Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2020 – 07:08 PM BST

PDB ID	:	6ZJS
Title	:	Cold-adapted beta-D-galactosidase from Arthrobacter sp. 32cB mutant E441Q in complex with galactose
Authors	:	Rutkiewicz, M.; Bujacz, A.; Bujacz, G.
Deposited on	:	2020-06-29
Resolution	:	1.50 Å(reported)

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

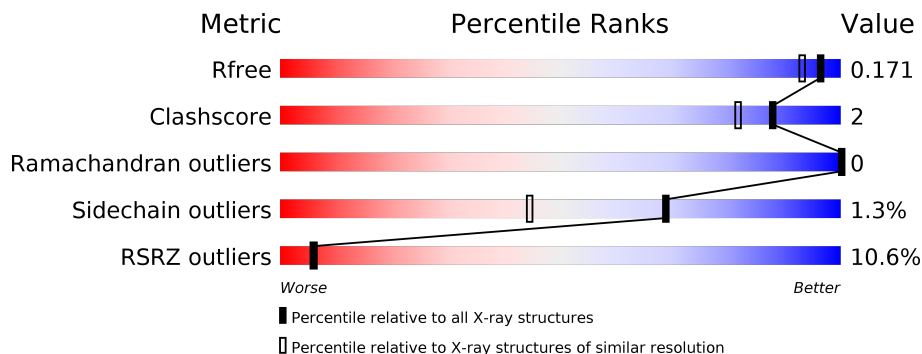|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.50 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	Percentile Ranks	Value
Rfree		0.171
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.3%
RSRZ outliers		10.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 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	1010	10% 95%

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
5	MLI	A	1132	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8588 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
1	A	987	Total	C	N	O	S	0	10	0
			7662	4824	1372	1446	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	GLN	GLU	engineered mutation	UNP A0A023UGN9

- Molecule 2 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by author).
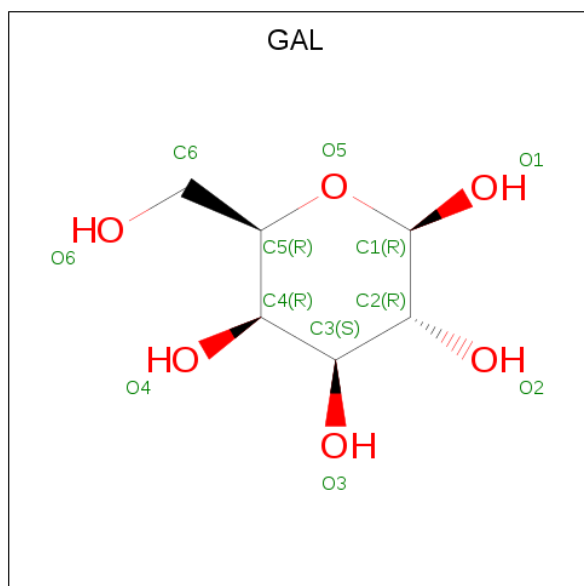
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			12	6	6		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

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

Continued on next page...

Continued from previous page...

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

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

MLI

O7

C1 C2

C3

O9 O6

O8
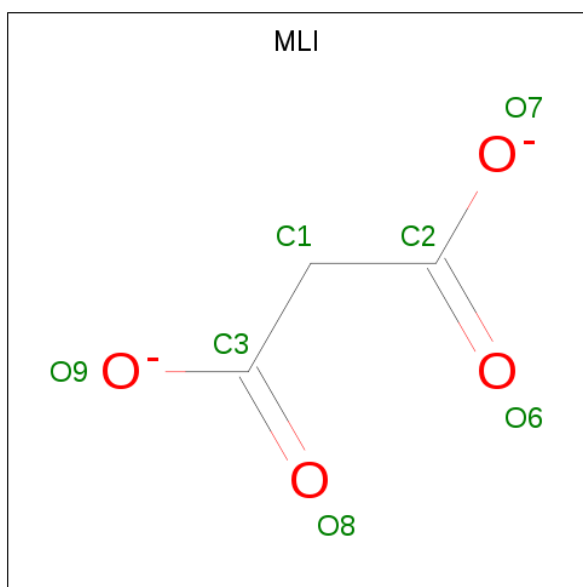
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 7	C 3	O 4	0	0
5	A	1	Total 7	C 3	O 4	0	0
5	A	1	Total 7	C 3	O 4	0	0
5	A	1	Total 7	C 3	O 4	0	0

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).

FMT

C

OH O2

O

O1
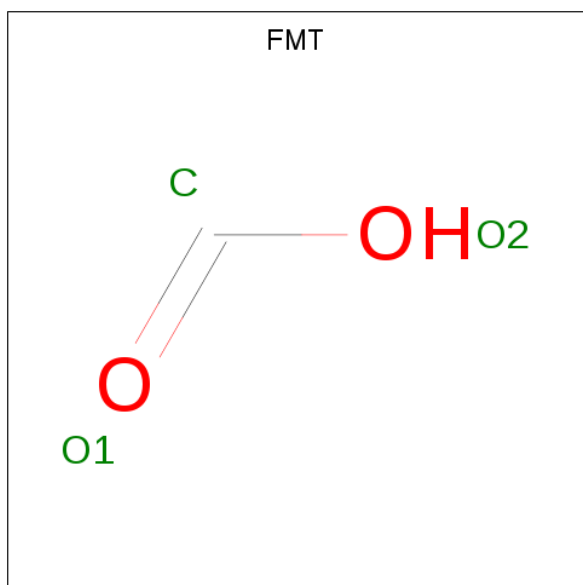
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 3	C 1	O 2	0	0
6	A	1	Total 3	C 1	O 2	0	0

- Molecule 7 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: $C_4H_6O_5$).
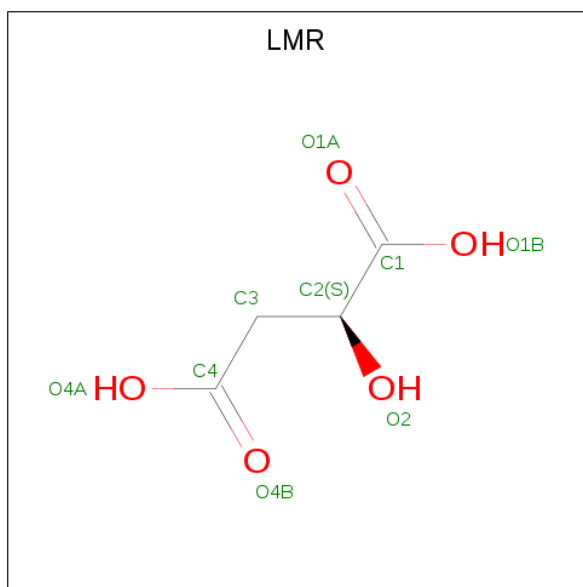
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 9	C 4	O 5	0	0
7	A	1	Total 9	C 4	O 5	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	720	Total 721	O 721	0	1

3 Residue-property plots ⓘ

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
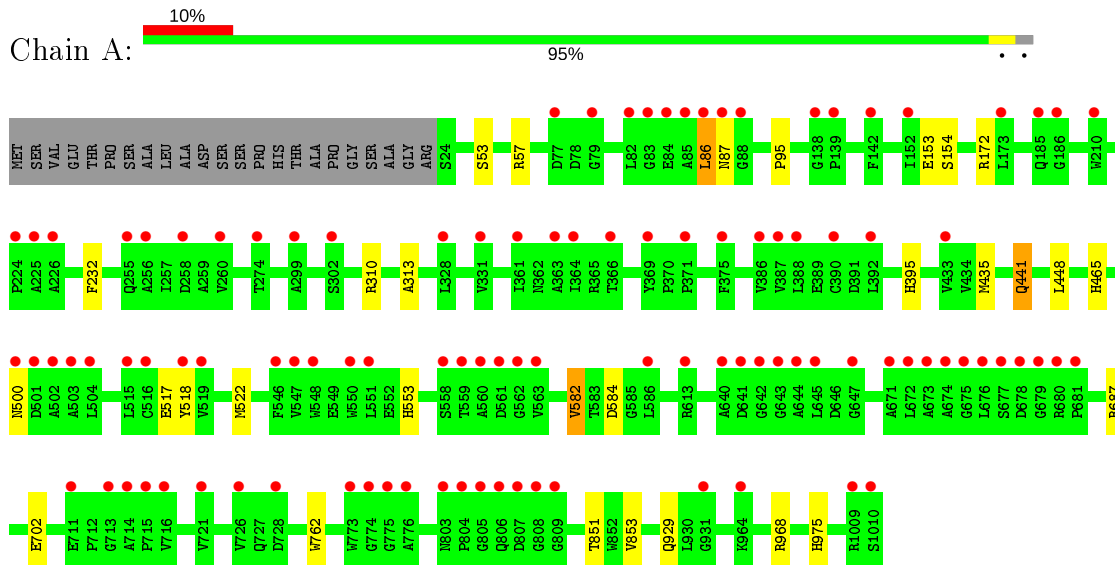
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.38Å 138.38Å 127.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.94 – 1.50 46.94 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.94-1.50) 99.9 (46.94-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	0.97 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.143 , 0.161 0.155 , 0.171	Depositor DCC
R_{free} test set	2359 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 56.1	EDS
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	8588	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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, FMT, MLI, GAL, ACT, LMR

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 RMSZ	Bond lengths $\#|Z| > 5$	Bond angles RMSZ	Bond angles $\#|Z| > 5$
1	A	0.45	0/7882	0.65	0/10738

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	7662	0	7385	27	0
2	A	84	0	83	4	0
3	A	5	0	0	0	0
4	A	64	0	48	4	0
5	A	28	0	8	1	0
6	A	6	0	2	0	0
7	A	18	0	8	1	0
8	A	721	0	0	7	0
All	All	8588	0	7534	31	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 (31) 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:86[A]:LEU:HD22	1:A:87:ASN:N	1.66	1.09
2:A:1107:GAL:H62	8:A:1263:HOH:O	1.54	1.07
1:A:86[A]:LEU:HD13	1:A:86[A]:LEU:H	1.23	1.00
1:A:86[A]:LEU:CD1	1:A:86[A]:LEU:H	1.98	0.77
1:A:500:ASN:H	4:A:1117:ACT:H1	1.49	0.76
1:A:86[A]:LEU:HD13	1:A:86[A]:LEU:N	2.02	0.73
1:A:968:ARG:NH1	8:A:1202:HOH:O	2.20	0.72
1:A:86[A]:LEU:CD2	1:A:87:ASN:N	2.51	0.72
1:A:395:HIS:CE1	1:A:441[B]:GLN:OE1	2.52	0.61
1:A:57[A]:ARG:NH1	8:A:1201:HOH:O	2.20	0.60
4:A:1118:ACT:H1	8:A:1542:HOH:O	2.00	0.60
1:A:313:ALA:HA	7:A:1136:LMR:H3A	1.90	0.53
2:A:1107:GAL:C6	8:A:1263:HOH:O	2.31	0.52
1:A:86[A]:LEU:HD22	1:A:86[A]:LEU:C	2.30	0.50
4:A:1127:ACT:H3	8:A:1478:HOH:O	2.13	0.49
1:A:435[B]:MET:HE1	1:A:465:HIS:HB2	1.95	0.48
1:A:57[B]:ARG:HB3	1:A:57[B]:ARG:CZ	2.44	0.48
1:A:687[A]:ARG:HD2	1:A:702:GLU:OE2	2.14	0.47
1:A:86[B]:LEU:HD12	1:A:86[B]:LEU:HA	1.76	0.46
1:A:553:HIS:HB2	1:A:582:VAL:HG22	1.98	0.45
1:A:851:THR:HG22	1:A:853:VAL:HG23	1.98	0.45
1:A:86[A]:LEU:CD2	1:A:86[A]:LEU:C	2.86	0.44
1:A:975:HIS:NE2	5:A:1130:MLI:H12	2.33	0.44
1:A:153:GLU:HA	1:A:154:SER:HA	1.75	0.42
1:A:95:PRO:HG3	2:A:1105:GAL:H62	2.01	0.42
1:A:517:GLU:OE2	8:A:1203:HOH:O	2.22	0.42
1:A:448:LEU:HB3	4:A:1121:ACT:H3	2.02	0.41
1:A:57[B]:ARG:CB	1:A:57[B]:ARG:NH2	2.84	0.41
1:A:522:MET:HA	1:A:584:ASP:HA	2.03	0.40
1:A:95:PRO:HG3	2:A:1105:GAL:C6	2.51	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	995/1010 (98%)	974 (98%)	21 (2%)	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	785/793 (99%)	773 (98%)	12 (2%)	65 39

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	86[A]	LEU
1	A	86[B]	LEU
1	A	172	ARG
1	A	232	PHE
1	A	310	ARG
1	A	441[A]	GLN
1	A	441[B]	GLN
1	A	518	TYR
1	A	582	VAL
1	A	762	TRP
1	A	929	GLN

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 5 are monoatomic - leaving 31 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	1128	-	1,3,3	5.62	1 (100%)	0,3,3	0.00	-
5	MLI	A	1130	-	0,6,6	0.00	-	0,7,7	0.00	-
4	ACT	A	1116	-	1,3,3	8.41	1 (100%)	0,3,3	0.00	-
4	ACT	A	1123	-	1,3,3	7.54	1 (100%)	0,3,3	0.00	-
4	ACT	A	1121	-	1,3,3	7.85	1 (100%)	0,3,3	0.00	-
4	ACT	A	1115	-	1,3,3	5.23	1 (100%)	0,3,3	0.00	-
2	GAL	A	1103	-	12,12,12	0.78	0	17,17,17	0.71	0
4	ACT	A	1114	-	1,3,3	5.20	1 (100%)	0,3,3	0.00	-
6	FMT	A	1133	-	0,2,2	0.00	-	0,1,1	0.00	-
4	ACT	A	1117	-	1,3,3	7.53	1 (100%)	0,3,3	0.00	-
6	FMT	A	1134	-	0,2,2	0.00	-	0,1,1	0.00	-
7	LMR	A	1135	-	2,8,8	0.66	0	3,10,10	0.43	0
7	LMR	A	1136	-	2,8,8	0.65	0	3,10,10	1.32	1 (33%)
2	GAL	A	1102	3	12,12,12	0.53	0	17,17,17	0.71	0
2	GAL	A	1106	-	12,12,12	0.98	1 (8%)	17,17,17	1.61	3 (17%)
4	ACT	A	1119	-	1,3,3	6.14	1 (100%)	0,3,3	0.00	-
2	GAL	A	1107	-	12,12,12	0.58	0	17,17,17	1.00	0
4	ACT	A	1127	-	1,3,3	5.40	1 (100%)	0,3,3	0.00	-
2	GAL	A	1104	-	12,12,12	0.64	0	17,17,17	0.86	0
4	ACT	A	1125	-	1,3,3	5.41	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	ACT	A	1122	-	1,3,3	7.04	1 (100%)	0,3,3	0.00	-
4	ACT	A	1126	-	1,3,3	6.73	1 (100%)	0,3,3	0.00	-
5	MLI	A	1132	-	0,6,6	0.00	-	0,7,7	0.00	-
4	ACT	A	1118	-	1,3,3	6.53	1 (100%)	0,3,3	0.00	-
5	MLI	A	1129	-	0,6,6	0.00	-	0,7,7	0.00	-
4	ACT	A	1120	-	1,3,3	6.73	1 (100%)	0,3,3	0.00	-
4	ACT	A	1124	-	1,3,3	8.61	1 (100%)	0,3,3	0.00	-
2	GAL	A	1101	-	12,12,12	0.56	0	17,17,17	0.75	0
5	MLI	A	1131	-	0,6,6	0.00	-	0,7,7	0.00	-
2	GAL	A	1105	-	12,12,12	0.80	0	17,17,17	0.99	0
4	ACT	A	1113	-	1,3,3	7.68	1 (100%)	0,3,3	0.00	-

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	GAL	A	1107	-	-	0/2/22/22	0/1/1/1
5	MLI	A	1130	-	-	0/0/4/4	-
2	GAL	A	1104	-	-	2/2/22/22	0/1/1/1
5	MLI	A	1129	-	-	0/0/4/4	-
7	LMR	A	1135	-	-	0/2/8/8	-
2	GAL	A	1101	-	-	1/2/22/22	0/1/1/1
7	LMR	A	1136	-	-	2/2/8/8	-
2	GAL	A	1102	3	-	1/2/22/22	0/1/1/1
2	GAL	A	1105	-	-	1/2/22/22	0/1/1/1
2	GAL	A	1106	-	-	0/2/22/22	0/1/1/1
5	MLI	A	1131	-	-	0/0/4/4	-
2	GAL	A	1103	-	-	2/2/22/22	0/1/1/1
5	MLI	A	1132	-	-	0/0/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1124	ACT	CH3-C	8.61	1.59	1.48
4	A	1116	ACT	CH3-C	8.41	1.59	1.48
4	A	1121	ACT	CH3-C	7.85	1.58	1.48
4	A	1113	ACT	CH3-C	7.68	1.58	1.48
4	A	1123	ACT	CH3-C	7.54	1.58	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1117	ACT	CH3-C	7.53	1.58	1.48
4	A	1122	ACT	CH3-C	7.04	1.57	1.48
4	A	1126	ACT	CH3-C	6.73	1.57	1.48
4	A	1120	ACT	CH3-C	6.73	1.57	1.48
4	A	1118	ACT	CH3-C	6.53	1.57	1.48
4	A	1119	ACT	CH3-C	6.14	1.56	1.48
4	A	1128	ACT	CH3-C	5.62	1.55	1.48
4	A	1125	ACT	CH3-C	5.41	1.55	1.48
4	A	1127	ACT	CH3-C	5.40	1.55	1.48
4	A	1115	ACT	CH3-C	5.23	1.55	1.48
4	A	1114	ACT	CH3-C	5.20	1.55	1.48
2	A	1106	GAL	C4-C5	2.42	1.58	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1106	GAL	O5-C5-C4	4.70	118.23	109.69
7	A	1136	LMR	C3-C2-C1	-2.21	108.28	111.10
2	A	1106	GAL	C1-O5-C5	2.15	117.72	113.66
2	A	1106	GAL	C3-C4-C5	2.01	113.82	110.24

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1136	LMR	C1-C2-C3-C4
7	A	1136	LMR	O2-C2-C3-C4
2	A	1104	GAL	O5-C5-C6-O6
2	A	1103	GAL	O5-C5-C6-O6
2	A	1104	GAL	C4-C5-C6-O6
2	A	1103	GAL	C4-C5-C6-O6
2	A	1101	GAL	O5-C5-C6-O6
2	A	1102	GAL	O5-C5-C6-O6
2	A	1105	GAL	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1130	MLI	1	0
4	A	1121	ACT	1	0

Continued from previous page...

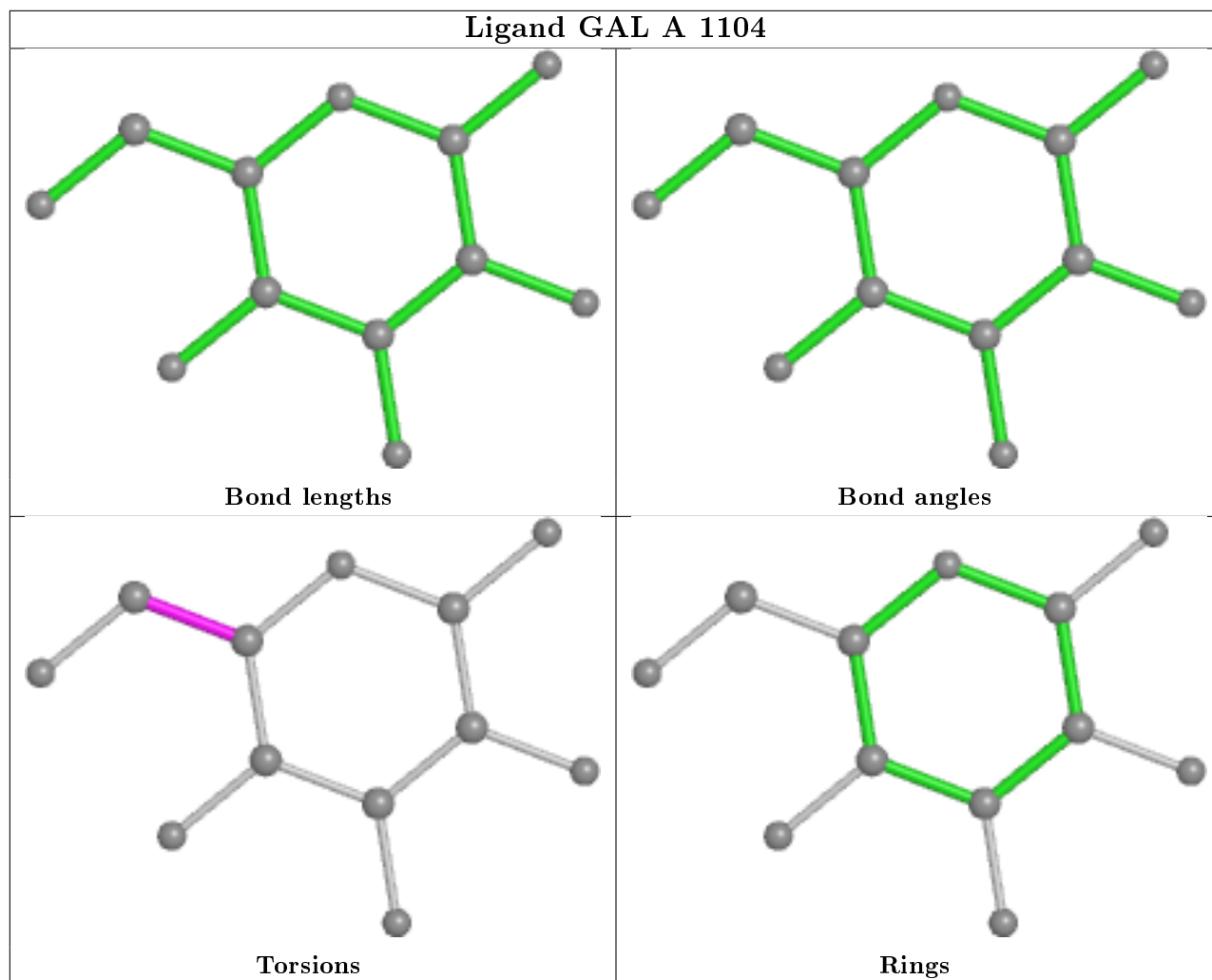| Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1117	ACT	1	0
7	A	1136	LMR	1	0
2	A	1107	GAL	2	0
4	A	1127	ACT	1	0
4	A	1118	ACT	1	0
2	A	1105	GAL	2	0

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.
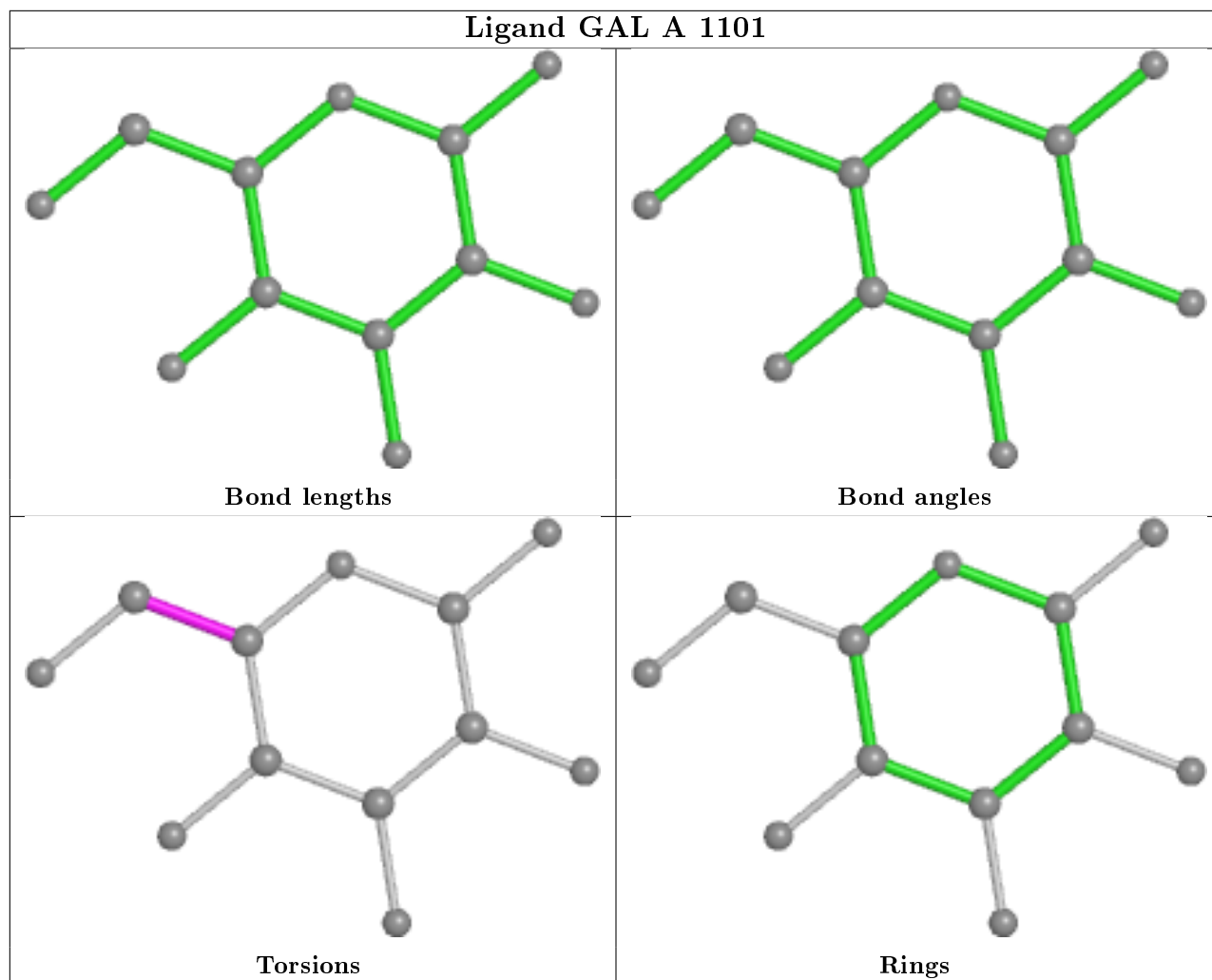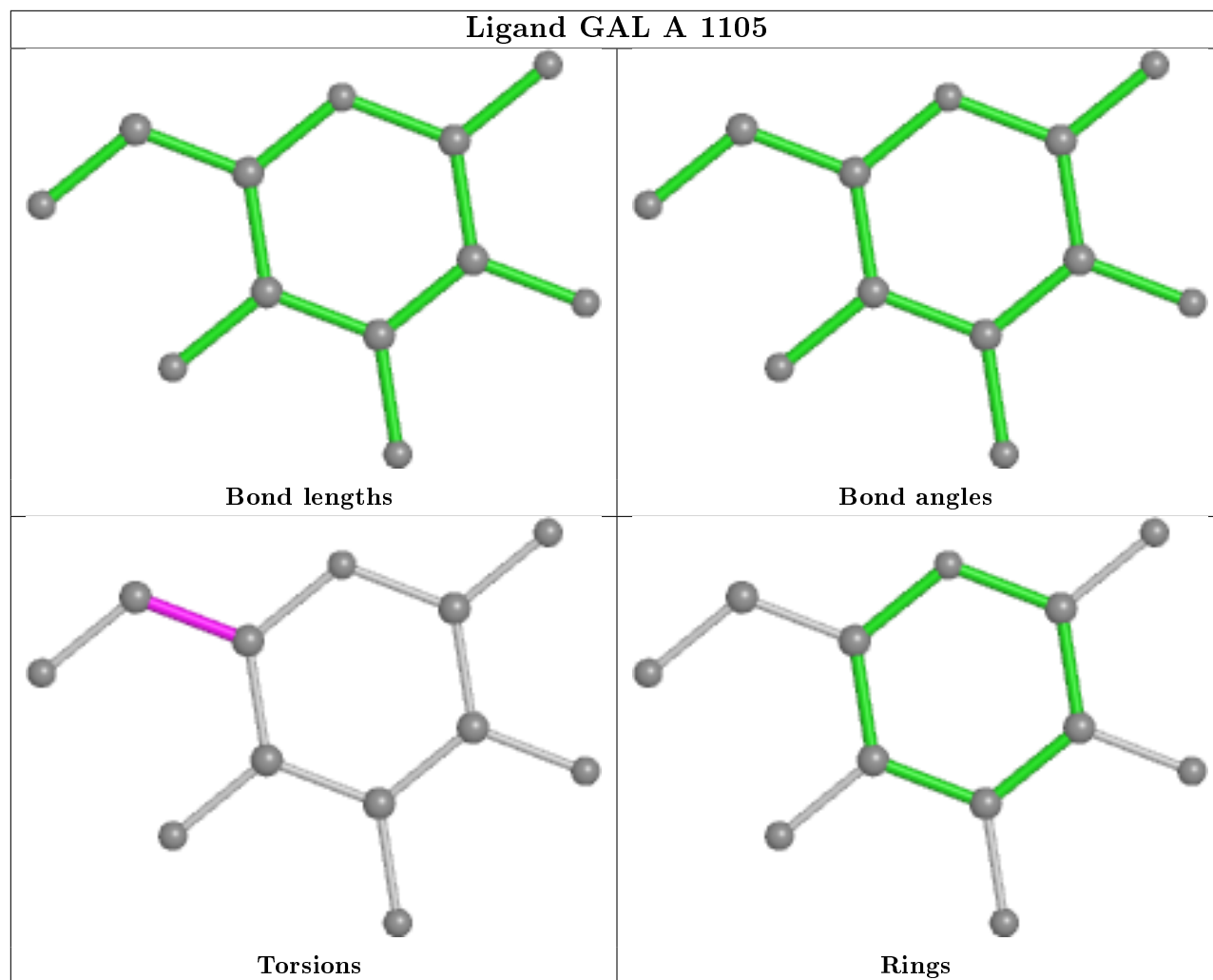
Ligand GAL A 1103

Bond lengths

Bond angles

Torsions

Rings

Ligand GAL A 1102

Bond lengths

Bond angles

Torsions

Rings

Ligand GAL A 1106

Bond lengths

Bond angles

Torsions

Rings

Ligand GAL A 1107

Bond lengths

Bond angles

Torsions

Rings

Ligand GAL A 1104

Bond lengths

Bond angles

Torsions

Rings

Ligand GAL A 1101

Bond lengths

Bond angles

Torsions

Rings

Ligand GAL A 1105

Bond lengths

Bond angles

Torsions

Rings

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(Å²)	Q<0.9
1	A	987/1010 (97%)	0.32	105 (10%) 6 6	19, 29, 58, 98	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86[A]	LEU	13.0
1	A	676	LEU	12.2
1	A	775	GLY	10.2
1	A	560	ALA	10.1
1	A	563	VAL	8.9
1	A	561	ASP	8.4
1	A	677	SER	8.2
1	A	674	ALA	7.9
1	A	642	GLY	7.9
1	A	678	ASP	7.9
1	A	87	ASN	7.8
1	A	776	ALA	7.6
1	A	562	GLY	7.2
1	A	679	GLY	7.2
1	A	716	VAL	6.9
1	A	559	THR	6.8
1	A	774	GLY	6.5
1	A	675	GLY	6.4
1	A	645	LEU	6.3
1	A	672	LEU	6.2
1	A	673	ALA	5.9
1	A	640	ALA	5.7
1	A	680	ARG	5.6
1	A	85	ALA	5.4
1	A	641	ASP	5.3
1	A	773	TRP	5.3
1	A	643	GLY	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	671	ALA	5.0
1	A	931	GLY	4.4
1	A	502	ALA	4.4
1	A	258	ASP	4.4
1	A	804	PRO	4.2
1	A	808	GLY	4.2
1	A	715	PRO	4.2
1	A	84	GLU	3.9
1	A	83	GLY	3.9
1	A	714	ALA	3.8
1	A	88	GLY	3.8
1	A	364	ILE	3.7
1	A	713	GLY	3.6
1	A	299	ALA	3.6
1	A	558	SER	3.5
1	A	82	LEU	3.5
1	A	807	ASP	3.3
1	A	721	VAL	3.3
1	A	644	ALA	3.3
1	A	331	VAL	3.2
1	A	388	LEU	3.2
1	A	369	TYR	3.2
1	A	613	ARG	3.0
1	A	260	VAL	2.9
1	A	255	GLN	2.9
1	A	806	GLN	2.9
1	A	500	ASN	2.9
1	A	392	LEU	2.8
1	A	547	VAL	2.8
1	A	503	ALA	2.8
1	A	185	GLN	2.8
1	A	226	ALA	2.8
1	A	386	VAL	2.8
1	A	728	ASP	2.7
1	A	225	ALA	2.7
1	A	256	ALA	2.7
1	A	711	GLU	2.7
1	A	546	PHE	2.6
1	A	1009	ARG	2.6
1	A	519	VAL	2.6
1	A	366	THR	2.6
1	A	964	LYS	2.6

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	726	VAL	2.6
1	A	328	LEU	2.5
1	A	152	ILE	2.5
1	A	550	TRP	2.5
1	A	387	VAL	2.5
1	A	647	GLY	2.5
1	A	803	ASN	2.5
1	A	1010	SER	2.4
1	A	173	LEU	2.4
1	A	363	ALA	2.4
1	A	548	TRP	2.4
1	A	551	LEU	2.4
1	A	79	GLY	2.4
1	A	516	CYS	2.3
1	A	186	GLY	2.3
1	A	433	VAL	2.2
1	A	302[A]	SER	2.2
1	A	805	GLY	2.2
1	A	224	PRO	2.2
1	A	77	ASP	2.2
1	A	515	LEU	2.2
1	A	586	LEU	2.2
1	A	375	PHE	2.1
1	A	138	GLY	2.1
1	A	518	TYR	2.1
1	A	274	THR	2.1
1	A	501	ASP	2.1
1	A	142	PHE	2.1
1	A	504	LEU	2.1
1	A	139	PRO	2.0
1	A	361	ILE	2.0
1	A	681	PRO	2.0
1	A	390	CYS	2.0
1	A	210	TRP	2.0
1	A	809	GLY	2.0
1	A	371	PRO	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	1127	4/4	0.35	0.27	71,73,73,73	0
2	GAL	A	1107	12/12	0.46	0.27	85,90,91,92	0
5	MLI	A	1130	7/7	0.48	0.19	74,74,76,76	0
4	ACT	A	1122	4/4	0.52	0.33	100,101,101,101	0
2	GAL	A	1106	12/12	0.53	0.32	104,105,107,107	0
4	ACT	A	1117	4/4	0.54	0.24	71,72,72,74	0
7	LMR	A	1135	9/9	0.57	0.29	87,88,89,89	0
7	LMR	A	1136	9/9	0.58	0.23	73,78,79,79	0
4	ACT	A	1118	4/4	0.58	0.22	57,61,61,65	0
4	ACT	A	1124	4/4	0.58	0.28	43,43,44,47	0
2	GAL	A	1104	12/12	0.59	0.19	63,70,71,72	0
5	MLI	A	1132	7/7	0.59	0.49	90,91,92,93	0
5	MLI	A	1129	7/7	0.64	0.22	72,74,78,80	0
6	FMT	A	1134	3/3	0.64	0.24	56,56,58,59	0
4	ACT	A	1126	4/4	0.65	0.15	57,58,58,58	0
2	GAL	A	1105	12/12	0.67	0.21	53,59,62,63	0
4	ACT	A	1119	4/4	0.68	0.16	79,79,80,81	0
2	GAL	A	1103	12/12	0.68	0.20	56,60,61,62	0
5	MLI	A	1131	7/7	0.73	0.17	68,69,75,75	0
4	ACT	A	1125	4/4	0.73	0.16	65,66,66,66	0
4	ACT	A	1121	4/4	0.82	0.12	32,35,35,38	0
2	GAL	A	1102	12/12	0.84	0.19	47,48,50,53	0
6	FMT	A	1133	3/3	0.86	0.13	51,51,54,56	0
4	ACT	A	1113	4/4	0.87	0.15	59,60,60,63	0
4	ACT	A	1123	4/4	0.88	0.13	42,47,49,50	0
4	ACT	A	1120	4/4	0.88	0.16	69,69,70,71	0
4	ACT	A	1128	4/4	0.91	0.13	58,61,64,64	0
4	ACT	A	1116	4/4	0.94	0.09	32,33,34,36	0
4	ACT	A	1115	4/4	0.95	0.12	34,36,36,37	0
3	NA	A	1112	1/1	0.96	0.10	47,47,47,47	0
3	NA	A	1110	1/1	0.96	0.12	43,43,43,43	0
2	GAL	A	1101	12/12	0.96	0.07	22,23,27,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	A	1114	4/4	0.97	0.08	30,31,32,33	0
3	NA	A	1108	1/1	0.99	0.09	24,24,24,24	0
3	NA	A	1111	1/1	1.00	0.05	30,30,30,30	0
3	NA	A	1109	1/1	1.00	0.06	26,26,26,26	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:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative)
and green (positive)
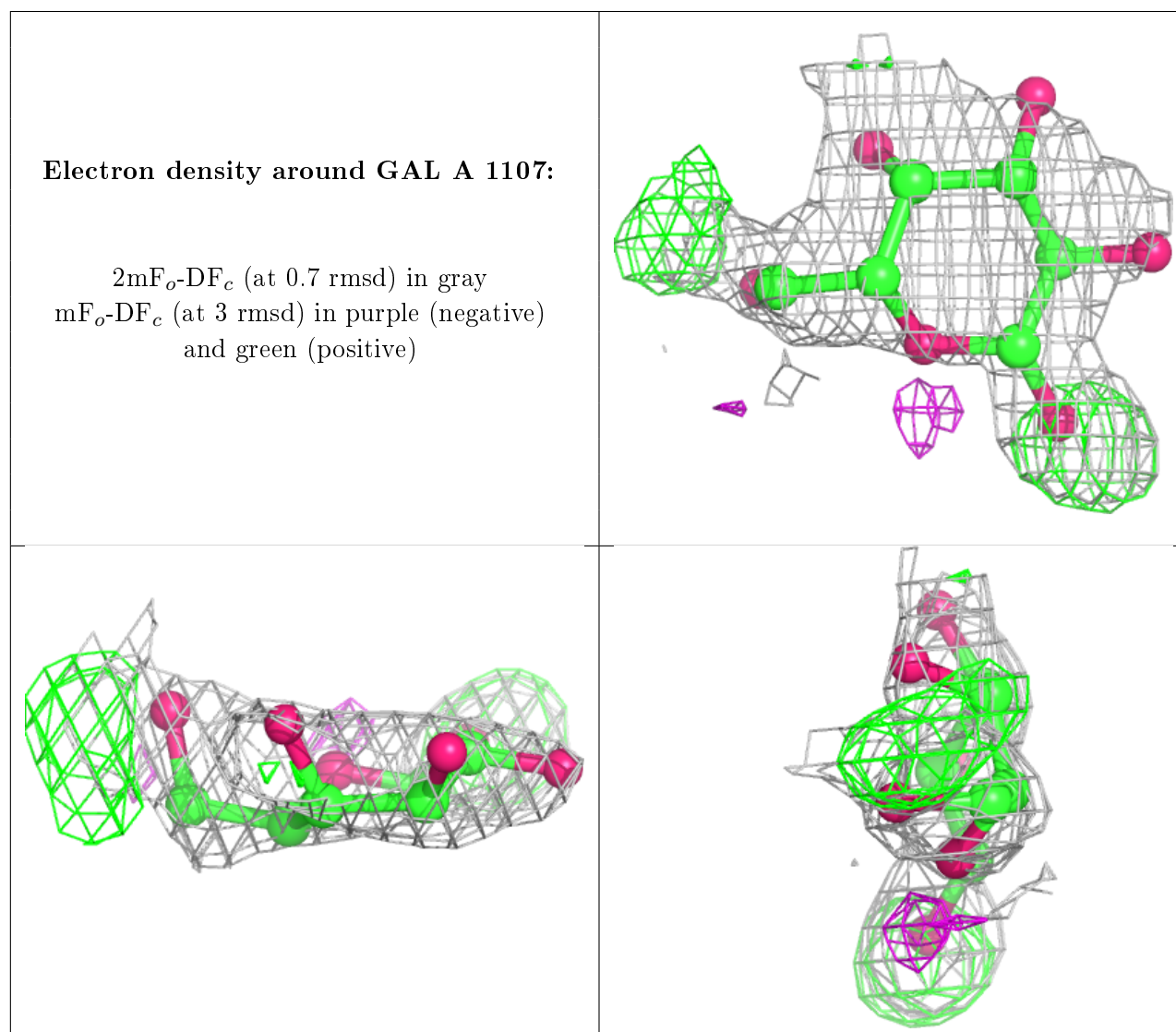
Electron density around GAL A 1106:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
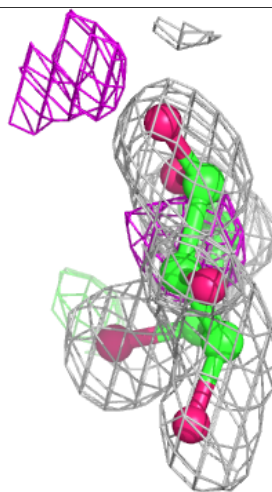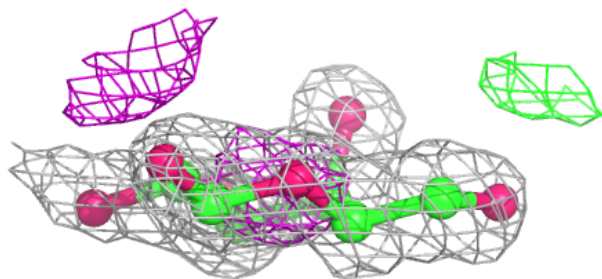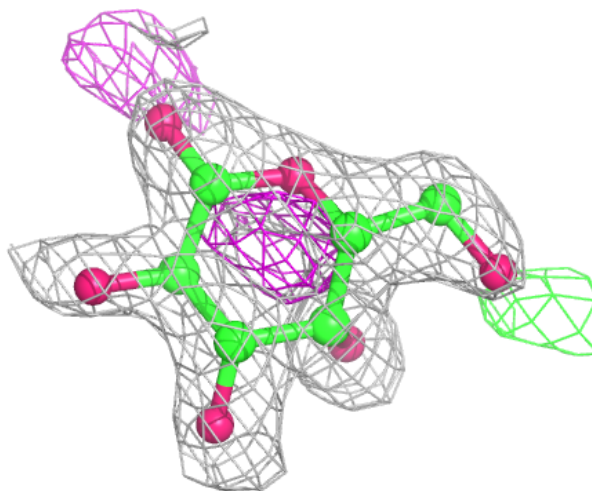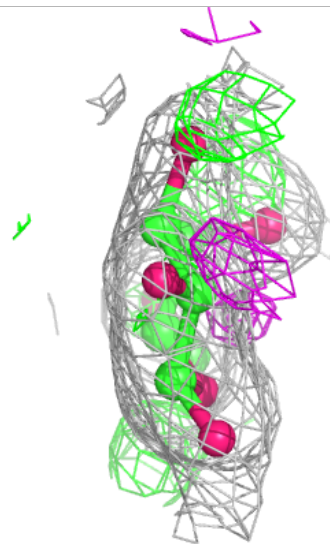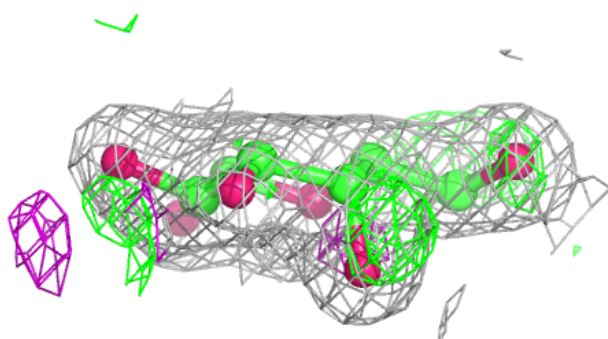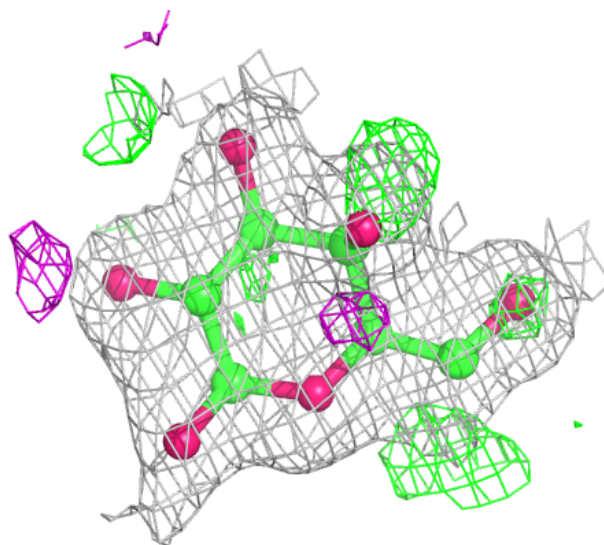and green (positive)
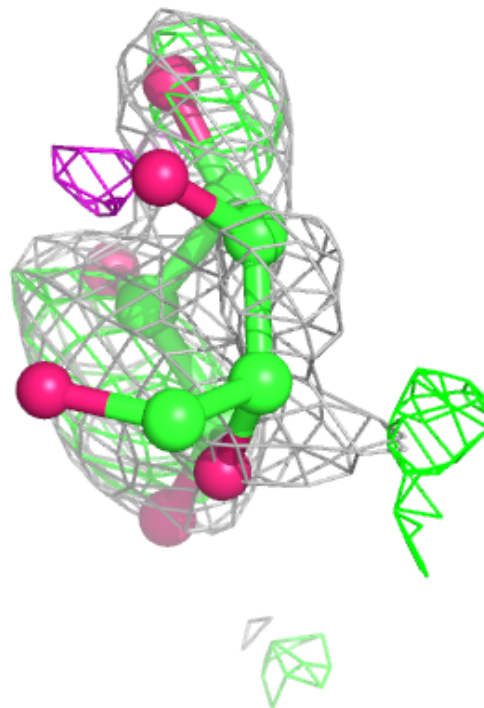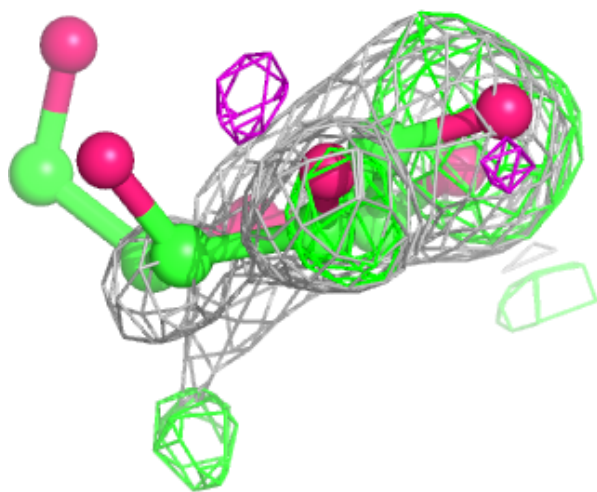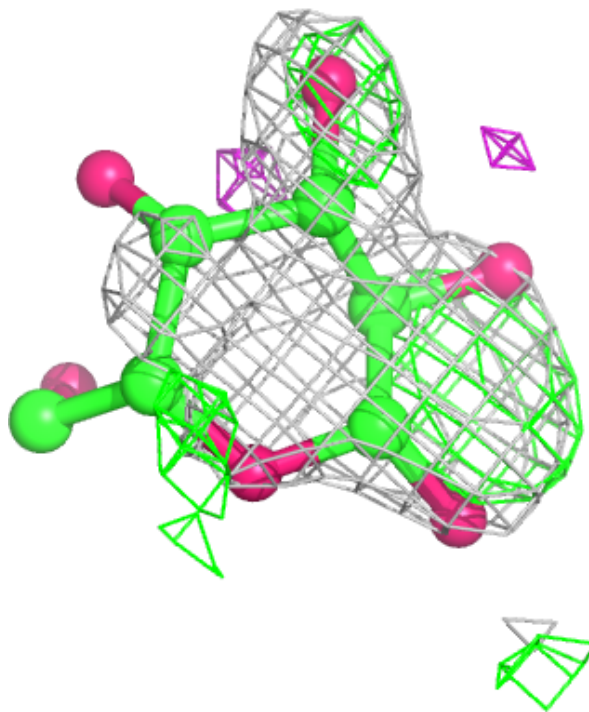
Electron density around GAL A 1104:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
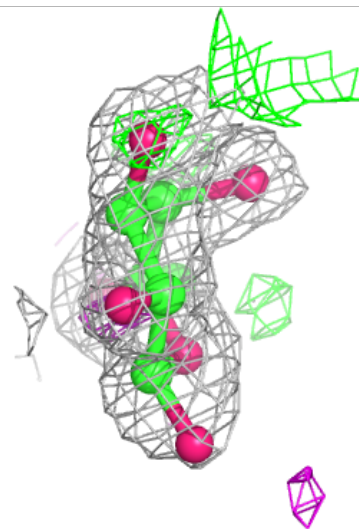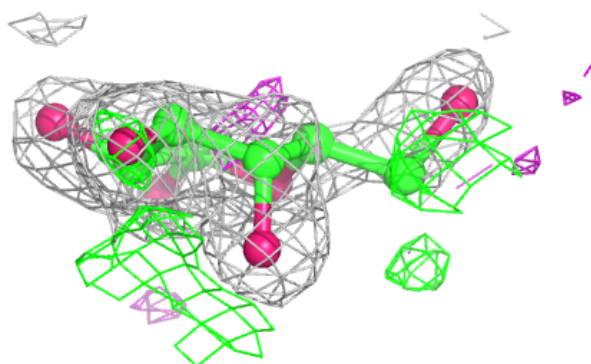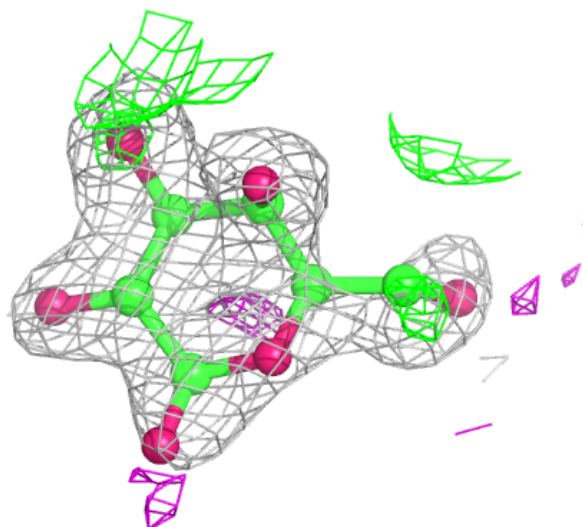
Electron density around GAL A 1105:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
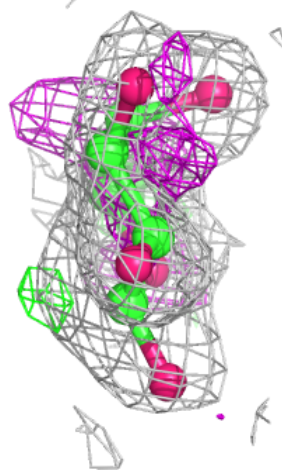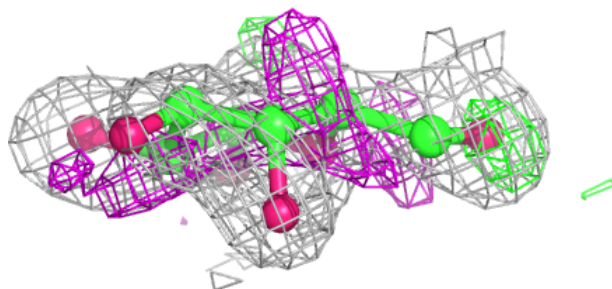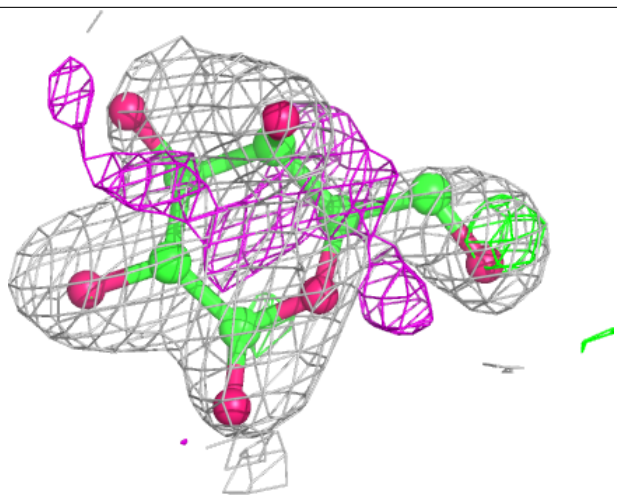
Electron density around GAL A 1103:

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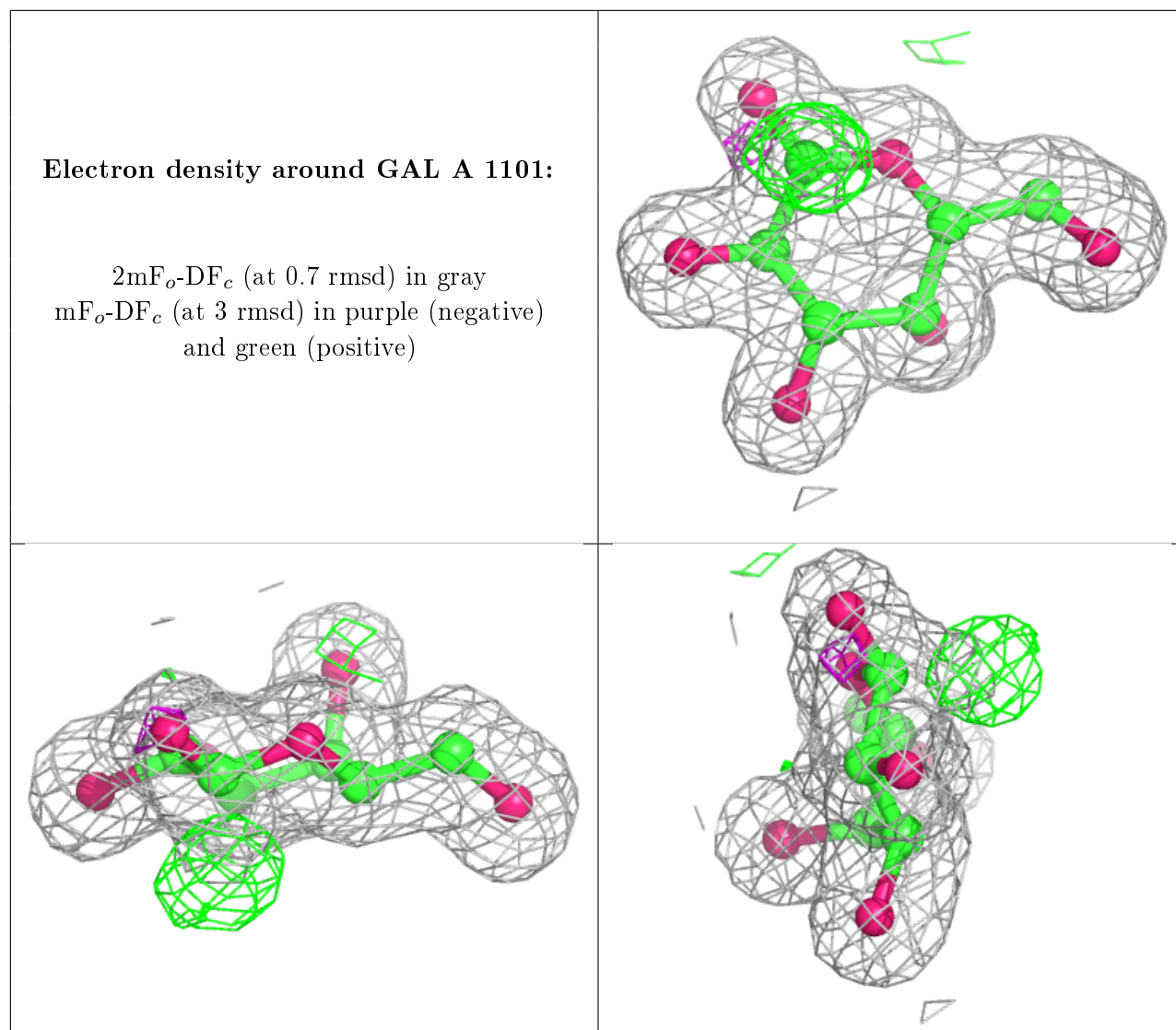and green (positive)

Electron density around GAL A 1102:

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

Electron density around GAL A 1101:

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

6.5 Other polymers (i)

There are no such residues in this entry.