



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:51 PM GMT

PDB ID : 2QT6
Title : Crystal Structure Determination of a Blue Laccase from Lentinus Tigrinus
Authors : Ferraroni, M.; Briganti, F.; Scozzafava, A.
Deposited on : 2007-08-01
Resolution : 1.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

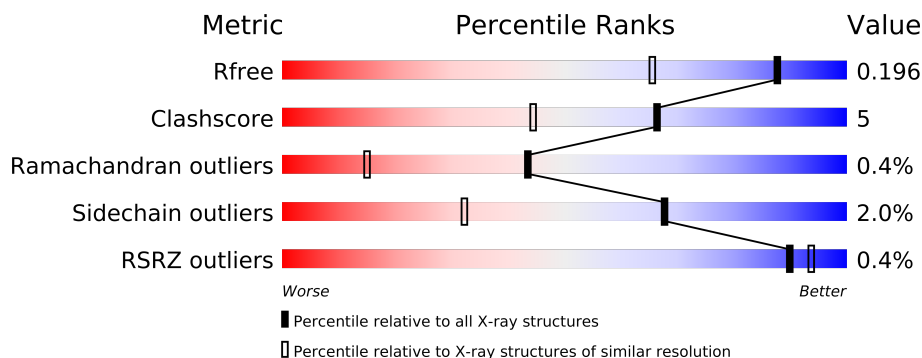
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **FAILED**
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.50 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}	66092	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	498	
1	B	498	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
11	GOL	A	3611	-	X
11	GOL	B	3710	-	X
4	NAG	A	605	-	X
5	MAN	A	3612	-	X
5	MAN	B	3711	-	X
7	CA	A	3717	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
7	CA	B	3712	-	X
9	PER	B	503	-	X

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 10085 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

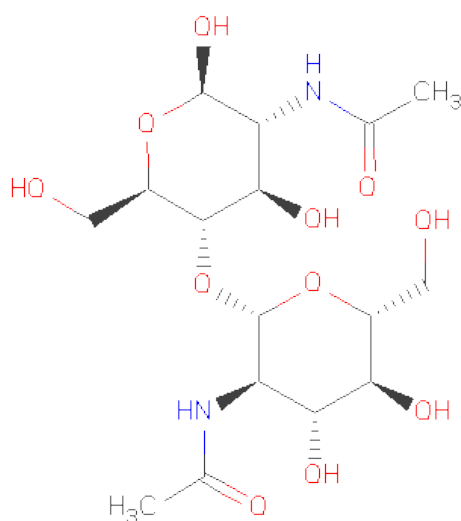
- Molecule 1 is a protein called Laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	10	0
			3836	2430	641	750	15			
1	B	498	Total	C	N	O	S	0	8	0
			3828	2427	640	746	15			

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

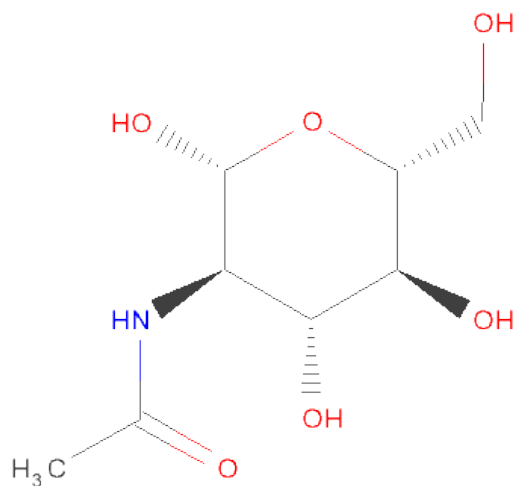
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			72	40	2	30		
2	B	5	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 3 is SUGAR (DI(N-ACETYL-D-GLUCOSAMINE)) (three-letter code: CBS) (formula: C₁₆H₂₈N₂O₁₁).



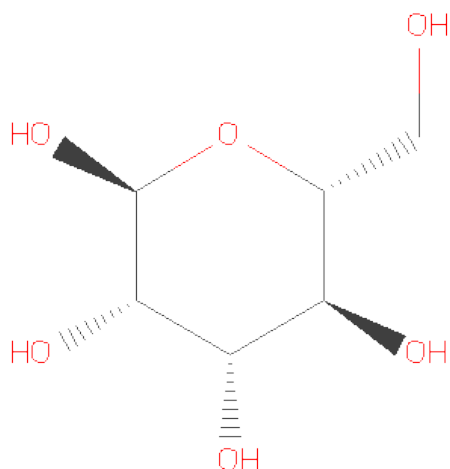
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	16	2	10		
3	B	1	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	5	Total	Ca	0	0
			5	5		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		

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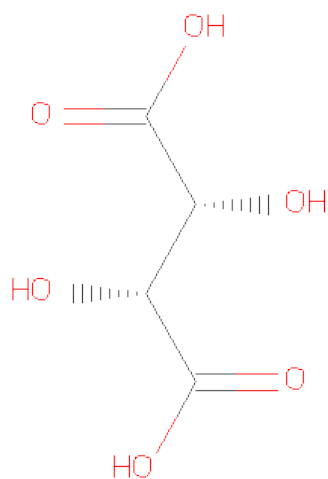
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Cl	0	0
			2	2		

- Molecule 9 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



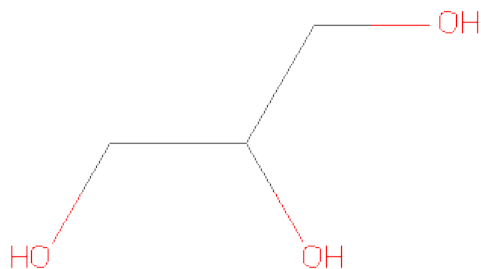
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	O	0	0
			2	2		

- Molecule 10 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 12 is water.

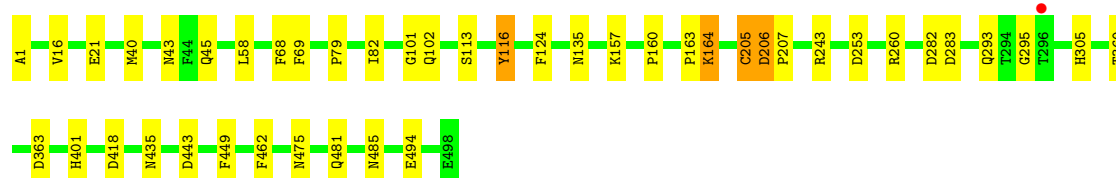
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1154	Total	O	0	6
			1160	1160		
12	B	980	Total	O	0	4
			984	984		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

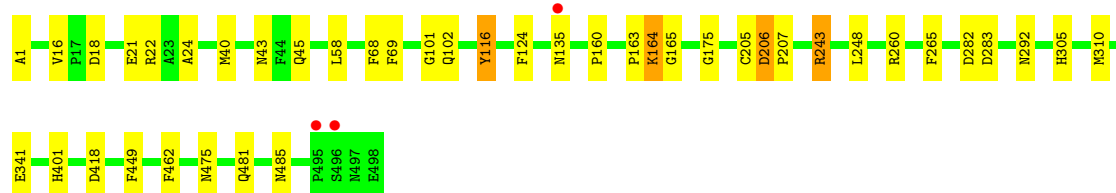
● Molecule 1: Laccase

Chain A: 



● Molecule 1: Laccase

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.22Å 111.61Å 97.09Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 25.35 – 1.42	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-1.50) 98.0 (25.35-1.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.150 , 0.182 0.164 , 0.196	Depositor DCC
R_{free} test set	1065 reflections (0.51%)	DCC
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10085	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: GOL, BMA, NAG, CL, CA, PER, CBS, TLA, 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	0.71	0/4001	0.81	4/5497 (0.1%)
1	B	0.69	0/3983	0.76	2/5476 (0.0%)
All	All	0.70	0/7984	0.79	6/10973 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ASP	CB-CG-OD2	-7.43	111.62	118.30
1	A	253	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	205[A]	CYS	CA-CB-SG	-5.17	104.70	114.00
1	A	205[B]	CYS	CA-CB-SG	-5.17	104.70	114.00
1	B	260	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	243	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	401	HIS	Peptide
1	B	401	HIS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3836	0	3593	38	0
1	B	3828	0	3589	34	0
2	A	72	0	62	1	0
2	B	72	0	62	1	0
3	A	28	0	26	1	0
3	B	28	0	26	0	0
4	A	14	0	13	0	0
5	A	11	0	10	3	0
5	B	11	0	10	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	5	0	0	0	0
7	B	1	0	0	0	0
8	A	2	0	0	1	0
8	B	1	0	0	0	0
9	B	2	0	0	0	0
10	A	10	0	3	0	0
11	A	6	0	8	3	0
11	B	6	0	8	0	0
12	A	1160	0	0	15	2
12	B	984	0	0	12	3
All	All	10085	0	7410	78	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (78) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:164:LYS:H	1:A:164:LYS:HD3	1.18	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1:ALA:HA	12:A:3936:HOH:O	1.58	1.03
1:A:157:LYS:HE2	12:A:3902:HOH:O	1.68	0.93
1:A:164:LYS:H	1:A:164:LYS:CD	1.81	0.89
1:B:164:LYS:H	1:B:164:LYS:CD	1.79	0.89
1:B:24:ALA:HA	12:B:3911:HOH:O	1.72	0.89
1:A:164:LYS:N	1:A:164:LYS:HD3	1.95	0.81
1:B:16:VAL:HG11	12:B:4412:HOH:O	1.82	0.80
1:B:164:LYS:H	1:B:164:LYS:HD2	1.47	0.80
1:B:22:ARG:NH2	12:B:3911:HOH:O	2.18	0.74
1:B:341:GLU:OE1	12:B:3883[A]:HOH:O	2.04	0.74
1:B:248:LEU:HG	12:B:3943:HOH:O	1.87	0.74
1:B:16:VAL:HG23	12:B:4154:HOH:O	1.89	0.73
1:A:16:VAL:HG12	1:A:21:GLU:HA	1.70	0.72
11:A:3611:GOL:H31	12:A:4383:HOH:O	1.91	0.71
1:A:260:ARG:NE	1:A:293[A]:GLN:HG2	2.05	0.71
1:B:40[B]:MET:HE2	1:B:101:GLY:HA2	1.73	0.70
1:B:43:ASN:ND2	1:B:45:GLN:HE21	1.90	0.68
1:B:164:LYS:HD2	1:B:164:LYS:N	2.04	0.68
1:B:16:VAL:HG12	1:B:21:GLU:HA	1.74	0.68
5:A:3612:MAN:C1	12:A:4863:HOH:O	2.43	0.66
1:A:16:VAL:HG12	1:A:21:GLU:CA	2.25	0.65
1:A:16:VAL:HG23	12:A:4328:HOH:O	1.96	0.65
1:A:157:LYS:CE	12:A:3902:HOH:O	2.36	0.65
1:A:16:VAL:HG11	12:A:4719:HOH:O	1.97	0.65
1:B:1:ALA:HA	12:B:3722:HOH:O	1.98	0.62
1:B:305:HIS:HE1	12:B:4045:HOH:O	1.82	0.62
1:A:164:LYS:N	1:A:164:LYS:CD	2.60	0.61
3:A:604:CBS:H61A	12:A:4332:HOH:O	2.01	0.61
1:B:164:LYS:NZ	12:B:3884:HOH:O	2.29	0.60
1:A:305:HIS:HE1	12:A:4177:HOH:O	1.84	0.60
1:A:43:ASN:HD21	1:A:45:GLN:HE21	1.48	0.59
1:B:305:HIS:HD2	1:B:418:ASP:O	1.86	0.59
1:A:305:HIS:HD2	1:A:418:ASP:O	1.85	0.59
1:B:16:VAL:HG12	1:B:21:GLU:CA	2.32	0.58
1:A:40[B]:MET:HE2	1:A:101:GLY:HA2	1.86	0.58
1:A:69:PHE:H	1:A:102:GLN:HE22	1.50	0.58
1:A:293[A]:GLN:HG3	12:A:4206:HOH:O	2.03	0.57
1:B:164:LYS:H	1:B:164:LYS:CE	2.17	0.57
1:B:116:TYR:CE1	1:B:205[A]:CYS:SG	2.98	0.57
1:A:113:SER:H	11:A:3611:GOL:C3	2.18	0.56
1:B:69:PHE:H	1:B:102:GLN:HE22	1.53	0.56
1:A:443:ASP:HB2	8:A:3720:CL:CL	2.43	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:113:SER:H	11:A:3611:GOL:H32	1.72	0.55
2:B:707:BMA:H62	12:B:4698:HOH:O	2.07	0.54
1:A:282:ASP:O	1:A:283:ASP:HB2	2.09	0.53
1:A:160:PRO:HG2	1:A:164:LYS:HD2	1.91	0.51
1:B:160:PRO:HG2	1:B:164:LYS:CE	2.40	0.51
1:A:163:PRO:HA	1:A:164:LYS:HD3	1.93	0.51
1:B:163:PRO:HA	1:B:164:LYS:HE3	1.94	0.50
1:A:481:GLN:HE21	1:A:485:ASN:HD21	1.60	0.49
1:B:43:ASN:HD21	1:B:45:GLN:HE21	1.61	0.49
1:B:310[A]:MET:HE2	12:B:4483:HOH:O	2.12	0.49
5:A:3612:MAN:O6	12:A:4858[A]:HOH:O	2.20	0.48
1:B:16:VAL:HG23	1:B:16:VAL:O	2.14	0.48
1:B:160:PRO:HG2	1:B:164:LYS:HE3	1.96	0.47
1:A:116:TYR:CE1	1:A:205[A]:CYS:SG	3.07	0.47
1:A:481:GLN:HE21	1:A:485:ASN:ND2	2.14	0.46
1:A:360[B]:THR:HG23	1:A:363:ASP:H	1.81	0.45
1:A:135:ASN:ND2	12:A:3930:HOH:O	2.31	0.44
1:B:68:PHE:HA	1:B:102:GLN:HE22	1.84	0.43
1:B:165:GLY:HA2	1:B:265:PHE:CE2	2.55	0.42
1:A:295:GLY:HA3	12:A:4366:HOH:O	2.18	0.42
1:A:79:PRO:HB2	1:A:82:ILE:HB	2.02	0.42
1:B:475:ASN:ND2	12:B:4462:HOH:O	2.52	0.42
2:A:607:BMA:O3	5:A:3612:MAN:C1	2.68	0.42
1:A:16:VAL:HG13	12:A:4408:HOH:O	2.19	0.42
1:A:43:ASN:ND2	1:A:45:GLN:HE21	2.15	0.42
1:A:206:ASP:HB3	1:A:207:PRO:CD	2.50	0.42
1:B:164:LYS:H	1:B:164:LYS:HE3	1.83	0.41
1:A:260:ARG:CD	1:A:293[A]:GLN:HG2	2.50	0.41
1:A:40[B]:MET:CE	12:A:4679:HOH:O	2.68	0.41
1:B:206:ASP:HB3	1:B:207:PRO:CD	2.50	0.41
1:A:68:PHE:HA	1:A:102:GLN:HE22	1.86	0.41
1:B:18:ASP:HA	1:B:175:GLY:O	2.21	0.40
1:B:282:ASP:O	1:B:283:ASP:HB2	2.22	0.40
1:B:481:GLN:HE21	1:B:485:ASN:HD21	1.69	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:B:3887:HOH:O	12:B:4541:HOH:O[2_745]	2.03	0.17
12:A:4834:HOH:O	12:B:4203:HOH:O[2_645]	2.05	0.15
12:A:3937:HOH:O	12:B:4054:HOH:O[2_645]	2.07	0.13

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	505/498 (101%)	492 (97%)	11 (2%)	2 (0%)	43	15
1	B	504/498 (101%)	489 (97%)	13 (3%)	2 (0%)	43	15
All	All	1009/996 (101%)	981 (97%)	24 (2%)	4 (0%)	43	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASP
1	B	206	ASP
1	B	58	LEU
1	A	58	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	429/420 (102%)	419 (98%)	10 (2%)	63	26
1	B	427/420 (102%)	419 (98%)	8 (2%)	69	35
All	All	856/840 (102%)	838 (98%)	18 (2%)	68	30

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

Mol	Chain	Res	Type
1	A	116	TYR
1	A	124	PHE
1	A	164	LYS
1	A	243	ARG
1	A	435	ASN

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Mol	Chain	Res	Type
1	A	449	PHE
1	A	462	PHE
1	A	475	ASN
1	A	494[A]	GLU
1	A	494[B]	GLU
1	B	116	TYR
1	B	124	PHE
1	B	135	ASN
1	B	164	LYS
1	B	243	ARG
1	B	292	ASN
1	B	449	PHE
1	B	462	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	43	ASN
1	A	70	GLN
1	A	91	ASN
1	A	102	GLN
1	A	305	HIS
1	A	315	ASN
1	A	485	ASN
1	B	39	ASN
1	B	43	ASN
1	B	70	GLN
1	B	91	ASN
1	B	102	GLN
1	B	135	ASN
1	B	292	ASN
1	B	305	HIS
1	B	315	ASN
1	B	485	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

10 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	CBS	A	603	1,2	27,29,30	0.69	0	37,41,43	1.40	6 (16%)
2	BMA	A	606	2	10,11,12	0.70	0	11,15,17	1.90	2 (18%)
2	BMA	A	607	2	10,11,12	0.87	0	11,15,17	2.13	1 (9%)
2	BMA	A	608	2	10,11,12	0.82	0	11,15,17	1.63	2 (18%)
2	BMA	A	609	2	10,11,12	0.83	0	11,15,17	1.78	2 (18%)
2	CBS	B	704	1,2	27,29,30	0.65	0	37,41,43	1.44	8 (21%)
2	BMA	B	706	2	10,11,12	0.61	0	11,15,17	1.71	3 (27%)
2	BMA	B	707	2	10,11,12	0.75	0	11,15,17	1.89	4 (36%)
2	BMA	B	708	2	10,11,12	0.70	0	11,15,17	2.46	2 (18%)
2	BMA	B	709	2	10,11,12	0.72	0	11,15,17	1.10	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	CBS	A	603	1,2	-	0/16/53/56	0/2/2/2
2	BMA	A	606	2	-	0/2/19/22	0/1/1/1
2	BMA	A	607	2	-	0/2/19/22	0/1/1/1
2	BMA	A	608	2	-	0/2/19/22	0/1/1/1
2	BMA	A	609	2	-	0/2/19/22	0/1/1/1
2	CBS	B	704	1,2	-	0/16/53/56	0/2/2/2
2	BMA	B	706	2	-	0/2/19/22	0/1/1/1
2	BMA	B	707	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	B	708	2	-	0/2/19/22	0/1/1/1
2	BMA	B	709	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	607	BMA	O5-C5-C6	5.54	112.79	106.98
2	B	708	BMA	O3-C3-C2	5.53	120.06	109.94
2	B	708	BMA	O5-C5-C6	5.36	112.61	106.98
2	A	606	BMA	O3-C3-C4	-5.00	99.14	110.35
2	A	603	CBS	O5B-C5B-C6B	4.54	111.75	106.98
2	A	609	BMA	O5-C5-C6	4.36	111.56	106.98
2	A	608	BMA	O5-C5-C6	3.63	110.79	106.98
2	B	704	CBS	O1A-C1A-O5A	-3.62	101.67	110.69
2	B	707	BMA	O5-C5-C6	3.54	110.70	106.98
2	B	706	BMA	O3-C3-C2	3.42	116.19	109.94
2	B	707	BMA	C3-C4-C5	3.33	116.15	110.20
2	A	603	CBS	O1A-C1A-O5A	-3.28	102.51	110.69
2	B	704	CBS	O7B-C7B-N2B	2.98	128.12	121.90
2	B	706	BMA	O3-C3-C4	-2.70	104.31	110.35
2	A	609	BMA	C3-C4-C5	2.68	115.00	110.20
2	B	704	CBS	O1A-C4B-C5B	-2.64	102.46	109.33
2	B	706	BMA	O5-C5-C6	2.59	109.70	106.98
2	A	606	BMA	O5-C5-C6	2.54	109.65	106.98
2	A	603	CBS	O1A-C4B-C3B	2.42	113.37	107.16
2	A	603	CBS	C1A-C2A-N2A	-2.32	106.62	111.02
2	B	704	CBS	C8A-C7A-N2A	-2.25	111.71	116.11
2	B	704	CBS	O7B-C7B-C8B	-2.23	117.68	122.04
2	B	707	BMA	C4-C3-C2	2.22	113.49	110.50
2	B	704	CBS	C1A-C2A-N2A	-2.18	106.89	111.02
2	A	608	BMA	C3-C4-C5	2.15	114.04	110.20
2	B	704	CBS	C1A-O1A-C4B	-2.09	112.65	117.99
2	B	707	BMA	O5-C5-C4	2.05	113.25	110.65
2	A	603	CBS	C3B-C4B-C5B	-2.04	106.26	110.85
2	B	704	CBS	O1A-C4B-C3B	2.04	112.38	107.16
2	A	603	CBS	C1A-O1A-C4B	-2.00	112.88	117.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 17 are monoatomic - leaving 9 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	$\# Z > 2$
10	TLA	A	3610	7	9,9,9	1.03	0	12,12,12	0.95	0
11	GOL	A	3611	-	5,5,5	0.41	0	5,5,5	0.65	0
5	MAN	A	3612	-	10,11,12	0.86	0	11,15,17	1.50	3 (27%)
3	CBS	A	604	1	27,29,30	0.56	0	37,41,43	1.32	4 (10%)
4	NAG	A	605	1,7	12,14,15	0.85	0	15,19,21	1.53	4 (26%)
11	GOL	B	3710	-	5,5,5	0.38	0	5,5,5	0.76	0
5	MAN	B	3711	-	10,11,12	0.75	0	11,15,17	0.75	0
9	PER	B	503	6	1,1,1	1.03	0	0,0,0	0.00	-
3	CBS	B	705	1	27,29,30	0.40	0	37,41,43	0.93	2 (5%)

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
10	TLA	A	3610	7	-	0/12/12/12	0/0/0/0
11	GOL	A	3611	-	-	0/4/4/4	0/0/0/0
5	MAN	A	3612	-	1/1/4/5	0/2/19/22	0/1/1/1
3	CBS	A	604	1	-	0/16/53/56	0/2/2/2
4	NAG	A	605	1,7	-	0/6/23/26	0/1/1/1
11	GOL	B	3710	-	-	0/4/4/4	0/0/0/0
5	MAN	B	3711	-	1/1/4/5	0/2/19/22	0/1/1/1
9	PER	B	503	6	-	0/0/0/0	0/0/0/0
3	CBS	B	705	1	-	0/16/53/56	0/2/2/2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	CBS	O5B-C5B-C6B	3.86	111.03	106.98
3	A	604	CBS	C4A-C3A-C2A	3.39	115.26	110.44
3	B	705	CBS	O5B-C5B-C6B	2.97	110.10	106.98
4	A	605	NAG	C3-C2-N2	-2.85	107.42	111.76
4	A	605	NAG	O3-C3-C2	2.81	115.00	109.09
5	A	3612	MAN	O5-C5-C6	2.67	109.78	106.98
3	A	604	CBS	C3A-C4A-C5A	2.57	114.79	110.20
5	A	3612	MAN	C4-C3-C2	2.54	113.92	110.50
4	A	605	NAG	C8-C7-N2	-2.42	111.38	116.11
3	B	705	CBS	C1A-O1A-C4B	-2.34	112.02	117.99
4	A	605	NAG	O4-C4-C3	-2.20	105.41	110.35
5	A	3612	MAN	C3-C4-C5	2.19	114.12	110.20
3	A	604	CBS	O3A-C3A-C2A	-2.14	105.21	109.61

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	3711	MAN	C5
5	A	3612	MAN	C5

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	498/498 (100%)	-0.48	1 (0%) 93 95	15, 19, 27, 35	0
1	B	498/498 (100%)	-0.23	3 (0%) 86 91	16, 23, 33, 40	0
All	All	996/996 (100%)	-0.35	4 (0%) 90 94	15, 20, 30, 40	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	THR	3.6
1	B	496	SER	2.7
1	B	495	PRO	2.5
1	B	135	ASN	2.4

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

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

6.3 Carbohydrates ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	BMA	A	609	11/12	0.18	17.57	40,42,47,49	0
2	BMA	B	707	11/12	0.27	17.07	48,51,54,57	0
2	BMA	B	706	11/12	0.18	12.60	31,37,40,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BMA	B	709	11/12	0.20	5.98	43,46,48,48	0
2	BMA	A	608	11/12	0.25	5.57	51,53,55,56	0
2	BMA	A	606	11/12	0.11	4.31	24,28,33,34	0
2	CBS	B	704	28/29	0.08	0.29	19,22,26,28	0
2	CBS	A	603	28/29	0.06	-0.27	16,18,20,21	0
2	BMA	B	708	11/12	0.23	-	45,48,49,51	0
2	BMA	A	607	11/12	0.21	-	35,37,43,49	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	CA	A	3717	1/1	0.16	20.98	29,29,29,29	0
5	MAN	B	3711	11/12	0.30	18.07	98,98,99,99	0
5	MAN	A	3612	11/12	0.28	17.20	45,51,53,56	0
9	PER	B	503	2/2	0.12	14.90	23,23,23,33	2
11	GOL	B	3710	6/6	0.11	6.61	24,29,30,31	0
11	GOL	A	3611	6/6	0.14	6.46	25,32,34,36	0
7	CA	B	3712	1/1	0.10	3.92	19,19,19,19	1
4	NAG	A	605	14/15	0.20	3.65	21,30,36,41	0
3	CBS	B	705	28/29	0.15	1.60	31,38,47,49	0
3	CBS	A	604	28/29	0.09	1.52	18,24,34,39	0
10	TLA	A	3610	10/10	0.08	1.24	21,23,25,29	0
8	CL	A	3720	1/1	0.08	0.55	37,37,37,37	0
7	CA	A	3716	1/1	0.02	-2.32	18,18,18,18	0
8	CL	A	3719	1/1	0.05	-2.37	29,29,29,29	0
8	CL	B	3718	1/1	0.05	-2.81	32,32,32,32	0
7	CA	A	3714	1/1	0.03	-2.86	18,18,18,18	0
6	CU	B	502	1/1	0.03	-3.57	24,24,24,24	1
6	CU	A	502	1/1	0.03	-4.12	21,21,21,21	1
7	CA	A	3715	1/1	0.02	-4.77	20,20,20,20	0
6	CU	A	500	1/1	0.01	-4.82	19,19,19,19	1
7	CA	A	3713	1/1	0.02	-5.07	20,20,20,20	0
6	CU	A	499	1/1	0.02	-5.23	19,19,19,19	1
6	CU	A	501	1/1	0.01	-5.59	22,22,22,22	1
6	CU	B	501	1/1	0.02	-6.31	26,26,26,26	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	CU	B	499	1/1	0.01	-6.68	24,24,24,24	1
6	CU	B	500	1/1	0.02	-14.76	23,23,23,23	1

6.5 Other polymers ⓘ

There are no such residues in this entry.