



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2017 – 06:51 AM EST

PDB ID : 4PSP  
Title : Crystal Structure of GH29 family alpha-L-fucosidase from *Fusarium graminearum* in the open form  
Authors : Cao, H.; Walton, J.; Brumm, P.; Phillips Jr., G.N.  
Deposited on : unknown  
Resolution : 1.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
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-20030345

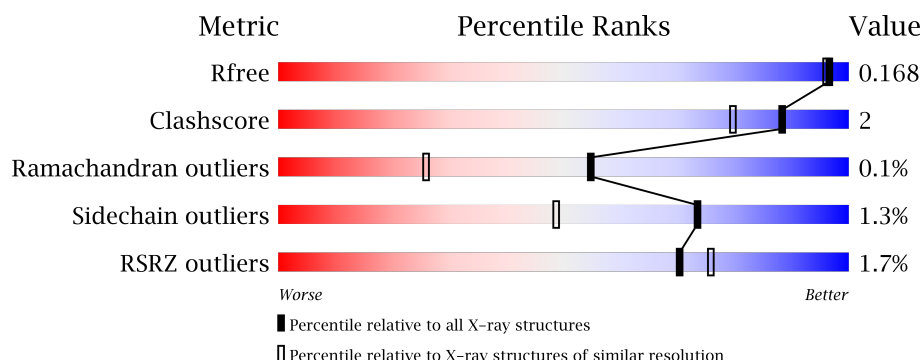
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1088 (1.56-1.56)
Clashscore	112137	1132 (1.56-1.56)
Ramachandran outliers	110173	1110 (1.56-1.56)
Sidechain outliers	110143	1108 (1.56-1.56)
RSRZ outliers	101464	1089 (1.56-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	585	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	B	585	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div></div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	A	606	-	-	-	X
4	MAN	A	607	-	-	-	X
4	MAN	A	612	-	-	-	X
5	TRS	A	616	-	-	-	X
5	TRS	A	618	-	-	-	X
5	TRS	B	604	-	-	-	X
7	GOL	A	621	-	-	-	X
7	GOL	A	622	-	-	-	X
7	GOL	B	607	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 21369 atoms, of which 9559 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 Alpha-fucosidase GH29.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	581	Total	C	H	N	O	S	0	49	0
			9481	3072	4626	829	944	10			
1	B	583	Total	C	H	N	O	S	0	56	0
			9540	3094	4643	830	963	10			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



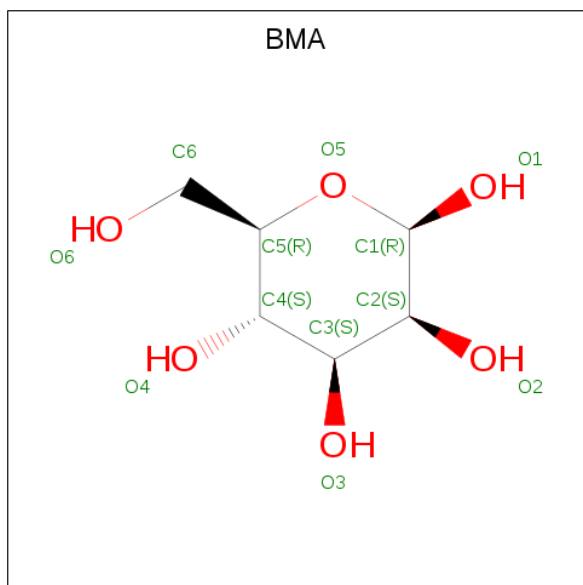
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 8	H 13	N 1	O 5	0	0
2	A	1	Total 27	C 8	H 13	N 1	O 5	0	0
2	A	1	Total 28	C 8	H 14	N 1	O 5	0	0
2	A	1	Total 28	C 8	H 14	N 1	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
2	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			20	6	9	5		
3	A	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			22	6	11	5		
4	A	1	Total	C	H	O	0	0
			21	6	10	5		
4	A	1	Total	C	H	O	0	0
			21	6	10	5		
4	A	1	Total	C	H	O	0	0
			22	6	11	5		
4	A	1	Total	C	H	O	0	0
			21	6	10	5		
4	A	1	Total	C	H	O	0	0
			22	6	11	5		
4	A	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).

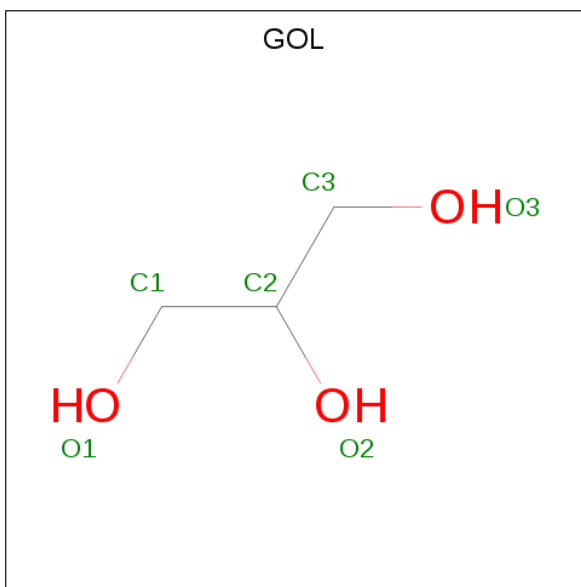


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
5	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
5	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
5	B	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
5	B	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
5	B	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

- 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: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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	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		

- Molecule 8 is water.

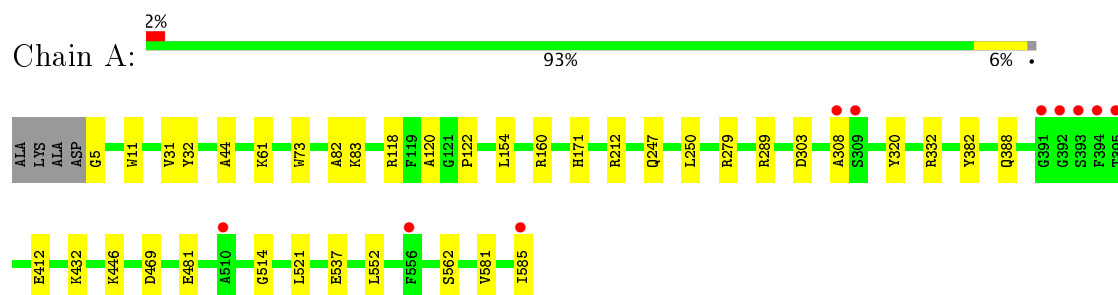
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	868	Total	O	0	0
			868	868		
8	B	918	Total	O	0	0
			918	918		



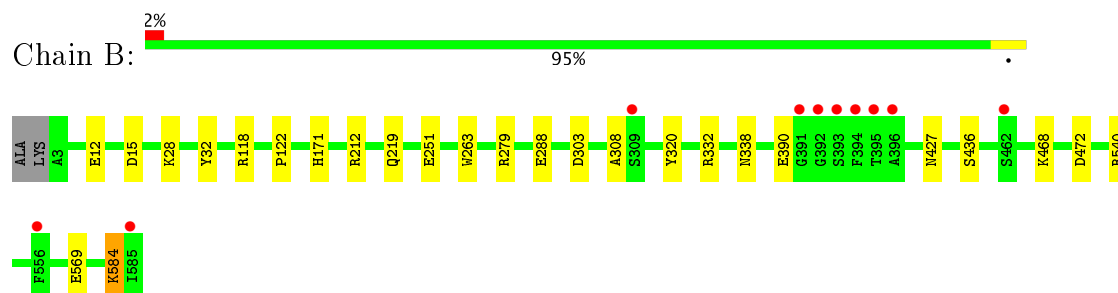
### 3 Residue-property plots [i](#)

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



- Molecule 1: Alpha-fucosidase GH29



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.87Å 75.89Å 80.84Å 105.91° 107.23° 106.75°	Depositor
Resolution (Å)	41.23 – 1.56 41.24 – 1.56	Depositor EDS
% Data completeness (in resolution range)	96.8 (41.23-1.56) 80.9 (41.24-1.56)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 1.56Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.135 , 0.169 0.134 , 0.168	Depositor DCC
$R_{free}$ test set	7207 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.7	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 50.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	21369	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, NA, TRS, 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	0.46	0/5202	0.64	3/7046 (0.0%)
1	B	0.47	0/5244	0.65	3/7106 (0.0%)
All	All	0.47	0/10446	0.65	6/14152 (0.0%)

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	B	15	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	154[A]	LEU	CA-CB-CG	5.98	129.05	115.30
1	A	154[B]	LEU	CA-CB-CG	5.98	129.05	115.30
1	A	154[C]	LEU	CA-CB-CG	5.98	129.05	115.30
1	B	212[A]	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	B	212[B]	ARG	NE-CZ-NH2	-5.83	117.38	120.30

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 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4855	4626	4432	26	0
1	B	4897	4643	4447	15	1
2	A	84	80	74	0	0
2	B	14	14	13	0	0
3	A	22	19	17	0	0
4	A	77	73	66	1	0
5	A	24	36	36	0	0
5	B	24	36	36	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	A	18	24	24	3	0
7	B	6	8	8	0	0
8	A	868	0	0	13	3
8	B	918	0	0	10	4
All	All	11810	9559	9153	45	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (45) 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:308[A]:ALA:HB2	1:A:320:TYR:CE2	2.26	0.70
1:A:412:GLU:OE1	8:A:1341:HOH:O	2.12	0.67
1:A:82:ALA:HB1	7:A:621:GOL:H11	1.75	0.67
1:A:118[B]:ARG:NH2	8:A:1122:HOH:O	2.25	0.67
1:B:251:GLU:OE1	8:B:1107:HOH:O	2.13	0.66
1:B:569:GLU:OE1	8:B:1586:HOH:O	2.14	0.64
1:B:584[A]:LYS:NZ	8:B:1499:HOH:O	2.29	0.64
1:B:308[A]:ALA:HB2	1:B:320:TYR:CZ	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLY:N	8:A:1414:HOH:O	2.32	0.62
1:A:382:TYR:OH	1:A:388[A]:GLN:OE1	2.10	0.61
1:A:514:GLY:O	8:A:1485:HOH:O	2.16	0.60
1:B:303[B]:ASP:OD1	8:B:1570:HOH:O	2.13	0.60
1:B:540:ARG:NH1	8:B:1569:HOH:O	2.26	0.58
1:B:332[B]:ARG:NH1	8:B:795:HOH:O	2.37	0.57
7:A:621:GOL:O1	8:A:1473:HOH:O	2.18	0.56
1:B:308[A]:ALA:HB2	1:B:320:TYR:CE2	2.41	0.55
1:A:432:LYS:NZ	1:A:469[B]:ASP:OD1	2.41	0.53
1:A:581:VAL:HG21	4:A:606:MAN:H62	1.91	0.53
1:A:537:GLU:OE2	8:A:1070:HOH:O	2.18	0.52
1:B:308[A]:ALA:HB2	1:B:320:TYR:OH	2.11	0.51
1:A:585:ILE:O	8:A:1004:HOH:O	2.20	0.51
1:A:308[A]:ALA:HB2	1:A:320:TYR:CZ	2.46	0.49
1:A:247[B]:GLN:NE2	8:A:1470:HOH:O	2.33	0.48
1:B:279[B]:ARG:NH1	8:B:1411:HOH:O	2.26	0.48
1:A:332[B]:ARG:NH1	8:A:1082:HOH:O	2.49	0.46
1:A:303[B]:ASP:OD1	8:A:1068:HOH:O	2.20	0.45
1:A:11:TRP:CD2	1:A:250:LEU:HD21	2.51	0.45
1:A:308[A]:ALA:HB2	1:A:320:TYR:HE2	1.79	0.44
1:A:289:ARG:HH12	1:A:308[A]:ALA:HA	1.82	0.44
1:B:118[B]:ARG:NH1	8:B:1160:HOH:O	2.51	0.43
1:A:11:TRP:CE3	1:A:279[B]:ARG:HD3	2.54	0.43
1:A:552:LEU:O	1:A:562:SER:HA	2.19	0.42
1:B:28:LYS:HA	1:B:338:ASN:OD1	2.20	0.42
1:A:83:LYS:H	7:A:621:GOL:C1	2.33	0.41
1:A:289:ARG:NH1	8:A:1356:HOH:O	2.52	0.41
1:A:31:VAL:O	1:A:120:ALA:HA	2.20	0.41
1:B:219:GLN:HA	1:B:263:TRP:CH2	2.55	0.41
1:B:436:SER:OG	1:B:468:LYS:HA	2.21	0.41
1:A:212[B]:ARG:NH1	8:A:1379:HOH:O	2.53	0.40
1:A:308[A]:ALA:HB2	1:A:320:TYR:OH	2.21	0.40

All (4) 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)
8:A:1282:HOH:O	8:B:1219:HOH:O[1_666]	2.13	0.07
8:A:1429:HOH:O	8:B:1568:HOH:O[1_656]	2.15	0.05
8:A:1087:HOH:O	8:B:1132:HOH:O[1_666]	2.16	0.04
1:B:12[B]:GLU:OE1	8:B:1077:HOH:O[1_655]	2.17	0.03

## 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	633/585 (108%)	616 (97%)	16 (2%)	1 (0%)	51	23
1	B	638/585 (109%)	620 (97%)	18 (3%)	0	100	100
All	All	1271/1170 (109%)	1236 (97%)	34 (3%)	1 (0%)	55	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	ALA

### 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	541/492 (110%)	532 (98%)	9 (2%)	66	36
1	B	545/492 (111%)	537 (98%)	8 (2%)	70	41
All	All	1086/984 (110%)	1069 (98%)	17 (2%)	73	39

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	A	61	LYS
1	A	73	TRP
1	A	160[A]	ARG
1	A	160[B]	ARG

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Mol	Chain	Res	Type
1	A	160[C]	ARG
1	A	171	HIS
1	A	446	LYS
1	A	481	GLU
1	B	32	TYR
1	B	171	HIS
1	B	288	GLU
1	B	390	GLU
1	B	427[A]	ASN
1	B	427[B]	ASN
1	B	584[A]	LYS
1	B	584[B]	LYS

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 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
2	NAG	A	601	1,2	14,14,15	0.52	0	15,19,21	0.46	0
2	NAG	A	602	3,2	14,14,15	0.46	0	15,19,21	0.48	0
3	BMA	A	603	2,4	11,11,12	0.85	0	13,15,17	0.83	0
4	MAN	A	604	3	11,11,12	0.87	0	13,15,17	1.19	2 (15%)
4	MAN	A	605	3,4	11,11,12	0.70	1 (9%)	13,15,17	1.20	1 (7%)
4	MAN	A	606	4	11,11,12	1.44	1 (9%)	13,15,17	0.94	1 (7%)
4	MAN	A	607	4	11,11,12	0.97	0	13,15,17	1.11	2 (15%)
2	NAG	A	608	1	14,14,15	0.21	0	15,19,21	0.54	0
2	NAG	A	609	1	14,14,15	0.34	0	15,19,21	0.50	0
4	MAN	A	610	3,4	11,11,12	0.94	1 (9%)	13,15,17	1.06	1 (7%)
4	MAN	A	611	4	11,11,12	0.87	0	13,15,17	0.95	1 (7%)
4	MAN	A	612	4	11,11,12	0.77	1 (9%)	13,15,17	1.19	1 (7%)
2	NAG	A	613	1,2	14,14,15	0.27	0	15,19,21	0.50	0
2	NAG	A	614	3,2	14,14,15	0.26	0	15,19,21	0.62	0
3	BMA	A	615	2,4	11,11,12	1.13	1 (9%)	13,15,17	0.89	0
5	TRS	A	616	-	7,7,7	0.58	0	9,9,9	1.00	0
5	TRS	A	617	-	7,7,7	0.96	1 (14%)	9,9,9	0.47	0
5	TRS	A	618	-	7,7,7	0.80	1 (14%)	9,9,9	0.67	0
7	GOL	A	620	-	5,5,5	0.33	0	5,5,5	0.31	0
7	GOL	A	621	-	5,5,5	0.21	0	5,5,5	0.73	0
7	GOL	A	622	-	5,5,5	0.30	0	5,5,5	0.27	0
2	NAG	B	601	1	14,14,15	0.50	0	15,19,21	0.49	0
5	TRS	B	602	-	7,7,7	0.77	0	9,9,9	0.79	0
5	TRS	B	603	-	7,7,7	0.91	1 (14%)	9,9,9	0.56	0
5	TRS	B	604	-	7,7,7	0.76	0	9,9,9	0.72	0
7	GOL	B	607	-	5,5,5	0.37	0	5,5,5	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	602	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	603	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	604	3	-	0/2/19/22	0/1/1/1
4	MAN	A	605	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	606	4	-	0/2/19/22	0/1/1/1
4	MAN	A	607	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	608	1	-	0/6/23/26	0/1/1/1
2	NAG	A	609	1	-	0/6/23/26	0/1/1/1
4	MAN	A	610	3,4	-	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
2	NAG	A	613	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	614	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	615	2,4	-	0/2/19/22	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
7	GOL	A	622	-	-	0/4/4/4	0/0/0/0
2	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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	606	MAN	O5-C1	-3.57	1.37	1.43
4	A	610	MAN	O5-C1	-2.74	1.39	1.43
5	A	617	TRS	C-N	-2.48	1.46	1.50
3	A	615	BMA	O5-C1	-2.42	1.39	1.43
5	B	603	TRS	C-N	-2.37	1.46	1.50
4	A	612	MAN	O5-C1	-2.15	1.40	1.43
5	A	618	TRS	C-N	-2.05	1.47	1.50
4	A	605	MAN	O5-C1	-2.01	1.40	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	612	MAN	O2-C2-C3	-2.82	104.63	110.17
4	A	604	MAN	O2-C2-C3	-2.58	105.10	110.17
4	A	607	MAN	O2-C2-C3	-2.46	105.34	110.17
4	A	606	MAN	O2-C2-C3	-2.44	105.38	110.17
4	A	607	MAN	C1-O5-C5	2.07	115.02	112.17
4	A	611	MAN	C1-O5-C5	2.12	115.08	112.17
4	A	610	MAN	C1-O5-C5	2.13	115.10	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	MAN	C1-O5-C5	2.29	115.32	112.17
4	A	605	MAN	C1-O5-C5	3.02	116.33	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	606	MAN	1	0
7	A	621	GOL	3	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	581/585 (99%)	-0.37	10 (1%) 70 76	9, 16, 35, 80	0
1	B	583/585 (99%)	-0.44	10 (1%) 70 76	8, 14, 31, 86	0
All	All	1164/1170 (99%)	-0.40	20 (1%) 70 76	8, 15, 33, 86	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	392	GLY	6.3
1	A	392	GLY	5.6
1	B	393	SER	4.9
1	A	556	PHE	4.9
1	B	395	THR	4.1
1	A	393	SER	3.7
1	A	394	PHE	3.7
1	B	391	GLY	3.5
1	A	585	ILE	3.2
1	A	391	GLY	3.0
1	B	585[A]	ILE	3.0
1	A	395	THR	2.9
1	B	556	PHE	2.7
1	B	396	ALA	2.7
1	B	394	PHE	2.6
1	A	510	ALA	2.4
1	B	309[A]	SER	2.2
1	A	308[A]	ALA	2.2
1	A	309[A]	SER	2.0
1	B	462	SER	2.0

## 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](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	A	621	6/6	0.83	0.35	10.26	32,45,57,58	0
4	MAN	A	607	11/12	0.76	0.23	9.72	32,48,66,68	0
5	TRS	B	604	8/8	0.93	0.12	7.62	15,23,29,33	0
4	MAN	A	606	11/12	0.89	0.12	5.69	20,34,42,44	0
5	TRS	A	616	8/8	0.93	0.10	4.80	20,27,41,41	0
4	MAN	A	612	11/12	0.93	0.11	4.55	18,25,36,43	0
7	GOL	A	622	6/6	0.94	0.14	3.50	25,35,60,65	0
5	TRS	A	618	8/8	0.90	0.19	3.01	28,43,49,52	0
7	GOL	B	607	6/6	0.92	0.12	2.85	23,33,41,46	0
4	MAN	A	611	11/12	0.90	0.18	1.87	29,48,68,81	0
5	TRS	A	617	8/8	0.87	0.13	1.71	23,36,49,59	0
6	NA	B	605	1/1	0.98	0.09	0.85	15,15,15,15	0
5	TRS	B	603	8/8	0.93	0.11	0.74	20,30,48,52	0
5	TRS	B	602	8/8	0.93	0.10	0.61	19,26,38,45	0
2	NAG	A	608	14/15	0.93	0.12	0.43	19,26,62,62	0
4	MAN	A	610	11/12	0.96	0.07	0.21	13,20,30,49	0
7	GOL	A	620	6/6	0.88	0.10	0.06	32,48,65,65	0
4	MAN	A	605	11/12	0.97	0.06	-0.10	12,18,33,40	0
6	NA	B	606	1/1	0.99	0.06	-0.37	12,12,12,12	0
2	NAG	A	613	14/15	0.97	0.07	-0.44	9,14,21,33	0
2	NAG	A	601	14/15	0.97	0.06	-0.49	12,16,26,32	0
2	NAG	B	601	14/15	0.96	0.08	-0.56	14,26,35,39	0
2	NAG	A	609	14/15	0.96	0.07	-0.57	18,25,31,35	0
6	NA	A	619	1/1	0.99	0.05	-0.91	16,16,16,16	0
3	BMA	A	603	11/12	0.96	0.06	-	14,18,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	A	604	11/12	0.84	0.17	-	31,54,65,76	0
2	NAG	A	614	14/15	0.97	0.06	-	11,17,28,28	0
2	NAG	A	602	14/15	0.97	0.07	-	13,18,29,29	0
3	BMA	A	615	11/12	0.94	0.09	-	13,18,27,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.