



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:41 pm GMT

PDB ID : 3X1B  
Title : Crystal structure of laccase from Lentinus sp. at 1.8 Å resolution  
Authors : Jeng, W.Y.; Shyur, L.F.; Wang, A.H.J.  
Deposited on : 2014-10-31  
Resolution : 1.80 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](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

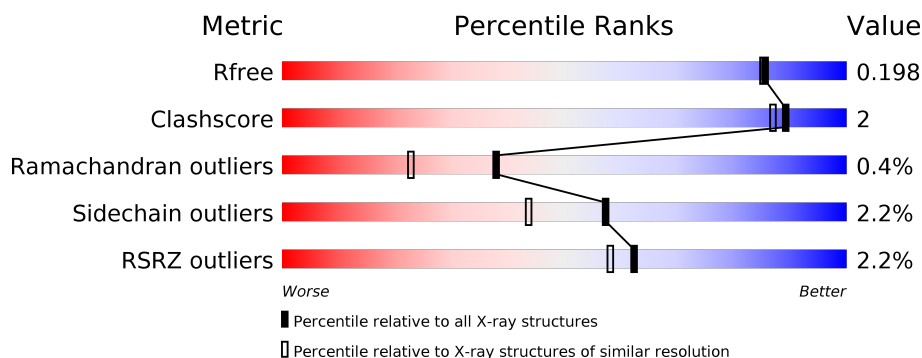
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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  $\geq 3$ , 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	521	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div></div> </div> </div>
1	B	521	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>7%</div> <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
2	MAN	A	612	-	-	-	X
2	NAG	B	602	-	-	-	X
3	NAG	A	613	-	-	-	X
3	NAG	B	614	-	-	-	X
5	MAN	B	612	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9079 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.

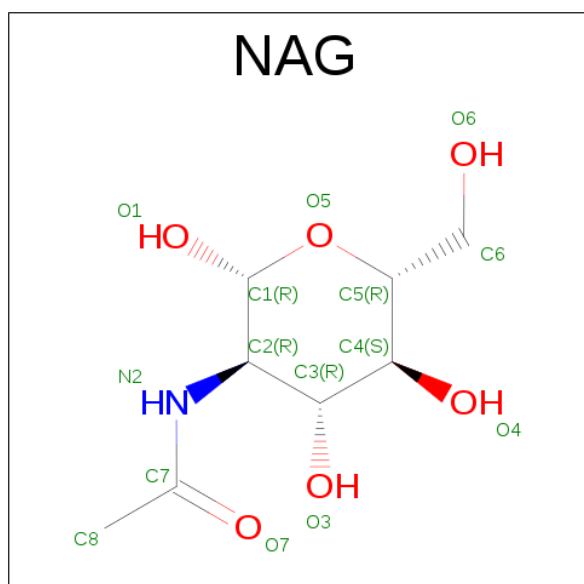
- Molecule 1 is a protein called laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	0	0
			3814	2435	648	724	7			
1	B	500	Total	C	N	O	S	0	0	0
			3814	2435	648	724	7			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	6	Total	C	N	O	0	0
			72	40	2	30		
2	A	6	Total	C	N	O	0	0
			72	40	2	30		
2	B	6	Total	C	N	O	0	0
			72	40	2	30		

- 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		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Cu	0	0
			4	4		
4	A	4	Total	Cu	0	0
			4	4		

- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	7	Total	C	N	O	0	0
			83	46	2	35		

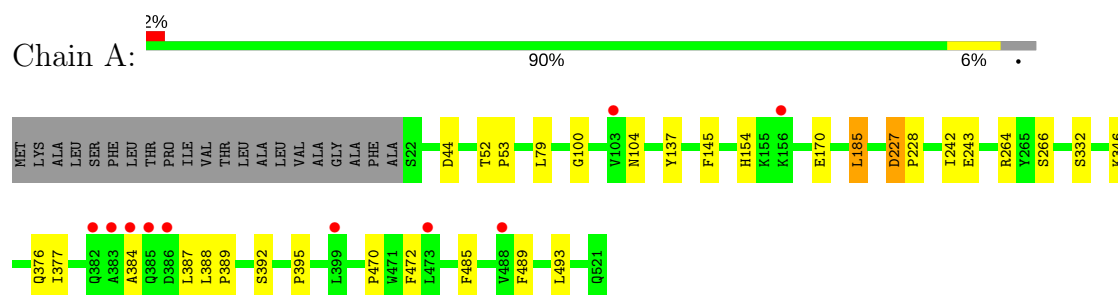
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	619	Total	O	0	0
			619	619		
6	B	497	Total	O	0	0
			497	497		

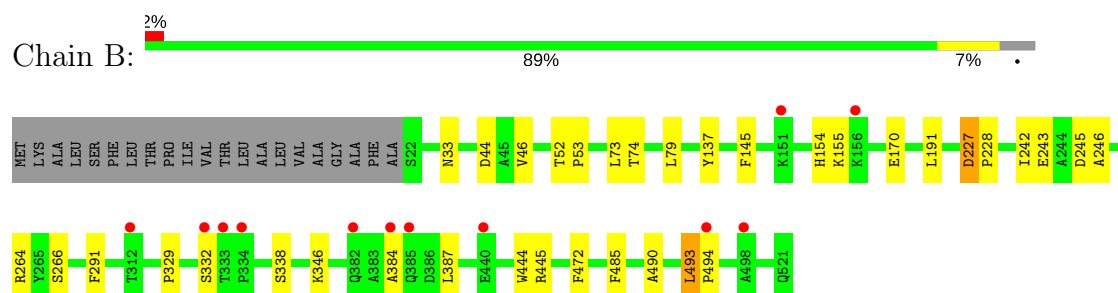
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: laccase



- Molecule 1: laccase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.27Å 188.68Å 65.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.98 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-1.80) 99.7 (29.98-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.145 , 0.197 0.146 , 0.198	Depositor DCC
$R_{free}$ test set	5719 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	1.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9079	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: BMA, NAG, CU, 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	0.40	0/3934	0.66	0/5401
1	B	0.37	0/3934	0.63	0/5401
All	All	0.38	0/7868	0.65	0/10802

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	3814	0	3625	15	0
1	B	3814	0	3625	17	0
2	A	144	0	122	3	0
2	B	72	0	61	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	B	83	0	70	0	0
6	A	619	0	0	2	0
6	B	497	0	0	1	0
All	All	9079	0	7529	34	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 2.

All (34) 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:376:GLN:HE22	1:A:388:LEU:H	1.14	0.89
2:A:610:MAN:H2	2:A:611:MAN:O2	1.76	0.85
1:A:170:GLU:OE1	6:A:1037:HOH:O	2.16	0.60
1:B:33:ASN:ND2	1:B:74:THR:H	2.00	0.60
1:B:170:GLU:HG2	1:B:191:LEU:HB2	1.83	0.60
1:B:44:ASP:OD2	6:B:1085:HOH:O	2.17	0.59
1:A:227:ASP:HB3	1:A:228:PRO:CD	2.35	0.56
1:A:389:PRO:HG2	1:A:392:SER:HB2	1.88	0.56
1:B:493:LEU:HB3	1:B:494:PRO:HD3	1.89	0.55
1:B:245:ASP:OD2	1:B:445:ARG:HB2	2.07	0.54
1:B:227:ASP:HB3	1:B:228:PRO:CD	2.38	0.54
1:A:44:ASP:OD2	6:A:1110:HOH:O	2.19	0.54
1:B:154:HIS:CD2	1:B:242:ILE:HB	2.43	0.54
1:B:227:ASP:HB3	1:B:228:PRO:HD3	1.94	0.50
1:B:243:GLU:HB3	1:B:266:SER:HB2	1.93	0.50
2:A:610:MAN:H2	2:A:611:MAN:C2	2.41	0.50
1:B:33:ASN:HD22	1:B:74:THR:H	1.58	0.49
1:A:243:GLU:HB3	1:A:266:SER:HB2	1.95	0.48
1:A:100:GLY:H	1:A:104:ASN:HD22	1.61	0.48
1:A:377:ILE:HG12	1:A:493:LEU:HD11	1.95	0.48
1:A:52:THR:HA	1:A:53:PRO:C	2.34	0.48
1:A:154:HIS:CD2	1:A:242:ILE:HB	2.49	0.48
1:A:227:ASP:HB3	1:A:228:PRO:HD3	1.96	0.47
1:B:490:ALA:HB1	1:B:493:LEU:HD23	1.97	0.46
1:A:185:LEU:HD22	1:B:291:PHE:H	1.82	0.45
2:A:610:MAN:H2	2:A:611:MAN:HO2	1.77	0.44
1:B:384:ALA:HA	1:B:387:LEU:HD12	2.01	0.43
1:B:46:VAL:HG13	1:B:73:LEU:HD21	2.01	0.43
1:B:52:THR:HA	1:B:53:PRO:C	2.39	0.43
1:A:384:ALA:HB3	1:A:395:PRO:HD3	2.01	0.42
1:B:329:PRO:HG3	1:B:444:TRP:HD1	1.85	0.41
1:A:384:ALA:HA	1:A:387:LEU:HD12	2.03	0.41
1:A:470:PRO:HA	1:A:489:PHE:O	2.20	0.41
1:B:243:GLU:OE2	1:B:246:ALA:HA	2.22	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	498/521 (96%)	488 (98%)	8 (2%)	2 (0%)	38	23
1	B	498/521 (96%)	485 (97%)	11 (2%)	2 (0%)	38	23
All	All	996/1042 (96%)	973 (98%)	19 (2%)	4 (0%)	38	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	ASP
1	B	227	ASP
1	B	79	LEU
1	A	79	LEU

### 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	411/426 (96%)	403 (98%)	8 (2%)	62	50
1	B	411/426 (96%)	401 (98%)	10 (2%)	54	40
All	All	822/852 (96%)	804 (98%)	18 (2%)	57	44

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	TYR
1	A	145	PHE

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Mol	Chain	Res	Type
1	A	185	LEU
1	A	264	ARG
1	A	332	SER
1	A	346	LYS
1	A	472	PHE
1	A	485	PHE
1	B	137	TYR
1	B	145	PHE
1	B	155	LYS
1	B	264	ARG
1	B	332	SER
1	B	338	SER
1	B	346	LYS
1	B	472	PHE
1	B	485	PHE
1	B	493	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	64	ASN
1	A	104	ASN
1	A	288	ASN
1	A	376	GLN
1	B	33	ASN
1	B	60	ASN
1	B	293	ASN
1	B	411	ASN
1	B	521	GLN

### 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

25 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
2	NAG	A	601	1,2	14,14,15	0.51	0	15,19,21	1.28	3 (20%)
2	NAG	A	602	2	14,14,15	0.61	0	15,19,21	0.89	0
2	BMA	A	603	2	11,11,12	0.32	0	13,15,17	0.84	0
2	MAN	A	604	2	11,11,12	0.57	0	13,15,17	0.89	0
2	MAN	A	605	2	11,11,12	0.50	0	13,15,17	0.96	0
2	MAN	A	606	2	11,11,12	0.52	0	13,15,17	0.81	0
2	NAG	A	607	1,2	14,14,15	0.44	0	15,19,21	1.06	0
2	NAG	A	608	2	14,14,15	0.55	0	15,19,21	0.73	0
2	BMA	A	609	2	11,11,12	0.38	0	13,15,17	1.31	2 (15%)
2	MAN	A	610	2	11,11,12	0.64	0	13,15,17	1.43	2 (15%)
2	MAN	A	611	2	11,11,12	0.53	0	13,15,17	0.93	0
2	MAN	A	612	2	11,11,12	0.56	0	13,15,17	1.04	1 (7%)
2	NAG	B	601	1,2	14,14,15	0.53	0	15,19,21	1.23	3 (20%)
2	NAG	B	602	2	14,14,15	0.50	0	15,19,21	1.04	1 (6%)
2	BMA	B	603	2	11,11,12	0.31	0	13,15,17	0.88	0
2	MAN	B	604	2	11,11,12	0.66	0	13,15,17	1.09	1 (7%)
2	MAN	B	605	2	11,11,12	0.58	0	13,15,17	1.03	1 (7%)
2	MAN	B	606	2	11,11,12	0.65	0	13,15,17	1.34	1 (7%)
5	NAG	B	607	1,5	14,14,15	0.46	0	15,19,21	1.17	2 (13%)
5	NAG	B	608	5	14,14,15	0.59	0	15,19,21	0.77	0
5	BMA	B	609	5	11,11,12	0.34	0	13,15,17	0.71	0
5	MAN	B	610	5	11,11,12	0.60	0	13,15,17	1.93	3 (23%)
5	MAN	B	611	5	11,11,12	0.60	0	13,15,17	2.35	4 (30%)
5	MAN	B	612	5	11,11,12	0.74	0	13,15,17	2.04	2 (15%)
5	MAN	B	613	5	11,11,12	0.60	0	13,15,17	0.83	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
2	NAG	A	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	602	2	-	0/6/23/26	0/1/1/1
2	BMA	A	603	2	-	0/2/19/22	0/1/1/1
2	MAN	A	604	2	-	0/2/19/22	0/1/1/1
2	MAN	A	605	2	-	0/2/19/22	0/1/1/1
2	MAN	A	606	2	-	0/2/19/22	0/1/1/1
2	NAG	A	607	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	608	2	-	0/6/23/26	0/1/1/1
2	BMA	A	609	2	-	0/2/19/22	0/1/1/1
2	MAN	A	610	2	-	0/2/19/22	0/1/1/1
2	MAN	A	611	2	-	0/2/19/22	1/1/1/1
2	MAN	A	612	2	-	0/2/19/22	0/1/1/1
2	NAG	B	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	602	2	-	0/6/23/26	0/1/1/1
2	BMA	B	603	2	-	0/2/19/22	0/1/1/1
2	MAN	B	604	2	-	0/2/19/22	0/1/1/1
2	MAN	B	605	2	-	0/2/19/22	0/1/1/1
2	MAN	B	606	2	-	0/2/19/22	0/1/1/1
5	NAG	B	607	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	608	5	-	0/6/23/26	0/1/1/1
5	BMA	B	609	5	-	0/2/19/22	0/1/1/1
5	MAN	B	610	5	-	0/2/19/22	0/1/1/1
5	MAN	B	611	5	-	0/2/19/22	1/1/1/1
5	MAN	B	612	5	-	0/2/19/22	0/1/1/1
5	MAN	B	613	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	611	MAN	C1-C2-C3	-5.86	102.23	109.65
5	B	611	MAN	C1-O5-C5	-3.59	107.22	112.17
5	B	610	MAN	O3-C3-C4	-2.94	103.95	110.36
2	A	601	NAG	O4-C4-C5	-2.63	102.66	109.28
2	A	609	BMA	O4-C4-C5	-2.58	102.78	109.28
2	B	601	NAG	O4-C4-C5	-2.46	103.08	109.28
2	B	602	NAG	C1-O5-C5	-2.46	108.77	112.17
2	B	601	NAG	O5-C1-C2	-2.35	108.21	111.47
2	A	601	NAG	C1-C2-N2	-2.15	106.82	110.49
5	B	611	MAN	C2-C3-C4	-2.11	107.19	110.88
2	A	601	NAG	O5-C1-C2	-2.03	108.65	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	607	NAG	C1-C2-N2	2.20	114.24	110.49
2	A	610	MAN	O3-C3-C2	2.26	114.14	110.02
2	A	609	BMA	C3-C4-C5	2.41	114.47	110.22
2	B	601	NAG	C1-O5-C5	2.52	115.64	112.17
2	B	605	MAN	C1-O5-C5	2.92	116.18	112.17
5	B	607	NAG	C1-O5-C5	2.92	116.19	112.17
2	B	604	MAN	C1-C2-C3	3.13	113.62	109.65
2	A	612	MAN	C1-O5-C5	3.31	116.72	112.17
2	A	610	MAN	C1-O5-C5	3.35	116.78	112.17
2	B	606	MAN	C1-C2-C3	3.57	114.17	109.65
5	B	611	MAN	O2-C2-C1	3.68	116.65	109.18
5	B	610	MAN	C1-O5-C5	3.84	117.46	112.17
5	B	612	MAN	C2-C3-C4	4.10	118.03	110.88
5	B	610	MAN	C3-C4-C5	4.23	117.68	110.22
5	B	612	MAN	C1-C2-C3	5.27	116.34	109.65

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	611	MAN	C1-C2-C3-C4-C5-O5
5	B	611	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	610	MAN	3	0
2	A	611	MAN	3	0

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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
3	NAG	A	613	1	14,14,15	0.46	0	15,19,21	0.84	0
3	NAG	B	614	1	14,14,15	0.46	0	15,19,21	1.28	1 (6%)

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	A	613	1	-	0/6/23/26	0/1/1/1
3	NAG	B	614	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	614	NAG	C1-O5-C5	3.05	116.37	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	500/521 (95%)	-0.42	10 (2%) 65 61	15, 24, 38, 64	0
1	B	500/521 (95%)	-0.36	12 (2%) 59 55	16, 27, 48, 62	0
All	All	1000/1042 (95%)	-0.39	22 (2%) 62 58	15, 25, 44, 64	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	GLN	6.1
1	A	384	ALA	4.6
1	A	386	ASP	4.2
1	A	382	GLN	4.1
1	B	334	PRO	4.1
1	B	333	THR	3.6
1	B	385	GLN	3.6
1	B	440	GLU	3.2
1	B	382	GLN	3.1
1	B	332	SER	2.8
1	B	384	ALA	2.7
1	B	156	LYS	2.7
1	B	494	PRO	2.7
1	A	156	LYS	2.4
1	B	498	ALA	2.4
1	A	103	VAL	2.4
1	A	399	LEU	2.4
1	B	312	THR	2.4
1	A	473	LEU	2.3
1	B	151	LYS	2.3
1	A	383	ALA	2.2
1	A	488	VAL	2.2



## 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
5	MAN	B	612	11/12	0.74	0.19	4.63	69,73,75,75	0
2	NAG	B	602	14/15	0.97	0.11	3.31	19,25,35,36	0
2	MAN	A	612	11/12	0.82	0.19	2.77	52,56,57,58	0
2	NAG	B	601	14/15	0.97	0.08	1.20	22,24,33,34	0
2	NAG	A	607	14/15	0.96	0.08	0.29	28,30,32,32	0
5	NAG	B	607	14/15	0.97	0.09	0.17	36,38,39,43	0
2	MAN	A	606	11/12	0.96	0.07	0.05	33,34,36,37	0
2	NAG	A	601	14/15	0.97	0.07	-0.01	19,21,30,32	0
2	NAG	A	602	14/15	0.97	0.06	-1.59	16,22,30,32	0
2	MAN	A	605	11/12	0.96	0.15	-	36,37,39,39	0
2	MAN	A	610	11/12	0.90	0.21	-	54,56,57,60	0
2	BMA	B	603	11/12	0.91	0.20	-	47,52,56,62	0
5	MAN	B	613	11/12	0.81	0.39	-	77,79,80,81	0
2	BMA	A	609	11/12	0.85	0.21	-	47,50,52,52	0
2	MAN	B	604	11/12	0.77	0.27	-	70,73,74,77	0
5	MAN	B	610	11/12	0.84	0.22	-	75,77,78,79	0
5	MAN	B	611	11/12	0.82	0.31	-	80,80,81,81	0
5	BMA	B	609	11/12	0.84	0.25	-	66,69,73,74	0
2	MAN	B	606	11/12	0.90	0.33	-	60,61,63,65	0
2	BMA	A	603	11/12	0.94	0.09	-	27,31,37,37	0
2	NAG	A	608	14/15	0.91	0.14	-	33,34,40,42	0
2	MAN	A	604	11/12	0.97	0.08	-	31,31,33,35	0
5	NAG	B	608	14/15	0.92	0.11	-	47,49,56,59	0
2	MAN	B	605	11/12	0.70	0.31	-	80,81,82,83	0
2	MAN	A	611	11/12	0.66	0.37	-	63,64,65,65	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
3	NAG	A	613	14/15	0.73	0.41	26.31	46,52,55,55	0
3	NAG	B	614	14/15	0.82	0.19	10.35	47,52,54,55	0
4	CU	A	617	1/1	0.99	0.04	-1.55	25,25,25,25	0
4	CU	B	618	1/1	0.99	0.02	-1.95	27,27,27,27	0
4	CU	A	616	1/1	1.00	0.05	-3.22	24,24,24,24	0
4	CU	A	615	1/1	1.00	0.03	-3.50	22,22,22,22	0
4	CU	B	616	1/1	1.00	0.03	-5.21	25,25,25,25	0
4	CU	B	617	1/1	1.00	0.06	-5.68	27,27,27,27	0
4	CU	B	615	1/1	1.00	0.02	-	31,31,31,31	0
4	CU	A	614	1/1	1.00	0.02	-	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.