



Full wwPDB X-ray Structure Validation Report

Sep 23, 2014 – 06:49 PM EDT

PDB ID : 4PSR
Title : Crystal Structure of alpha-L-fucosidase from Fusarium graminearum in the open form in complex with L-fucose
Authors : Cao, H.; Walton, J.; Brumm, P.; Phillips Jr., G.N.
Deposited on : 2014-03-07
Resolution : 1.38 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>

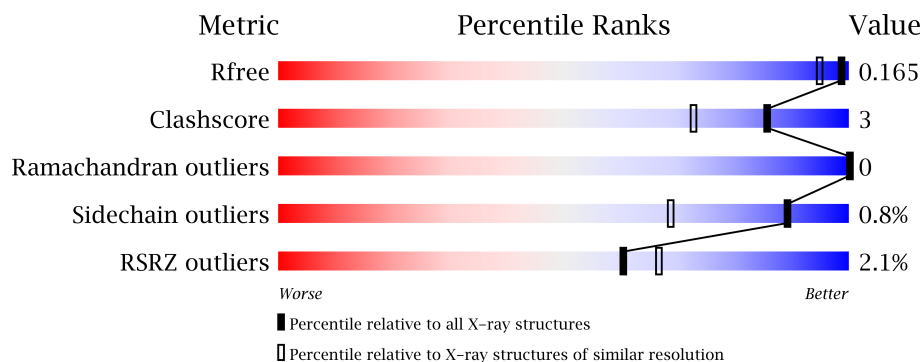
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
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) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 1.38 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	1348 (1.40-1.36)
Clashscore	79885	1515 (1.40-1.36)
Ramachandran outliers	78287	1473 (1.40-1.36)
Sidechain outliers	78261	1472 (1.40-1.36)
RSRZ outliers	66119	1348 (1.40-1.36)

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	585	
1	B	585	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	TRS	A	616	-	X
5	TRS	A	618	-	X
7	GOL	B	608	-	X

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 21517 atoms, of which 9640 are hydrogens 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.

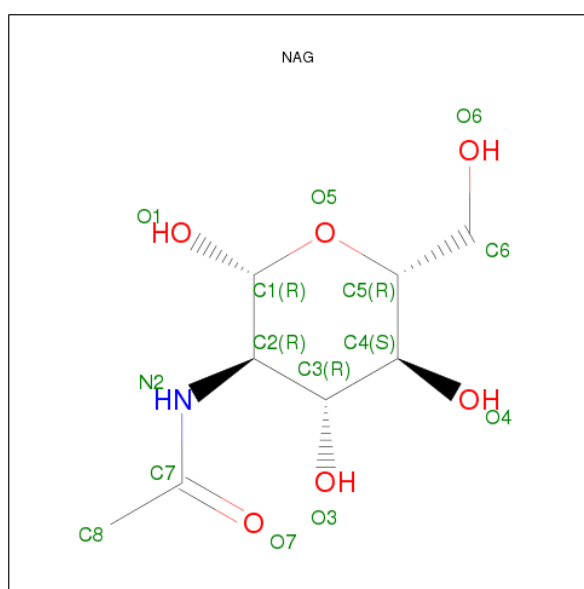
- Molecule 1 is a protein called Alpha-fucosidase GH29.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	581	Total	C	H	N	O	S	0	55	0
			9531	3091	4646	833	951	10			
1	B	583	Total	C	H	N	O	S	0	62	0
			9601	3110	4679	837	965	10			

- Molecule 2 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	7	Total	C	H	N	O	0	0
			156	46	73	2	35		

- 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	H	N	O	0	0
			28	8	14	1	5		

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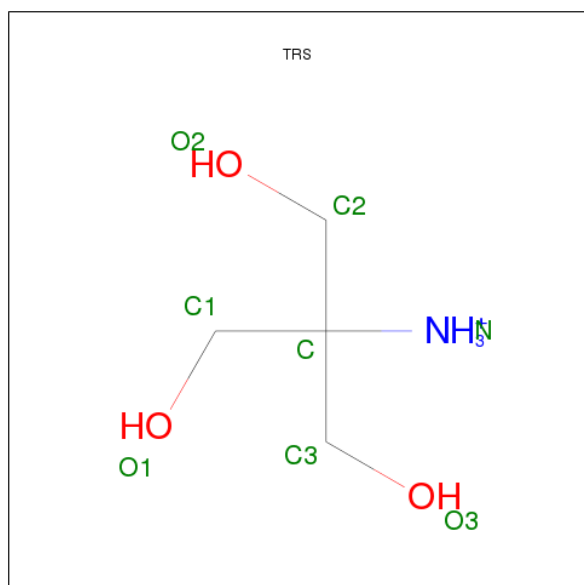
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	6	Total	C	H	N	O	0	1
			155	46	72	2	35		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).

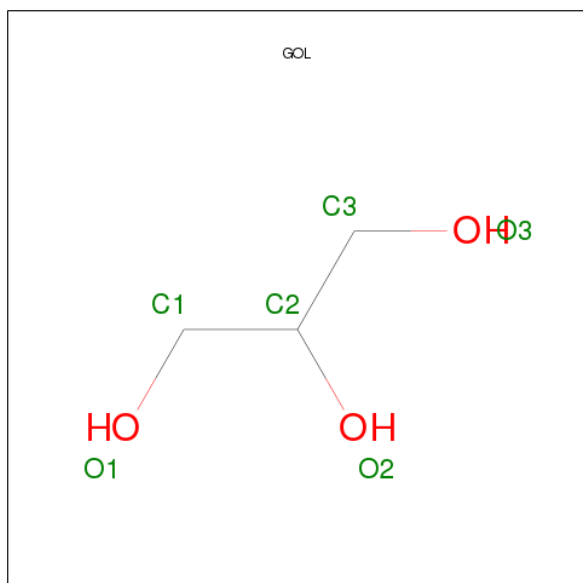


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
5	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
5	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
5	B	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
5	B	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
5	B	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

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

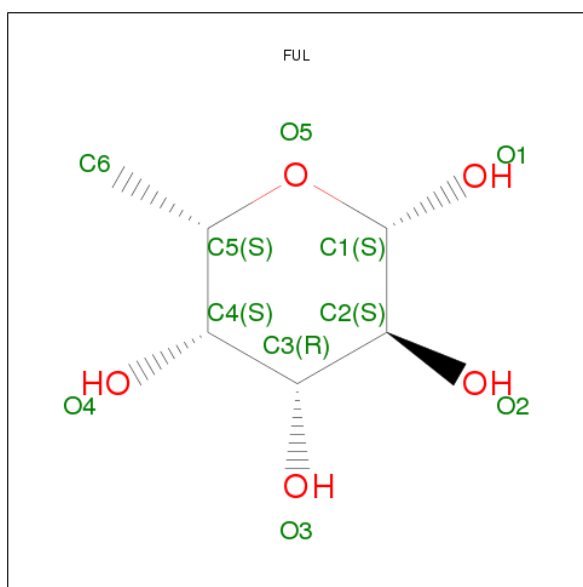
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Na	0	0
			2	2		
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	B	1	Total	C	H	O	0	0
			14	3	8	3		
7	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 8 is SUGAR (BETA-L-FUCOSE) (three-letter code: FUL) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			23	6	12	5		
8	B	1	Total	C	H	O	0	0
			23	6	12	5		

- Molecule 9 is water.

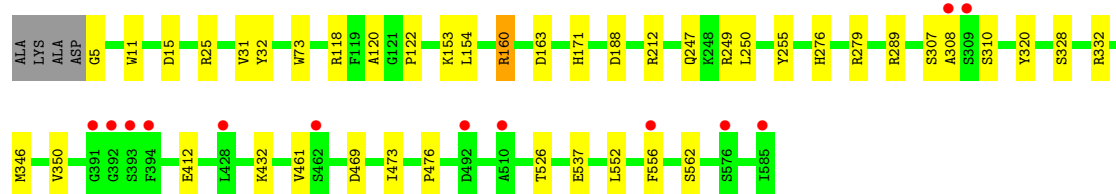
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	870	Total	O	0	0
			870	870		
9	B	895	Total	O	0	0
			895	895		

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.

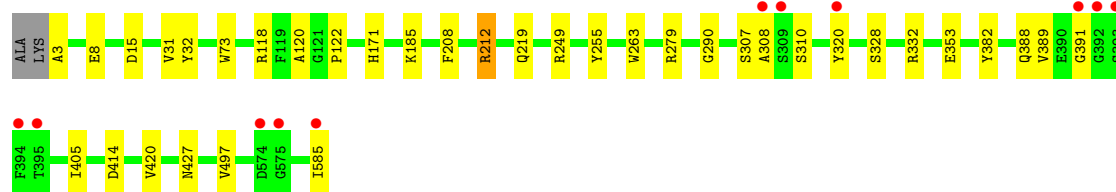
- Molecule 1: Alpha-fucosidase GH29

Chain A: 



- Molecule 1: Alpha-fucosidase GH29

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.15Å 75.99Å 80.97Å 105.69° 107.32° 106.93°	Depositor
Resolution (Å)	43.28 – 1.38 43.28 – 1.38	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.28-1.38) 91.7 (43.28-1.38)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.38Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.138 , 0.166 0.138 , 0.165	Depositor DCC
R_{free} test set	10215 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 47.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 214983 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	21517	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, NA, TRS, FUL, 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	0.53	0/5247	0.73	5/7108 (0.1%)
1	B	0.56	0/5287	0.79	9/7164 (0.1%)
All	All	0.54	0/10534	0.76	14/14272 (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 (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212[B]	ARG	NE-CZ-NH1	-14.53	113.03	120.30
1	B	212[C]	ARG	NE-CZ-NH1	-14.53	113.03	120.30
1	B	212[B]	ARG	NE-CZ-NH2	8.21	124.40	120.30
1	B	212[C]	ARG	NE-CZ-NH2	8.21	124.40	120.30
1	B	310[A]	SER	N-CA-CB	-7.26	99.61	110.50
1	B	310[B]	SER	N-CA-CB	-7.26	99.61	110.50
1	A	154[A]	LEU	CA-CB-CG	6.70	130.71	115.30
1	A	154[B]	LEU	CA-CB-CG	6.70	130.71	115.30
1	A	25	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	249	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	15	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	249	ARG	NE-CZ-NH1	5.24	122.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	15	ASP	CB-CG-OD1	5.08	122.87	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	PRO	Peptide
1	B	122	PRO	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	4885	4646	16	30	0
1	B	4922	4679	13	21	1
2	A	83	73	4	0	0
3	A	28	28	0	0	0
3	B	14	14	0	0	0
4	A	83	72	2	0	0
5	A	24	36	0	0	0
5	B	24	36	0	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	A	12	16	0	0	0
7	B	12	16	0	0	0
8	A	11	12	0	0	0
8	B	11	12	0	0	0
9	A	870	0	0	16	3
9	B	895	0	0	12	7
All	All	11877	9640	35	53	7

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 3.

All (53) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:160[C]:ARG:NH2	9:A:1527:HOH:O	2.15	0.80
1:A:5:GLY:N	9:A:1488:HOH:O	2.16	0.77
1:B:427[A]:ASN:ND2	9:B:1511:HOH:O	2.22	0.72
1:B:353:GLU:OE1	9:B:1325:HOH:O	2.09	0.70
1:A:188[A]:ASP:OD2	9:A:1114:HOH:O	2.10	0.69
1:A:537:GLU:OE2	9:A:1098:HOH:O	2.10	0.67
1:B:585:ILE:OXT	9:B:1570:HOH:O	2.13	0.67
1:B:3:ALA:N	9:B:1578:HOH:O	2.29	0.65
1:A:163[B]:ASP:OD1	9:A:940:HOH:O	2.16	0.61
1:B:279[B]:ARG:NH1	9:B:1135:HOH:O	2.24	0.61
1:A:289:ARG:HH12	1:A:308[A]:ALA:HA	1.67	0.60
1:B:382:TYR:OH	1:B:388[A]:GLN:NE2	2.34	0.59
1:A:308[A]:ALA:HB2	1:A:320:TYR:CE2	2.39	0.56
1:A:118[A]:ARG:NH2	9:A:1101:HOH:O	2.27	0.56
1:B:212[B]:ARG:NH1	9:B:1589:HOH:O	2.37	0.56
1:B:185:LYS:NZ	9:B:1407:HOH:O	2.33	0.56
1:B:308[A]:ALA:HB2	1:B:320:TYR:OH	2.06	0.55
1:B:308[A]:ALA:HB2	1:B:320:TYR:CZ	2.42	0.55
1:B:389[B]:VAL:HG12	1:B:391:GLY:H	1.72	0.54
1:A:412:GLU:OE1	9:A:938:HOH:O	2.19	0.53
1:A:308[A]:ALA:HB2	1:A:320:TYR:HE2	1.77	0.49
1:B:212[B]:ARG:HG2	1:B:255:TYR:CE1	2.48	0.49
1:A:247[B]:GLN:NE2	9:A:1335:HOH:O	2.45	0.48
1:A:432:LYS:NZ	1:A:469[B]:ASP:OD1	2.47	0.47
1:A:307[B]:SER:HB3	9:A:1526:HOH:O	2.14	0.47
1:A:188[B]:ASP:OD2	9:A:831:HOH:O	2.20	0.47
1:A:212[B]:ARG:HG3	1:A:255:TYR:CZ	2.49	0.47
1:B:307[B]:SER:HB3	9:B:1582:HOH:O	2.13	0.47
1:A:153[B]:LYS:HD3	9:A:1520:HOH:O	2.16	0.46
1:A:461:VAL:HG22	1:A:476:PRO:HD3	1.98	0.45
1:B:118[B]:ARG:NH2	9:B:1547:HOH:O	2.48	0.44
1:B:31:VAL:O	1:B:120:ALA:HA	2.17	0.44
1:B:497:VAL:HG22	9:B:1268:HOH:O	2.17	0.44
1:A:212[A]:ARG:NH2	9:A:1533:HOH:O	2.51	0.43
1:A:11:TRP:CD2	1:A:250:LEU:HD21	2.53	0.43
1:A:276:HIS:O	9:A:1536:HOH:O	2.22	0.43
1:B:219:GLN:HA	1:B:263:TRP:CH2	2.53	0.43
1:A:11:TRP:CE3	1:A:279[B]:ARG:HD3	2.54	0.43
1:B:290:GLY:HA2	1:B:332[B]:ARG:NH1	2.33	0.43
1:A:461:VAL:HG11	1:A:473:ILE:HG23	2.01	0.43
1:B:208:PHE:HE2	1:B:212[C]:ARG:CZ	2.32	0.42
1:A:332[B]:ARG:NH1	9:A:1099:HOH:O	2.52	0.42
1:A:346:MET:HE2	1:A:350:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:332[B]:ARG:NE	9:A:1099:HOH:O	2.49	0.42
1:A:328:SER:O	1:A:332[B]:ARG:HG2	2.19	0.41
1:A:552:LEU:O	1:A:562:SER:HA	2.20	0.41
1:B:328:SER:O	1:B:332[B]:ARG:HG2	2.21	0.41
1:A:153[A]:LYS:HE3	9:A:894:HOH:O	2.21	0.41
1:A:31:VAL:O	1:A:120:ALA:HA	2.21	0.40
1:B:405:ILE:HG22	1:B:420[B]:VAL:HG22	2.04	0.40
1:A:526:THR:HB	1:A:556:PHE:CD1	2.57	0.40

All (7) 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)
9:A:1354:HOH:O	9:B:1275:HOH:O[1_556]	2.02	0.18
9:B:1363:HOH:O	9:B:1412:HOH:O[1_445]	2.08	0.12
9:A:1122:HOH:O	9:B:1176:HOH:O[1_666]	2.09	0.11
9:B:1412:HOH:O	9:B:1457:HOH:O[1_665]	2.11	0.09
9:B:1036:HOH:O	9:B:1569:HOH:O[1_445]	2.13	0.07
9:A:1487:HOH:O	9:B:1289:HOH:O[1_666]	2.17	0.03
1:B:8[B]:GLU:OE1	9:B:1541:HOH:O[1_655]	2.19	0.01

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	638/585 (109%)	624 (98%)	14 (2%)	0	100	100
1	B	645/585 (110%)	630 (98%)	15 (2%)	0	100	100
All	All	1283/1170 (110%)	1254 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	545/492 (111%)	537 (98%)	8 (2%)	76	45
1	B	550/492 (112%)	547 (100%)	3 (0%)	94	79
All	All	1095/984 (111%)	1084 (99%)	11 (1%)	89	62

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

Mol	Chain	Res	Type
1	A	32	TYR
1	A	73	TRP
1	A	160[A]	ARG
1	A	160[B]	ARG
1	A	160[C]	ARG
1	A	171	HIS
1	A	310[A]	SER
1	A	310[B]	SER
1	B	32	TYR
1	B	73	TRP
1	B	171	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

14 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	12,14,15	0.37	0	15,19,21	0.37	0
2	NAG	A	602	2	12,14,15	0.41	0	15,19,21	0.47	0
2	BMA	A	603	2	10,11,12	0.68	0	11,15,17	0.96	1 (9%)
2	MAN	A	604	2	10,11,12	0.71	0	11,15,17	1.23	2 (18%)
2	MAN	A	605	2	10,11,12	0.64	0	11,15,17	1.08	1 (9%)
2	MAN	A	606	2	10,11,12	1.04	1 (10%)	11,15,17	0.92	1 (9%)
2	MAN	A	607	2	10,11,12	1.13	1 (10%)	11,15,17	0.91	1 (9%)
4	MAN	A	610[A]	4	10,11,12	0.95	1 (10%)	11,15,17	0.97	0
4	MAN	A	610[B]	4	10,11,12	0.59	0	11,15,17	0.95	1 (9%)
4	MAN	A	611	4	10,11,12	0.79	0	11,15,17	0.81	0
4	MAN	A	612	4	10,11,12	0.61	0	11,15,17	1.20	2 (18%)
4	NAG	A	613	1,4	12,14,15	0.47	0	15,19,21	0.54	0
4	NAG	A	614	4	12,14,15	0.36	0	15,19,21	0.39	0
4	BMA	A	615	4	10,11,12	0.78	0	11,15,17	1.14	1 (9%)

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	MAN	A	607	2	-	0/2/19/22	0/1/1/1
4	MAN	A	610[A]	4	-	0/2/19/22	0/1/1/1
4	MAN	A	610[B]	4	-	0/2/19/22	0/1/1/1
4	MAN	A	611	4	-	0/2/19/22	0/1/1/1
4	MAN	A	612	4	-	0/2/19/22	0/1/1/1
4	NAG	A	613	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	614	4	-	0/6/23/26	0/1/1/1
4	BMA	A	615	4	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	610[A]	MAN	O5-C5	-2.32	1.41	1.45
2	A	606	MAN	O2-C2	-2.29	1.38	1.43
2	A	607	MAN	O5-C5	2.03	1.49	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	MAN	O2-C2-C3	-2.87	104.01	110.10
2	A	604	MAN	O5-C5-C6	2.37	109.46	106.98
4	A	612	MAN	O2-C2-C3	-2.36	105.10	110.10
4	A	612	MAN	O5-C5-C6	2.25	109.34	106.98
2	A	606	MAN	O2-C2-C3	-2.20	105.43	110.10
4	A	615	BMA	C4-C3-C2	2.13	112.99	110.61
4	A	610[B]	MAN	O2-C2-C3	-2.11	105.64	110.10
2	A	603	BMA	O5-C5-C4	-2.10	107.99	110.65
2	A	607	MAN	O2-C2-C3	-2.03	105.79	110.10
2	A	604	MAN	O2-C2-C3	-2.03	105.81	110.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 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	608	1	12,14,15	0.40	0	15,19,21	0.29	0
3	NAG	A	609	1	12,14,15	0.46	0	15,19,21	0.56	0
5	TRS	A	616	-	7,7,7	0.79	0	9,9,9	0.76	0
5	TRS	A	617	-	7,7,7	0.76	0	9,9,9	0.92	1 (11%)
5	TRS	A	618	-	7,7,7	0.93	1 (14%)	9,9,9	0.85	0
7	GOL	A	620	-	5,5,5	0.28	0	5,5,5	0.13	0
7	GOL	A	621	-	5,5,5	0.31	0	5,5,5	0.29	0
8	FUL	A	622	-	11,11,11	0.50	0	16,16,16	1.23	2 (12%)
3	NAG	B	601	1	12,14,15	0.48	0	15,19,21	0.38	0
5	TRS	B	602	-	7,7,7	0.72	0	9,9,9	0.81	0
5	TRS	B	603	-	7,7,7	0.73	0	9,9,9	0.89	0
5	TRS	B	604	-	7,7,7	0.64	0	9,9,9	0.67	0
7	GOL	B	607	-	5,5,5	0.27	0	5,5,5	0.31	0
7	GOL	B	608	-	5,5,5	0.29	0	5,5,5	0.57	0
8	FUL	B	609	-	11,11,11	0.51	0	16,16,16	1.01	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	608	1	-	0/6/23/26	0/1/1/1
3	NAG	A	609	1	-	0/6/23/26	0/1/1/1
5	TRS	A	616	-	-	0/9/9/9	0/0/0/0
5	TRS	A	617	-	-	0/9/9/9	0/0/0/0
5	TRS	A	618	-	-	0/9/9/9	0/0/0/0
7	GOL	A	620	-	-	0/4/4/4	0/0/0/0
7	GOL	A	621	-	-	0/4/4/4	0/0/0/0
8	FUL	A	622	-	-	0/0/20/20	0/1/1/1
3	NAG	B	601	1	-	0/6/23/26	0/1/1/1
5	TRS	B	602	-	-	0/9/9/9	0/0/0/0
5	TRS	B	603	-	-	0/9/9/9	0/0/0/0
5	TRS	B	604	-	-	0/9/9/9	0/0/0/0
7	GOL	B	607	-	-	0/4/4/4	0/0/0/0
7	GOL	B	608	-	-	0/4/4/4	0/0/0/0
8	FUL	B	609	-	-	0/0/20/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	618	TRS	C-N	-2.41	1.47	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
8	A	622	FUL	C1-C2-C3	-3.05	105.96	110.48
8	B	609	FUL	C1-C2-C3	-2.77	106.38	110.48
5	A	617	TRS	O1-C1-C	-2.18	106.85	111.28
8	A	622	FUL	C1-O5-C5	-2.04	109.71	113.53

There are no chirality outliers.

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	581/585 (99%)	-0.07	13 (2%) 59 65	9, 15, 33, 73	0
1	B	583/585 (99%)	-0.21	11 (1%) 64 71	9, 14, 30, 77	0
All	All	1164/1170 (99%)	-0.14	24 (2%) 60 67	9, 15, 32, 77	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	556	PHE	4.8
1	A	391	GLY	4.5
1	B	392	GLY	4.2
1	A	585	ILE	3.9
1	A	308[A]	ALA	3.7
1	B	391	GLY	3.4
1	B	585	ILE	3.4
1	B	574	ASP	3.0
1	B	394	PHE	2.9
1	B	393	SER	2.9
1	B	395	THR	2.8
1	A	392	GLY	2.8
1	B	308[A]	ALA	2.7
1	A	428	LEU	2.7
1	A	462	SER	2.6
1	A	394	PHE	2.4
1	B	320	TYR	2.3
1	A	576	SER	2.2
1	B	309[A]	SER	2.2
1	A	393	SER	2.1
1	B	575	GLY	2.1
1	A	309[A]	SER	2.1
1	A	510	ALA	2.1
1	A	492[A]	ASP	2.0

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	MAN	A	607	11/12	0.25	15.33	31,49,62,69	0
4	MAN	A	612	11/12	0.17	7.93	16,23,34,34	0
2	MAN	A	606	11/12	0.13	6.11	21,32,40,42	0
4	BMA	A	615	11/12	0.10	4.40	15,18,25,26	0
4	NAG	A	614	14/15	0.07	2.78	13,18,29,29	0
2	MAN	A	604	11/12	0.19	2.54	32,51,62,72	0
4	MAN	A	611	11/12	0.20	2.52	23,37,58,70	0
4	MAN	A	610[B]	11/12	0.09	1.92	14,18,30,31	20
4	MAN	A	610[A]	11/12	0.09	1.79	14,18,38,38	20
4	NAG	A	613	14/15	0.07	-0.22	11,14,22,34	0
2	MAN	A	605	11/12	0.07	-0.29	14,18,38,38	0
2	NAG	A	601	14/15	0.06	-0.50	12,16,20,32	0
2	NAG	A	602	14/15	0.07	-0.64	14,18,30,30	0
2	BMA	A	603	11/12	0.06	-1.19	15,18,22,22	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(Å ²)	Q<0.9
5	TRS	A	616	8/8	0.16	9.80	21,28,38,38	0
5	TRS	A	618	8/8	0.21	3.08	29,39,45,49	0
7	GOL	B	608	6/6	0.18	2.04	39,55,66,76	0
5	TRS	A	617	8/8	0.13	1.93	17,24,44,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	TRS	B	603	8/8	0.13	1.83	16,21,46,48	0
7	GOL	A	620	6/6	0.15	1.68	36,44,57,59	0
5	TRS	B	604	8/8	0.11	1.58	16,22,26,29	0
7	GOL	B	607	6/6	0.16	1.50	33,48,63,65	0
8	FUL	B	609	11/11	0.07	0.86	12,15,18,18	0
5	TRS	B	602	8/8	0.10	0.58	21,27,42,51	0
7	GOL	A	621	6/6	0.15	0.22	40,49,56,65	0
3	NAG	A	608	14/15	0.10	0.14	16,23,56,56	0
6	NA	B	605	1/1	0.07	-0.09	17,17,17,17	0
3	NAG	A	609	14/15	0.07	-0.34	17,25,34,40	0
3	NAG	B	601	14/15	0.08	-0.56	14,25,38,47	0
6	NA	B	606	1/1	0.06	-0.59	13,13,13,13	0
6	NA	A	619	1/1	0.05	-0.76	15,15,15,15	0
8	FUL	A	622	11/11	0.06	-0.82	12,15,18,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.