



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 07:24 PM BST

PDB ID : 6ZJW
Title : Cold-adapted beta-D-galactosidase from *Arthrobacter* sp. 32cB mutant D207A in complex with galactose
Authors : Rutkiewicz, M.; Bujacz, A.; Bujacz, G.
Deposited on : 2020-06-29
Resolution : 2.12 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 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 : 2.13.1
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

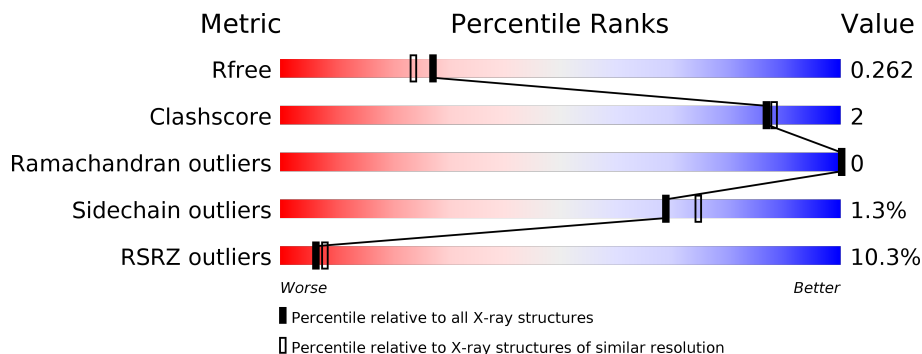
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 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 $\leq 5\%$. 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	1010	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7947 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.

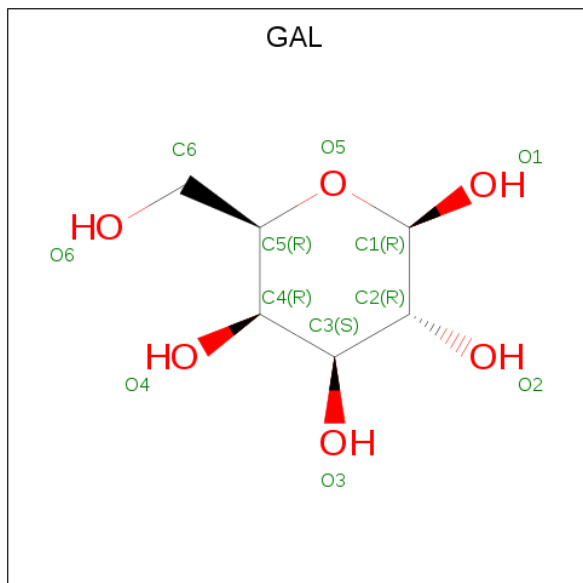
- Molecule 1 is a protein called Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	989	7620	4794	1362	1446	18	0	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	ALA	ASP	engineered mutation	UNP A0A023UGN9

- Molecule 2 is beta-D-galactopyranose (three-letter code: GAL) (formula: C₆H₁₂O₆) (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		

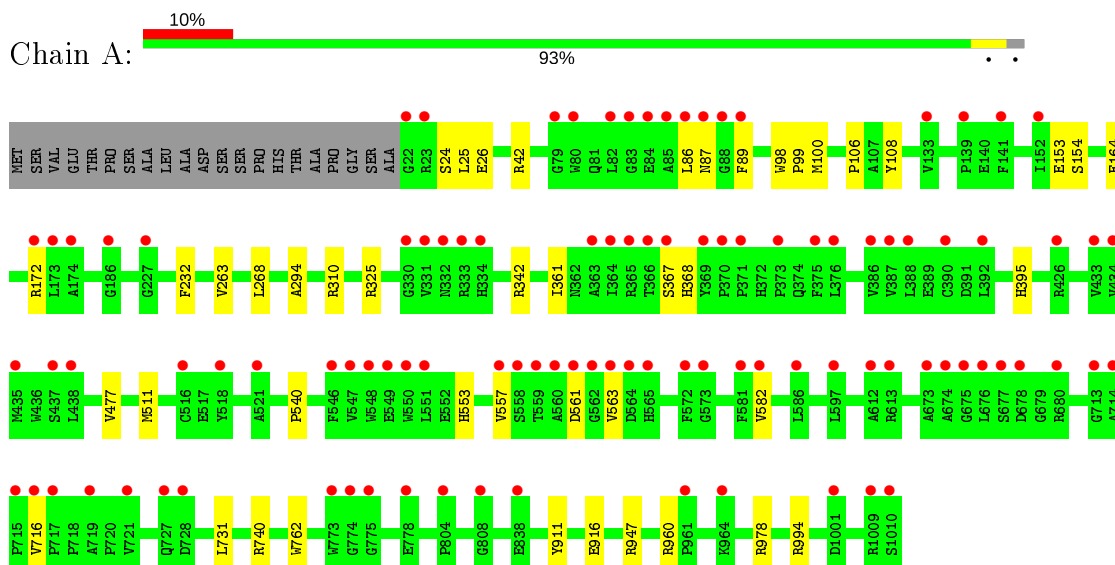
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	303	Total 303	O 303	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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.28Å 139.28Å 127.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.86 – 2.12 43.86 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.4 (43.86-2.12) 99.6 (43.86-2.12)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.12Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.223 , 0.257 0.226 , 0.262	Depositor DCC
R_{free} test set	2093 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtrriage
Anisotropy	0.473	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7947	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GAL

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	0.28	0/7825	0.49	0/10666

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	7620	0	7316	31	0
2	A	24	0	24	1	0
3	A	303	0	0	0	0
All	All	7947	0	7340	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:553:HIS:HB2	1:A:582:VAL:CG1	1.74	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:HIS:HB2	1:A:582:VAL:HG12	1.07	1.05
1:A:553:HIS:CB	1:A:582:VAL:HG12	1.98	0.90
1:A:108:TYR:CE1	1:A:582:VAL:HG22	2.24	0.72
1:A:108:TYR:CZ	1:A:582:VAL:HG22	2.29	0.67
1:A:553:HIS:CB	1:A:582:VAL:CG1	2.66	0.65
1:A:108:TYR:CD1	1:A:582:VAL:HG22	2.40	0.57
1:A:553:HIS:HB2	1:A:582:VAL:HG11	1.83	0.56
1:A:108:TYR:CD2	1:A:582:VAL:CG2	2.93	0.52
1:A:263:VAL:HG23	1:A:268:LEU:HB2	1.95	0.48
1:A:108:TYR:CE2	1:A:582:VAL:HG22	2.48	0.48
1:A:86:LEU:HD13	1:A:89:PHE:HB2	1.95	0.48
1:A:100:MET:CE	1:A:106:PRO:HG3	2.44	0.47
1:A:911:TYR:O	1:A:960:ARG:HD3	2.15	0.47
1:A:42:ARG:NH2	1:A:164:GLU:OE2	2.48	0.46
1:A:325[B]:ARG:HE	1:A:540:PRO:HA	1.81	0.46
1:A:108:TYR:CG	1:A:582:VAL:CG2	2.99	0.46
1:A:361:ILE:O	2:A:1101:GAL:O2	2.23	0.45
1:A:978:ARG:HH12	1:A:994:ARG:NH1	2.14	0.45
1:A:153:GLU:OE1	1:A:342:ARG:NH1	2.40	0.45
1:A:153:GLU:HA	1:A:154:SER:HA	1.76	0.44
1:A:716:VAL:O	1:A:716:VAL:HG23	2.18	0.44
1:A:263:VAL:HG12	1:A:294:ALA:HB2	2.00	0.43
1:A:108:TYR:CE2	1:A:582:VAL:CG2	3.01	0.43
1:A:24:SER:C	1:A:25:LEU:HD12	2.39	0.43
1:A:325[B]:ARG:NE	1:A:540:PRO:HA	2.34	0.43
1:A:731:LEU:HD13	1:A:740:ARG:HG3	2.01	0.43
1:A:367:SER:HA	1:A:368:HIS:HA	1.81	0.42
1:A:98:TRP:N	1:A:99:PRO:CD	2.83	0.41
1:A:916:GLU:OE1	1:A:947:ARG:NH2	2.48	0.41
1:A:477:VAL:C	1:A:511:MET:HE2	2.40	0.41

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	989/1010 (98%)	955 (97%)	34 (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	778/792 (98%)	768 (99%)	10 (1%)	69	74

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

Mol	Chain	Res	Type
1	A	26	GLU
1	A	87	ASN
1	A	172	ARG
1	A	232	PHE
1	A	310	ARG
1	A	395	HIS
1	A	557	VAL
1	A	561	ASP
1	A	563	VAL
1	A	762	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	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](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GAL	A	1101	-	12,12,12	0.36	0	17,17,17	0.62	0
2	GAL	A	1102	-	12,12,12	0.41	0	17,17,17	0.75	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
2	GAL	A	1101	-	-	0/2/22/22	0/1/1/1
2	GAL	A	1102	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

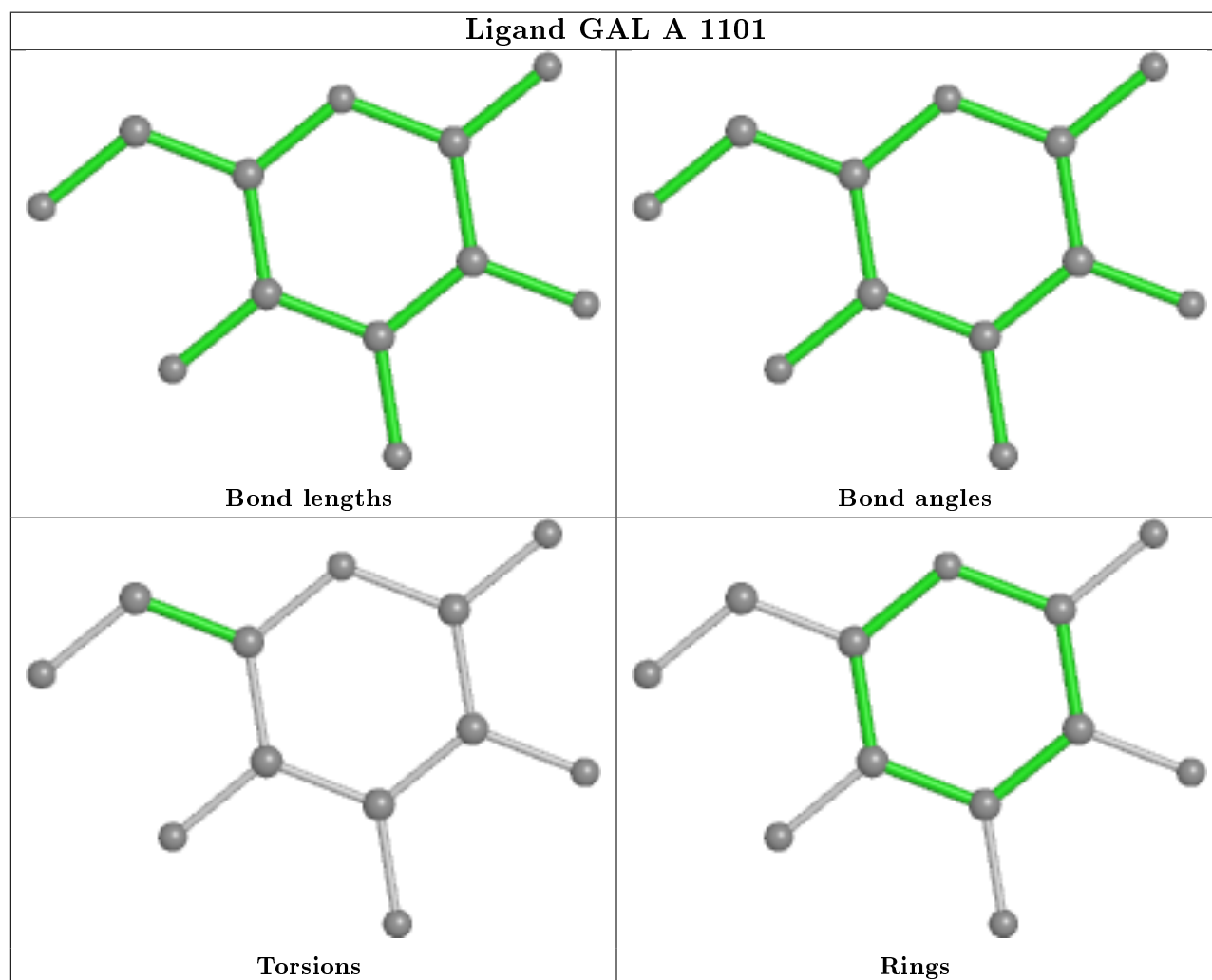
There are no torsion outliers.

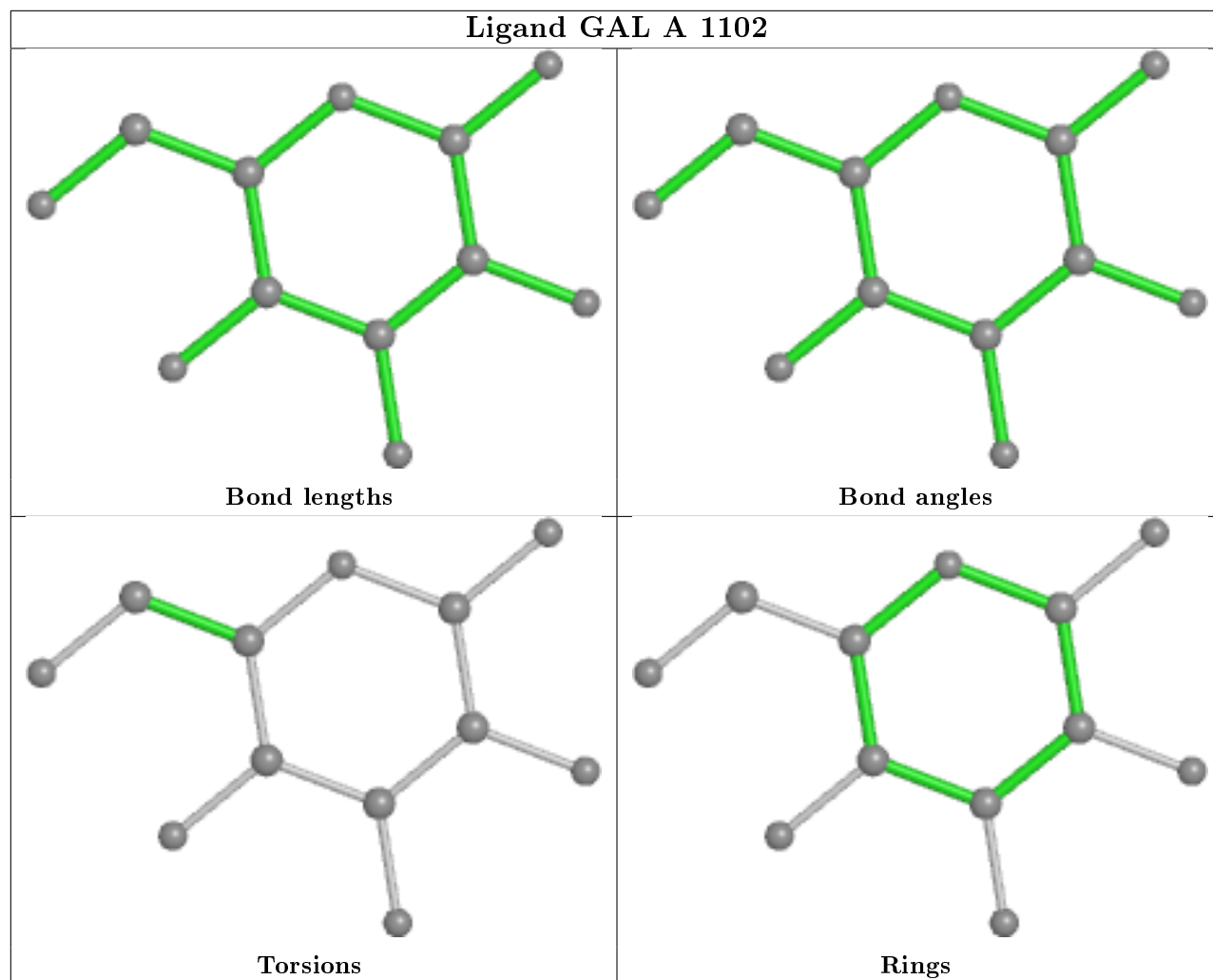
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	GAL	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 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 than 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.





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, 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	989/1010 (97%)	0.45	102 (10%) 6 8	33, 56, 86, 152	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	561	ASP	8.3
1	A	563	VAL	7.0
1	A	716	VAL	6.3
1	A	562	GLY	6.2
1	A	388	LEU	6.1
1	A	559	THR	6.0
1	A	676	LEU	5.4
1	A	714	ALA	5.2
1	A	678	ASP	5.2
1	A	560	ALA	5.0
1	A	331	VAL	4.9
1	A	364	ILE	4.9
1	A	677	SER	4.8
1	A	86	LEU	4.8
1	A	387	VAL	4.8
1	A	85	ALA	4.3
1	A	547	VAL	4.3
1	A	558	SER	4.2
1	A	773	TRP	4.1
1	A	386	VAL	4.1
1	A	80	TRP	4.1
1	A	390	CYS	4.1
1	A	808	GLY	4.0
1	A	369	TYR	3.9
1	A	673	ALA	3.9
1	A	141	PHE	3.9
1	A	87	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1010	SER	3.8
1	A	23	ARG	3.7
1	A	366	THR	3.7
1	A	521	ALA	3.5
1	A	186	GLY	3.5
1	A	371	PRO	3.4
1	A	674	ALA	3.3
1	A	557	VAL	3.3
1	A	774	GLY	3.2
1	A	437	SER	3.1
1	A	174	ALA	3.1
1	A	375	PHE	3.1
1	A	1009	ARG	3.1
1	A	370	PRO	3.0
1	A	550	TRP	3.0
1	A	88	GLY	3.0
1	A	22	GLY	3.0
1	A	333	ARG	2.9
1	A	365	ARG	2.9
1	A	516	CYS	2.9
1	A	964	LYS	2.9
1	A	715	PRO	2.9
1	A	804	PRO	2.9
1	A	775	GLY	2.8
1	A	433	VAL	2.8
1	A	572	PHE	2.8
1	A	330	GLY	2.7
1	A	376	LEU	2.7
1	A	79	GLY	2.7
1	A	613	ARG	2.7
1	A	961	PRO	2.6
1	A	426	ARG	2.6
1	A	434	VAL	2.6
1	A	518	TYR	2.6
1	A	565	HIS	2.6
1	A	713	GLY	2.6
1	A	582	VAL	2.6
1	A	546	PHE	2.6
1	A	838	GLU	2.6
1	A	173	LEU	2.6
1	A	586	LEU	2.6
1	A	172	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	82	LEU	2.5
1	A	573	GLY	2.5
1	A	728	ASP	2.5
1	A	152	ILE	2.5
1	A	680	ARG	2.5
1	A	133	VAL	2.4
1	A	1001	ASP	2.4
1	A	675	GLY	2.4
1	A	435	MET	2.4
1	A	334	HIS	2.4
1	A	367	SER	2.4
1	A	548	TRP	2.4
1	A	721	VAL	2.3
1	A	717	PRO	2.3
1	A	597	LEU	2.3
1	A	727	GLN	2.3
1	A	392	LEU	2.3
1	A	612	ALA	2.3
1	A	778	GLU	2.3
1	A	719	ALA	2.3
1	A	564	ASP	2.3
1	A	332	ASN	2.3
1	A	89	PHE	2.2
1	A	438	LEU	2.2
1	A	581	PHE	2.2
1	A	139	PRO	2.1
1	A	83	GLY	2.1
1	A	551	LEU	2.1
1	A	227	GLY	2.1
1	A	373	PRO	2.0
1	A	84	GLU	2.0
1	A	363	ALA	2.0
1	A	549	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](#)

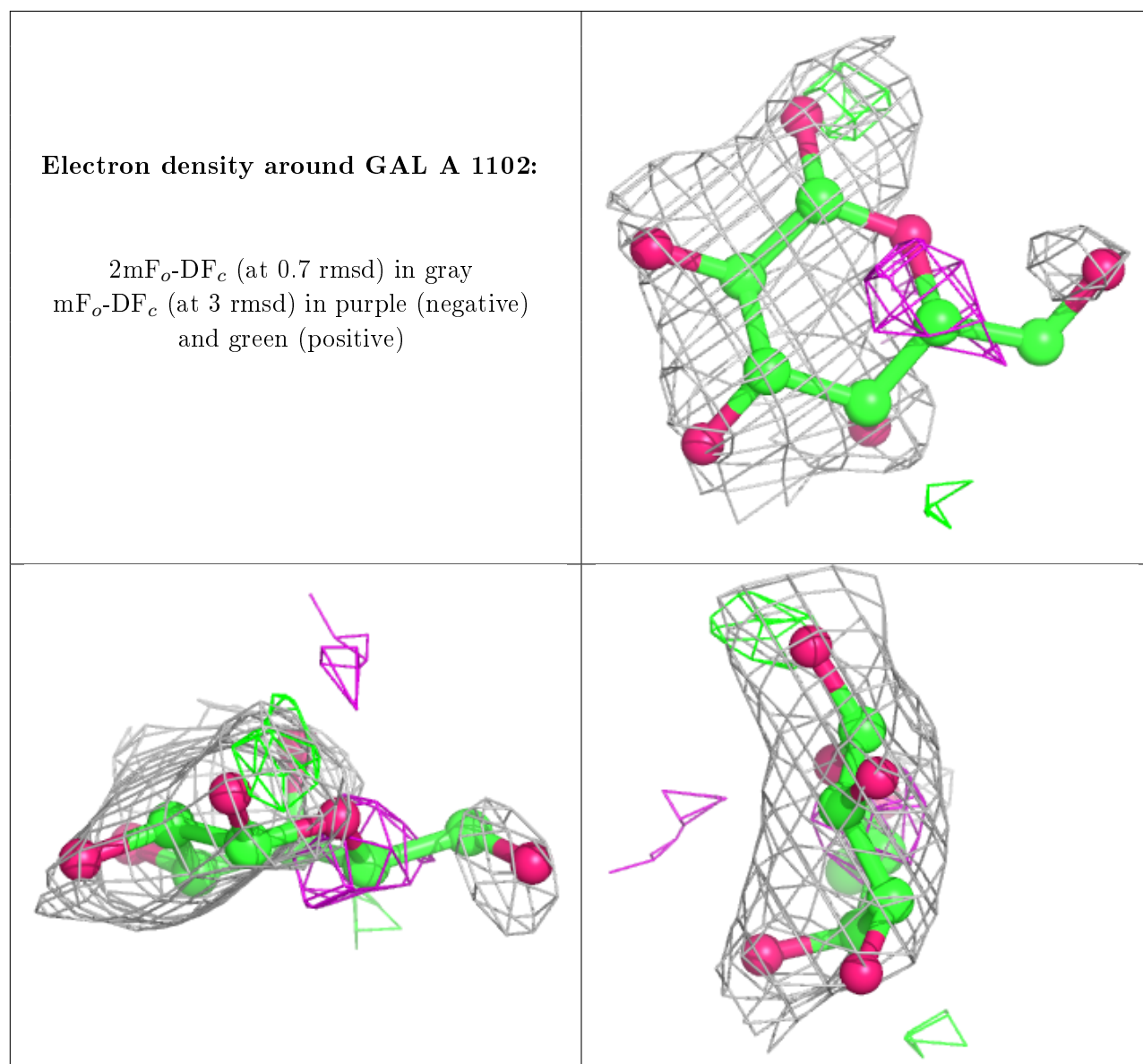
There are no monosaccharides in this entry.

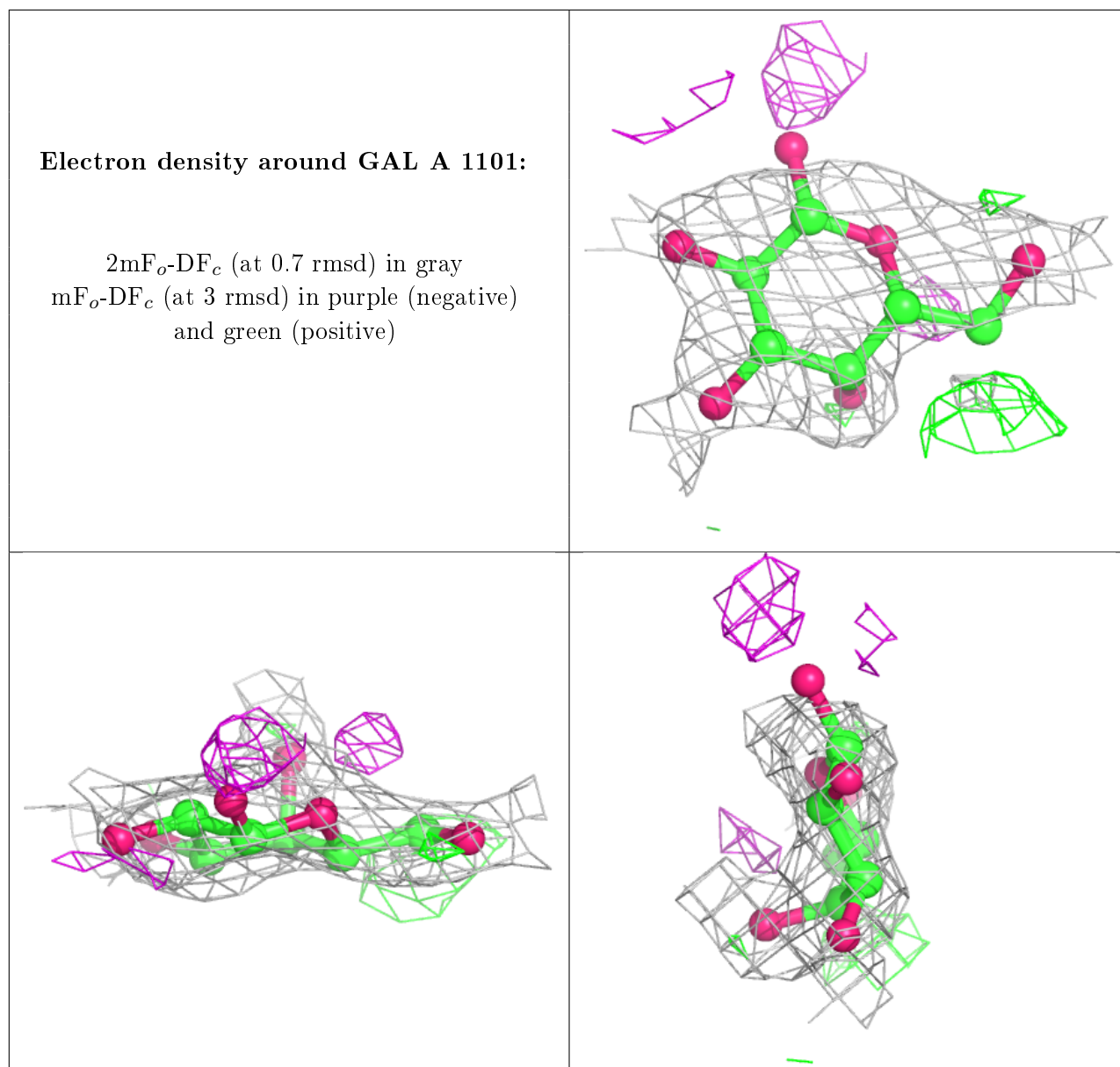
6.4 Ligands [\(i\)](#)

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
2	GAL	A	1102	12/12	0.56	0.36	99,106,113,113	12
2	GAL	A	1101	12/12	0.72	0.26	69,79,85,90	12

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.