Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:17 PM GMT

PDB ID	:	1EX1
Title	:	BETA-D-GLUCAN EXOHYDROLASE FROM BARLEY
Authors	:	Varghese, J.N.; Hrmova, M.; Fincher, G.B.
Deposited on	:	1998-11-10
Resolution	:	2.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

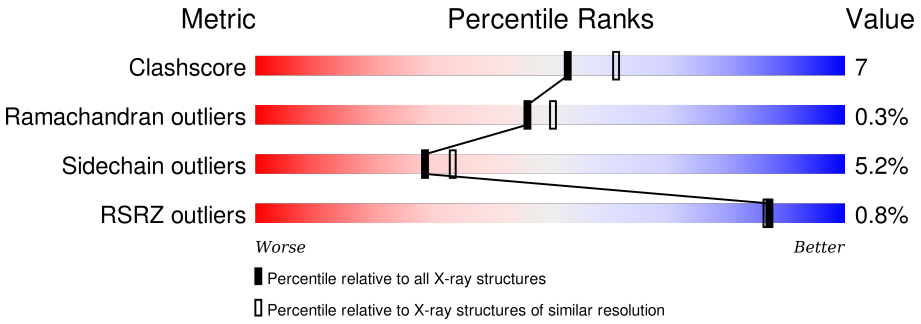
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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

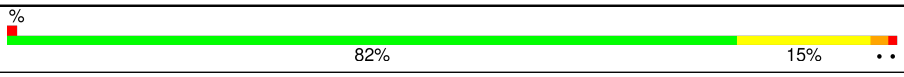
The reported resolution of this entry is 2.20 Å.

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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	605	

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
2	NAG	A	610	-	-	-	X
3	NAG	A	611	-	-	-	X
3	MAN	A	613	X	-	-	-
3	FCA	A	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	616	-	-	-	X
4	GLC	A	617	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4885 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.

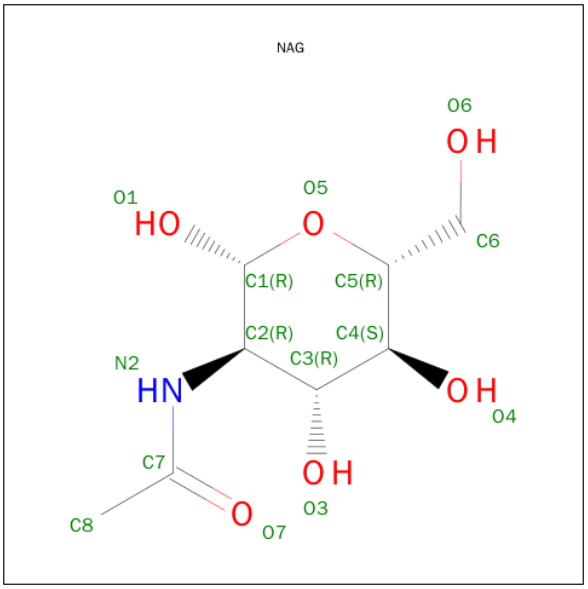
- Molecule 1 is a protein called PROTEIN (BETA-D-GLUCAN EXOHYDROLASE ISOENZYME EXO1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	602	4566	2891	787	862	26	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	LYS	ASN	CONFLICT	GB AAD23382

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

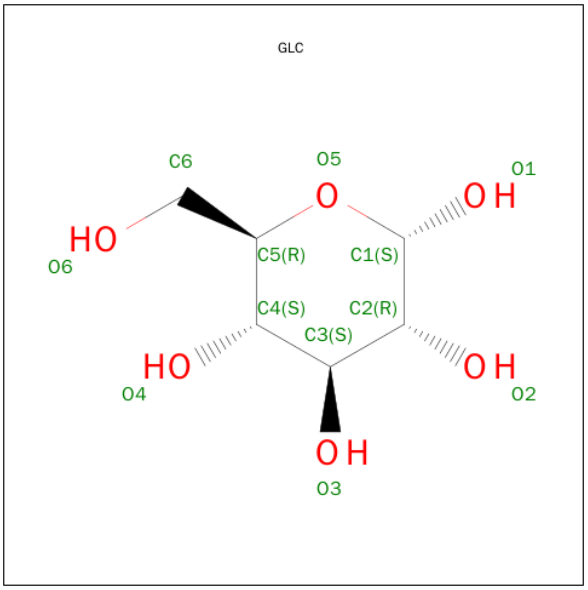


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (NAG-MAN-MAN-NAG-NAG-FC A).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	6	Total	C	N	O	0	0
			74	42	3	29		

- Molecule 4 is GLUCOSE (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



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

- Molecule 5 is water.

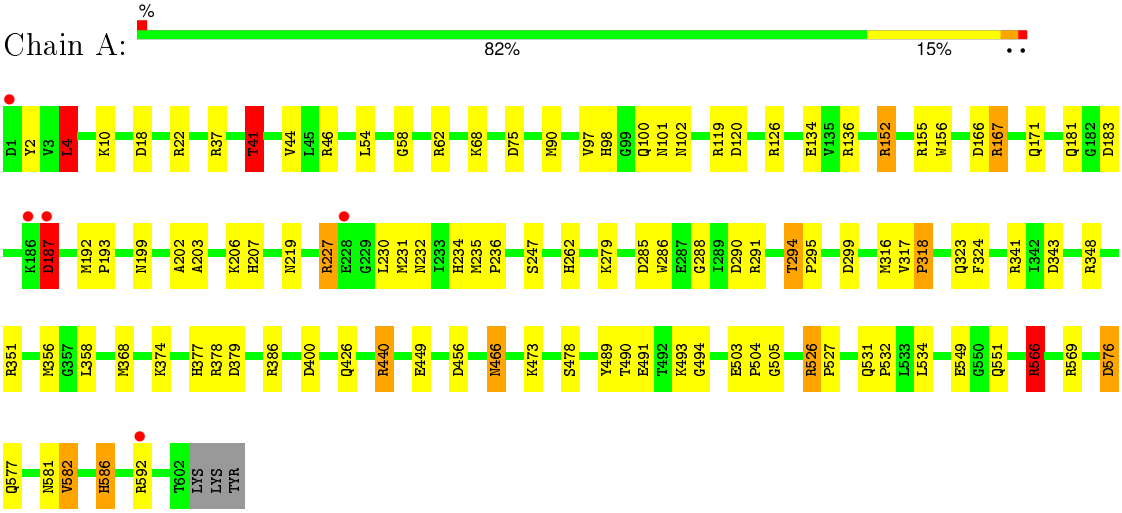
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	220	Total	O	0	0
			220	220		

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 (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: PROTEIN (BETA-D-GLUCAN EXOHYDROLASE ISOENZYME EXO1)

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	102.09Å 102.09Å 184.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 12.51 – 2.20	Depositor EDS
% Data completeness (in resolution range)	83.3 (20.00-2.20) 83.4 (12.51-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.202 0.146 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 60.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 41584 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4885	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FCA, GLC, NAG, 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	0.69	0/4663	1.47	53/6334 (0.8%)

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
3	A	6	0
All	All	6	1

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	ASP	CB-CG-OD1	13.13	130.11	118.30
1	A	152	ARG	NE-CZ-NH2	-12.92	113.84	120.30
1	A	62	ARG	NE-CZ-NH2	-12.44	114.08	120.30
1	A	386	ARG	NE-CZ-NH2	-12.33	114.13	120.30
1	A	566	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	A	22	ARG	NE-CZ-NH2	-11.33	114.63	120.30
1	A	379	ASP	CB-CG-OD1	9.79	127.11	118.30
1	A	37	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	A	440	ARG	CD-NE-CZ	9.52	136.93	123.60
1	A	566	ARG	CD-NE-CZ	9.43	136.80	123.60
1	A	343	ASP	CB-CG-OD1	9.15	126.53	118.30
1	A	449	GLU	OE1-CD-OE2	-8.68	112.89	123.30
1	A	119	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	18	ASP	CB-CG-OD2	7.76	125.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4	LEU	CA-CB-CG	7.53	132.61	115.30
1	A	119	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	566	ARG	CB-CA-C	-7.49	95.43	110.40
1	A	227	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	A	155	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	A	379	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	A	167	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	183	ASP	CB-CG-OD1	6.76	124.38	118.30
1	A	456	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	126	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	341	ARG	NE-CZ-NH1	-6.41	117.09	120.30
1	A	126	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	A	378	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	187	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	576	ASP	N-CA-CB	6.14	121.66	110.60
1	A	351	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	400	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	343	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	41	THR	N-CA-CB	-5.83	99.23	110.30
1	A	46	ARG	CD-NE-CZ	5.79	131.71	123.60
1	A	374	LYS	CA-CB-CG	5.78	126.12	113.40
1	A	166	ASP	OD1-CG-OD2	-5.72	112.43	123.30
1	A	348	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	526	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	155	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	592	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	A	75	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	37	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	378	ARG	CG-CD-NE	-5.42	100.41	111.80
1	A	576	ASP	CB-CA-C	-5.40	99.60	110.40
1	A	291	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	299	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	549	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	A	466	ASN	CA-CB-CG	-5.27	101.80	113.40
1	A	386	ARG	NH1-CZ-NH2	5.25	125.18	119.40
1	A	152	ARG	NH1-CZ-NH2	5.22	125.14	119.40
1	A	426	GLN	CA-CB-CG	5.16	124.75	113.40
1	A	120	ASP	CB-CG-OD2	-5.11	113.71	118.30
1	A	324	PHE	CB-CG-CD1	-5.09	117.24	120.80

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	613	MAN	C1
3	A	614	FCA	C2,C5,C3,C1,C4

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	ASP	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	4566	0	4551	60	0
2	A	14	0	13	0	0
3	A	74	0	64	1	0
4	A	11	0	10	2	0
5	A	220	0	0	5	0
All	All	4885	0	4638	61	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 7.

All (61) 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:181:GLN:HE21	1:A:203:ALA:H	1.20	0.88
1:A:41:THR:HG22	1:A:44:VAL:H	1.35	0.88
1:A:286:TRP:HB2	1:A:316:MET:HE1	1.56	0.87
1:A:316:MET:SD	5:A:869:HOH:O	2.34	0.84
1:A:286:TRP:HE3	1:A:316:MET:CE	1.90	0.83
1:A:58:GLY:H	1:A:102:ASN:ND2	1.81	0.78
1:A:156:TRP:HE1	1:A:219:ASN:HD22	1.32	0.77
1:A:262:HIS:HE1	1:A:285:ASP:H	1.31	0.76
1:A:4:LEU:HD13	1:A:10:LYS:HG3	1.68	0.74
1:A:566:ARG:HG3	1:A:566:ARG:HH11	1.55	0.72
1:A:54:LEU:CD1	1:A:316:MET:HE3	2.22	0.70
1:A:317:VAL:HB	1:A:318:PRO:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:TRP:CE3	1:A:316:MET:CE	2.78	0.66
1:A:286:TRP:HE3	1:A:316:MET:HE2	1.59	0.66
1:A:286:TRP:CE3	1:A:316:MET:HE2	2.30	0.65
1:A:566:ARG:HG3	1:A:566:ARG:NH1	2.12	0.65
1:A:54:LEU:HD11	1:A:316:MET:HE3	1.79	0.64
1:A:262:HIS:CE1	1:A:285:ASP:H	2.15	0.64
1:A:97:VAL:H	1:A:101:ASN:HD21	1.47	0.63
1:A:202:ALA:HB2	1:A:356:MET:HE2	1.85	0.58
1:A:58:GLY:H	1:A:102:ASN:HD21	1.51	0.58
1:A:68:LYS:HG3	5:A:852:HOH:O	2.03	0.57
1:A:316:MET:CE	4:A:617:GLC:H62	2.35	0.56
1:A:316:MET:HE3	4:A:617:GLC:H62	1.87	0.56
1:A:286:TRP:HB2	1:A:316:MET:CE	2.33	0.55
1:A:134:GLU:OE2	1:A:377:HIS:HD2	1.92	0.53
1:A:490:THR:HG22	1:A:491:GLU:HG3	1.93	0.51
1:A:136:ARG:HB3	1:A:368:MET:HE3	1.93	0.51
1:A:577:GLN:O	1:A:586:HIS:HE1	1.94	0.50
1:A:181:GLN:NE2	1:A:203:ALA:H	2.01	0.50
1:A:235:MET:N	1:A:236:PRO:CD	2.75	0.50
1:A:156:TRP:HE1	1:A:219:ASN:ND2	2.04	0.49
1:A:581:ASN:O	1:A:582:VAL:C	2.49	0.48
1:A:199:ASN:HD22	1:A:368:MET:CE	2.27	0.48
1:A:227:ARG:O	1:A:231:MET:HG2	2.14	0.47
1:A:234:HIS:HE1	5:A:872:HOH:O	1.96	0.47
1:A:54:LEU:HD11	1:A:316:MET:CE	2.43	0.47
1:A:97:VAL:H	1:A:101:ASN:ND2	2.14	0.46
1:A:192:MET:HE3	1:A:193:PRO:HD2	1.98	0.46
1:A:294:THR:HA	1:A:295:PRO:C	2.35	0.46
1:A:551:GLN:HG2	5:A:787:HOH:O	2.16	0.44
1:A:489:TYR:CD1	1:A:494:GLY:HA3	2.53	0.44
1:A:317:VAL:N	1:A:318:PRO:HA	2.32	0.44
1:A:181:GLN:HE22	1:A:247:SER:N	2.16	0.43
1:A:2:TYR:CE2	1:A:4:LEU:HB2	2.53	0.43
1:A:503:GLU:HA	1:A:504:PRO:C	2.37	0.43
1:A:206:LYS:HA	1:A:207:HIS:HA	1.85	0.43
1:A:527:PRO:HD3	1:A:569:ARG:HD3	1.99	0.43
1:A:586:HIS:H	1:A:586:HIS:CD2	2.37	0.43
1:A:181:GLN:HE22	1:A:247:SER:H	1.66	0.42
3:A:612:NAG:O3	3:A:615:MAN:H3	2.20	0.42
1:A:317:VAL:CB	1:A:318:PRO:HA	2.40	0.41
1:A:262:HIS:CE1	1:A:288:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD13	1:A:316:MET:HE3	2.01	0.41
1:A:202:ALA:HB2	1:A:356:MET:CE	2.51	0.41
1:A:526:ARG:HB2	1:A:527:PRO:HD2	2.02	0.41
1:A:134:GLU:OE2	1:A:377:HIS:CD2	2.72	0.40
1:A:167:ARG:HH11	1:A:171:GLN:HE22	1.68	0.40
1:A:286:TRP:HE3	1:A:316:MET:HE1	1.78	0.40
1:A:234:HIS:HD2	5:A:761:HOH:O	2.04	0.40
1:A:531:GLN:N	1:A:532:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

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	600/605 (99%)	574 (96%)	24 (4%)	2 (0%)	46 50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ASP
1	A	505	GLY

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	485/488 (99%)	460 (95%)	25 (5%)	29 33

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	41	THR
1	A	90	MET
1	A	98	HIS
1	A	100	GLN
1	A	152	ARG
1	A	187	ASP
1	A	230	LEU
1	A	232	ASN
1	A	279	LYS
1	A	290	ASP
1	A	294	THR
1	A	318	PRO
1	A	323	GLN
1	A	358	LEU
1	A	440	ARG
1	A	466	ASN
1	A	473	LYS
1	A	478	SER
1	A	493	LYS
1	A	534	LEU
1	A	566	ARG
1	A	576	ASP
1	A	582	VAL
1	A	586	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	102	ASN
1	A	171	GLN
1	A	181	GLN
1	A	199	ASN
1	A	219	ASN
1	A	234	HIS
1	A	262	HIS

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Mol	Chain	Res	Type
1	A	377	HIS
1	A	581	ASN
1	A	586	HIS

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)

6 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	$\#\|Z\| > 2$
3	NAG	A	611	1,3	14,14,15	1.26	1 (7%)	15,19,21	2.07	5 (33%)
3	NAG	A	612	3	14,14,15	1.15	1 (7%)	15,19,21	1.17	1 (6%)
3	MAN	A	613	3	11,11,12	0.83	0	14,15,17	1.28	2 (14%)
3	FCA	A	614	3	10,10,11	0.99	1 (10%)	14,14,16	2.04	4 (28%)
3	MAN	A	615	3	11,11,12	1.16	1 (9%)	14,15,17	1.81	4 (28%)
3	NAG	A	616	3	14,14,15	1.26	1 (7%)	15,19,21	1.71	2 (13%)

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	611	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	612	3	-	0/6/23/26	0/1/1/1
3	MAN	A	613	3	1/1/4/5	0/2/19/22	0/1/1/1
3	FCA	A	614	3	5/5/4/5	0/0/17/20	0/1/1/1
3	MAN	A	615	3	-	0/2/19/22	0/1/1/1
3	NAG	A	616	3	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	616	NAG	O7-C7	-3.85	1.14	1.23
3	A	611	NAG	O7-C7	-3.63	1.14	1.23
3	A	612	NAG	O7-C7	-3.24	1.15	1.23
3	A	614	FCA	O5-C1	-2.04	1.40	1.43
3	A	615	MAN	C1-C2	2.46	1.58	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	615	MAN	C3-C4-C5	-3.38	104.30	110.20
3	A	614	FCA	O5-C1-C2	-3.03	105.94	110.86
3	A	616	NAG	C4-C3-C2	-2.73	106.98	111.23
3	A	611	NAG	O5-C5-C6	-2.64	101.63	107.35
3	A	612	NAG	C6-C5-C4	-2.59	106.62	113.02
3	A	611	NAG	C6-C5-C4	-2.33	107.28	113.02
3	A	611	NAG	C4-C3-C2	-2.30	107.66	111.23
3	A	615	MAN	O6-C6-C5	-2.07	104.50	111.33
3	A	613	MAN	C3-C4-C5	-2.05	106.62	110.20
3	A	614	FCA	C2-C3-C4	2.19	114.77	111.04
3	A	613	MAN	O2-C2-C1	2.39	114.00	109.21
3	A	615	MAN	O3-C3-C2	2.67	114.82	110.00
3	A	614	FCA	C1-C2-C3	3.06	113.16	109.54
3	A	615	MAN	C1-O5-C5	3.54	116.74	112.25
3	A	616	NAG	C1-O5-C5	4.23	117.61	112.25
3	A	611	NAG	O3-C3-C2	4.35	117.72	109.11
3	A	611	NAG	C1-O5-C5	4.43	117.87	112.25
3	A	614	FCA	C1-O5-C5	5.21	120.43	112.38

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	613	MAN	C1

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Mol	Chain	Res	Type	Atom
3	A	614	FCA	C2
3	A	614	FCA	C5
3	A	614	FCA	C3
3	A	614	FCA	C1
3	A	614	FCA	C4

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	612	NAG	1	0
3	A	615	MAN	1	0

5.6 Ligand geometry (i)

2 ligands 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	610	1	14,14,15	1.19	1 (7%)	15,19,21	1.81	3 (20%)
4	GLC	A	617	-	11,11,12	1.81	3 (27%)	14,15,17	2.94	7 (50%)

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	610	1	-	0/6/23/26	0/1/1/1
4	GLC	A	617	-	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	610	NAG	O7-C7	-3.53	1.15	1.23
4	A	617	GLC	O5-C1	2.92	1.48	1.43
4	A	617	GLC	O4-C4	3.05	1.50	1.43
4	A	617	GLC	O6-C6	3.27	1.56	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	617	GLC	O3-C3-C4	-4.03	101.27	110.34
2	A	610	NAG	C4-C3-C2	-3.97	105.06	111.23
4	A	617	GLC	O5-C1-C2	-3.03	105.94	110.86
4	A	617	GLC	O4-C4-C5	-2.76	101.92	109.24
4	A	617	GLC	O2-C2-C3	-2.50	105.08	110.12
2	A	610	NAG	O7-C7-C8	2.21	126.12	122.06
4	A	617	GLC	O4-C4-C3	3.23	117.61	110.34
2	A	610	NAG	C1-O5-C5	3.46	116.64	112.25
4	A	617	GLC	C1-C2-C3	4.76	115.17	109.54
4	A	617	GLC	C1-O5-C5	6.33	120.28	112.25

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
4	A	617	GLC	2	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^{th} 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	602/605 (99%)	-0.94	5 (0%)	87	87	13, 23, 39, 63	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	ASP	4.0
1	A	186	LYS	3.3
1	A	228	GLU	3.1
1	A	592	ARG	2.4
1	A	1	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, 95^{th} 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	616	14/15	0.85	0.24	7.06	59,63,64,65	0
3	NAG	A	611	14/15	0.93	0.24	2.79	51,54,55,59	0
3	FCA	A	614	10/11	0.88	0.32	-	55,55,57,60	0
3	NAG	A	612	14/15	0.81	0.23	-	58,62,67,67	0
3	MAN	A	613	11/12	0.75	0.35	-	67,69,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MAN	A	615	11/12	0.75	0.27	-	63,66,67,67	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, 95^{th} 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
2	NAG	A	610	14/15	0.88	0.23	8.11	47,49,53,55	0
4	GLC	A	617	11/12	0.92	0.14	5.24	2,11,18,19	0

6.5 Other polymers

There are no such residues in this entry.