Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2023 – 08:12 AM EDT

PDB ID	:	3POC
Title	:	The crystal structure of the D307A mutant of alpha-Glucosidase (FAMILY 31) from Ruminococcus obeum ATCC 29174 in complex with acarbose
Authors	:	Tan, K.; Tesar, C.; Wilton, R.; Keigher, L.; Babnigg, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2010-11-22
Resolution	:	1.99 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

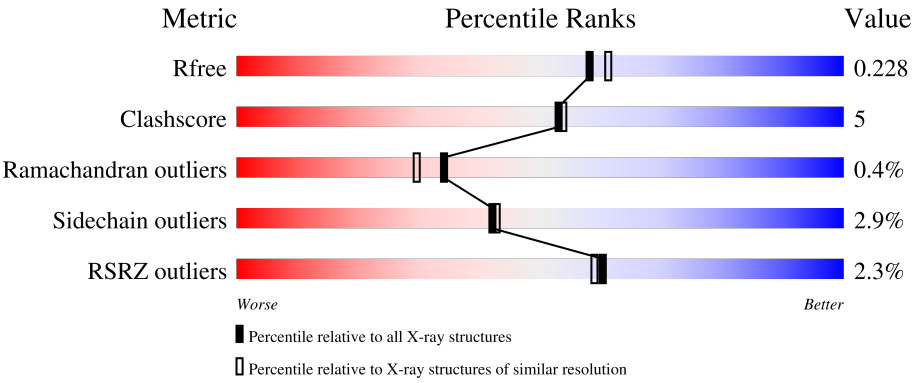
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

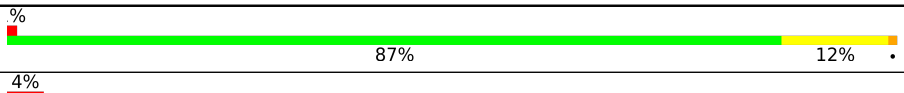
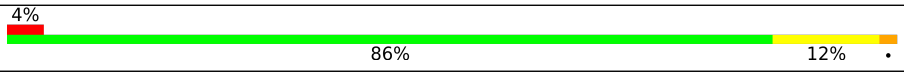
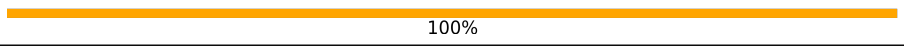
The reported resolution of this entry is 1.99 Å.

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	666	
1	B	666	
2	C	3	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11497 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 alpha-Glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	2	0
			5447	3496	895	1021	35			
1	B	664	Total	C	N	O	S	0	3	0
			5448	3496	892	1024	36			

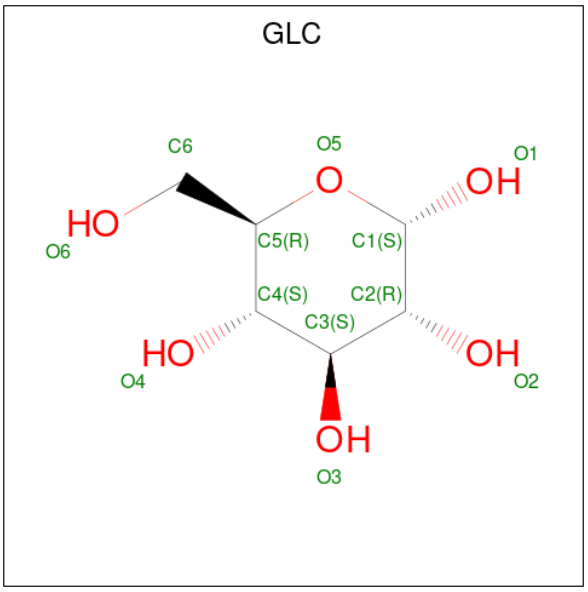
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A5ZY13
A	-1	ASN	-	expression tag	UNP A5ZY13
A	0	ALA	-	expression tag	UNP A5ZY13
A	307	ALA	ASP	engineered mutation	UNP A5ZY13
B	-2	SER	-	expression tag	UNP A5ZY13
B	-1	ASN	-	expression tag	UNP A5ZY13
B	0	ALA	-	expression tag	UNP A5ZY13
B	307	ALA	ASP	engineered mutation	UNP A5ZY13

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

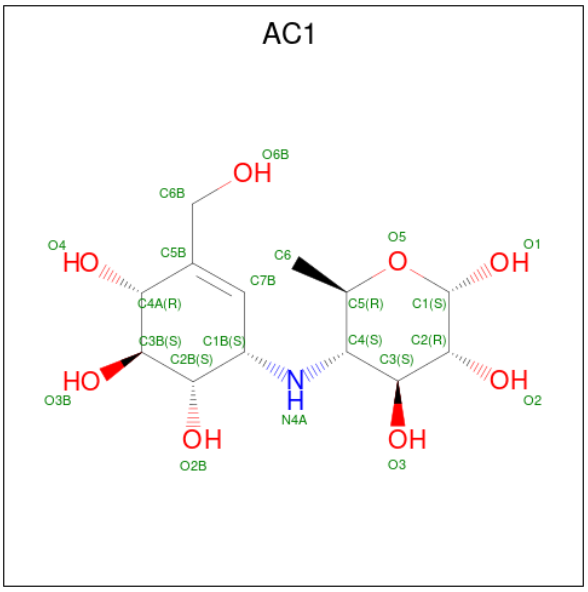
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 3 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



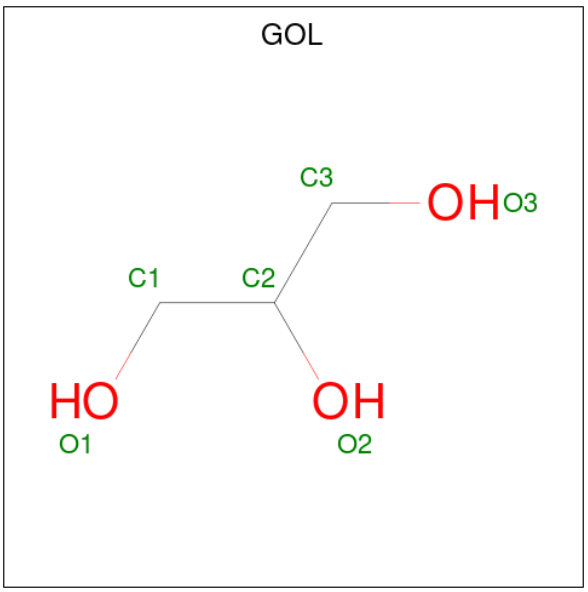
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0

- Molecule 4 is 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose (three-letter code: AC1) (formula: $C_{13}H_{23}NO_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 12 7 1 4	0	0
4	B	1	Total C N O 12 7 1 4	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

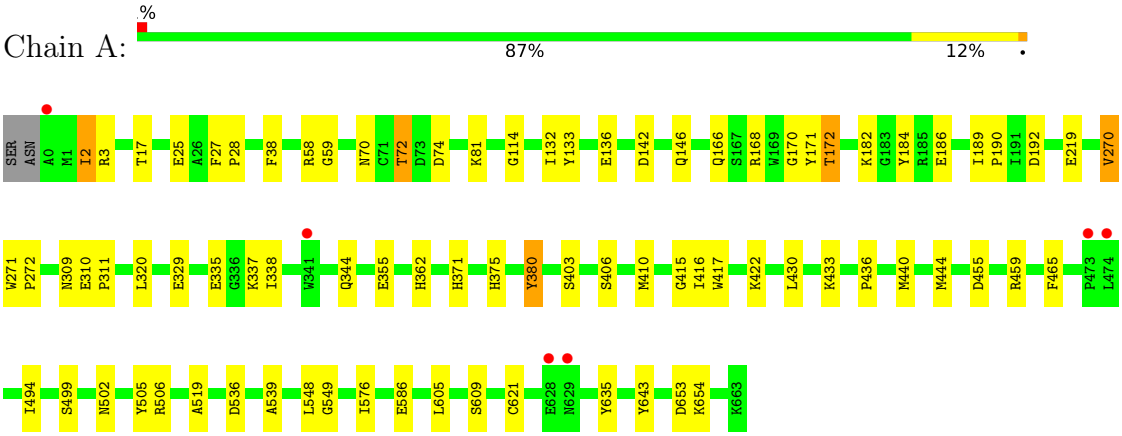
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	282	Total O 282 282	0	0
6	B	234	Total O 234 234	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

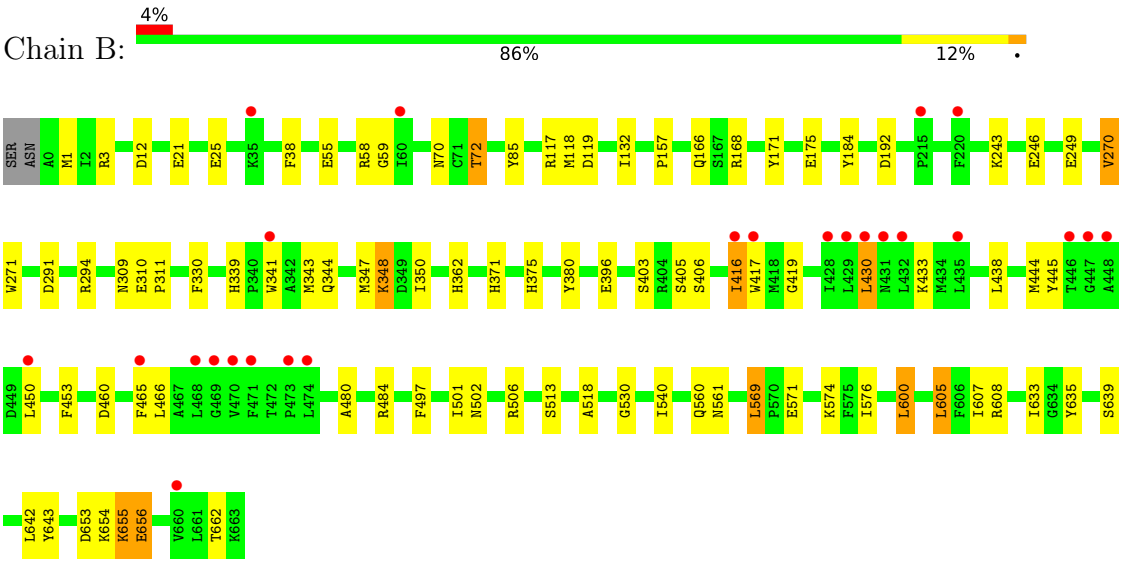
• Molecule 1: alpha-Glucosidase

Chain A:



• Molecule 1: alpha-Glucosidase

Chain B:



• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:


GLC1
GLC2
AC13

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.95Å 125.69Å 87.97Å 90.00° 107.62° 90.00°	Depositor
Resolution (Å)	41.37 – 1.99 41.36 – 1.99	Depositor EDS
% Data completeness (in resolution range)	84.1 (41.37-1.99) 95.1 (41.36-1.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.168 , 0.225 0.177 , 0.228	Depositor DCC
R_{free} test set	4584 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.877	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11497	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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, 0.333 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: GLC, GOL, AC1

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	0.37	0/5596	0.53	0/7543
1	B	0.34	0/5597	0.51	0/7546
All	All	0.35	0/11193	0.52	0/15089

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5447	0	5226	52	0
1	B	5448	0	5220	65	0
2	C	44	0	30	4	0
3	A	12	0	12	0	0
4	A	12	0	8	0	0
4	B	12	0	8	0	0
5	A	6	0	8	2	0
6	A	282	0	0	4	0
6	B	234	0	0	3	0
All	All	11497	0	10512	115	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 5.

All (115) 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:189:ILE:HD11	1:A:494:ILE:HD11	1.71	0.73
1:A:70:ASN:O	1:A:72:THR:HG23	1.89	0.72
1:B:270:VAL:HG12	1:B:271:TRP:H	1.53	0.72
1:B:655:LYS:HD3	1:B:656:GLU:N	2.05	0.72
1:B:330:PHE:CB	1:B:343:MET:HE3	2.22	0.69
1:A:170:GLY:O	1:A:172:THR:HG23	1.94	0.68
1:B:576:ILE:HB	1:B:605:LEU:HD12	1.77	0.67
6:A:859:HOH:O	1:B:118[A]:MET:HG2	1.96	0.66
1:B:396:GLU:OE2	2:C:2:GLC:H62	1.96	0.65
1:A:310:GLU:N	1:A:311:PRO:HA	2.13	0.64
1:A:621:CYS:SG	5:A:665:GOL:H31	2.38	0.64
1:B:362:HIS:NE2	1:B:371:HIS:HD2	1.95	0.64
1:B:310:GLU:N	1:B:311:PRO:HA	2.13	0.63
1:B:118[B]:MET:HG2	1:B:119:ASP:N	2.14	0.62
1:B:330:PHE:HB2	1:B:343:MET:HE3	1.82	0.61
1:A:219:GLU:HB2	6:A:902:HOH:O	2.01	0.60
1:B:70:ASN:O	1:B:72:THR:HG23	2.02	0.60
1:A:371:HIS:HE1	1:A:375:HIS:ND1	2.00	0.59
1:B:502:ASN:O	1:B:506:ARG:HG3	2.03	0.59
1:A:362:HIS:NE2	1:A:371:HIS:HD2	1.99	0.59
1:B:38:PHE:CZ	1:B:132:ILE:HD11	2.38	0.59
1:B:571:GLU:OE2	1:B:608:ARG:HD2	2.01	0.59
1:A:605:LEU:C	1:A:605:LEU:HD12	2.24	0.58
1:B:59:GLY:HA2	1:B:433:LYS:HD3	1.85	0.57
1:A:621:CYS:SG	5:A:665:GOL:C3	2.92	0.57
1:B:406:SER:OG	1:B:416:ILE:HD11	2.04	0.57
1:B:70:ASN:O	1:B:72:THR:CG2	2.53	0.57
1:B:168:ARG:HB3	1:B:171:TYR:CE1	2.39	0.57
1:B:653:ASP:HB2	2:C:1:GLC:O2	2.03	0.57
1:B:453:PHE:CZ	1:B:480:ALA:HB2	2.40	0.56
1:B:371:HIS:HE1	1:B:375:HIS:ND1	2.03	0.56
1:A:410:MET:CE	1:A:416:ILE:HD11	2.36	0.56
1:B:1:MET:CE	1:B:3:ARG:HG3	2.36	0.56
1:B:576:ILE:HB	1:B:605:LEU:CD1	2.36	0.55
1:A:609:SER:HA	1:A:635:TYR:CE2	2.42	0.55
1:B:497:PHE:O	1:B:501:ILE:HG12	2.07	0.54
1:B:655:LYS:HD3	1:B:656:GLU:H	1.73	0.54
1:A:371:HIS:CE1	1:A:375:HIS:ND1	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLY:HA2	1:A:433:LYS:HD3	1.90	0.54
1:B:55:GLU:HB2	1:B:438:LEU:HD21	1.90	0.54
1:B:639:SER:OG	1:B:662:THR:HG22	2.09	0.53
1:B:453:PHE:CE1	1:B:480:ALA:HB2	2.44	0.52
1:B:460:ASP:HB3	1:B:600:LEU:HD11	1.91	0.52
1:A:436:PRO:O	1:A:440:MET:HG3	2.09	0.52
1:A:410:MET:HE1	1:A:416:ILE:HD11	1.91	0.52
1:B:344:GLN:HG3	6:B:667:HOH:O	2.09	0.52
1:B:569:LEU:HD23	1:B:569:LEU:N	2.25	0.52
1:A:2:ILE:HD11	1:A:133:TYR:HD1	1.73	0.52
1:A:548:LEU:HD23	1:A:549:GLY:N	2.26	0.51
1:B:21:GLU:HG2	6:B:741:HOH:O	2.08	0.51
1:A:190:PRO:HB2	1:A:505:TYR:CE1	2.47	0.50
1:A:422:LYS:HD2	1:A:455:ASP:OD2	2.12	0.50
1:A:415:GLY:O	1:A:416:ILE:HD13	2.11	0.50
1:A:309:ASN:ND2	1:A:403:SER:OG	2.44	0.50
1:A:410:MET:HE1	1:A:416:ILE:CD1	2.43	0.49
1:A:403:SER:HB3	1:A:410:MET:HE1	1.95	0.49
1:B:168:ARG:HB3	1:B:171:TYR:CZ	2.48	0.49
1:A:406:SER:HB3	1:A:416:ILE:HD11	1.94	0.48
1:A:444:MET:HE1	1:A:519:ALA:HA	1.95	0.48
1:B:484:ARG:HD3	6:B:868:HOH:O	2.12	0.48
1:A:114:GLY:HA3	6:A:836:HOH:O	2.12	0.48
1:B:166:GLN:NE2	1:B:184:TYR:OH	2.46	0.48
1:A:344:GLN:NE2	1:B:348:LYS:HG2	2.29	0.47
1:A:499:SER:HB3	6:A:803:HOH:O	2.13	0.47
1:A:166:GLN:NE2	1:A:184:TYR:OH	2.43	0.47
1:B:444:MET:HE1	1:B:518:ALA:HB3	1.97	0.47
1:B:270:VAL:HG12	1:B:271:TRP:N	2.27	0.47
1:B:309:ASN:ND2	1:B:403:SER:OG	2.47	0.47
1:A:459:ARG:HD3	1:B:118[A]:MET:SD	2.54	0.47
1:A:335:GLU:HB2	1:A:337:LYS:HE2	1.96	0.46
1:B:38:PHE:HZ	1:B:132:ILE:HD11	1.77	0.46
1:B:85:TYR:CE2	1:B:419:GLY:HA3	2.50	0.46
1:A:271:TRP:N	1:A:272:PRO:CD	2.79	0.46
1:A:81:LYS:HA	1:A:81:LYS:HD2	1.71	0.46
1:A:344:GLN:HE22	1:B:348:LYS:HG2	1.80	0.45
1:B:1:MET:HE1	1:B:3:ARG:HG3	1.97	0.45
1:B:605:LEU:HD12	1:B:605:LEU:C	2.37	0.45
1:B:117:ARG:HG2	1:B:119:ASP:OD1	2.16	0.45
1:A:182:LYS:HE3	1:A:186:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLU:N	1:B:311:PRO:CA	2.80	0.45
1:B:371:HIS:CE1	1:B:375:HIS:ND1	2.85	0.45
1:B:406:SER:CB	1:B:416:ILE:HD11	2.47	0.45
1:A:38:PHE:CZ	1:A:132:ILE:HD11	2.51	0.44
1:B:430:LEU:HD23	1:B:430:LEU:HA	1.81	0.44
1:B:157:PRO:HG3	1:B:445:TYR:CD1	2.53	0.44
1:A:27:PHE:HA	1:A:28:PRO:HD3	1.71	0.43
1:A:329:GLU:HB3	1:A:338:ILE:CD1	2.47	0.43
1:A:74:ASP:OD1	1:A:81:LYS:HE2	2.18	0.43
1:B:513:SER:HB2	1:B:642:LEU:HD12	1.99	0.43
1:A:310:GLU:N	1:A:311:PRO:CA	2.81	0.43
1:A:643:TYR:CD2	1:A:643:TYR:C	2.91	0.43
1:A:136:GLU:O	1:A:146:GLN:NE2	2.52	0.43
1:A:576:ILE:CD1	1:A:586:GLU:HG2	2.48	0.43
1:B:450:LEU:HD13	1:B:466:LEU:HD23	2.01	0.42
1:B:243:LYS:HE2	1:B:249:GLU:OE2	2.19	0.42
1:A:502:ASN:O	1:A:506:ARG:HG3	2.19	0.42
1:B:117:ARG:HD3	1:B:119:ASP:OD1	2.19	0.42
1:A:536:ASP:HB3	1:A:539:ALA:HB3	2.01	0.42
1:B:530:GLY:HA2	1:B:540:ILE:HG22	2.00	0.42
1:A:2:ILE:HD12	1:A:3:ARG:N	2.34	0.42
2:C:3:AC1:O2B	2:C:3:AC1:C4	2.68	0.41
1:B:560:GLN:O	1:B:561:ASN:HB2	2.20	0.41
1:A:380:TYR:CD1	1:A:380:TYR:C	2.93	0.41
1:B:339:HIS:CG	1:B:341:TRP:CZ2	3.09	0.41
1:B:571:GLU:OE2	1:B:608:ARG:CD	2.67	0.41
1:B:574:LYS:HG3	1:B:635:TYR:CE2	2.55	0.41
1:A:70:ASN:O	1:A:72:THR:CG2	2.63	0.41
1:B:607:ILE:CD1	1:B:633:ILE:HG22	2.50	0.41
1:A:168:ARG:HB3	1:A:171:TYR:CE1	2.55	0.41
1:A:142:ASP:O	1:A:146:GLN:HG3	2.21	0.41
1:A:410:MET:HE2	1:A:416:ILE:HD11	2.03	0.41
1:B:291:ASP:HB3	1:B:294:ARG:NH1	2.36	0.41
1:B:347:MET:O	1:B:350:ILE:HG12	2.21	0.40
1:B:396:GLU:CD	2:C:2:GLC:H62	2.41	0.40
1:B:643:TYR:CD2	1:B:643:TYR:C	2.94	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	664/666 (100%)	636 (96%)	25 (4%)	3 (0%)	29	23
1	B	665/666 (100%)	632 (95%)	31 (5%)	2 (0%)	41	37
All	All	1329/1332 (100%)	1268 (95%)	56 (4%)	5 (0%)	34	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	654	LYS
1	A	58	ARG
1	B	58	ARG
1	A	270	VAL
1	B	270	VAL

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	573/574 (100%)	559 (98%)	14 (2%)	49	51
1	B	574/574 (100%)	555 (97%)	19 (3%)	38	37
All	All	1147/1148 (100%)	1114 (97%)	33 (3%)	42	43

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE

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Mol	Chain	Res	Type
1	A	17	THR
1	A	25	GLU
1	A	72	THR
1	A	172	THR
1	A	192	ASP
1	A	270	VAL
1	A	320	LEU
1	A	355	GLU
1	A	380	TYR
1	A	417	TRP
1	A	430	LEU
1	A	465	PHE
1	A	653	ASP
1	B	12	ASP
1	B	25	GLU
1	B	72	THR
1	B	175	GLU
1	B	192	ASP
1	B	246	GLU
1	B	348	LYS
1	B	380	TYR
1	B	405	SER
1	B	416	ILE
1	B	417	TRP
1	B	430	LEU
1	B	465	PHE
1	B	569	LEU
1	B	600	LEU
1	B	605	LEU
1	B	654	LYS
1	B	655	LYS
1	B	656	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	344	GLN
1	A	371	HIS
1	B	89	ASN
1	B	166	GLN
1	B	306	ASN

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Mol	Chain	Res	Type
1	B	344	GLN
1	B	371	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)

3 monosaccharides 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	GLC	C	1	2	12,12,12	0.51	0	17,17,17	1.44	3 (17%)
2	GLC	C	2	2	11,11,12	0.39	0	15,15,17	1.75	3 (20%)
2	AC1	C	3	2	21,22,23	0.77	0	22,32,34	1.66	4 (18%)

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	GLC	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	AC1	C	3	2	-	2/6/43/46	0/2/2/2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	GLC	C1-O5-C5	5.53	119.68	112.19
2	C	3	AC1	C1-O5-C5	3.88	121.57	112.78
2	C	3	AC1	C1-C2-C3	3.37	113.81	109.67
2	C	1	GLC	O1-C1-O5	-3.34	100.34	110.38
2	C	1	GLC	C4-C3-C2	-3.12	105.38	110.82
2	C	3	AC1	C2B-C3B-C4A	3.06	115.03	110.18
2	C	2	GLC	C1-C2-C3	2.90	113.23	109.67
2	C	1	GLC	O4-C4-C3	2.88	117.01	110.35
2	C	3	AC1	O5-C1-C2	2.28	114.30	110.77
2	C	2	GLC	O5-C1-C2	2.01	113.88	110.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	AC1	C7B-C5B-C6B-O6B
2	C	1	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	C	3	AC1	C2B-C1B-N4A-C4

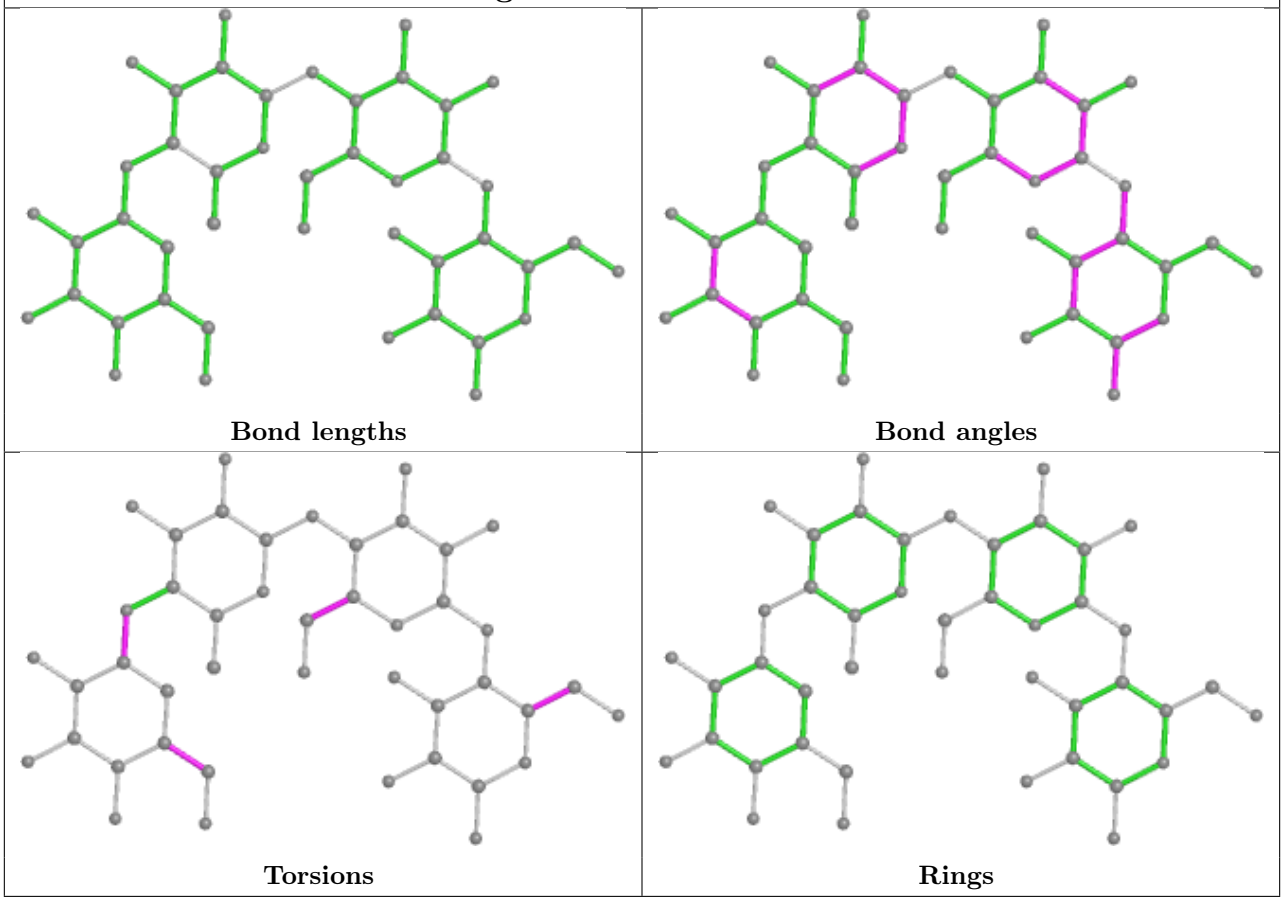
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	AC1	1	0
2	C	2	GLC	2	0
2	C	1	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C



5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
4	AC1	B	664	-	12,12,23	0.76	0	11,17,34	1.57	2 (18%)
3	GLC	A	664	-	12,12,12	0.54	0	17,17,17	1.03	1 (5%)
5	GOL	A	665	-	5,5,5	0.34	0	5,5,5	0.33	0
4	AC1	A	664(A)	-	12,12,23	0.79	0	11,17,34	1.86	2 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AC1	B	664	-	-	0/2/22/46	0/1/1/2
3	GLC	A	664	-	-	2/2/22/22	0/1/1/1
5	GOL	A	665	-	-	2/4/4/4	-
4	AC1	A	664(A)	-	-	1/2/22/46	0/1/1/2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	664(A)	AC1	O6B-C6B-C5B	-4.90	100.76	112.50
4	B	664	AC1	O6B-C6B-C5B	-3.73	103.57	112.50
3	A	664	GLC	O1-C1-O5	-3.59	99.60	110.38
4	A	664(A)	AC1	C7B-C1B-N4A	-2.74	105.77	110.71
4	B	664	AC1	C7B-C1B-N4A	-2.51	106.19	110.71

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	664(A)	AC1	C7B-C5B-C6B-O6B
5	A	665	GOL	O1-C1-C2-O2
3	A	664	GLC	O5-C5-C6-O6
3	A	664	GLC	C4-C5-C6-O6
5	A	665	GOL	O1-C1-C2-C3

There are no ring outliers.

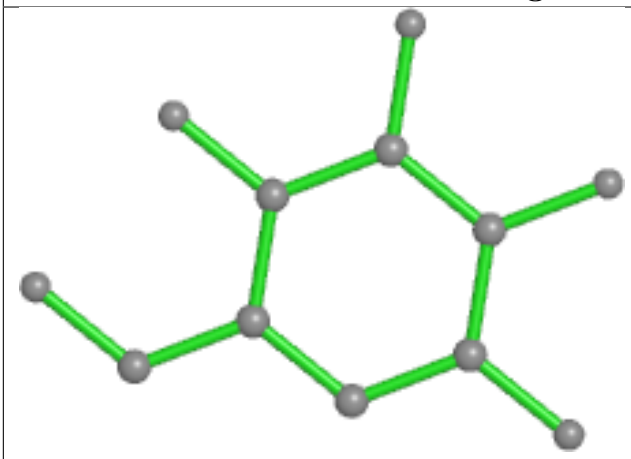
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	665	GOL	2	0

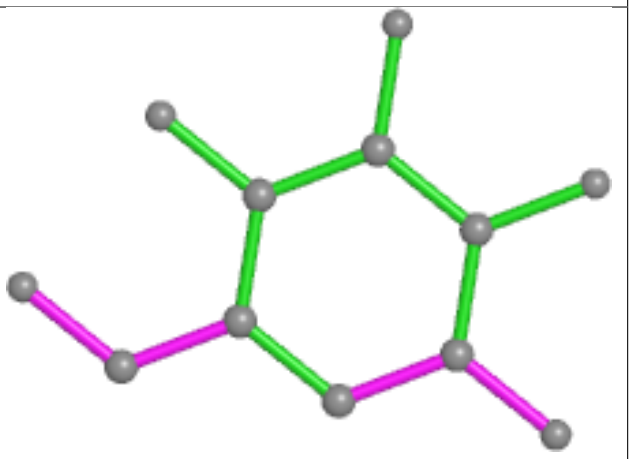
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

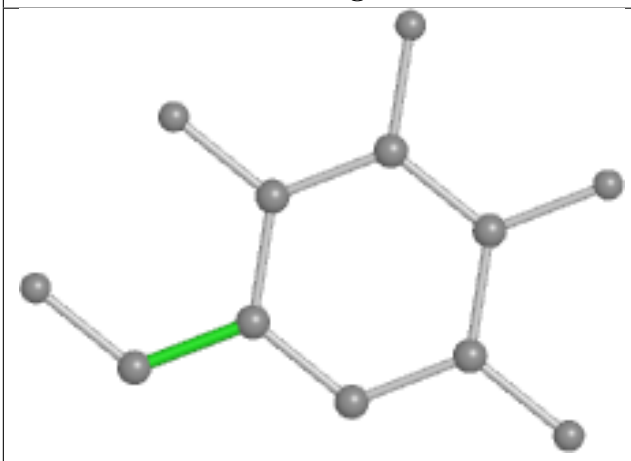
Ligand AC1 B 664



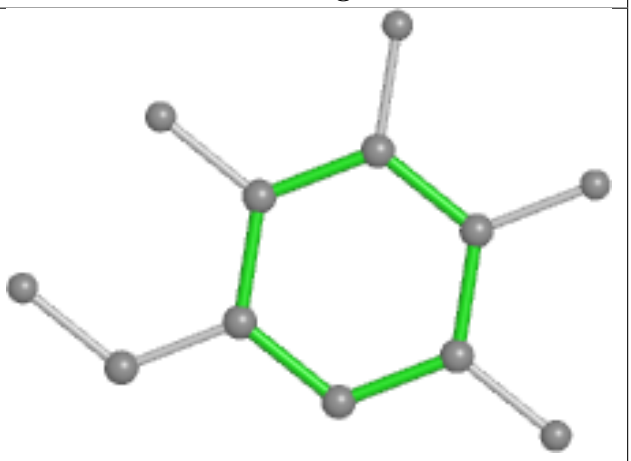
Bond lengths



Bond angles

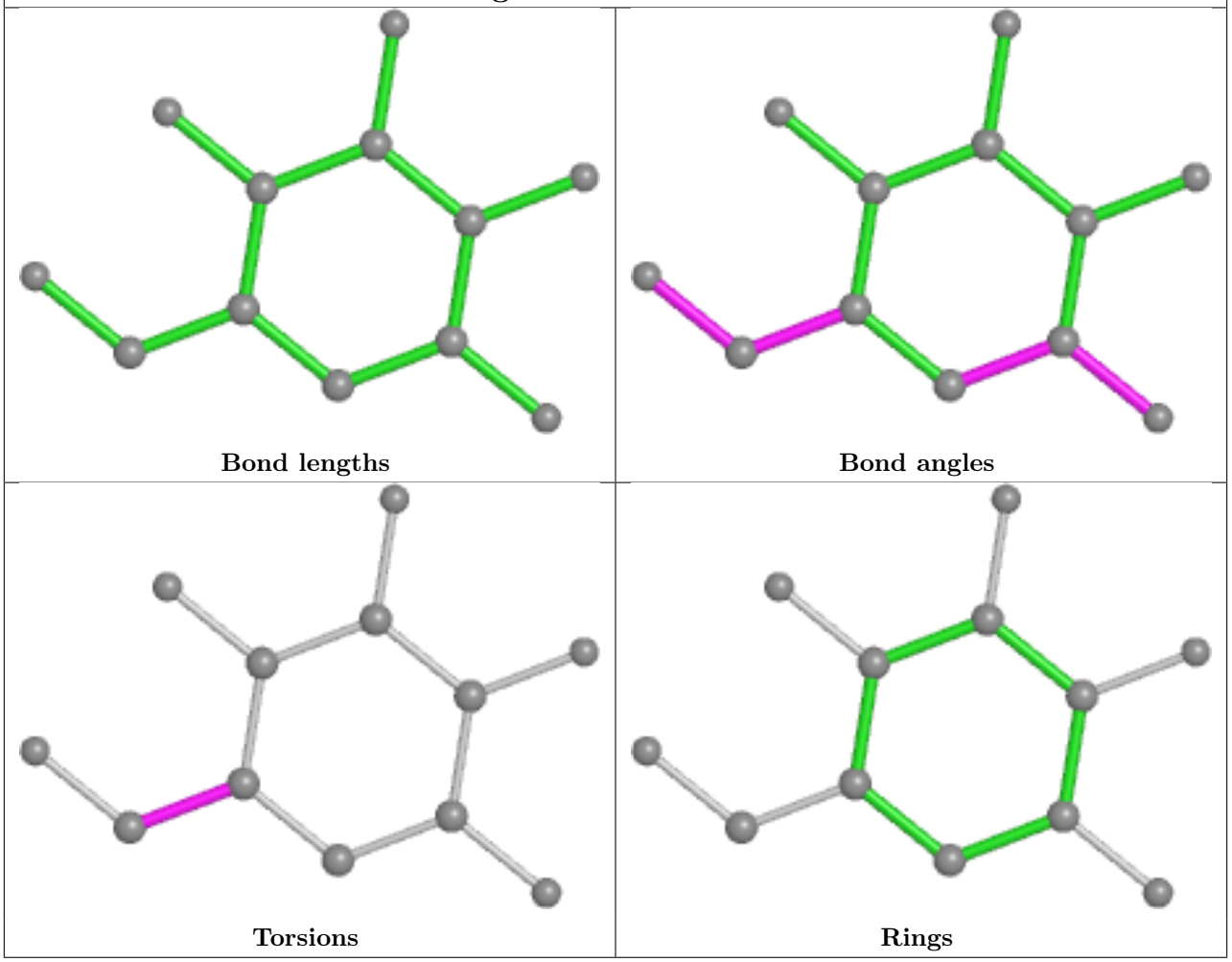


Torsions



Rings

Ligand AC1 A 664A



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	664/666 (99%)	-0.11	6 (0%)	84	83	24, 37, 64, 97	1 (0%)
1	B	664/666 (99%)	0.02	25 (3%)	40	39	27, 41, 65, 91	0
All	All	1328/1332 (99%)	-0.04	31 (2%)	60	59	24, 39, 65, 97	1 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	448	ALA	4.0
1	B	430	LEU	3.7
1	B	470	VAL	3.4
1	B	432	LEU	3.1
1	A	629	ASN	3.1
1	B	474	LEU	3.0
1	A	0	ALA	2.9
1	B	469	GLY	2.9
1	B	468	LEU	2.8
1	B	435	LEU	2.7
1	B	428	ILE	2.5
1	B	446	THR	2.5
1	B	341	TRP	2.5
1	A	474	LEU	2.5
1	B	416	ILE	2.5
1	B	450	LEU	2.4
1	B	660	VAL	2.4
1	A	341	TRP	2.3
1	B	471	PHE	2.3
1	B	447	GLY	2.2
1	A	628	GLU	2.2
1	A	473	PRO	2.2
1	B	473	PRO	2.2
1	B	431	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	35	LYS	2.1
1	B	215	PRO	2.1
1	B	465	PHE	2.1
1	B	220	PHE	2.0
1	B	417	TRP	2.0
1	B	429	LEU	2.0
1	B	60	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

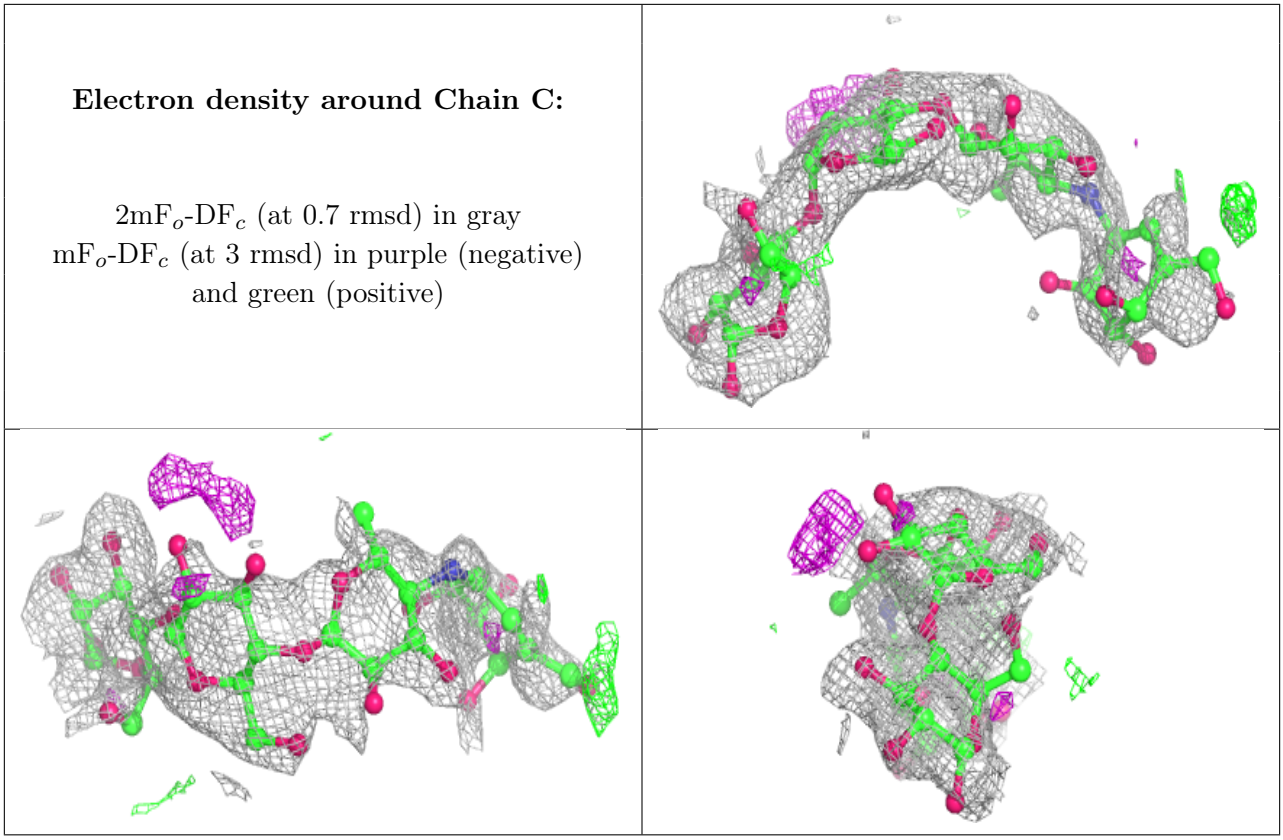
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

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. 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	B-factors(Å^2)	Q<0.9
2	AC1	C	3	21/22	0.68	0.23	108,117,128,129	0
2	GLC	C	1	12/12	0.75	0.29	72,89,96,98	0
2	GLC	C	2	11/12	0.86	0.23	90,96,101,106	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands

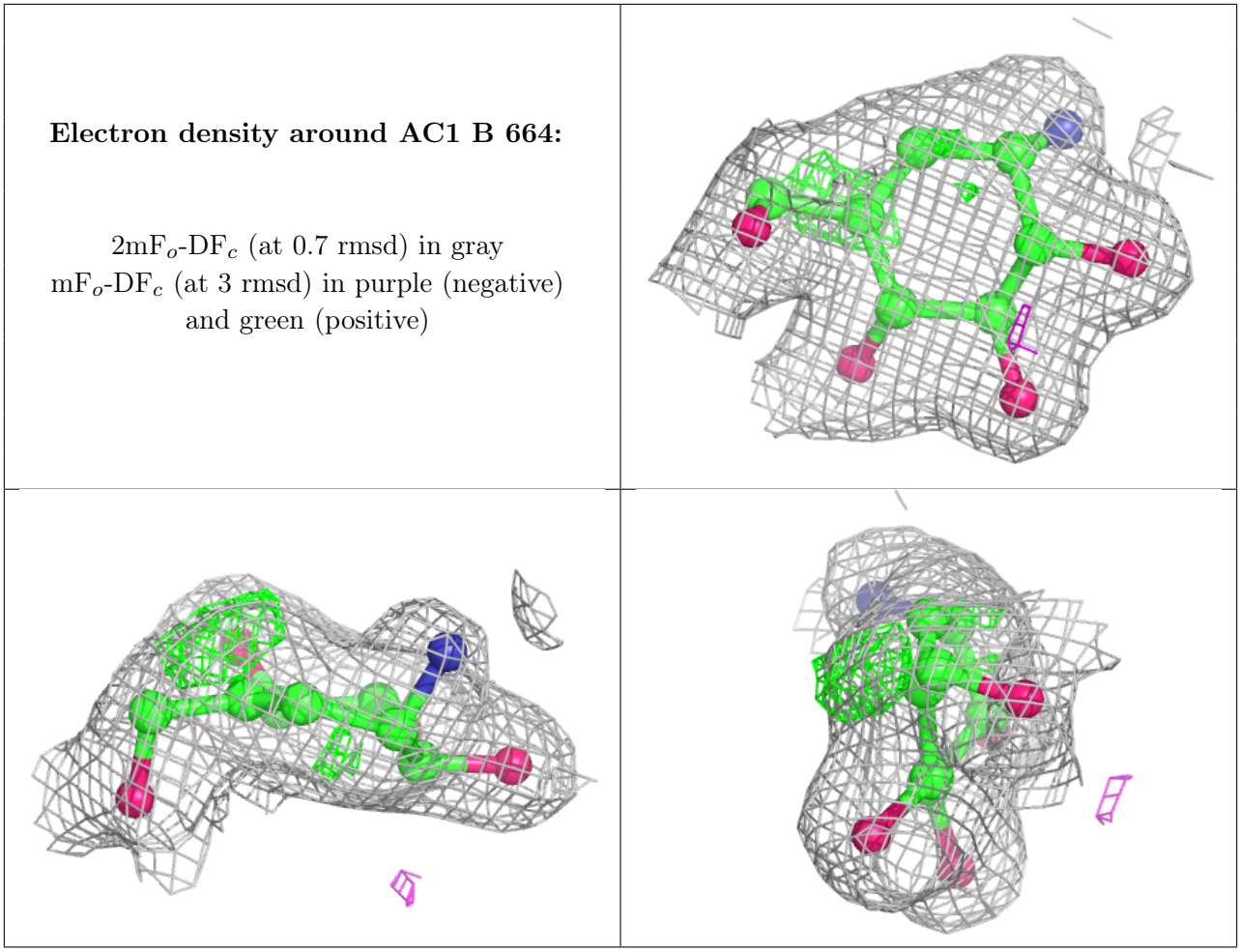
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	A	664	12/12	0.68	0.23	84,109,111,113	0
5	GOL	A	665	6/6	0.83	0.14	62,71,74,76	0
4	AC1	B	664	12/22	0.93	0.19	35,41,50,51	0
4	AC1	A	664(A)	12/22	0.93	0.10	23,32,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

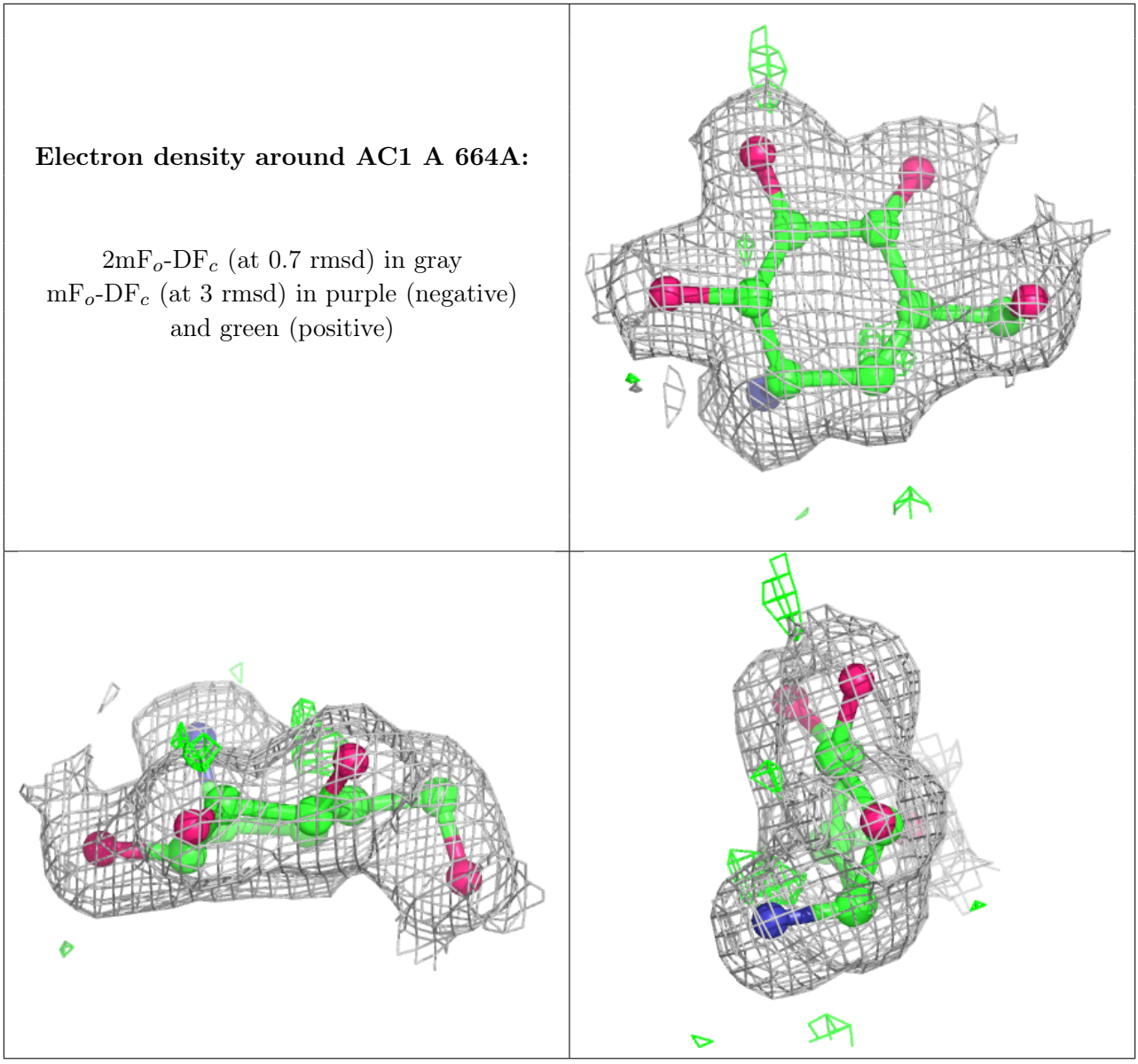
Electron density around AC1 B 664:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around AC1 A 664A:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.