



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:40 AM GMT

PDB ID : 2XYB
Title : CRYSTAL STRUCTURE OF A FULLY FUNCTIONAL LACCASE FROM
THE LIGNINOLYTIC FUNGUS PYCNOPORUS CINNABARINUS
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Deposited on : 2010-11-17
Resolution : 1.75 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

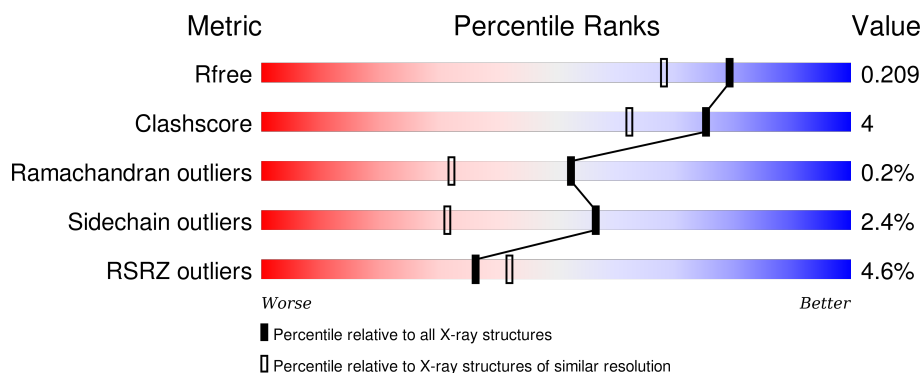
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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 $\leq 5\%$. 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	497	<div> <div>5%</div> <div>91%</div> <div>8%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SO4	A	603	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	GOL	A	610	-	-	-	X
11	GOL	A	612	-	-	-	X
11	GOL	A	613	-	-	-	X
13	NA	A	718	-	-	-	X
4	NAG	A	511	-	-	-	X
5	NAG	A	530	-	-	-	X

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 4791 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.

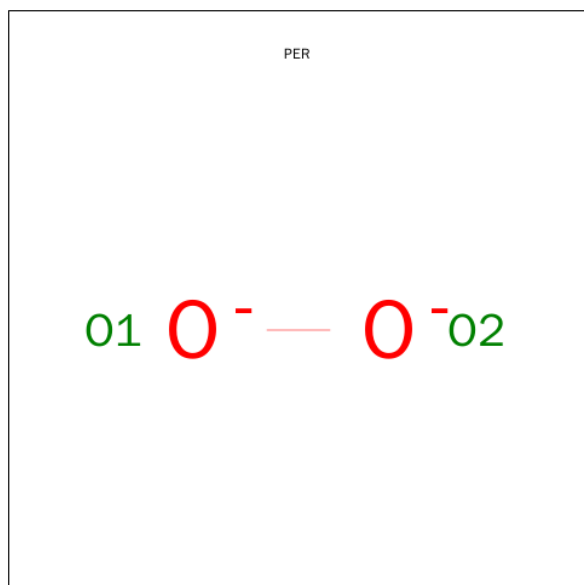
- Molecule 1 is a protein called LACCASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	8	0
			3859	2465	648	734	12			

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

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

- Molecule 3 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			2	2		

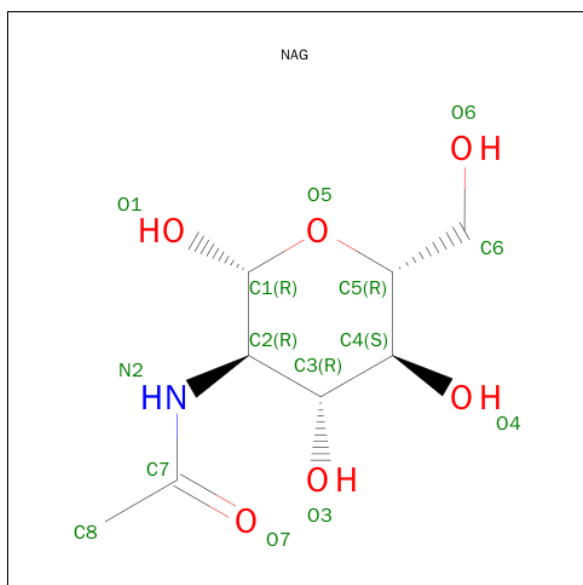
- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

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

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

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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

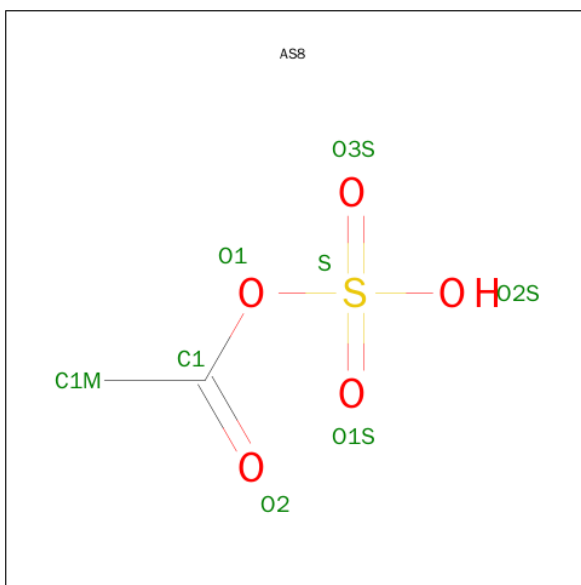


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

- Molecule 8 is ACETYSULFATE (three-letter code: AS8) (formula: $C_2H_4O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O	S	0	0
			8	2	5	1		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- 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	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	8	Total	Zn	0	0
			8	8		

- Molecule 13 is SODIUM ION (three-letter code: NA) (formula: Na).

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

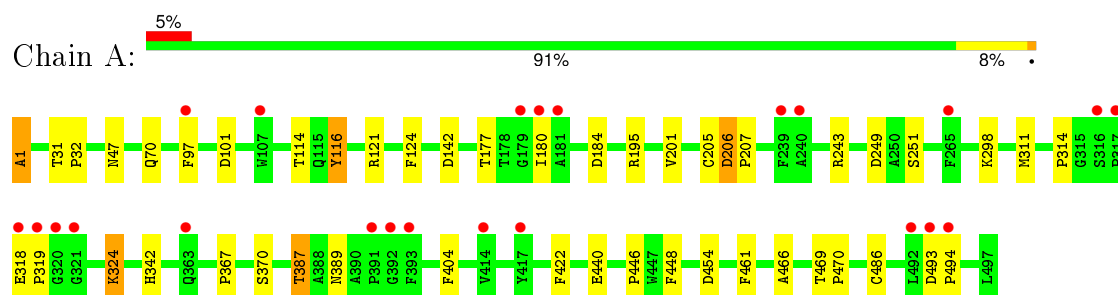
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	712	Total	O	0	0
			712	712		

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 ($\text{RSRZ} > 2$). 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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.30Å 62.90Å 91.42Å 90.00° 126.70° 90.00°	Depositor
Resolution (Å)	72.55 – 1.75 45.67 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (72.55-1.75) 99.6 (45.67-1.75)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.164 , 0.208 0.165 , 0.209	Depositor DCC
R_{free} test set	3365 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.2	EDS
Estimated twinning fraction	0.016 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 66425 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4791	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, BMA, NAG, NA, AS8, PER, SO4, ACT, 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	0.88	2/4008 (0.0%)	0.83	4/5504 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	486	CYS	CB-SG	5.50	1.91	1.82
1	A	1	ALA	N-CA	5.22	1.56	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	ALA	N-CA-C	7.09	130.15	111.00
1	A	121	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	A	121	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	201	VAL	CB-CA-C	-5.07	101.77	111.40

There are no chirality outliers.

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	3859	0	3669	26	1
2	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
4	A	50	0	43	1	0
5	A	56	0	50	2	0
6	A	14	0	13	0	0
7	A	39	0	34	2	0
8	A	8	0	4	0	0
9	A	4	0	3	0	0
10	A	10	0	0	0	0
11	A	24	0	32	2	0
12	A	8	0	0	0	0
13	A	1	0	0	0	0
14	A	712	0	0	8	0
All	All	4791	0	3848	31	1

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 4.

All (31) 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:493:ASP:OD1	1:A:494:PRO:HD2	1.78	0.84
1:A:440[B]:GLU:OE2	14:A:2593:HOH:O	1.98	0.81
7:A:561:NAG:O3	7:A:562:BMA:H2	1.86	0.76
1:A:311[B]:MET:HE2	14:A:2228:HOH:O	1.94	0.67
1:A:101:ASP:HB3	14:A:2205:HOH:O	1.98	0.63
1:A:311[B]:MET:HE3	14:A:2383:HOH:O	2.02	0.60
1:A:367:PRO:HG2	1:A:370:SER:HB2	1.83	0.59
5:A:530:NAG:H61	5:A:531:NAG:C1	2.34	0.57
1:A:324[B]:LYS:CE	14:A:2502:HOH:O	2.53	0.57
5:A:540:NAG:O4	5:A:541:NAG:H83	2.05	0.56
1:A:1:ALA:N	1:A:142:ASP:OD2	2.39	0.55
1:A:31:THR:HA	1:A:32:PRO:C	2.26	0.55
1:A:249:ASP:O	11:A:612:GOL:H32	2.09	0.53
1:A:342:HIS:CE1	14:A:2693:HOH:O	2.63	0.51
1:A:469:THR:N	1:A:470:PRO:CD	2.75	0.49
1:A:324[B]:LYS:HE3	14:A:2502:HOH:O	2.13	0.49
1:A:446:PRO:HA	1:A:466:ALA:HA	1.94	0.48
1:A:387:THR:OG1	1:A:389:ASN:HB2	2.12	0.48
1:A:101:ASP:OD1	1:A:101:ASP:N	2.47	0.47
1:A:318:GLU:O	1:A:319:PRO:C	2.53	0.47
4:A:512:BMA:H61	4:A:513:MAN:O2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASP:HB3	1:A:207:PRO:CD	2.46	0.45
1:A:251:SER:OG	11:A:612:GOL:O2	2.36	0.44
1:A:404:PHE:O	1:A:422:PHE:HA	2.18	0.43
1:A:114:THR:HA	1:A:454:ASP:OD2	2.18	0.42
1:A:116:TYR:CE1	1:A:205[B]:CYS:SG	3.13	0.41
1:A:70:GLN:HE22	1:A:97:PHE:CB	2.33	0.41
1:A:47:ASN:ND2	14:A:2106:HOH:O	2.53	0.41
1:A:314:PRO:HG3	1:A:440[A]:GLU:HG2	2.02	0.41
7:A:561:NAG:H4	7:A:562:BMA:O2	2.20	0.41

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ASP:OD2	1:A:195[A]:ARG:NH2[4_545]	2.06	0.14

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	503/497 (101%)	492 (98%)	10 (2%)	1 (0%)	52 32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASP

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	428/420 (102%)	417 (97%)	11 (3%)	54 28

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	TYR
1	A	124	PHE
1	A	177	THR
1	A	180	ILE
1	A	243	ARG
1	A	298	LYS
1	A	324[A]	LYS
1	A	324[B]	LYS
1	A	387	THR
1	A	448	PHE
1	A	461	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	70	GLN
1	A	71	GLN
1	A	252	GLN
1	A	336	ASN
1	A	360	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 ⓘ

11 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$
4	NAG	A	510	1,4	14,14,15	0.75	0	15,19,21	1.72	3 (20%)
4	NAG	A	511	4	14,14,15	1.03	0	15,19,21	1.79	5 (33%)
4	BMA	A	512	4	11,11,12	0.59	0	14,15,17	2.02	3 (21%)
4	MAN	A	513	4	11,11,12	0.54	0	14,15,17	2.06	5 (35%)
5	NAG	A	530	1,5	14,14,15	0.71	0	15,19,21	1.38	2 (13%)
5	NAG	A	531	5	14,14,15	0.44	0	15,19,21	1.43	2 (13%)
5	NAG	A	540	1,5	14,14,15	0.70	0	15,19,21	1.25	1 (6%)
5	NAG	A	541	5	14,14,15	0.41	0	15,19,21	2.06	4 (26%)
7	NAG	A	560	1,7	14,14,15	0.87	1 (7%)	15,19,21	1.44	1 (6%)
7	NAG	A	561	7	14,14,15	0.60	0	15,19,21	1.71	3 (20%)
7	BMA	A	562	7	11,11,12	0.54	0	14,15,17	1.06	1 (7%)

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	NAG	A	510	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	511	4	-	0/6/23/26	0/1/1/1
4	BMA	A	512	4	-	0/2/19/22	0/1/1/1
4	MAN	A	513	4	-	0/2/19/22	1/1/1/1
5	NAG	A	530	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	531	5	-	0/6/23/26	0/1/1/1
5	NAG	A	540	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	541	5	-	0/6/23/26	0/1/1/1
7	NAG	A	560	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	561	7	-	0/6/23/26	0/1/1/1
7	BMA	A	562	7	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	560	NAG	C1-C2	2.59	1.56	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	513	MAN	C2-C3-C4	-4.69	103.08	111.04
5	A	541	NAG	C2-N2-C7	-4.25	117.58	123.04
4	A	513	MAN	C1-C2-C3	-3.99	104.82	109.54
4	A	512	BMA	C2-C3-C4	-3.46	105.17	111.04
5	A	530	NAG	C3-C4-C5	-3.40	104.26	110.20
7	A	560	NAG	C2-N2-C7	-3.38	118.69	123.04
7	A	561	NAG	C1-O5-C5	-3.27	108.10	112.25
4	A	511	NAG	O4-C4-C5	-3.09	101.04	109.24
4	A	510	NAG	O4-C4-C5	-3.04	101.18	109.24
4	A	510	NAG	O7-C7-C8	-2.91	116.72	122.06
4	A	513	MAN	C1-O5-C5	-2.76	108.74	112.25
5	A	531	NAG	C2-N2-C7	-2.72	119.55	123.04
4	A	511	NAG	C4-C3-C2	-2.66	107.10	111.23
5	A	540	NAG	C3-C2-N2	-2.64	104.23	110.56
4	A	511	NAG	C8-C7-N2	-2.40	111.51	116.11
4	A	511	NAG	C1-O5-C5	-2.40	109.21	112.25
5	A	541	NAG	C6-C5-C4	-2.35	107.21	113.02
7	A	561	NAG	O4-C4-C5	-2.21	103.37	109.24
4	A	513	MAN	O5-C5-C6	2.01	111.69	107.35
4	A	513	MAN	O4-C4-C3	2.01	114.86	110.34
4	A	510	NAG	C1-O5-C5	2.18	115.01	112.25
4	A	512	BMA	C3-C4-C5	2.25	114.11	110.20
7	A	562	BMA	C1-O5-C5	2.37	115.26	112.25
5	A	530	NAG	O5-C5-C6	2.77	113.34	107.35
4	A	511	NAG	O7-C7-N2	3.06	128.10	121.86
7	A	561	NAG	C4-C3-C2	3.31	116.38	111.23
5	A	541	NAG	C3-C4-C5	3.66	116.58	110.20
5	A	531	NAG	C1-O5-C5	3.76	117.02	112.25
5	A	541	NAG	C1-O5-C5	4.09	117.44	112.25
4	A	512	BMA	C1-O5-C5	5.35	119.04	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	513	MAN	C1-C2-C3-C4-C5-O5

8 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	512	BMA	1	0
4	A	513	MAN	1	0
5	A	530	NAG	1	0
5	A	531	NAG	1	0
5	A	540	NAG	1	0
5	A	541	NAG	1	0
7	A	561	NAG	2	0
7	A	562	BMA	2	0

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 13 are monoatomic - leaving 10 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	PER	A	505	2	0,1,1	0.00	-	0,0,0	0.00	-
6	NAG	A	550	1	14,14,15	0.75	0	15,19,21	1.46	3 (20%)
8	AS8	A	601	-	6,7,7	1.83	1 (16%)	4,10,10	2.14	2 (50%)
9	ACT	A	602	12	1,3,3	1.94	0	0,3,3	0.00	-
10	SO4	A	603	-	4,4,4	0.34	0	6,6,6	0.31	0
10	SO4	A	604	12	4,4,4	0.16	0	6,6,6	0.17	0
11	GOL	A	610	-	5,5,5	0.34	0	5,5,5	1.01	0
11	GOL	A	611	-	5,5,5	0.39	0	5,5,5	0.46	0
11	GOL	A	612	-	5,5,5	0.42	0	5,5,5	0.29	0
11	GOL	A	613	-	5,5,5	0.28	0	5,5,5	0.21	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	PER	A	505	2	-	0/0/0/0	0/0/0/0
6	NAG	A	550	1	-	0/6/23/26	0/1/1/1
8	AS8	A	601	-	-	0/0/5/5	0/0/0/0
9	ACT	A	602	12	-	0/0/0/0	0/0/0/0
10	SO4	A	603	-	-	0/0/0/0	0/0/0/0
10	SO4	A	604	12	-	0/0/0/0	0/0/0/0
11	GOL	A	610	-	-	0/4/4/4	0/0/0/0
11	GOL	A	611	-	-	0/4/4/4	0/0/0/0
11	GOL	A	612	-	-	0/4/4/4	0/0/0/0
11	GOL	A	613	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	601	AS8	O1-S	-4.13	1.56	1.63

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	601	AS8	O2S-S-O1S	-2.96	97.41	108.56
8	A	601	AS8	O2S-S-O3S	-2.56	98.94	108.56
6	A	550	NAG	C1-O5-C5	2.64	115.60	112.25
6	A	550	NAG	C2-N2-C7	2.74	126.56	123.04
6	A	550	NAG	C4-C3-C2	3.06	115.99	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	612	GOL	2	0

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	497/497 (100%)	0.04	23 (4%)	36 42	18, 27, 41, 71	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	ILE	10.9
1	A	316	SER	4.5
1	A	181	ALA	4.4
1	A	414	VAL	3.8
1	A	494	PRO	3.2
1	A	363	GLN	2.9
1	A	318	GLU	2.8
1	A	493	ASP	2.6
1	A	317	PRO	2.6
1	A	240	ALA	2.5
1	A	392	GLY	2.5
1	A	320	GLY	2.4
1	A	417	TYR	2.4
1	A	107	TRP	2.4
1	A	391	PRO	2.2
1	A	265	PHE	2.2
1	A	97	PHE	2.2
1	A	239	PHE	2.2
1	A	321	GLY	2.2
1	A	492	LEU	2.1
1	A	319	PRO	2.1
1	A	393	PHE	2.1
1	A	179	GLY	2.1

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, 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
5	NAG	A	530	14/15	0.91	0.17	6.74	43,49,55,64	0
4	NAG	A	511	14/15	0.95	0.14	4.92	24,30,41,45	0
4	NAG	A	510	14/15	0.96	0.09	0.40	22,28,37,37	0
7	NAG	A	560	14/15	0.92	0.08	-0.88	30,38,43,44	0
5	NAG	A	541	14/15	0.70	0.32	-	68,74,75,75	0
7	BMA	A	562	11/12	0.74	0.32	-	73,77,79,80	0
4	BMA	A	512	11/12	0.79	0.26	-	54,64,71,78	0
5	NAG	A	531	14/15	0.79	0.29	-	57,72,75,78	0
7	NAG	A	561	14/15	0.87	0.25	-	40,51,57,67	0
5	NAG	A	540	14/15	0.92	0.08	-	46,54,57,60	0
4	MAN	A	513	11/12	0.77	0.38	-	83,85,88,89	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, 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
11	GOL	A	613	6/6	0.88	0.22	13.21	30,41,45,45	0
13	NA	A	718	1/1	0.84	0.22	4.38	43,43,43,43	0
11	GOL	A	612	6/6	0.91	0.16	3.43	47,53,55,55	0
10	SO4	A	603	5/5	0.86	0.17	2.51	56,62,67,68	0
11	GOL	A	610	6/6	0.93	0.12	2.42	30,41,46,46	0
8	AS8	A	601	8/8	0.97	0.17	0.99	26,35,42,47	0
11	GOL	A	611	6/6	0.97	0.08	0.73	32,34,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PER	A	505	2/2	0.99	0.09	-1.13	27,27,27,30	0
12	ZN	A	710	1/1	0.99	0.03	-1.30	33,33,33,33	0
2	CU	A	503	1/1	1.00	0.08	-2.02	25,25,25,25	0
2	CU	A	502	1/1	0.99	0.06	-2.11	29,29,29,29	0
2	CU	A	501	1/1	0.99	0.06	-2.99	29,29,29,29	0
2	CU	A	504	1/1	0.99	0.02	-3.96	35,35,35,35	0
12	ZN	A	717	1/1	0.89	0.21	-	84,84,84,84	0
12	ZN	A	711	1/1	0.94	0.04	-	38,38,38,38	0
12	ZN	A	716	1/1	0.92	0.08	-	63,63,63,63	0
12	ZN	A	713	1/1	0.95	0.11	-	61,61,61,61	0
10	SO4	A	604	5/5	0.96	0.13	-	63,70,72,73	0
9	ACT	A	602	4/4	0.95	0.09	-	27,33,34,35	0
12	ZN	A	712	1/1	0.98	0.03	-	42,42,42,42	0
12	ZN	A	714	1/1	0.98	0.08	-	53,53,53,53	0
6	NAG	A	550	14/15	0.70	0.41	-	69,78,79,79	0
12	ZN	A	715	1/1	0.97	0.12	-	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.