



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:46 PM GMT

PDB ID : 1QK0
Title : CEL6A (Y169F) WITH A NON-HYDROLYSABLE CELLOTETRAOSE
Authors : Zou, J.-Y.; Jones, T.A.
Deposited on : 1999-07-08
Resolution : 2.10 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

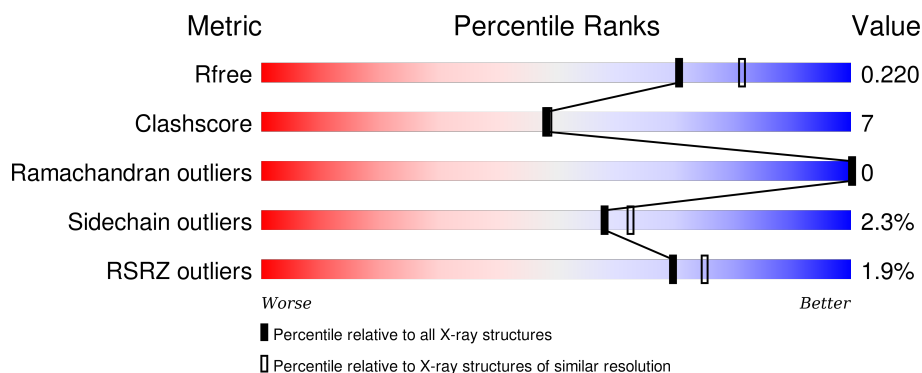
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	363	<div> <div>2%</div> <div>86%</div> <div>13%</div> </div>
1	B	363	<div> <div>2%</div> <div>81%</div> <div>18%</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
2	NAG	A	501	-	-	-	X
2	NAG	B	501	-	-	-	X
3	MAN	B	503	-	-	-	X
3	MAN	B	504	-	-	-	X
3	MAN	B	509	-	-	-	X
7	IOD	B	899	-	-	X	-
8	XYS	B	902	-	-	-	X
8	GLC	B	903	X	-	-	-

2 Entry composition [i](#)

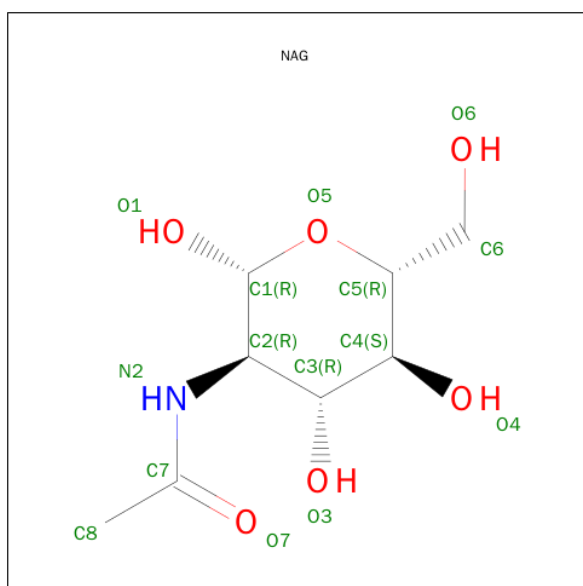
There are 9 unique types of molecules in this entry. The entry contains 6276 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CELLOBIOHYDROLASE CEL6A (FORMERLY CALLED CBH II).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2747	1743	463	531	10			
1	B	363	Total	C	N	O	S	0	0	0
			2747	1743	463	531	10			

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



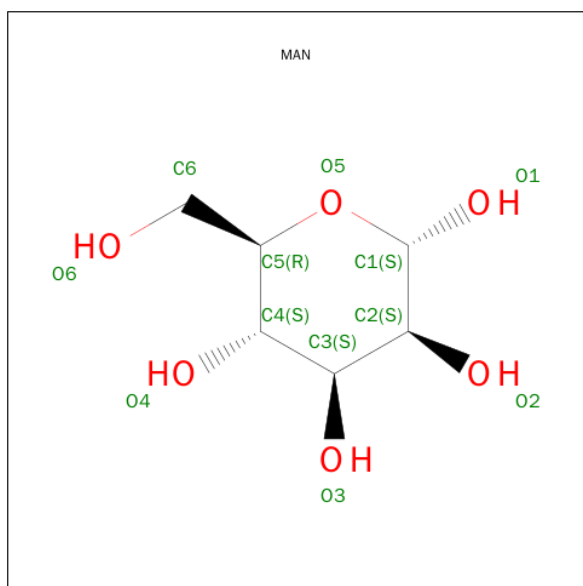
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

Continued on next page...

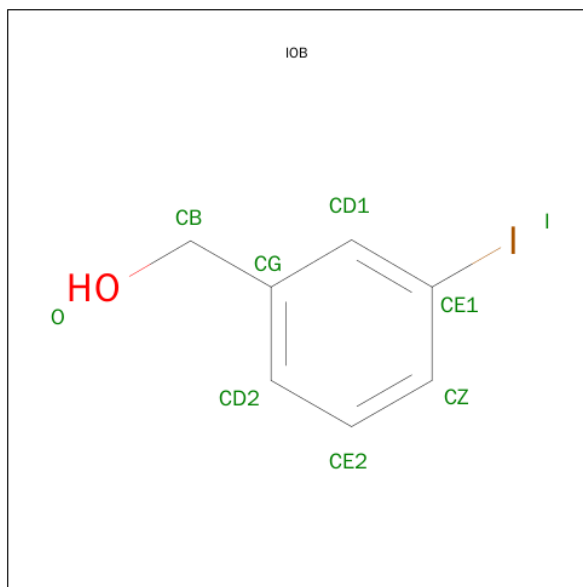
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Co	0	0
			1	1		
4	A	1	Total	Co	0	0
			1	1		

- Molecule 5 is 3-IODO-BENZYL ALCOHOL (three-letter code: IOB) (formula: C₇H₇IO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	I	O	0	0
			9	7	1	1		
5	B	1	Total	C	I	O	0	0
			9	7	1	1		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	2	Total	C	O	0	0
			20	11	9		

- Molecule 7 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	I	0	0
			1	1		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	2	Total	C	O	0	0
			20	11	9		

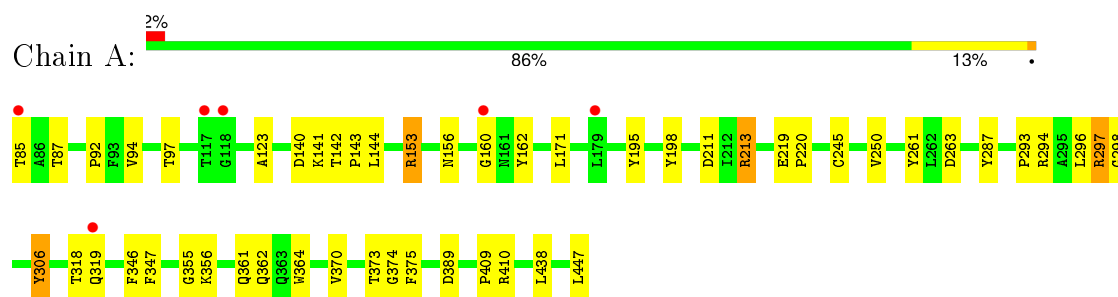
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	275	Total	O	0	0
			275	275		
9	B	236	Total	O	0	0
			236	236		

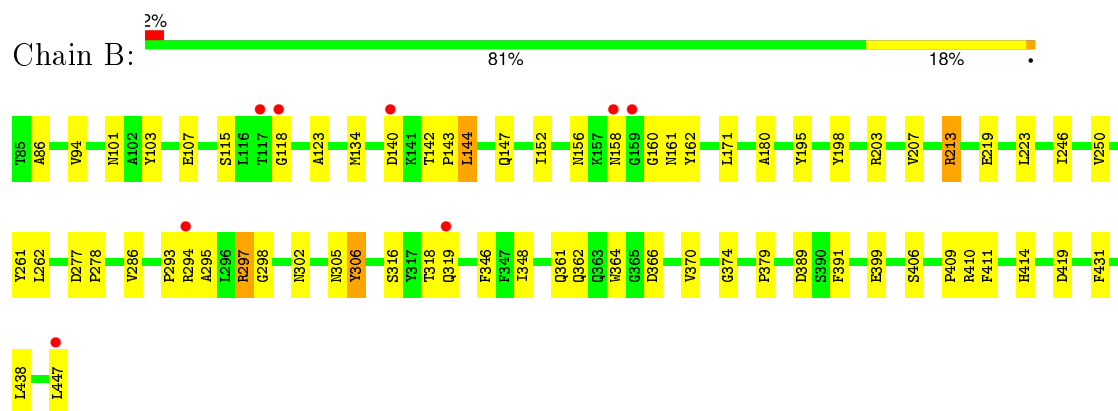
3 Residue-property plots

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: CELLOBIOHYDROLASE CEL6A (FORMERLY CALLED CBH II)



- Molecule 1: CELLOBIOHYDROLASE CEL6A (FORMERLY CALLED CBH II)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.50 Å 74.69 Å 91.14 Å 90.00° 103.19° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 39.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.10) 99.0 (39.91-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.95 (at 2.10 Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.181 , 0.221 0.178 , 0.220	Depositor DCC
R_{free} test set	1427 reflections (4.07%)	DCC
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.4	EDS
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 36535 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6276	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.70 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4819e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: XYP, XYS, CO, NAG, GLC, BGC, IOD, IOB, 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	0.32	0/2823	0.58	0/3870
1	B	0.30	0/2823	0.58	0/3870
All	All	0.31	0/5646	0.58	0/7740

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
8	B	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	903	GLC	C1

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	2747	0	2606	33	0
1	B	2747	0	2606	47	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
3	A	77	0	70	2	0
3	B	77	0	70	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	9	0	6	0	0
5	B	9	0	6	1	0
6	A	20	0	17	0	0
7	B	1	0	0	2	0
8	B	20	0	17	0	0
9	A	275	0	0	1	0
9	B	236	0	0	2	0
All	All	6276	0	5450	82	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 (82) 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:297:ARG:HD3	1:A:389:ASP:OD2	1.73	0.88
1:B:297:ARG:HD3	1:B:389:ASP:OD2	1.73	0.87
1:B:305:ASN:ND2	1:B:306:TYR:H	1.86	0.73
1:B:316:SER:HA	1:B:319:GLN:NE2	2.04	0.73
3:A:504:MAN:O2	3:A:504:MAN:H61	1.92	0.70
1:B:305:ASN:HD22	1:B:306:TYR:H	1.40	0.69
1:B:161:ASN:HB3	3:B:504:MAN:O2	1.94	0.68
1:A:261:TYR:CZ	1:A:297:ARG:HG2	2.32	0.64
1:B:362:GLN:HG2	1:B:419:ASP:HB3	1.80	0.64
1:A:153:ARG:HD2	1:A:211:ASP:OD2	1.98	0.62
1:B:134:MET:CE	1:B:144:LEU:HD22	2.31	0.60
1:A:85:THR:HB	1:A:211:ASP:HA	1.84	0.59
1:B:414:HIS:NE2	9:B:2200:HOH:O	2.32	0.59
1:B:294:ARG:HG3	1:B:295:ALA:N	2.18	0.59
1:B:134:MET:HE1	1:B:144:LEU:HD22	1.85	0.58
1:B:147:GLN:NE2	9:B:2032:HOH:O	2.36	0.57
1:B:94:VAL:O	1:B:213:ARG:NH2	2.37	0.56
1:A:297:ARG:HG3	1:A:297:ARG:O	2.04	0.56
1:A:409:PRO:O	1:A:410:ARG:HB2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:TYR:CE2	1:B:297:ARG:HG2	2.41	0.56
1:A:361:GLN:HG3	1:A:370:VAL:HG11	1.87	0.55
1:B:250:VAL:HG12	1:B:293:PRO:HG2	1.87	0.55
1:B:261:TYR:CZ	1:B:297:ARG:HG2	2.42	0.54
7:B:899:IOD:I	5:B:901:IOB:HB2	2.77	0.54
1:B:180:ALA:O	7:B:899:IOD:I	2.97	0.53
1:B:277:ASP:HB3	1:B:278:PRO:HD3	1.91	0.53
1:A:141:LYS:HE3	1:A:144:LEU:CD1	2.40	0.52
1:B:156:ASN:HA	1:B:160:GLY:O	2.11	0.51
1:A:261:TYR:CE2	1:A:297:ARG:HG2	2.44	0.51
1:B:171:LEU:HG	1:B:219:GLU:CD	2.31	0.51
1:A:250:VAL:HG12	1:A:293:PRO:HG2	1.92	0.51
1:A:250:VAL:CG1	1:A:293:PRO:HG2	2.41	0.51
1:A:140:ASP:O	1:A:143:PRO:HD2	2.11	0.51
1:B:297:ARG:O	1:B:297:ARG:HG3	2.11	0.51
1:B:103:TYR:CD1	1:B:144:LEU:HD11	2.46	0.50
1:B:361:GLN:HG3	1:B:370:VAL:HG11	1.92	0.50
1:B:366:ASP:OD2	1:B:419:ASP:OD2	2.30	0.50
1:B:140:ASP:O	1:B:143:PRO:HD2	2.13	0.49
1:B:195:TYR:O	1:B:198:TYR:HB3	2.12	0.48
1:A:94:VAL:O	1:A:213:ARG:NH2	2.44	0.48
1:A:220:PRO:HA	1:A:263:ASP:CG	2.34	0.48
1:B:374:GLY:HA2	1:B:438:LEU:HA	1.95	0.48
1:B:203:ARG:O	1:B:207:VAL:HG23	2.13	0.48
1:B:302:ASN:OD1	1:B:305:ASN:HB3	2.14	0.48
1:B:250:VAL:CG1	1:B:293:PRO:HG2	2.43	0.48
1:B:223:LEU:HD21	1:B:246:ILE:HD12	1.96	0.47
1:B:123:ALA:HB2	1:B:447:LEU:HD23	1.96	0.47
1:A:374:GLY:HA2	1:A:438:LEU:HA	1.95	0.47
1:B:262:LEU:HD11	1:B:286:VAL:HG11	1.96	0.47
1:B:115:SER:HB3	3:B:508:MAN:H5	1.96	0.47
1:A:287:TYR:HD1	1:A:296:LEU:HD23	1.81	0.46
1:A:298:GLY:HA3	1:A:346:PHE:O	2.16	0.46
1:A:318:THR:HA	1:A:364:TRP:CE3	2.52	0.45
1:A:195:TYR:O	1:A:198:TYR:HB3	2.17	0.45
1:A:87:THR:HB	3:A:503:MAN:H2	1.73	0.45
1:B:261:TYR:CE2	1:B:348:ILE:HG23	2.52	0.45
1:B:142:THR:OG1	1:B:143:PRO:HD3	2.17	0.45
1:B:118:GLY:O	3:B:509:MAN:H2	2.18	0.44
1:A:141:LYS:HE3	1:A:144:LEU:HD12	1.99	0.44
1:B:101:ASN:OD1	1:B:103:TYR:HB3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:TYR:CD2	1:A:373:THR:HG21	2.53	0.44
1:A:171:LEU:HG	1:A:219:GLU:CD	2.38	0.43
1:B:362:GLN:HA	1:B:362:GLN:HE21	1.84	0.43
1:A:195:TYR:CD2	1:A:245:CYS:HB3	2.53	0.43
1:B:298:GLY:HA3	1:B:346:PHE:O	2.18	0.43
1:A:92:PRO:HD3	1:A:297:ARG:HD2	2.00	0.43
1:A:97:THR:O	1:A:162:TYR:HA	2.19	0.43
1:B:409:PRO:O	1:B:410:ARG:HB2	2.19	0.43
1:A:355:GLY:HA3	1:A:375:PHE:O	2.18	0.43
1:A:156:ASN:HA	1:A:160:GLY:CA	2.50	0.42
1:B:152:ILE:HG23	1:B:162:TYR:HB2	2.01	0.42
1:A:141:LYS:HE3	1:A:144:LEU:HD13	2.01	0.42
1:B:107:GLU:OE1	1:B:399:GLU:OE2	2.38	0.42
1:B:318:THR:HA	1:B:364:TRP:CE3	2.55	0.42
1:A:142:THR:OG1	1:A:143:PRO:HD3	2.20	0.41
1:A:356:LYS:HE3	9:A:2200:HOH:O	2.19	0.41
1:A:347:PHE:N	1:A:347:PHE:CD1	2.88	0.41
1:A:123:ALA:HB2	1:A:447:LEU:HD23	2.02	0.41
1:B:406:SER:HA	1:B:411:PHE:CG	2.56	0.41
1:B:86:ALA:O	1:B:213:ARG:HD3	2.21	0.41
1:B:379:PRO:HA	1:B:391:PHE:O	2.21	0.41
1:B:115:SER:HB3	3:B:508:MAN:C5	2.52	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	361/363 (99%)	346 (96%)	15 (4%)	0	100	100
1	B	361/363 (99%)	347 (96%)	14 (4%)	0	100	100
All	All	722/726 (99%)	693 (96%)	29 (4%)	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	284/284 (100%)	277 (98%)	7 (2%)	55	59
1	B	284/284 (100%)	278 (98%)	6 (2%)	61	66
All	All	568/568 (100%)	555 (98%)	13 (2%)	58	62

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ARG
1	A	213	ARG
1	A	294	ARG
1	A	297	ARG
1	A	306	TYR
1	A	319	GLN
1	A	362	GLN
1	B	144	LEU
1	B	158	ASN
1	B	213	ARG
1	B	297	ARG
1	B	306	TYR
1	B	431	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	237	ASN
1	A	239	GLN
1	A	339	ASN
1	B	147	GLN
1	B	158	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	197	ASN
1	B	237	ASN
1	B	239	GLN
1	B	305	ASN
1	B	362	GLN
1	B	422	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 ⓘ

4 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$
6	XYP	A	902	5,6	9,9,10	0.59	0	12,12,14	0.81	0
6	BGC	A	903	6	11,11,12	0.42	0	14,15,17	0.76	1 (7%)
8	XYS	B	902	8,5	9,9,10	0.89	0	12,12,14	1.72	3 (25%)
8	GLC	B	903	8	11,11,12	0.45	0	14,15,17	0.78	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
6	XYP	A	902	5,6	-	0/0/14/17	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BGC	A	903	6	-	0/2/19/22	0/1/1/1
8	XYS	B	902	8,5	-	0/0/14/17	0/1/1/1
8	GLC	B	903	8	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	903	GLC	C1-O5-C5	2.04	114.84	112.25
6	A	903	BGC	C1-O5-C5	2.25	115.11	112.25
8	B	902	XYS	O5-C1-C2	2.58	115.12	110.31
8	B	902	XYS	C5-O5-C1	3.00	116.40	111.57
8	B	902	XYS	C1-C2-C3	3.96	114.23	109.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	903	GLC	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 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	501	1	14,14,15	0.45	0	15,19,21	0.97	2 (13%)
2	NAG	A	502	1	14,14,15	0.48	0	15,19,21	0.84	1 (6%)
3	MAN	A	503	1	11,11,12	0.51	0	14,15,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	A	504	1	11,11,12	0.54	0	14,15,17	1.15	1 (7%)
3	MAN	A	505	1	11,11,12	0.53	0	14,15,17	0.75	1 (7%)
3	MAN	A	506	1	11,11,12	0.52	0	14,15,17	0.71	0
3	MAN	A	507	1	11,11,12	0.47	0	14,15,17	0.80	1 (7%)
3	MAN	A	508	1	11,11,12	0.46	0	14,15,17	0.67	0
3	MAN	A	509	1	11,11,12	0.52	0	14,15,17	0.70	0
5	IOB	A	901	6	9,9,9	1.39	1 (11%)	11,11,11	0.80	0
2	NAG	B	501	1	14,14,15	0.50	0	15,19,21	0.81	0
2	NAG	B	502	1	14,14,15	0.49	0	15,19,21	0.71	0
3	MAN	B	503	1	11,11,12	0.46	0	14,15,17	0.67	0
3	MAN	B	504	1	11,11,12	0.45	0	14,15,17	0.62	0
3	MAN	B	505	1	11,11,12	0.50	0	14,15,17	0.81	1 (7%)
3	MAN	B	506	1	11,11,12	0.53	0	14,15,17	0.69	0
3	MAN	B	507	1	11,11,12	0.47	0	14,15,17	0.70	0
3	MAN	B	508	1	11,11,12	0.48	0	14,15,17	0.70	0
3	MAN	B	509	1	11,11,12	0.49	0	14,15,17	0.71	1 (7%)
5	IOB	B	901	8	9,9,9	1.66	1 (11%)	11,11,11	0.94	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	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	MAN	A	503	1	-	0/2/19/22	0/1/1/1
3	MAN	A	504	1	-	0/2/19/22	1/1/1/1
3	MAN	A	505	1	-	0/2/19/22	0/1/1/1
3	MAN	A	506	1	-	0/2/19/22	0/1/1/1
3	MAN	A	507	1	-	0/2/19/22	0/1/1/1
3	MAN	A	508	1	-	0/2/19/22	0/1/1/1
3	MAN	A	509	1	-	0/2/19/22	0/1/1/1
5	IOB	A	901	6	-	0/2/2/2	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	502	1	-	0/6/23/26	0/1/1/1
3	MAN	B	503	1	-	0/2/19/22	0/1/1/1
3	MAN	B	504	1	-	0/2/19/22	0/1/1/1
3	MAN	B	505	1	-	0/2/19/22	0/1/1/1
3	MAN	B	506	1	-	0/2/19/22	0/1/1/1
3	MAN	B	507	1	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	B	508	1	-	0/2/19/22	0/1/1/1
3	MAN	B	509	1	-	0/2/19/22	0/1/1/1
5	IOB	B	901	8	-	0/2/2/2	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	IOB	CD1-CE1	2.60	1.43	1.38
5	B	901	IOB	CD1-CE1	2.68	1.43	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	NAG	C2-N2-C7	-2.28	120.11	123.04
2	A	501	NAG	C2-N2-C7	-2.22	120.19	123.04
3	B	509	MAN	C1-O5-C5	2.03	114.82	112.25
3	A	505	MAN	C1-O5-C5	2.17	115.00	112.25
2	A	501	NAG	C1-O5-C5	2.38	115.26	112.25
3	B	505	MAN	C1-O5-C5	2.40	115.29	112.25
3	A	507	MAN	C1-O5-C5	2.41	115.31	112.25
5	B	901	IOB	O-CB-CG	2.42	121.71	111.77
3	A	504	MAN	C1-O5-C5	3.85	117.13	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	MAN	1	0
3	A	504	MAN	1	0
3	B	504	MAN	1	0
3	B	508	MAN	2	0
3	B	509	MAN	1	0
5	B	901	IOB	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	363/363 (100%)	-0.12	6 (1%) 73 78	10, 15, 24, 34	0
1	B	363/363 (100%)	-0.09	8 (2%) 65 71	11, 18, 27, 40	0
All	All	726/726 (100%)	-0.11	14 (1%) 70 75	10, 16, 25, 40	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	158	ASN	6.3
1	B	159	GLY	3.9
1	B	447	LEU	2.8
1	A	85	THR	2.6
1	A	160	GLY	2.5
1	B	294	ARG	2.5
1	A	118	GLY	2.4
1	A	319	GLN	2.3
1	B	140	ASP	2.3
1	A	117	THR	2.2
1	B	319	GLN	2.2
1	B	117	THR	2.2
1	A	179	LEU	2.2
1	B	118	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
8	XYS	B	902	9/10	0.92	0.13	3.99	21,23,24,25	0
8	GLC	B	903	11/12	0.95	0.11	0.47	18,18,19,19	0
6	BGC	A	903	11/12	0.97	0.11	0.00	15,16,17,17	0
6	XYP	A	902	9/10	0.94	0.10	-0.39	18,18,19,19	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MAN	B	509	11/12	0.68	0.46	12.84	35,37,38,38	0
2	NAG	B	501	14/15	0.90	0.23	5.27	31,32,33,33	0
2	NAG	A	501	14/15	0.84	0.23	4.46	30,31,33,34	0
3	MAN	B	503	11/12	0.88	0.17	2.10	30,31,31,32	0
3	MAN	B	504	11/12	0.78	0.35	2.01	29,32,33,33	0
5	IOB	B	901	9/9	0.98	0.12	1.78	28,31,32,34	0
3	MAN	A	504	11/12	0.79	0.25	1.65	27,29,30,30	0
3	MAN	A	509	11/12	0.76	0.20	0.38	28,28,29,30	0
3	MAN	A	507	11/12	0.92	0.12	0.26	23,24,24,26	0
3	MAN	B	506	11/12	0.94	0.16	0.20	23,23,24,24	0
3	MAN	A	506	11/12	0.91	0.12	0.10	19,20,22,22	0
7	IOD	B	899	1/1	1.00	0.10	-0.10	46,46,46,46	0
2	NAG	B	502	14/15	0.94	0.10	-0.34	20,21,22,22	0
2	NAG	A	502	14/15	0.94	0.11	-0.37	16,17,19,20	0
5	IOB	A	901	9/9	0.99	0.10	-0.44	20,21,22,24	0
3	MAN	A	503	11/12	0.62	0.34	-	36,38,39,40	0
3	MAN	A	505	11/12	0.90	0.11	-	21,22,22,22	0
3	MAN	B	508	11/12	0.82	0.22	-	35,36,37,38	0
3	MAN	B	507	11/12	0.88	0.18	-	27,28,28,29	0
4	CO	A	900	1/1	0.96	0.05	-	32,32,32,32	0
3	MAN	A	508	11/12	0.95	0.09	-	19,19,20,20	0
4	CO	B	900	1/1	0.96	0.05	-	43,43,43,43	0
3	MAN	B	505	11/12	0.90	0.13	-	24,25,25,26	0

6.5 Other polymers

There are no such residues in this entry.