Full wwPDB X-ray Structure Validation Report (i)

May 17, 2017 – 11:33 AM EDT

PDB ID	:	5MIB
Title	:	The study of the X-ray induced enzymatic reduction of molecular oxygen to water for laccase from Steccherinum murashkinskyi.The 12-th structure of the series with total exposition time 333 min.
Authors	:	Polyakov, K.M.; Gavryushov, S.; Fedorova, T.V.; Glazunova, O.A.; Popov, A.N.
Deposited on	:	2016-11-28
Resolution	:	1.35 Å(reported)

The following versions of software and data (see references (i)) 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	:	rb-20029077
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)	:	rb-20029077

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 1.35 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	Percentile Ranks	Value
Rfree		0.148
Clashscore		3
Ramachandran outliers		0.4%
Sidechain outliers		1.0%
RSRZ outliers		2.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
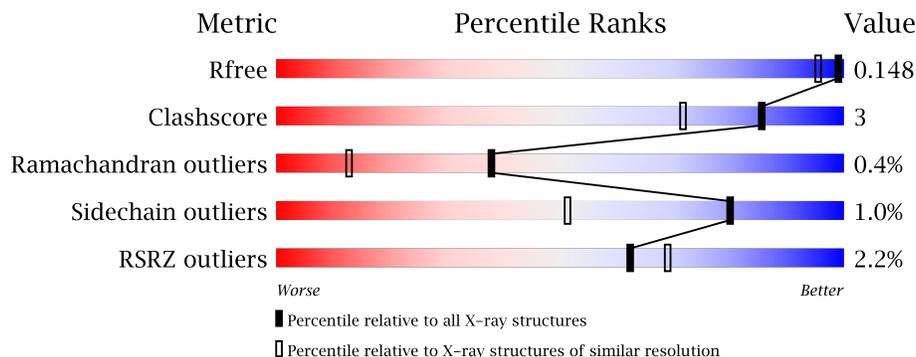
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	1024 (1.38-1.34)
Clashscore	112137	1063 (1.38-1.34)
Ramachandran outliers	110173	1048 (1.38-1.34)
Sidechain outliers	110143	1048 (1.38-1.34)
RSRZ outliers	101464	1025 (1.38-1.34)

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.

Mol	Chain	Length	Quality of chain
1	A	546	2% · 85% · 5% · 9%

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	607	-	-	-	X
4	OXY	A	609	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OXY	A	610	-	-	-	X
5	CIT	A	611	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8087 atoms, of which 3385 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 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	499	7290	2466	3385	662	767	10	79	35	0

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
2	A	4	6	6	0	2

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

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

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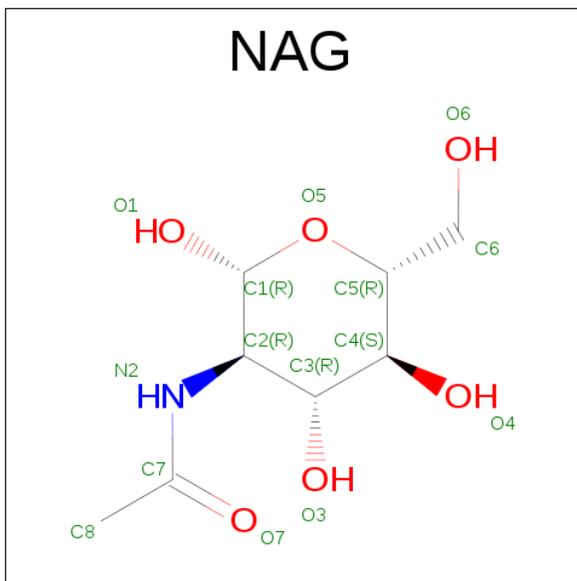
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).
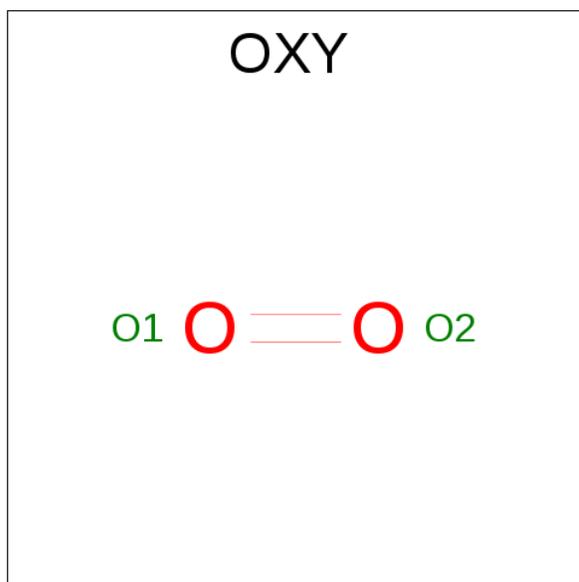
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 2	O 2	0	0
4	A	1	Total 2	O 2	0	0

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).
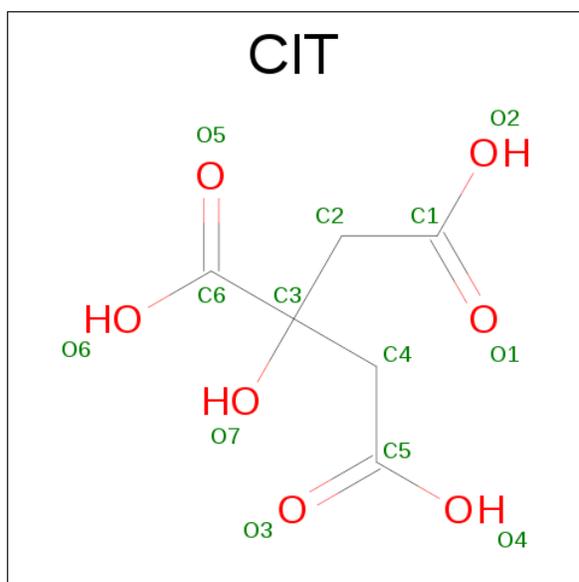
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 13	C 6	O 7	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Na 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	707	Total 717	O 717	0	10

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Laccase 2
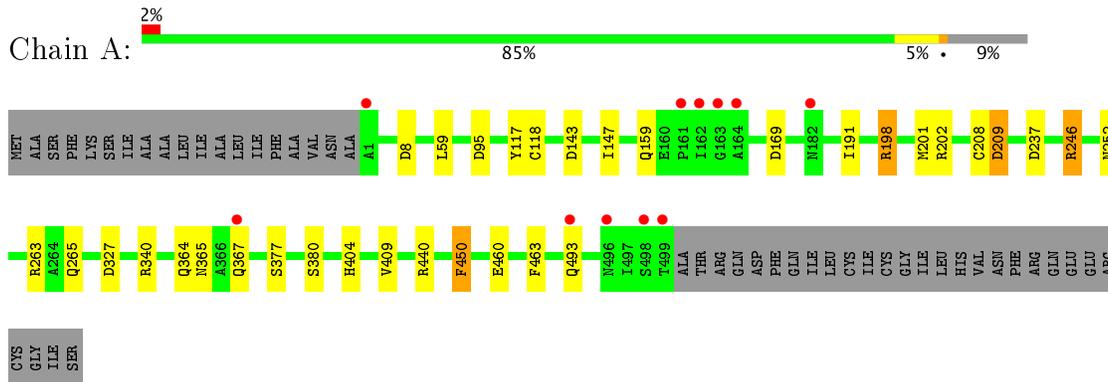
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.44Å 84.45Å 112.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.54 – 1.35 19.48 – 1.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (67.54-1.35) 98.0 (19.48-1.35)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.130 , 0.148 0.131 , 0.148	Depositor DCC
R_{free} test set	5828 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	9.2	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 53.7	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	8087	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, NAG, OXY, CU, CIT

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	0.96	5/4171 (0.1%)	1.00	23/5738 (0.4%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377[A]	SER	CB-OG	-8.96	1.30	1.42
1	A	377[B]	SER	CB-OG	-8.96	1.30	1.42
1	A	380[A]	SER	CB-OG	-5.49	1.35	1.42
1	A	380[B]	SER	CB-OG	-5.49	1.35	1.42
1	A	460	GLU	CG-CD	-5.16	1.44	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	ASP	CB-CG-OD1	10.87	128.09	118.30
1	A	95	ASP	CB-CG-OD1	7.44	125.00	118.30
1	A	340	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	450	PHE	CB-CG-CD2	-6.82	116.03	120.80
1	A	409[A]	VAL	CA-CB-CG2	6.73	120.99	110.90
1	A	409[B]	VAL	CA-CB-CG2	6.73	120.99	110.90
1	A	198[A]	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	198[B]	ARG	NE-CZ-NH2	-6.49	117.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	327	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	209	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	169	ASP	CB-CG-OD2	6.24	123.91	118.30
1	A	198[A]	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	198[B]	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	450	PHE	CB-CG-CD1	6.03	125.02	120.80
1	A	202	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	8	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	409[A]	VAL	CG1-CB-CG2	-5.48	102.13	110.90
1	A	409[B]	VAL	CG1-CB-CG2	-5.48	102.13	110.90
1	A	143	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	263	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	340	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	246	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	440	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	404	HIS	Peptide

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	3905	3385	3674	18	0
2	A	6	0	0	0	0
3	A	56	0	50	0	0
4	A	4	0	0	1	0
5	A	13	0	5	0	0
6	A	1	0	0	0	0
7	A	717	0	0	11	0
All	All	4702	3385	3729	19	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 3.

All (19) 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:364:GLN:OE1	7:A:708:HOH:O	1.62	1.15
1:A:159[B]:GLN:HG3	7:A:759:HOH:O	1.55	1.05
1:A:159[B]:GLN:CG	7:A:759:HOH:O	2.19	0.83
1:A:265[C]:GLN:OE1	7:A:707:HOH:O	1.97	0.81
4:A:609:OXY:O2	7:A:702:HOH:O	2.03	0.75
1:A:493:GLN:HG2	7:A:1180:HOH:O	1.87	0.74
1:A:198[B]:ARG:CZ	7:A:709:HOH:O	2.36	0.74
1:A:147:ILE:HD11	1:A:201[B]:MET:HE2	1.70	0.72
1:A:198[B]:ARG:NE	7:A:709:HOH:O	2.33	0.61
1:A:365:ASN:HD21	1:A:367:GLN:HB2	1.65	0.60
1:A:118:CYS:SG	1:A:208[B]:CYS:HB3	2.43	0.57
1:A:265[C]:GLN:CD	7:A:707:HOH:O	2.41	0.57
1:A:118:CYS:HA	1:A:208[B]:CYS:SG	2.48	0.53
1:A:198[B]:ARG:HG2	1:A:252[B]:ASN:ND2	2.24	0.52
1:A:147:ILE:HD11	1:A:201[B]:MET:CE	2.39	0.49
1:A:198[B]:ARG:HE	1:A:252[B]:ASN:HD22	1.66	0.44
1:A:364:GLN:HB3	7:A:1090:HOH:O	2.17	0.43
1:A:364:GLN:NE2	7:A:717[A]:HOH:O	2.53	0.41

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	535/546 (98%)	523 (98%)	10 (2%)	2 (0%)	38	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	ASP

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Mol	Chain	Res	Type
1	A	59	LEU

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	443/447 (99%)	439 (99%)	4 (1%)	82	55

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	TYR
1	A	246	ARG
1	A	450	PHE
1	A	463	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	182	ASN
1	A	364	GLN
1	A	365	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	NAG	A	605	1,3	14,14,15	1.65	2 (14%)	15,19,21	1.18	1 (6%)
3	NAG	A	606	3	14,14,15	1.36	2 (14%)	15,19,21	2.29	4 (26%)
3	NAG	A	607	1,3	14,14,15	0.87	0	15,19,21	1.08	2 (13%)
3	NAG	A	608	3	14,14,15	0.91	0	15,19,21	2.04	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	605	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	606	3	-	0/6/23/26	0/1/1/1
3	NAG	A	607	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	608	3	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	NAG	O5-C1	-3.91	1.37	1.43
3	A	606	NAG	C1-C2	2.32	1.55	1.52
3	A	605	NAG	C1-C2	2.93	1.56	1.52
3	A	606	NAG	C2-N2	3.28	1.52	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	608	NAG	C1-O5-C5	-6.24	103.57	112.17
3	A	606	NAG	O7-C7-C8	-4.93	113.09	122.06
3	A	608	NAG	O4-C4-C3	-2.65	104.58	110.36
3	A	608	NAG	C3-C4-C5	-2.48	105.85	110.22
3	A	605	NAG	O7-C7-C8	-2.26	117.94	122.06
3	A	607	NAG	O5-C1-C2	-2.26	108.33	111.47
3	A	607	NAG	C1-C2-N2	-2.05	106.99	110.49
3	A	608	NAG	C1-C2-N2	2.25	114.34	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	606	NAG	C1-C2-N2	2.94	115.51	110.49
3	A	606	NAG	C8-C7-N2	3.95	123.25	116.11
3	A	606	NAG	C3-C4-C5	4.16	117.54	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	605	1,3	14,14,15	1.65	2 (14%)	15,19,21	1.18	1 (6%)
3	NAG	A	606	3	14,14,15	1.36	2 (14%)	15,19,21	2.29	4 (26%)
3	NAG	A	607	1,3	14,14,15	0.87	0	15,19,21	1.08	2 (13%)
3	NAG	A	608	3	14,14,15	0.91	0	15,19,21	2.04	4 (26%)
4	OXY	A	609	2	1,1,1	0.28	0	0,0,0	0.00	-
4	OXY	A	610	-	1,1,1	0.02	0	0,0,0	0.00	-
5	CIT	A	611	-	3,12,12	1.25	1 (33%)	3,17,17	0.71	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	NAG	A	605	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	606	3	-	0/6/23/26	0/1/1/1
3	NAG	A	607	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	608	3	-	0/6/23/26	0/1/1/1
4	OXY	A	609	2	-	0/0/0/0	0/0/0/0
4	OXY	A	610	-	-	0/0/0/0	0/0/0/0
5	CIT	A	611	-	-	0/6/16/16	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	NAG	O5-C1	-3.91	1.37	1.43
5	A	611	CIT	O7-C3	2.13	1.46	1.43
3	A	606	NAG	C1-C2	2.32	1.55	1.52
3	A	605	NAG	C1-C2	2.93	1.56	1.52
3	A	606	NAG	C2-N2	3.28	1.52	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	608	NAG	C1-O5-C5	-6.24	103.57	112.17
3	A	606	NAG	O7-C7-C8	-4.93	113.09	122.06
3	A	608	NAG	O4-C4-C3	-2.65	104.58	110.36
3	A	608	NAG	C3-C4-C5	-2.48	105.85	110.22
3	A	605	NAG	O7-C7-C8	-2.26	117.94	122.06
3	A	607	NAG	O5-C1-C2	-2.26	108.33	111.47
3	A	607	NAG	C1-C2-N2	-2.05	106.99	110.49
3	A	608	NAG	C1-C2-N2	2.25	114.34	110.49
3	A	606	NAG	C1-C2-N2	2.94	115.51	110.49
3	A	606	NAG	C8-C7-N2	3.95	123.25	116.11
3	A	606	NAG	C3-C4-C5	4.16	117.54	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	609	OXY	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	499/546 (91%)	-0.47	11 (2%)	62	69	5, 9, 18, 47	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162[A]	ILE	5.2
1	A	499	THR	5.0
1	A	498	SER	4.6
1	A	1	ALA	4.3
1	A	163[A]	GLY	3.2
1	A	496	ASN	3.0
1	A	182	ASN	2.4
1	A	367	GLN	2.4
1	A	161[A]	PRO	2.3
1	A	164[A]	ALA	2.1
1	A	493	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	607	14/15	0.97	0.06	2.91	9,10,13,14	0
3	NAG	A	605	14/15	0.97	0.06	0.43	11,12,15,15	0
3	NAG	A	606	14/15	0.82	0.20	-	19,27,33,34	0
3	NAG	A	608	14/15	0.96	0.08	-	11,14,23,26	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

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, 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	OXY	A	610	2/2	0.97	0.10	7.85	14,14,14,16	2
5	CIT	A	611	13/13	0.89	0.16	6.16	19,25,31,34	0
3	NAG	A	607	14/15	0.97	0.06	2.91	9,10,13,14	0
4	OXY	A	609	2/2	0.99	0.05	2.52	6,6,6,6	2
3	NAG	A	605	14/15	0.97	0.06	0.43	11,12,15,15	0
2	CU	A	603	1/1	1.00	0.04	0.09	6,6,6,6	1
2	CU	A	604	1/1	1.00	0.04	-1.20	6,6,6,6	0
2	CU	A	602[B]	1/1	1.00	0.04	-1.61	5,5,5,5	1
2	CU	A	602[A]	1/1	1.00	0.04	-1.69	13,13,13,13	1
2	CU	A	601[A]	1/1	1.00	0.04	-1.75	6,6,6,6	1
2	CU	A	601[B]	1/1	1.00	0.04	-2.49	7,7,7,7	1
3	NAG	A	606	14/15	0.82	0.20	-	19,27,33,34	0
3	NAG	A	608	14/15	0.96	0.08	-	11,14,23,26	0
6	NA	A	612	1/1	0.97	0.09	-	16,16,16,16	1

6.5 Other polymers (i)

There are no such residues in this entry.