Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 04:53 PM EDT

PDB ID	:	6ZJQ
Title	:	Cold-adapted beta-D-galactosidase from Arthrobacter sp. 32cB mutant E517Q in complex with galactose
Authors	:	Rutkiewicz, M.; Bujacz, A.; Bujacz, G.
Deposited on	:	2020-06-29
Resolution	:	1.70 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 (i) 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 (i)) were used in the production of this report:

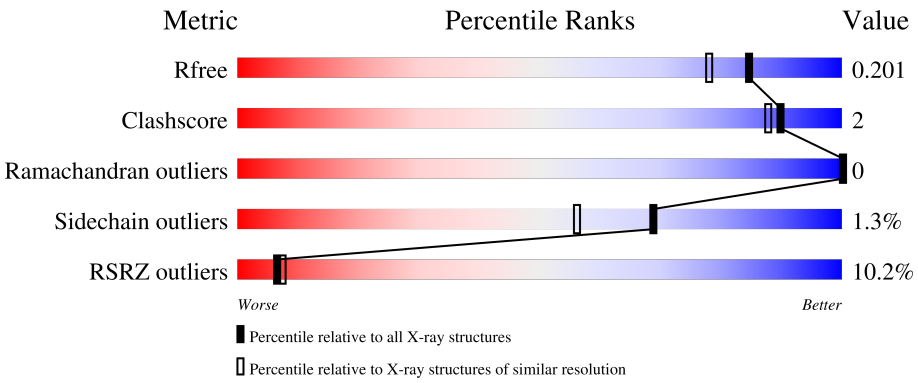
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

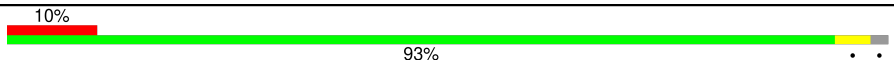
The reported resolution of this entry is 1.70 Å.

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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	1012	

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	ACT	A	1108	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8396 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	987	7624	4797	1363	1445	19	0	4	0

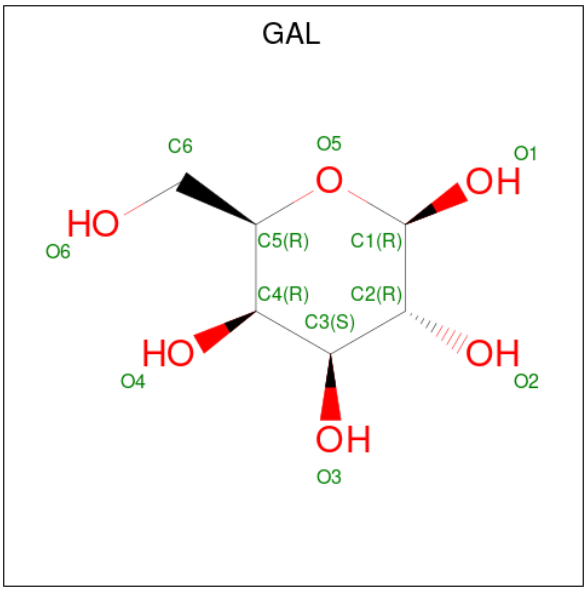
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLU	-	expression tag	UNP A0A023UGN9
A	0	GLN	-	expression tag	UNP A0A023UGN9
A	517	GLN	GLU	engineered mutation	UNP A0A023UGN9

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

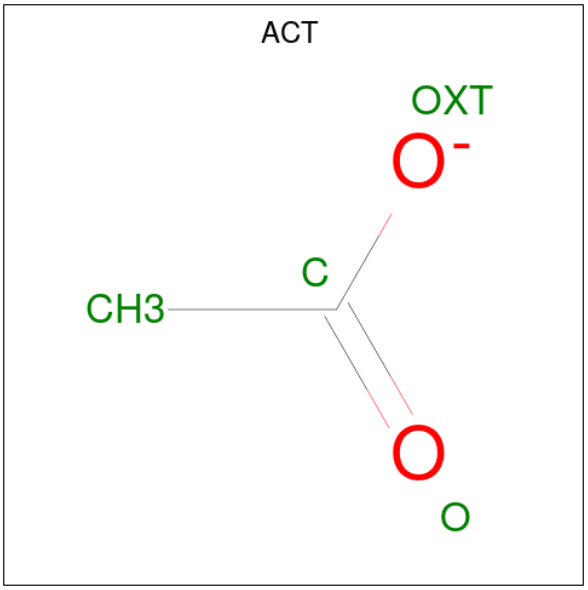
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	5	5	5	0	0

- Molecule 3 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	A	1	4	2	2	0	0

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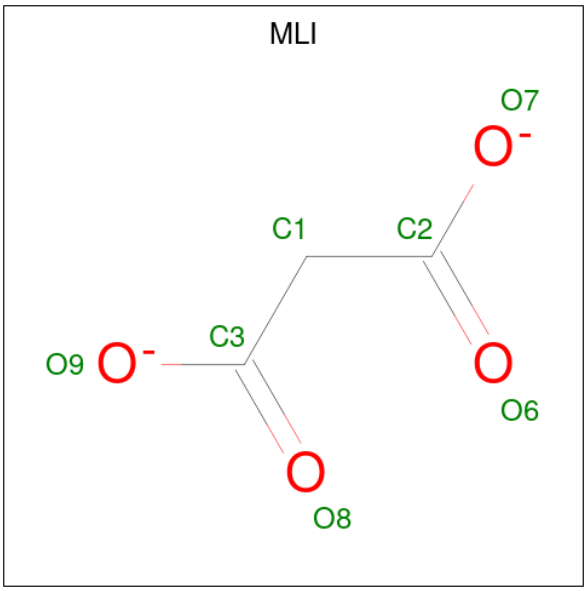
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0
4	A	1	4	2	2		0	0

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	7	3	4	0	0
5	A	1	7	3	4	0	0
5	A	1	7	3	4	0	0
5	A	1	7	3	4	0	0
5	A	1	7	3	4	0	0
5	A	1	7	3	4	0	0

- Molecule 6 is water.

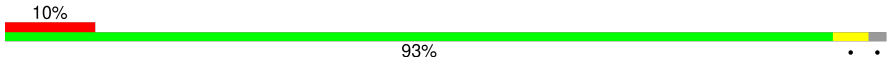
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	621	621	621	0	0

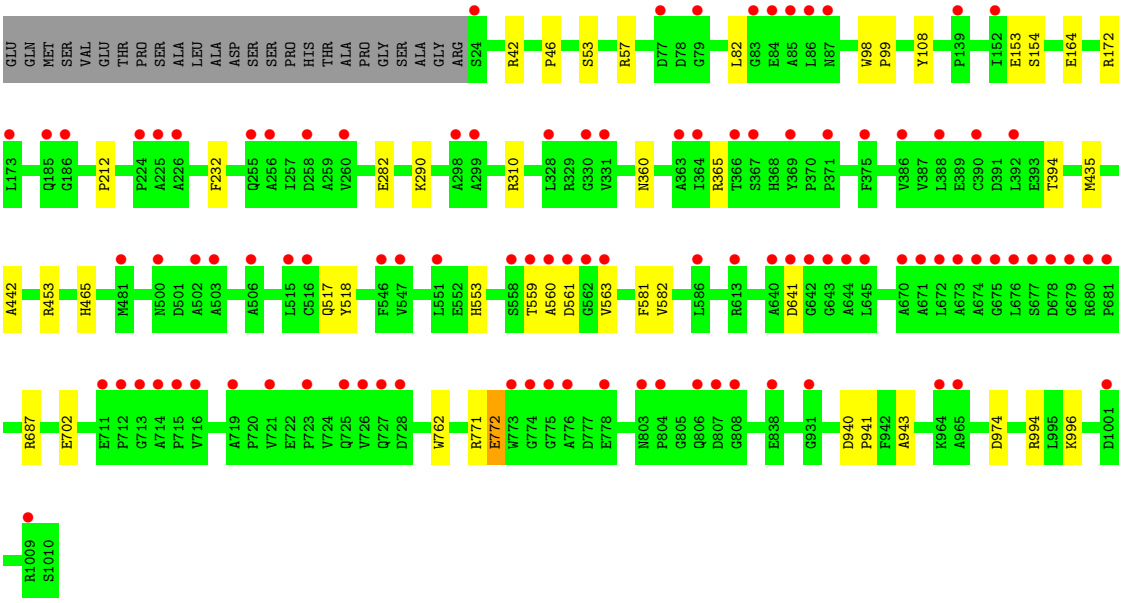
3 Residue-property plots (i)

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: Beta-galactosidase

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.61Å 138.61Å 127.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.72 – 1.70 46.95 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.72-1.70) 99.8 (46.95-1.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.165 , 0.196 0.172 , 0.201	Depositor DCC
R_{free} test set	2101 reflections (1.35%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 56.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	8396	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ACT, GAL, MLI

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	0.49	0/7829	0.64	0/10671

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 (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	7624	0	7322	25	0
2	A	5	0	0	0	0
3	A	24	0	23	1	0
4	A	80	0	60	4	0
5	A	42	0	12	0	0
6	A	621	0	0	7	0
All	All	8396	0	7417	28	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 2.

All (28) 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:365:ARG:HH12	1:A:517:GLN:HE21	1.35	0.74
4:A:1108:ACT:H3	6:A:1233:HOH:O	1.93	0.69
1:A:435[B]:MET:HE1	1:A:465:HIS:HB2	1.76	0.67
1:A:46:PRO:HA	4:A:1108:ACT:H2	1.77	0.65
4:A:1123:ACT:H3	6:A:1432:HOH:O	1.95	0.64
1:A:772:GLU:HB2	6:A:1292:HOH:O	2.00	0.60
1:A:453:ARG:HD3	6:A:1713:HOH:O	2.04	0.58
1:A:559:THR:OG1	1:A:563:VAL:HG12	2.05	0.56
1:A:42:ARG:NH2	1:A:164:GLU:OE2	2.37	0.54
1:A:772:GLU:OE2	1:A:994:ARG:NH1	2.37	0.52
1:A:435[B]:MET:CE	1:A:465:HIS:HB2	2.43	0.49
1:A:394:THR:OG1	1:A:442:ALA:HA	2.14	0.47
1:A:687:ARG:HD2	1:A:702:GLU:OE2	2.15	0.47
1:A:153:GLU:HA	1:A:154:SER:HA	1.74	0.44
1:A:772:GLU:CB	6:A:1292:HOH:O	2.62	0.43
1:A:108:TYR:CZ	1:A:582:VAL:HB	2.54	0.43
1:A:553:HIS:HB2	1:A:582:VAL:HG22	2.00	0.43
1:A:560:ALA:O	1:A:561:ASP:HB2	2.18	0.43
4:A:1108:ACT:CH3	6:A:1249:HOH:O	2.66	0.43
1:A:641:ASP:N	1:A:641:ASP:OD1	2.51	0.42
1:A:82:LEU:HD22	1:A:82:LEU:N	2.35	0.42
1:A:57:ARG:NH1	6:A:1207:HOH:O	2.42	0.41
1:A:771:ARG:HH11	1:A:771:ARG:HG3	1.85	0.41
1:A:282:GLU:HB2	1:A:290:LYS:HG2	2.02	0.41
1:A:943:ALA:HB3	1:A:974:ASP:HB2	2.02	0.41
1:A:940:ASP:O	1:A:941:PRO:C	2.60	0.40
1:A:360:ASN:HA	3:A:1107:GAL:O3	2.21	0.40
1:A:99:PRO:HG2	1:A:212:PRO:HD2	2.03	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	989/1012 (98%)	959 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	779/795 (98%)	769 (99%)	10 (1%)	69	56

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	98	TRP
1	A	172	ARG
1	A	232	PHE
1	A	310	ARG
1	A	518	TYR
1	A	581	PHE
1	A	762	TRP
1	A	772	GLU
1	A	996	LYS

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 5 are monoatomic - leaving 28 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	$\#\|Z\| > 2$
4	ACT	A	1123	-	3,3,3	1.36	0	3,3,3	1.38	0
4	ACT	A	1109	-	3,3,3	1.58	1 (33%)	3,3,3	1.27	0
4	ACT	A	1121	-	3,3,3	1.55	1 (33%)	3,3,3	1.45	0
4	ACT	A	1125	-	3,3,3	1.59	1 (33%)	3,3,3	1.35	0
3	GAL	A	1107	-	12,12,12	0.71	0	17,17,17	0.75	0
5	MLI	A	1132	-	6,6,6	1.37	0	7,7,7	1.27	0
5	MLI	A	1128	-	6,6,6	1.41	0	7,7,7	1.36	0
5	MLI	A	1129	-	6,6,6	1.36	0	7,7,7	0.96	0
5	MLI	A	1130	-	6,6,6	1.40	0	7,7,7	1.31	0
4	ACT	A	1112	-	3,3,3	1.69	1 (33%)	3,3,3	1.56	0
5	MLI	A	1131	-	6,6,6	1.39	0	7,7,7	1.28	1 (14%)
5	MLI	A	1133	-	6,6,6	1.47	0	7,7,7	1.33	1 (14%)
4	ACT	A	1113	-	3,3,3	1.57	1 (33%)	3,3,3	1.41	0
4	ACT	A	1116	-	3,3,3	1.76	1 (33%)	3,3,3	1.34	0
4	ACT	A	1115	-	3,3,3	1.57	1 (33%)	3,3,3	1.44	0
4	ACT	A	1110	-	3,3,3	0.94	0	3,3,3	1.55	1 (33%)
4	ACT	A	1122	-	3,3,3	1.50	1 (33%)	3,3,3	1.57	0
4	ACT	A	1127	-	3,3,3	1.84	1 (33%)	3,3,3	1.49	1 (33%)
4	ACT	A	1108	-	3,3,3	0.67	0	3,3,3	1.43	0
4	ACT	A	1117	-	3,3,3	1.48	1 (33%)	3,3,3	1.55	0
4	ACT	A	1111	-	3,3,3	1.45	1 (33%)	3,3,3	1.51	0
4	ACT	A	1114	-	3,3,3	1.38	0	3,3,3	1.33	0
3	GAL	A	1106	2	12,12,12	0.85	0	17,17,17	0.82	0
4	ACT	A	1124	-	3,3,3	1.67	1 (33%)	3,3,3	1.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACT	A	1126	-	3,3,3	1.53	1 (33%)	3,3,3	1.45	0
4	ACT	A	1118	-	3,3,3	1.52	0	3,3,3	1.45	0
4	ACT	A	1119	-	3,3,3	1.46	0	3,3,3	1.45	0
4	ACT	A	1120	-	3,3,3	1.32	0	3,3,3	1.37	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
5	MLI	A	1133	-	-	2/4/4/4	-
5	MLI	A	1129	-	-	0/4/4/4	-
3	GAL	A	1107	-	-	1/2/22/22	0/1/1/1
5	MLI	A	1132	-	-	2/4/4/4	-
3	GAL	A	1106	2	-	1/2/22/22	0/1/1/1
5	MLI	A	1128	-	-	2/4/4/4	-
5	MLI	A	1130	-	-	2/4/4/4	-
5	MLI	A	1131	-	-	2/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1127	ACT	CH3-C	2.92	1.60	1.49
4	A	1116	ACT	CH3-C	2.57	1.59	1.49
4	A	1124	ACT	CH3-C	2.54	1.59	1.49
4	A	1112	ACT	CH3-C	2.45	1.58	1.49
4	A	1125	ACT	CH3-C	2.39	1.58	1.49
4	A	1121	ACT	CH3-C	2.36	1.58	1.49
4	A	1113	ACT	CH3-C	2.33	1.58	1.49
4	A	1122	ACT	CH3-C	2.32	1.58	1.49
4	A	1109	ACT	CH3-C	2.30	1.58	1.49
4	A	1117	ACT	CH3-C	2.23	1.57	1.49
4	A	1115	ACT	CH3-C	2.18	1.57	1.49
4	A	1111	ACT	CH3-C	2.15	1.57	1.49
4	A	1126	ACT	CH3-C	2.13	1.57	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1110	ACT	OXT-C-O	2.08	129.76	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1131	MLI	O9-C3-C1	2.06	120.89	114.51
5	A	1133	MLI	O7-C2-C1	2.01	120.74	114.51
4	A	1127	ACT	O-C-CH3	-2.00	114.31	122.53

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1107	GAL	O5-C5-C6-O6
3	A	1106	GAL	O5-C5-C6-O6
5	A	1130	MLI	C3-C1-C2-O6
5	A	1130	MLI	C3-C1-C2-O7
5	A	1132	MLI	C3-C1-C2-O7
5	A	1131	MLI	C2-C1-C3-O8
5	A	1128	MLI	C3-C1-C2-O6
5	A	1131	MLI	C2-C1-C3-O9
5	A	1132	MLI	C3-C1-C2-O6
5	A	1128	MLI	C3-C1-C2-O7
5	A	1133	MLI	C3-C1-C2-O6
5	A	1133	MLI	C3-C1-C2-O7

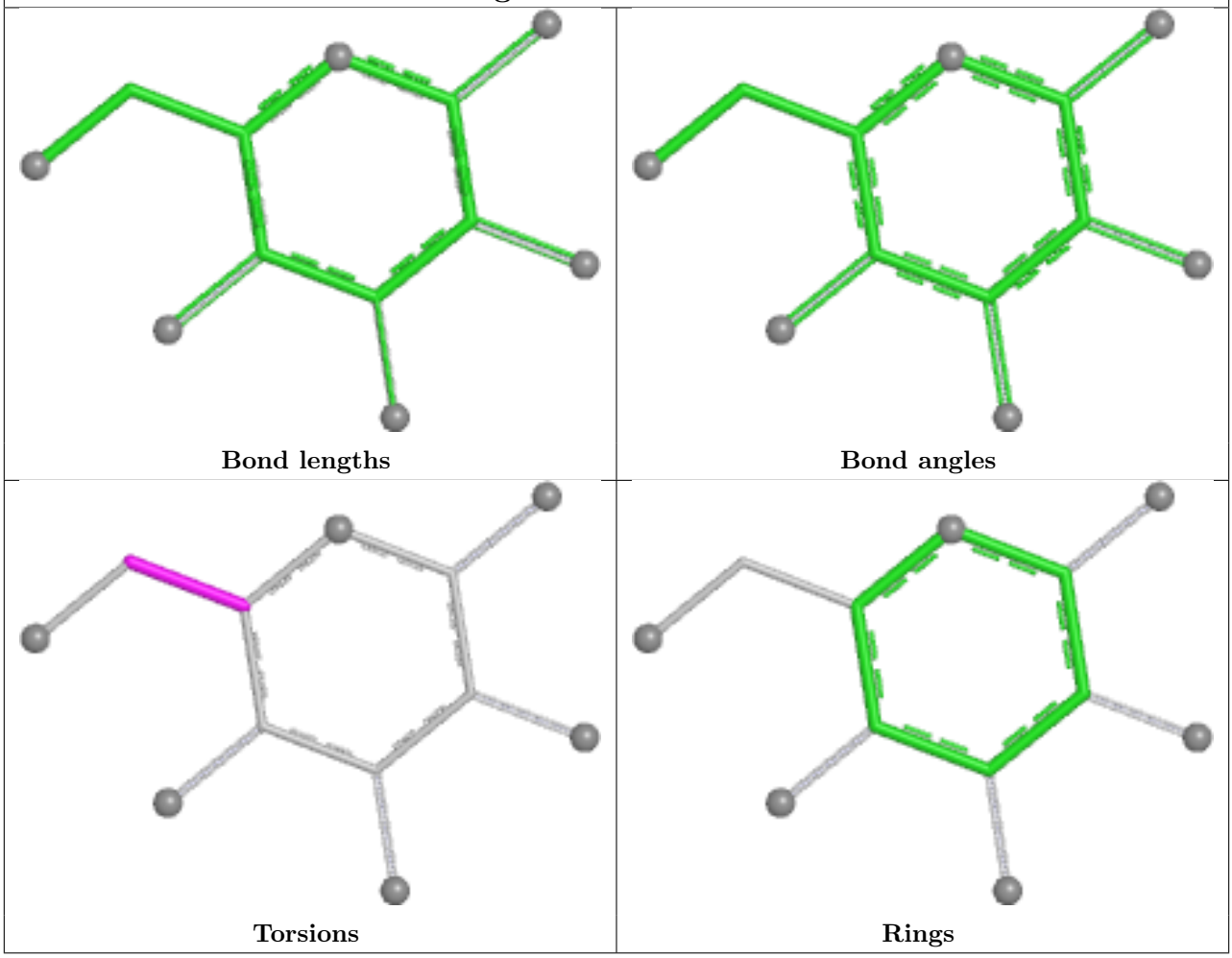
There are no ring outliers.

3 monomers are involved in 5 short contacts:

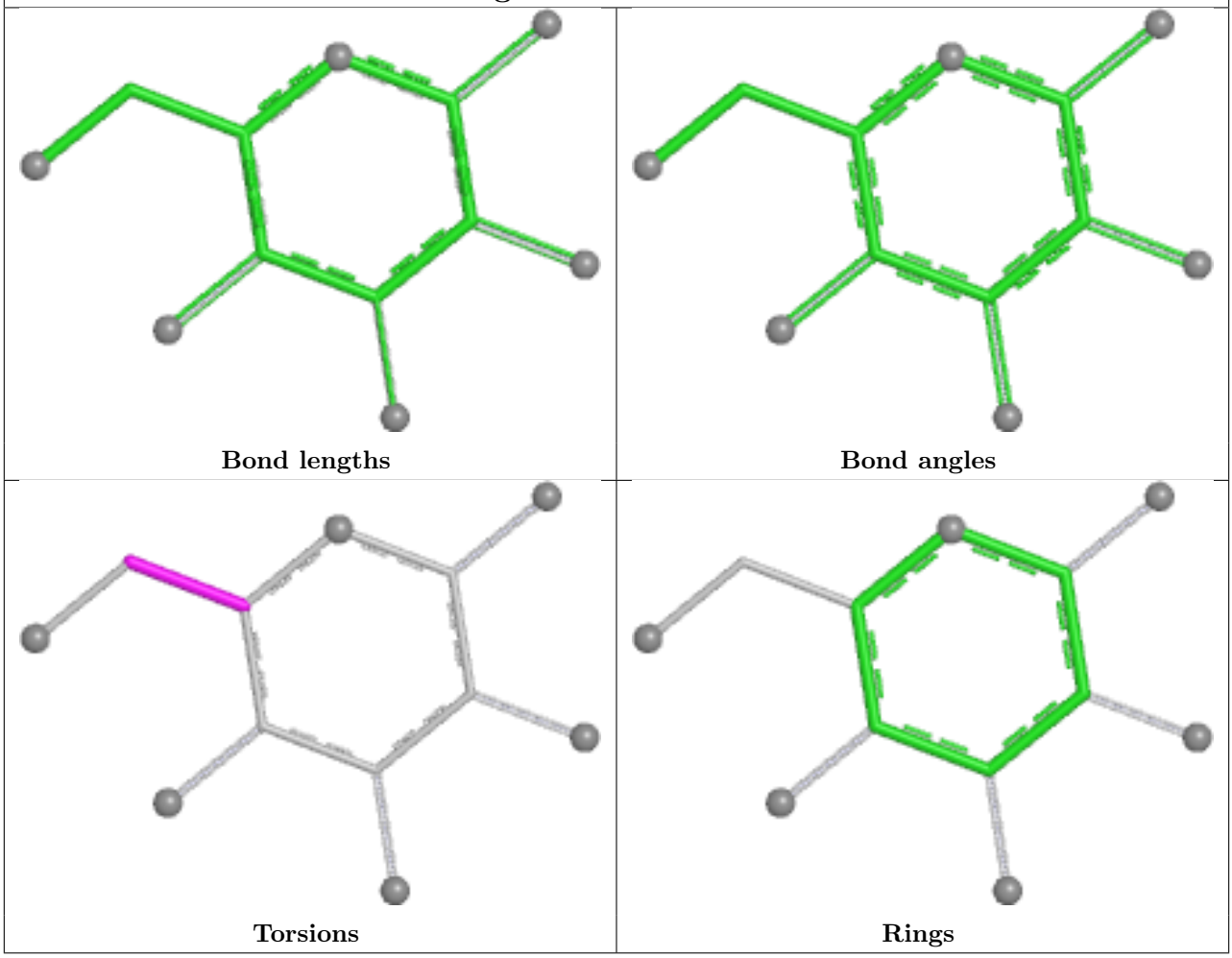
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1123	ACT	1	0
3	A	1107	GAL	1	0
4	A	1108	ACT	3	0

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 GAL A 1107



Ligand GAL A 1106



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 (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	987/1012 (97%)	0.33	101 (10%) 6 7	23, 34, 59, 97	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	561	ASP	9.3
1	A	676	LEU	8.9
1	A	560	ALA	8.5
1	A	775	GLY	8.4
1	A	716	VAL	8.3
1	A	87	ASN	8.2
1	A	642	GLY	8.1
1	A	678	ASP	7.6
1	A	563	VAL	7.5
1	A	673	ALA	7.2
1	A	677	SER	7.1
1	A	679	GLY	6.9
1	A	85	ALA	6.6
1	A	776	ALA	6.3
1	A	643	GLY	6.1
1	A	774	GLY	6.0
1	A	674	ALA	6.0
1	A	83	GLY	6.0
1	A	559	THR	5.9
1	A	562	GLY	5.7
1	A	675	GLY	5.7
1	A	672	LEU	5.2
1	A	645	LEU	5.2
1	A	680	ARG	5.1
1	A	804	PRO	4.9
1	A	641	ASP	4.9
1	A	481	MET	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	640	ALA	4.7
1	A	258	ASP	4.7
1	A	502	ALA	4.5
1	A	86	LEU	4.4
1	A	715	PRO	4.3
1	A	84	GLU	4.3
1	A	613[A]	ARG	4.1
1	A	1009	ARG	4.0
1	A	671	ALA	4.0
1	A	808	GLY	4.0
1	A	721	VAL	4.0
1	A	299	ALA	3.8
1	A	773	TRP	3.8
1	A	255	GLN	3.6
1	A	714	ALA	3.5
1	A	719	ALA	3.5
1	A	807	ASP	3.5
1	A	806	GLN	3.3
1	A	388	LEU	3.3
1	A	713	GLY	3.3
1	A	931	GLY	3.3
1	A	558	SER	3.2
1	A	726	VAL	3.2
1	A	1001	ASP	3.2
1	A	79	GLY	3.2
1	A	369	TYR	3.2
1	A	503	ALA	3.1
1	A	364	ILE	3.1
1	A	964	LYS	3.0
1	A	331	VAL	3.0
1	A	728	ASP	2.9
1	A	225	ALA	2.9
1	A	173	LEU	2.8
1	A	260	VAL	2.8
1	A	506	ALA	2.8
1	A	392	LEU	2.8
1	A	226	ALA	2.7
1	A	77	ASP	2.6
1	A	386	VAL	2.6
1	A	725	GLN	2.6
1	A	366	THR	2.6
1	A	778	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	500	ASN	2.6
1	A	711	GLU	2.5
1	A	298	ALA	2.5
1	A	727	GLN	2.5
1	A	803	ASN	2.5
1	A	681	PRO	2.5
1	A	390	CYS	2.5
1	A	139	PRO	2.4
1	A	551	LEU	2.4
1	A	256	ALA	2.4
1	A	516	CYS	2.4
1	A	152	ILE	2.4
1	A	375	PHE	2.4
1	A	547	VAL	2.3
1	A	328	LEU	2.3
1	A	586	LEU	2.2
1	A	363	ALA	2.2
1	A	185	GLN	2.2
1	A	24	SER	2.2
1	A	546	PHE	2.2
1	A	515	LEU	2.2
1	A	723	PRO	2.2
1	A	186	GLY	2.2
1	A	330	GLY	2.2
1	A	644	ALA	2.2
1	A	670	ALA	2.2
1	A	965	ALA	2.1
1	A	224	PRO	2.1
1	A	712	PRO	2.1
1	A	367	SER	2.1
1	A	371	PRO	2.1
1	A	838	GLU	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 monosaccharides 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. 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.

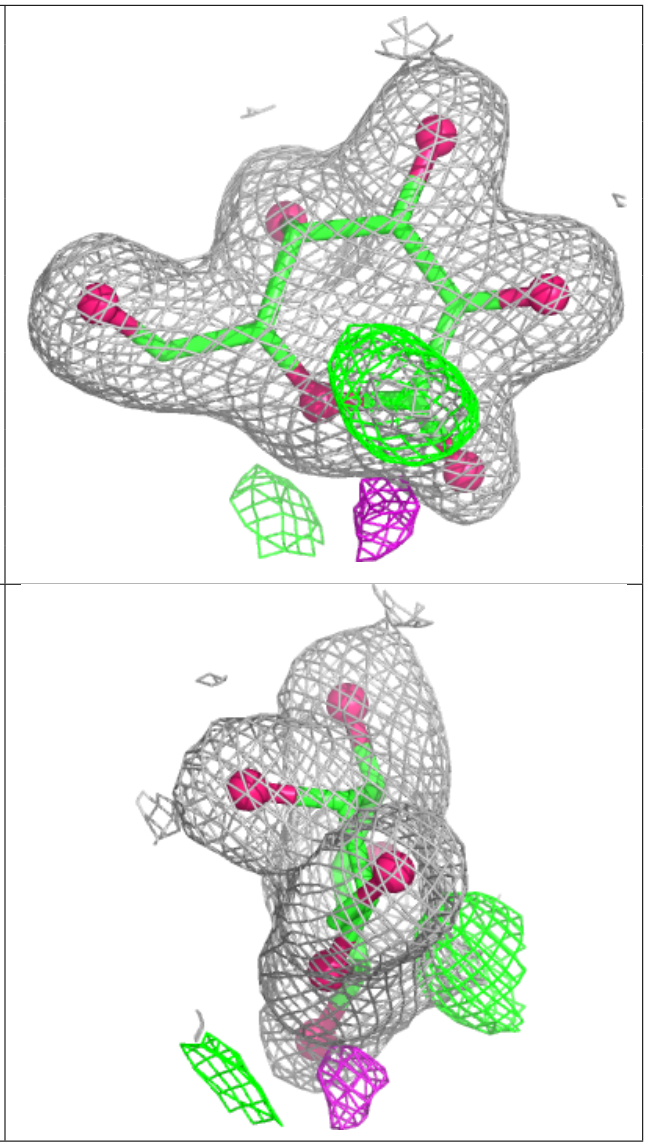
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	A	1124	4/4	0.48	0.23	59,61,62,68	0
4	ACT	A	1125	4/4	0.55	0.14	59,69,70,72	0
4	ACT	A	1121	4/4	0.62	0.21	53,62,66,68	0
4	ACT	A	1115	4/4	0.68	0.27	59,59,61,66	0
4	ACT	A	1119	4/4	0.72	0.15	58,59,64,70	0
5	MLI	A	1129	7/7	0.74	0.20	59,65,73,76	0
5	MLI	A	1133	7/7	0.79	0.23	60,67,73,75	0
4	ACT	A	1113	4/4	0.80	0.24	55,64,70,70	0
5	MLI	A	1131	7/7	0.80	0.53	58,64,72,77	0
4	ACT	A	1123	4/4	0.80	0.26	51,67,74,78	0
4	ACT	A	1112	4/4	0.81	0.24	55,57,58,64	0
5	MLI	A	1132	7/7	0.81	0.27	45,58,71,75	0
4	ACT	A	1117	4/4	0.81	0.41	61,62,69,71	0
5	MLI	A	1128	7/7	0.82	0.34	58,62,71,79	0
4	ACT	A	1126	4/4	0.83	0.20	59,61,66,70	0
4	ACT	A	1114	4/4	0.83	0.14	61,64,71,76	0
4	ACT	A	1109	4/4	0.86	0.20	58,61,66,70	0
4	ACT	A	1120	4/4	0.88	0.11	54,61,72,72	0
4	ACT	A	1110	4/4	0.90	0.13	27,40,44,58	0
4	ACT	A	1108	4/4	0.91	0.14	48,54,67,70	0
5	MLI	A	1130	7/7	0.92	0.20	42,51,70,73	0
2	NA	A	1103	1/1	0.93	0.13	48,48,48,48	0
2	NA	A	1105	1/1	0.94	0.09	64,64,64,64	0
4	ACT	A	1127	4/4	0.94	0.11	29,35,47,49	0
4	ACT	A	1122	4/4	0.95	0.13	30,46,50,65	0
3	GAL	A	1107	12/12	0.95	0.08	27,28,30,40	0
4	ACT	A	1116	4/4	0.95	0.10	30,32,44,61	0
3	GAL	A	1106	12/12	0.96	0.14	27,27,27,29	0
4	ACT	A	1111	4/4	0.96	0.20	32,41,45,47	0
4	ACT	A	1118	4/4	0.96	0.12	42,54,63,67	0
2	NA	A	1104	1/1	0.99	0.05	31,31,31,31	0
2	NA	A	1102	1/1	0.99	0.10	29,29,29,29	0
2	NA	A	1101	1/1	0.99	0.12	27,27,27,27	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.

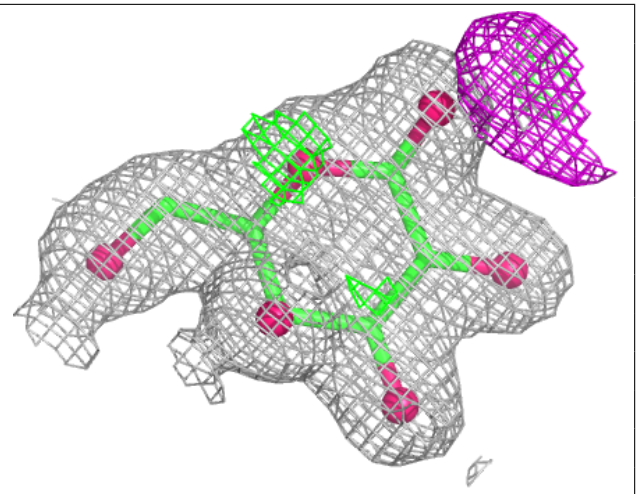
Electron density around GAL A 1107:

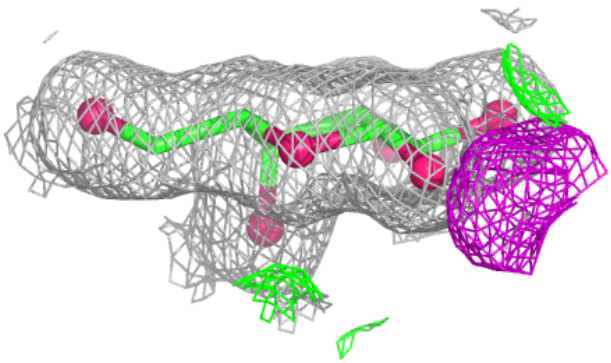
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

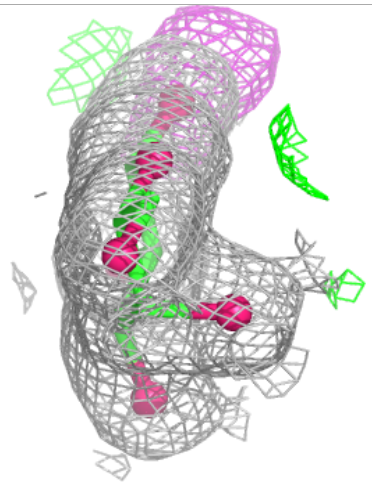


Electron density around GAL A 1106:

$2mF_o$-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 (i)

There are no such residues in this entry.