	1.42	0.83
2:B:34:TRP:CZ2	2:B:111:LYS:HE3	2.15	0.82
2:B:224:ASN:HD22	2:B:224:ASN:C	1.83	0.82
2:B:97:ASN:ND2	2:B:100:SER:H	1.79	0.80
1:A:127:ILE:HD12	1:A:127:ILE:N	1.96	0.79
1:A:120:ARG:CD	1:A:120:ARG:H	1.96	0.79
2:B:224:ASN:HD22	2:B:226:LEU:H	1.29	0.77
2:B:64:TYR:HE1	8:B:1014:BGC:H1	1.50	0.75
1:A:114:GLU:OE2	1:A:114:GLU:N	2.21	0.74
1:A:25:ARG:HD2	1:A:161:ALA:O	1.87	0.73
2:B:17:ASN:HD21	2:B:36:SER:HB3	1.53	0.72
1:A:3:ARG:HG3	1:A:27:TYR:CE2	2.25	0.72
8:B:1014:BGC:H4	8:B:1015:GAL:O2	1.88	0.71
1:A:182:PRO:HB3	1:A:186:MET:SD	2.31	0.70
2:B:181:GLN:OE1	2:B:181:GLN:HA	1.91	0.70
1:A:120:ARG:HD3	1:A:120:ARG:H	1.57	0.70
2:B:73:MET:CE	8:B:1015:GAL:H5	2.21	0.69
1:A:10:SER:H	1:A:12:THR:CG2	2.05	0.69
2:B:144:PHE:HE2	2:B:233:PRO:HD3	1.59	0.68
1:A:139:PHE:CB	1:A:140:PRO:HD2	2.12	0.68
6:B:259:NAG:H3	6:B:259:NAG:C8	2.19	0.68
2:B:1:CYS:N	10:B:1016:HOH:O	2.21	0.68
2:B:221:ASN:HD22	2:B:224:ASN:H	1.41	0.66
1:A:127:ILE:HD11	1:A:177:GLY:HA2	1.76	0.66
2:B:133:ASP:HB3	2:B:137:ARG:HH12	1.60	0.66
2:B:81:VAL:HG12	2:B:83:GLU:HG2	1.76	0.66
1:A:197:SER:OG	1:A:236:MET:HB3	1.95	0.66
1:A:53:VAL:HG12	1:A:69:ILE:HG13	1.78	0.66
1:A:166:ILE:HG23	1:A:186:MET:HE2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLY:HA3	4:A:1001:P6C:H61	1.80	0.64
2:B:148:CYS:O	2:B:158:VAL:HA	1.98	0.63
2:B:166:ASN:C	2:B:166:ASN:HD22	2.00	0.63
1:A:220:PHE:N	1:A:220:PHE:CD1	2.66	0.63
1:A:87:PHE:HZ	1:A:94:HIS:O	1.82	0.62
2:B:34:TRP:CZ3	2:B:111:LYS:HG2	2.34	0.62
2:B:197:ILE:HB	2:B:238:ILE:O	1.99	0.62
1:A:105:PRO:HG2	1:A:116:TYR:CE2	2.35	0.62
2:B:195:ALA:HB2	10:B:1036:HOH:O	2.00	0.61
1:A:120:ARG:NE	1:A:120:ARG:H	1.99	0.61
1:A:155:GLN:HG2	1:A:190:GLU:OE2	2.01	0.61
2:B:133:ASP:HB3	2:B:137:ARG:NH1	2.15	0.61
1:A:11:GLN:NE2	10:A:1038:HOH:O	2.12	0.60
6:B:259:NAG:H83	6:B:259:NAG:C3	2.23	0.60
1:A:110:TYR:HD2	10:A:1014:HOH:O	1.84	0.60
1:A:52:PHE:CD2	1:A:95:LEU:HD21	2.37	0.60
1:A:18:PHE:CB	1:A:167:LEU:HD21	2.18	0.60
1:A:96:PHE:O	1:A:99:THR:HB	2.02	0.59
2:B:34:TRP:CH2	2:B:111:LYS:HE3	2.37	0.59
1:A:52:PHE:CG	1:A:95:LEU:HD21	2.38	0.58
2:B:193:SER:O	2:B:194:VAL:CG2	2.51	0.58
1:A:220:PHE:H	1:A:220:PHE:HD1	1.50	0.58
1:A:101:ARG:CG	1:A:101:ARG:HH11	2.09	0.58
2:B:224:ASN:ND2	2:B:224:ASN:C	2.56	0.57
1:A:59:ASN:HD22	1:A:59:ASN:C	2.07	0.57
2:B:18:VAL:HG12	2:B:46:TRP:CZ2	2.39	0.57
6:B:260:MAN:H2	6:B:261:BMA:O2	2.05	0.56
1:A:94:HIS:O	1:A:95:LEU:HB2	2.06	0.56
2:B:193:SER:O	2:B:194:VAL:HG22	2.05	0.56
1:A:9:THR:O	1:A:9:THR:HG23	2.06	0.55
1:A:3:ARG:HG3	1:A:27:TYR:CZ	2.42	0.55
1:A:1:TYR:HD2	1:A:2:GLU:H	1.53	0.55
1:A:48:GLU:HG3	1:A:49:ALA:H	1.72	0.55
2:B:37:LYS:HZ3	2:B:43:ASN:HD21	1.55	0.55
1:A:101:ARG:HG2	1:A:101:ARG:NH1	2.11	0.54
1:A:196:GLN:HB3	1:A:233:LEU:HD22	1.90	0.54
1:A:166:ILE:HG12	1:A:186:MET:HG3	1.89	0.54
1:A:139:PHE:O	1:A:141:GLY:N	2.40	0.54
2:B:169:TRP:CZ3	2:B:187:LEU:HD13	2.42	0.54
1:A:70:ASP:OD1	1:A:72:THR:HB	2.08	0.54
2:B:188:THR:HG23	2:B:209:GLN:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:VAL:HG13	2:B:9:ARG:O	2.09	0.53
2:B:17:ASN:HD21	2:B:36:SER:CB	2.20	0.53
1:A:69:ILE:CG2	1:A:76:VAL:HG22	2.39	0.52
1:A:93:THR:OG1	10:A:1006:HOH:O	2.19	0.52
1:A:70:ASP:HB3	1:A:73:ASN:OD1	2.09	0.52
1:A:93:THR:HB	1:A:94:HIS:CD2	2.44	0.52
1:A:220:PHE:O	1:A:221:VAL:HG23	2.10	0.52
2:B:192:ASP:N	2:B:192:ASP:OD1	2.41	0.52
2:B:166:ASN:ND2	2:B:166:ASN:C	2.62	0.52
1:A:127:ILE:O	1:A:131:ILE:HD13	2.10	0.52
1:A:139:PHE:HB3	1:A:140:PRO:CD	2.31	0.52
2:B:195:ALA:HA	2:B:239:ILE:HB	1.91	0.51
1:A:48:GLU:CG	1:A:49:ALA:N	2.71	0.51
2:B:37:LYS:NZ	2:B:43:ASN:HD21	2.09	0.51
2:B:232:ASN:HB3	2:B:234:GLY:H	1.74	0.51
2:B:22:ASP:O	2:B:23:ASP:HB2	2.09	0.51
1:A:48:GLU:CG	1:A:49:ALA:H	2.22	0.51
2:B:34:TRP:CE2	9:B:1013:GAL:C1	2.94	0.51
2:B:71:TYR:HA	2:B:116:THR:HG22	1.93	0.51
2:B:168:ARG:NH1	10:B:1021:HOH:O	2.35	0.50
1:A:146:GLN:O	1:A:150:ILE:HG12	2.11	0.50
1:A:17:TYR:O	1:A:21:ILE:HG12	2.12	0.50
2:B:21:ARG:NH2	2:B:112:GLY:O	2.45	0.50
2:B:34:TRP:CZ2	9:B:1013:GAL:C1	2.95	0.50
2:B:144:PHE:HB2	2:B:248:ASN:HA	1.93	0.49
1:A:105:PRO:HB2	1:A:116:TYR:OH	2.12	0.49
1:A:101:ARG:CG	1:A:101:ARG:NH1	2.72	0.49
2:B:224:ASN:HD22	2:B:225:GLY:N	2.09	0.49
1:A:87:PHE:CZ	1:A:94:HIS:O	2.64	0.49
5:B:256:NAG:C6	5:B:257:NAG:H2	2.12	0.49
1:A:43:SER:O	1:A:44:GLY:C	2.50	0.49
1:A:205:GLU:HB2	2:B:89:ILE:HB	1.94	0.49
1:A:150:ILE:O	1:A:153:LEU:N	2.45	0.48
1:A:164:ASN:N	1:A:165:PRO:CD	2.76	0.48
2:B:42:PRO:HG2	7:B:262:NAG:H82	1.94	0.48
1:A:120:ARG:NE	1:A:120:ARG:N	2.61	0.48
1:A:93:THR:HB	1:A:94:HIS:HD2	1.78	0.48
2:B:165:GLN:NE2	2:B:180:GLU:OE2	2.46	0.48
2:B:32:GLN:NE2	9:B:1013:GAL:H4	2.16	0.48
1:A:120:ARG:CD	1:A:120:ARG:N	2.72	0.48
2:B:24:ASP:HB3	2:B:29:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:VAL:HG23	8:B:1015:GAL:O4	2.14	0.48
2:B:231:ALA:O	2:B:232:ASN:HB2	2.12	0.48
1:A:220:PHE:N	1:A:220:PHE:HD1	2.06	0.47
1:A:110:TYR:O	1:A:111:PRO:C	2.52	0.47
2:B:144:PHE:CE2	2:B:233:PRO:HD3	2.44	0.47
2:B:22:ASP:N	9:B:1013:GAL:O4	2.47	0.47
1:A:162:ARG:HD3	1:A:193:TRP:CD2	2.49	0.47
2:B:244:THR:HG22	2:B:249:GLN:NE2	2.30	0.47
1:A:159:GLU:HA	1:A:159:GLU:OE1	2.15	0.46
1:A:59:ASN:HD21	1:A:63:ASP:H	1.63	0.46
2:B:213:PHE:CD1	2:B:219:ILE:HG12	2.50	0.46
1:A:20:PHE:HZ	1:A:55:VAL:HG21	1.81	0.46
1:A:127:ILE:CD1	1:A:127:ILE:N	2.73	0.46
2:B:133:ASP:CB	2:B:137:ARG:HH12	2.28	0.46
1:A:134:VAL:CG2	1:A:135:THR:N	2.78	0.46
2:B:97:ASN:HD22	2:B:100:SER:H	1.62	0.45
2:B:73:MET:HE1	8:B:1015:GAL:H5	1.95	0.45
1:A:240:CYS:HB2	2:B:1:CYS:HB2	1.75	0.45
2:B:213:PHE:CE1	2:B:219:ILE:HG12	2.51	0.45
2:B:64:TYR:CE1	8:B:1014:BGC:H1	2.39	0.45
1:A:20:PHE:HZ	1:A:55:VAL:CG2	2.29	0.45
2:B:103:ALA:HB2	2:B:120:LEU:HD12	1.99	0.45
2:B:62:THR:CG2	8:B:1015:GAL:H62	2.47	0.45
2:B:241:TYR:CG	2:B:242:PRO:HD2	2.52	0.45
1:A:23:LEU:HD13	1:A:23:LEU:HA	1.85	0.45
1:A:69:ILE:HA	1:A:75:TYR:O	2.16	0.45
1:A:110:TYR:CD2	1:A:111:PRO:HD3	2.52	0.45
2:B:34:TRP:CH2	2:B:111:LYS:CE	2.99	0.45
2:B:166:ASN:ND2	2:B:166:ASN:N	2.63	0.45
1:A:159:GLU:HG3	1:A:190:GLU:HG2	1.98	0.45
2:B:8:VAL:HG13	2:B:131:GLY:H	1.82	0.45
2:B:193:SER:C	2:B:194:VAL:HG23	2.37	0.44
1:A:166:ILE:HG23	1:A:186:MET:CE	2.45	0.44
2:B:193:SER:C	2:B:194:VAL:CG2	2.86	0.44
2:B:188:THR:HA	2:B:208:GLY:O	2.18	0.44
2:B:213:PHE:CE1	2:B:219:ILE:HD11	2.53	0.44
2:B:31:ILE:HG22	2:B:115:LEU:HD22	2.00	0.44
1:A:162:ARG:HH12	4:A:1001:P6C:C1	2.31	0.44
2:B:166:ASN:HD22	2:B:166:ASN:N	2.13	0.43
1:A:159:GLU:OE2	1:A:190:GLU:HG2	2.18	0.43
1:A:10:SER:H	1:A:12:THR:HG22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:ARG:C	2:B:15:GLY:H	2.22	0.43
2:B:34:TRP:CD1	2:B:35:PRO:HD2	2.53	0.43
2:B:62:THR:HG22	8:B:1015:GAL:H62	1.99	0.43
2:B:8:VAL:HG11	2:B:130:ALA:HB1	2.00	0.43
2:B:226:LEU:HB2	2:B:240:ILE:HG23	1.99	0.43
2:B:20:VAL:O	2:B:20:VAL:HG22	2.18	0.42
1:A:18:PHE:C	1:A:18:PHE:HD1	2.22	0.42
1:A:85:SER:OG	1:A:99:THR:HG22	2.19	0.42
1:A:196:GLN:HB3	1:A:233:LEU:CD2	2.49	0.42
1:A:204:THR:OG1	1:A:205:GLU:N	2.52	0.42
1:A:221:VAL:HG12	1:A:221:VAL:O	2.18	0.42
2:B:41:ASP:HA	2:B:42:PRO:HD2	1.83	0.42
1:A:86:TYR:HB3	1:A:104:LEU:CD2	2.49	0.42
1:A:213:ARG:HG2	10:A:1054:HOH:O	2.18	0.42
1:A:204:THR:C	1:A:206:GLY:H	2.23	0.42
2:B:18:VAL:HG12	2:B:46:TRP:CE2	2.55	0.42
1:A:129:GLN:HB3	1:A:152:ILE:HD13	2.01	0.42
1:A:18:PHE:C	1:A:18:PHE:CD1	2.93	0.41
1:A:76:VAL:HG23	1:A:154:ILE:HD13	2.02	0.41
1:A:86:TYR:HB3	1:A:104:LEU:HD21	2.01	0.41
1:A:13:THR:O	1:A:16:GLU:HB2	2.21	0.41
1:A:188:GLU:HB3	1:A:214:LEU:HD22	2.02	0.41
1:A:3:ARG:HH11	1:A:3:ARG:HA	1.85	0.41
2:B:166:ASN:HD22	2:B:167:ASP:N	2.18	0.41
2:B:46:TRP:HA	2:B:55:ARG:O	2.19	0.41
1:A:127:ILE:O	1:A:128:ASP:C	2.59	0.41
2:B:186:CYS:O	2:B:199:ILE:HA	2.20	0.41
1:A:204:THR:HG21	2:B:6:PRO:HD2	2.02	0.41
2:B:162:VAL:HG12	2:B:163:SER:N	2.35	0.41
2:B:246:LYS:HB3	2:B:247:PRO:CD	2.50	0.41
1:A:116:TYR:HD2	1:A:143:THR:CG2	2.34	0.41
1:A:159:GLU:CA	1:A:159:GLU:OE1	2.69	0.41
1:A:130:LEU:HA	1:A:130:LEU:HD12	1.92	0.41
2:B:164:GLN:O	2:B:164:GLN:HG3	2.16	0.41
1:A:94:HIS:N	1:A:94:HIS:CD2	2.88	0.41
2:B:133:ASP:HB3	2:B:137:ARG:NH2	2.37	0.40
6:B:259:NAG:C3	6:B:259:NAG:C8	2.86	0.40
2:B:26:HIS:O	2:B:27:ASP:C	2.59	0.40
1:A:7:ASP:HB2	1:A:20:PHE:CD1	2.56	0.40
2:B:20:VAL:HB	2:B:31:ILE:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	238/240 (99%)	200 (84%)	27 (11%)	11 (5%)	3 9
2	B	253/255 (99%)	223 (88%)	21 (8%)	9 (4%)	4 14
All	All	491/495 (99%)	423 (86%)	48 (10%)	20 (4%)	3 11

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	TYR
1	A	140	PRO
1	A	143	THR
1	A	204	THR
1	A	217	PRO
1	A	221	VAL
2	B	165	GLN
1	A	92	GLY
1	A	141	GLY
1	A	235	ILE
2	B	91	GLY
1	A	93	THR
2	B	39	ASN
2	B	144	PHE
2	B	197	ILE
2	B	243	ALA
2	B	232	ASN
2	B	207	SER
1	A	150	ILE
2	B	194	VAL

5.3.2 Protein sidechains

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	205/205 (100%)	158 (77%)	47 (23%)	1 3
2	B	211/211 (100%)	178 (84%)	33 (16%)	3 9
All	All	416/416 (100%)	336 (81%)	80 (19%)	2 5

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	5	ASP
1	A	6	LEU
1	A	12	THR
1	A	15	GLU
1	A	18	PHE
1	A	23	LEU
1	A	24	LEU
1	A	25	ARG
1	A	32	SER
1	A	47	VAL
1	A	53	VAL
1	A	54	LEU
1	A	57	LEU
1	A	59	ASN
1	A	60	GLU
1	A	69	ILE
1	A	72	THR
1	A	74	LEU
1	A	85	SER
1	A	88	LEU
1	A	93	THR
1	A	101	ARG
1	A	104	LEU
1	A	109	SER
1	A	114	GLU
1	A	120	ARG
1	A	127	ILE
1	A	130	LEU
1	A	131	ILE
1	A	132	GLN

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Mol	Chain	Res	Type
1	A	133	SER
1	A	144	ARG
1	A	145	THR
1	A	148	ARG
1	A	151	LEU
1	A	159	GLU
1	A	167	LEU
1	A	169	ARG
1	A	171	ARG
1	A	181	LEU
1	A	205	GLU
1	A	213	ARG
1	A	216	ILE
1	A	219	ASN
1	A	220	PHE
1	A	221	VAL
2	B	8	VAL
2	B	17	ASN
2	B	20	VAL
2	B	23	ASP
2	B	36	SER
2	B	38	SER
2	B	45	LEU
2	B	50	ARG
2	B	83	GLU
2	B	110	ILE
2	B	115	LEU
2	B	119	THR
2	B	120	LEU
2	B	129	LEU
2	B	158	VAL
2	B	164	GLN
2	B	166	ASN
2	B	180	GLU
2	B	182	ASN
2	B	191	ARG
2	B	192	ASP
2	B	197	ILE
2	B	198	ASN
2	B	200	VAL
2	B	212	VAL
2	B	224	ASN

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Mol	Chain	Res	Type
2	B	228	MET
2	B	232	ASN
2	B	235	LEU
2	B	237	GLN
2	B	238	ILE
2	B	240	ILE
2	B	250	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	94	HIS
1	A	115	GLN
1	A	119	HIS
2	B	17	ASN
2	B	32	GLN
2	B	43	ASN
2	B	97	ASN
2	B	145	ASN
2	B	165	GLN
2	B	166	ASN
2	B	185	GLN
2	B	198	ASN
2	B	215	ASN
2	B	221	ASN
2	B	224	ASN
2	B	232	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

13 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	$\#\|Z\| > 2$
8	BGC	B	1014	8	12,12,12	0.92	0	17,17,17	2.12	7 (41%)
8	GAL	B	1015	8	11,11,12	0.63	0	14,15,17	2.20	5 (35%)
5	NAG	B	256	2,5	14,14,15	0.87	0	15,19,21	3.13	8 (53%)
5	NAG	B	257	5	14,14,15	0.72	0	15,19,21	1.67	2 (13%)
6	NAG	B	258	2,6	14,14,15	0.76	0	15,19,21	1.62	3 (20%)
6	NAG	B	259	6	14,14,15	0.56	0	15,19,21	2.02	5 (33%)
6	MAN	B	260	6	11,11,12	0.58	0	14,15,17	2.43	4 (28%)
6	BMA	B	261	6	11,11,12	0.54	0	14,15,17	1.55	3 (21%)
7	NAG	B	262	2,7	14,14,15	0.55	0	15,19,21	1.96	4 (26%)
7	NAG	B	263	7	14,14,15	0.69	0	15,19,21	1.84	3 (20%)
7	MAN	B	264	7	11,11,12	0.46	0	14,15,17	1.70	3 (21%)
8	BGC	B	265	8	12,12,12	0.55	0	17,17,17	2.35	5 (29%)
8	GAL	B	266	8	11,11,12	0.55	0	14,15,17	2.24	4 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BGC	B	1014	8	-	0/2/22/22	0/1/1/1
8	GAL	B	1015	8	-	0/2/19/22	0/1/1/1
5	NAG	B	256	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	257	5	-	0/6/23/26	0/1/1/1
6	NAG	B	258	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	259	6	-	0/6/23/26	0/1/1/1
6	MAN	B	260	6	2/2/4/5	0/2/19/22	0/1/1/1
6	BMA	B	261	6	-	0/2/19/22	0/1/1/1
7	NAG	B	262	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	263	7	-	0/6/23/26	0/1/1/1
7	MAN	B	264	7	1/1/4/5	0/2/19/22	1/1/1/1
8	BGC	B	265	8	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GAL	B	266	8	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	259	NAG	C3-C4-C5	-4.51	102.33	110.20
7	B	263	NAG	C1-O5-C5	-4.49	106.55	112.25
8	B	1015	GAL	C1-O5-C5	-4.34	106.74	112.25
5	B	256	NAG	C3-C4-C5	-4.29	102.71	110.20
5	B	256	NAG	O7-C7-C8	-3.55	115.55	122.06
8	B	1015	GAL	O3-C3-C2	-3.48	103.72	110.00
6	B	258	NAG	C3-C4-C5	-3.46	104.17	110.20
8	B	1015	GAL	O2-C2-C3	-3.12	103.84	110.12
7	B	264	MAN	O5-C1-C2	-3.02	105.96	110.86
7	B	264	MAN	C2-C3-C4	-2.72	106.43	111.04
8	B	1014	BGC	O2-C2-C3	-2.67	104.32	110.34
5	B	256	NAG	C4-C3-C2	-2.36	107.55	111.23
6	B	259	NAG	C1-O5-C5	-2.36	109.25	112.25
6	B	258	NAG	O4-C4-C3	-2.32	105.11	110.34
7	B	262	NAG	C3-C2-N2	-2.26	105.15	110.56
7	B	262	NAG	C2-N2-C7	-2.00	120.47	123.04
8	B	1015	GAL	C2-C3-C4	2.04	114.50	111.04
8	B	1014	BGC	O5-C5-C6	2.13	111.73	106.36
6	B	261	BMA	O2-C2-C1	2.39	113.99	109.21
6	B	259	NAG	O4-C4-C5	2.49	115.85	109.24
8	B	266	GAL	C2-C3-C4	2.56	115.38	111.04
6	B	258	NAG	C1-O5-C5	2.57	115.51	112.25
8	B	1014	BGC	O3-C3-C4	2.66	116.34	110.34
6	B	260	MAN	O5-C5-C6	2.69	113.18	107.35
8	B	1014	BGC	O2-C2-C1	2.74	115.84	109.82
5	B	256	NAG	C8-C7-N2	2.76	121.39	116.11
5	B	256	NAG	C2-N2-C7	2.78	126.61	123.04
7	B	264	MAN	O2-C2-C1	2.86	114.94	109.21
8	B	265	BGC	C4-C3-C2	2.86	116.13	110.79
7	B	262	NAG	C4-C3-C2	2.87	115.69	111.23
7	B	263	NAG	O4-C4-C5	2.89	116.90	109.24
5	B	257	NAG	O3-C3-C2	2.98	115.01	109.11
8	B	1015	GAL	C3-C4-C5	3.00	115.43	110.20
6	B	259	NAG	C6-C5-C4	3.02	120.46	113.02
8	B	1014	BGC	O5-C1-C2	3.20	114.91	109.80
6	B	259	NAG	O5-C5-C6	3.22	114.33	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	266	GAL	C1-C2-C3	3.29	113.43	109.54
6	B	261	BMA	C1-C2-C3	3.30	113.44	109.54
8	B	266	GAL	C3-C4-C5	3.36	116.05	110.20
6	B	261	BMA	O5-C5-C6	3.38	114.66	107.35
5	B	256	NAG	O3-C3-C2	3.58	116.21	109.11
8	B	265	BGC	O5-C5-C4	3.64	116.52	109.68
8	B	1014	BGC	C1-C2-C3	3.68	115.90	110.43
6	B	260	MAN	C2-C3-C4	3.84	117.57	111.04
8	B	265	BGC	C1-O5-C5	3.89	120.66	113.47
8	B	1014	BGC	C3-C4-C5	3.96	117.09	110.20
7	B	263	NAG	C4-C3-C2	4.07	117.55	111.23
5	B	257	NAG	C4-C3-C2	4.28	117.89	111.23
6	B	260	MAN	O3-C3-C4	4.43	120.31	110.34
7	B	262	NAG	C1-O5-C5	4.62	118.12	112.25
8	B	265	BGC	O5-C1-C2	4.87	117.56	109.80
5	B	256	NAG	C3-C2-N2	5.09	122.76	110.56
8	B	266	GAL	C1-O5-C5	5.39	119.09	112.25
8	B	265	BGC	C1-C2-C3	5.51	118.63	110.43
6	B	260	MAN	O3-C3-C2	5.75	120.39	110.00
5	B	256	NAG	C1-O5-C5	7.13	121.30	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	260	MAN	C3
6	B	260	MAN	C1
7	B	264	MAN	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	264	MAN	C1-C2-C3-C4-C5-O5

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1014	BGC	3	0
8	B	1015	GAL	6	0
5	B	256	NAG	2	0
5	B	257	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	259	NAG	4	0
6	B	260	MAN	1	0
6	B	261	BMA	1	0
7	B	262	NAG	1	0

5.6 Ligand geometry

3 ligands 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	$\#\|Z\| > 2$
4	P6C	A	1001	-	14,18,18	2.64	2 (14%)	16,26,26	4.36	8 (50%)
3	NAG	A	1003	1	14,14,15	0.57	0	15,19,21	1.88	3 (20%)
9	GAL	B	1013	-	11,11,12	0.53	0	14,15,17	2.80	8 (57%)

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
4	P6C	A	1001	-	-	0/4/8/8	0/2/2/2
3	NAG	A	1003	1	1/1/5/7	0/6/23/26	0/1/1/1
9	GAL	B	1013	-	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	P6C	C8-C9	3.09	1.47	1.42
4	A	1001	P6C	C8-C5	8.52	1.63	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1001	P6C	C11-C12-N13	-4.45	119.44	123.65
9	B	1013	GAL	C1-C2-C3	-4.29	104.47	109.54
3	A	1003	NAG	C4-C3-C2	-2.68	107.06	111.23
4	A	1001	P6C	C9-C14-N13	-2.66	116.98	121.81
4	A	1001	P6C	C9-C14-N15	-2.50	118.06	122.11
9	B	1013	GAL	C2-C3-C4	2.46	115.22	111.04
9	B	1013	GAL	O2-C2-C1	2.52	114.25	109.21
9	B	1013	GAL	C1-O5-C5	2.88	115.90	112.25
3	A	1003	NAG	O3-C3-C2	2.97	115.00	109.11
9	B	1013	GAL	O3-C3-C4	3.38	117.94	110.34
4	A	1001	P6C	C6-C5-C8	3.44	117.45	111.26
9	B	1013	GAL	O5-C5-C6	3.62	115.18	107.35
3	A	1003	NAG	C1-O5-C5	4.23	117.61	112.25
9	B	1013	GAL	C3-C4-C5	4.31	117.70	110.20
9	B	1013	GAL	O4-C4-C3	4.85	121.27	110.34
4	A	1001	P6C	C12-N13-C14	5.45	123.35	116.93
4	A	1001	P6C	N13-C14-N15	6.16	124.96	116.14
4	A	1001	P6C	C11-N10-C9	8.75	123.73	118.33
4	A	1001	P6C	C4-C5-C8	10.26	129.74	111.26

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1003	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	P6C	2	0
9	B	1013	GAL	5	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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.