Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 04:41 PM JST

PDB ID	:	7EXG
Title	:	Crystal structure of D383A mutant from Arabidopsis thaliana complexed with Galactose.
Authors	:	Chuankhayan, P.; Guan, H.H.; Lin, C.C.; Chen, N.C.; Huang, Y.C.; Yoshimura, M.; Nakagawa, A.; Lee, R.H.; Chen, C.J.
Deposited on	:	2021-05-27
Resolution	:	2.05 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:

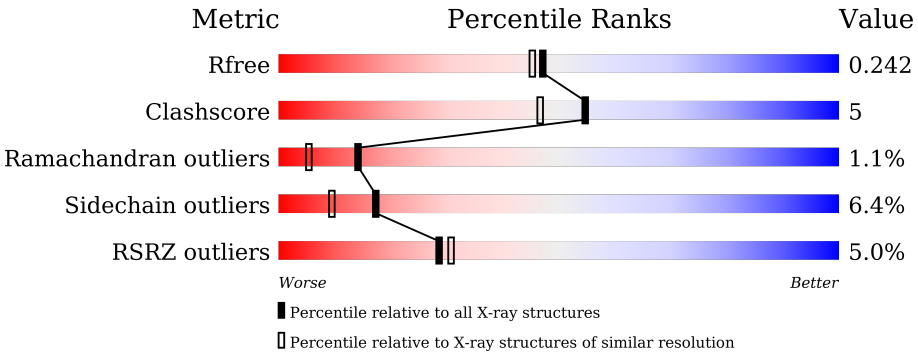
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	749	7% 79% 15%
1	B	749	3% 82% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11821 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.

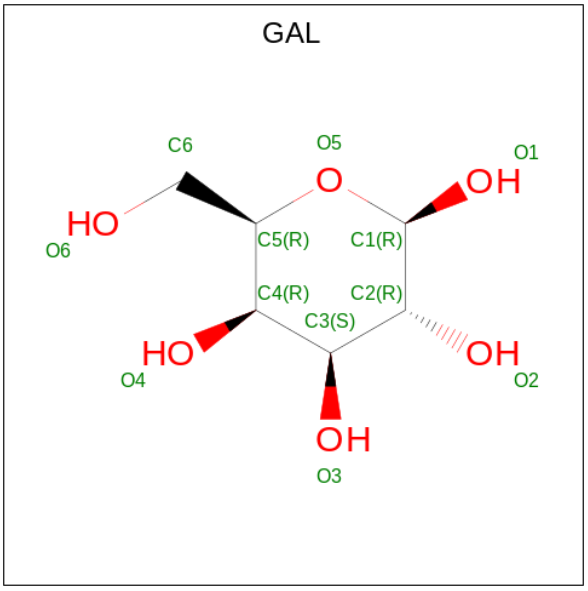
- Molecule 1 is a protein called Probable galactinol–sucrose galactosyltransferase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	716	Total	C	N	O	S	0	0	0
			5610	3567	967	1047	29			
1	A	716	Total	C	N	O	S	0	0	0
			5610	3567	967	1047	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	302	ARG	LYS	conflict	UNP Q8RX87
B	383	ALA	ASP	engineered mutation	UNP Q8RX87
A	302	ARG	LYS	conflict	UNP Q8RX87
A	383	ALA	ASP	engineered mutation	UNP Q8RX87

- Molecule 2 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
2	B	1	Total C O 11 5 6	0	0
2	A	1	Total C O 11 6 5	0	0

- Molecule 3 is water.

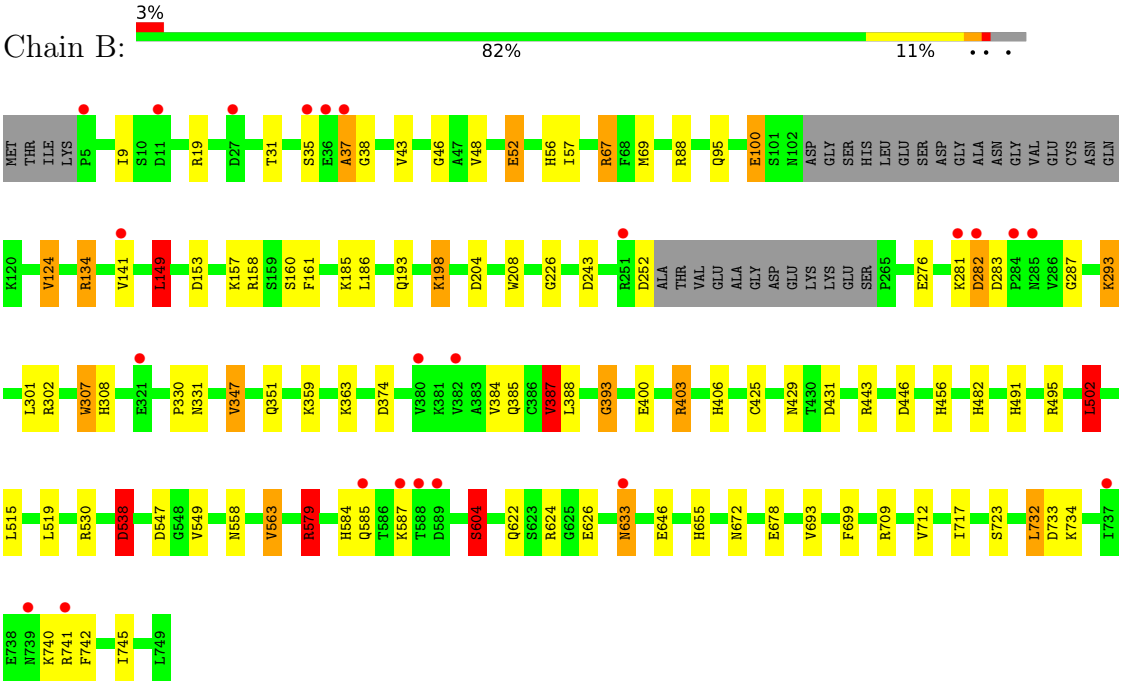
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	359	Total O 359 359	0	0
3	A	220	Total O 220 220	0	0

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.

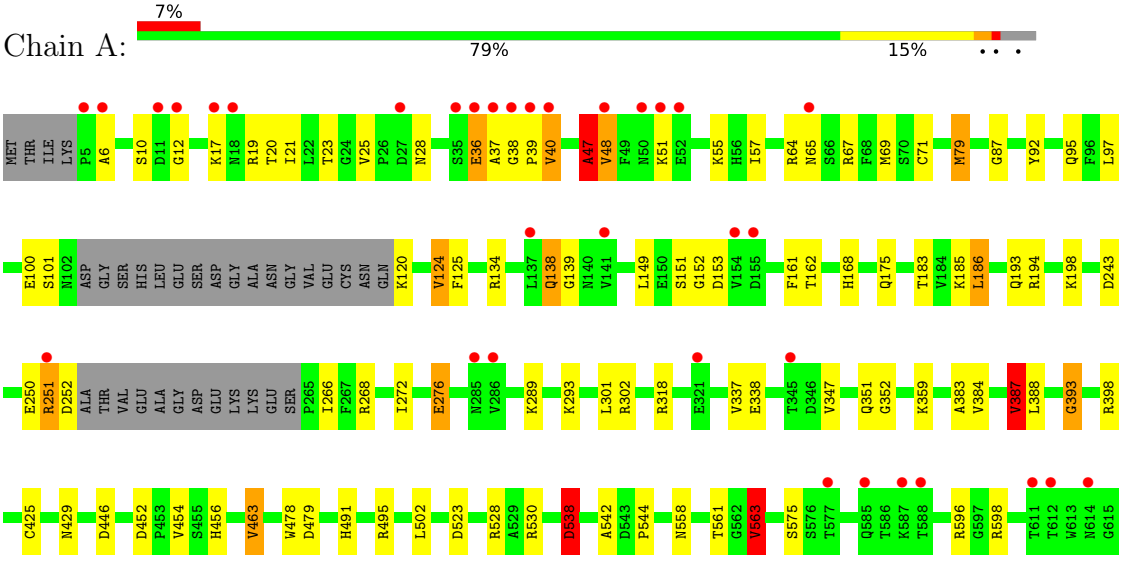
• Molecule 1: Probable galactinol–sucrose galactosyltransferase 6

Chain B:



• Molecule 1: Probable galactinol–sucrose galactosyltransferase 6

Chain A:




D616
C617
A618
S621
Q622
S623
R624
G625
E626
L627
I628
Y632
N633
V634
S635
E646
V657
D658
G659
V660
S661
N672
E678
R681
A684
E685
K686
M687
K708
S714
N715
E720
T729
L732
D733
K734
I737
E738
N739
K740
R741
F742
L749

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.03Å 103.74Å 182.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.05 29.87 – 2.05	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-2.05) 92.9 (29.87-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.184 , 0.235 0.194 , 0.242	Depositor DCC
R_{free} test set	5259 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11821	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: 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	0.86	0/5744	1.01	21/7778 (0.3%)
1	B	1.00	4/5744 (0.1%)	1.04	24/7778 (0.3%)
All	All	0.93	4/11488 (0.0%)	1.03	45/15556 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	604	SER	CB-OG	-7.19	1.32	1.42
1	B	646	GLU	CG-CD	6.61	1.61	1.51
1	B	307	TRP	CB-CG	6.17	1.61	1.50
1	B	374	ASP	CB-CG	5.24	1.62	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	528	ARG	NE-CZ-NH2	-13.91	113.34	120.30
1	A	528	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	B	204	ASP	CB-CG-OD1	8.99	126.39	118.30
1	B	579	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	B	547	ASP	CB-CG-OD1	8.02	125.51	118.30
1	B	302	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	B	387	VAL	CB-CA-C	-7.45	97.25	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	563	VAL	CB-CA-C	-7.30	97.53	111.40
1	B	538	ASP	CB-CG-OD1	-7.29	111.74	118.30
1	A	530	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	B	124	VAL	CB-CA-C	-7.21	97.70	111.40
1	A	563	VAL	CB-CA-C	-7.03	98.05	111.40
1	B	443	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	387	VAL	CB-CA-C	-6.75	98.58	111.40
1	B	502	LEU	CA-CB-CG	6.56	130.38	115.30
1	B	547	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	124	VAL	CB-CA-C	-6.50	99.04	111.40
1	B	579	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	B	563	VAL	CG1-CB-CG2	6.13	120.71	110.90
1	A	446	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	A	528	ARG	CG-CD-NE	-6.04	99.12	111.80
1	B	67	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	B	530	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	194	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	B	530	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	79	MET	CG-SD-CE	5.84	109.55	100.20
1	A	138	GLN	CB-CA-C	-5.82	98.77	110.40
1	A	681	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	149	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	528	ARG	CD-NE-CZ	5.58	131.41	123.60
1	A	251	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	523	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	302	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	646	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	B	403	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	363	LYS	CD-CE-NZ	-5.33	99.45	111.70
1	A	538	ASP	CB-CA-C	-5.21	99.99	110.40
1	A	616	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	47	ALA	C-N-CA	5.13	134.54	121.70
1	A	186	LEU	CB-CG-CD1	5.12	119.70	111.00
1	B	633	ASN	N-CA-C	5.11	124.79	111.00
1	B	387	VAL	N-CA-CB	5.08	122.67	111.50
1	A	616	ASP	CB-CG-OD1	5.06	122.86	118.30
1	B	134	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	B	204	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	ALA	Peptide

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	5610	0	5533	64	0
1	B	5610	0	5533	54	0
2	A	11	0	10	0	0
2	B	11	0	8	1	0
3	A	220	0	0	5	0
3	B	359	0	0	14	0
All	All	11821	0	11084	116	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 (116) 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:B:252:ASP:C	3:B:902:HOH:O	1.69	1.25
2:B:801:GAL:O6	2:B:801:GAL:C5	2.06	1.04
1:B:287:GLY:N	3:B:901:HOH:O	1.88	1.00
1:A:558:ASN:HD21	1:A:672:ASN:HD21	1.12	0.95
1:B:709:ARG:HD3	3:B:1208:HOH:O	1.67	0.95
1:A:624:ARG:NH2	1:A:626:GLU:OE2	2.10	0.83
1:A:95:GLN:HE21	1:A:134:ARG:HH21	1.25	0.82
1:B:95:GLN:HE21	1:B:134:ARG:HH21	1.29	0.81
1:A:71:CYS:HB3	1:A:79:MET:HE2	1.64	0.80
1:B:502:LEU:HD21	1:B:519:LEU:HD22	1.65	0.77
1:A:47:ALA:HA	1:A:48:VAL:HG12	1.67	0.77
1:A:71:CYS:HB3	1:A:79:MET:CE	2.15	0.76
1:A:71:CYS:CB	1:A:79:MET:CE	2.64	0.76
1:B:52:GLU:HA	1:B:52:GLU:OE1	1.88	0.74
1:A:71:CYS:CB	1:A:79:MET:HE2	2.18	0.73
1:A:153:ASP:OD1	1:A:393:GLY:O	2.09	0.71
1:B:331:ASN:HB3	3:B:1174:HOH:O	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ASP:OD1	1:A:454:VAL:HG12	1.94	0.68
1:A:463:VAL:HG13	1:A:478:TRP:CE2	2.30	0.66
1:B:95:GLN:HE22	1:B:429:ASN:HA	1.61	0.65
1:A:678:GLU:HG3	1:A:742:PHE:CE1	2.32	0.65
1:A:276:GLU:H	1:A:276:GLU:CD	1.98	0.65
1:B:558:ASN:HD21	1:B:672:ASN:HD21	1.45	0.64
1:A:21:ILE:HD11	1:A:101:SER:OG	1.98	0.64
1:B:9:ILE:HD12	1:B:31:THR:CG2	2.28	0.62
1:B:515:LEU:C	1:B:515:LEU:HD23	2.19	0.62
1:A:71:CYS:HB2	1:A:79:MET:CE	2.29	0.62
1:B:678:GLU:HG3	1:B:742:PHE:CE1	2.33	0.62
1:A:71:CYS:CB	1:A:79:MET:HE1	2.29	0.62
1:B:400:GLU:OE1	1:B:403:ARG:NH1	2.32	0.61
1:A:491:HIS:HD1	1:A:495:ARG:HH12	1.47	0.61
1:B:491:HIS:HD1	1:B:495:ARG:HH12	1.48	0.61
1:A:621:SER:HB2	1:A:646:GLU:OE1	2.01	0.61
1:A:720:GLU:HB2	1:A:729:THR:HG22	1.83	0.60
1:A:28:ASN:O	1:A:48:VAL:HG12	2.02	0.60
1:A:558:ASN:ND2	1:A:672:ASN:HD21	1.93	0.60
1:B:198:LYS:HE2	3:B:1014:HOH:O	2.01	0.60
1:A:463:VAL:HG13	1:A:478:TRP:CD2	2.38	0.59
1:A:168:HIS:HE1	3:A:968:HOH:O	1.85	0.59
1:A:563:VAL:HG13	3:A:978:HOH:O	2.01	0.59
1:A:138:GLN:HG3	3:A:927:HOH:O	2.03	0.59
1:A:71:CYS:HB2	1:A:79:MET:HE1	1.85	0.58
1:B:456:HIS:HE1	3:B:1020:HOH:O	1.87	0.57
1:A:456:HIS:HE1	3:A:1073:HOH:O	1.85	0.57
1:B:52:GLU:OE1	1:B:52:GLU:CA	2.51	0.57
1:B:693:VAL:HG21	1:B:745:ILE:HD12	1.85	0.57
1:B:709:ARG:CD	3:B:1208:HOH:O	2.37	0.56
1:A:95:GLN:HE22	1:A:429:ASN:HA	1.71	0.56
1:A:12:GLY:O	1:A:25:VAL:HG23	2.06	0.55
1:A:28:ASN:O	1:A:48:VAL:CG1	2.55	0.55
1:B:56:HIS:HE1	1:B:158:ARG:O	1.89	0.55
1:B:693:VAL:CG2	1:B:745:ILE:HD12	2.37	0.55
1:B:741:ARG:HB3	1:A:741:ARG:HE	1.70	0.55
1:A:67:ARG:HD3	1:A:100:GLU:OE1	2.09	0.53
1:B:252:ASP:O	3:B:902:HOH:O	2.04	0.53
1:B:48:VAL:HG12	1:B:160:SER:CB	2.39	0.53
1:B:385:GLN:HG3	1:B:425:CYS:O	2.09	0.52
1:A:47:ALA:O	1:A:161:PHE:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ILE:HD12	1:B:31:THR:HG23	1.92	0.52
1:B:740:LYS:O	1:B:741:ARG:HB3	2.10	0.52
1:B:741:ARG:CB	1:A:741:ARG:HE	2.22	0.52
1:B:482:HIS:HD2	3:B:1079:HOH:O	1.92	0.51
1:A:618:ALA:HB1	1:A:627:LEU:HD11	1.93	0.51
1:A:20:THR:HG21	1:A:23:THR:HG22	1.92	0.51
1:B:624:ARG:HD2	1:B:626:GLU:OE2	2.12	0.50
1:A:71:CYS:C	1:A:79:MET:HE2	2.32	0.50
1:A:87:GLY:O	1:A:139:GLY:HA3	2.12	0.50
1:A:463:VAL:CG1	1:A:478:TRP:CD2	2.95	0.48
1:B:347:VAL:HG22	1:B:351:GLN:NE2	2.29	0.48
1:A:138:GLN:CG	3:A:927:HOH:O	2.59	0.48
1:A:37:ALA:HB3	1:A:38:GLY:HA2	1.95	0.48
1:A:55:LYS:HE2	1:A:57:ILE:HD11	1.96	0.48
1:B:331:ASN:CB	3:B:1174:HOH:O	2.57	0.47
1:A:384:VAL:HG12	1:A:387:VAL:HG22	1.96	0.47
1:A:628:ILE:N	1:A:628:ILE:HD12	2.29	0.47
1:A:251:ARG:O	1:A:252:ASP:C	2.52	0.47
1:B:699:PHE:HB2	1:B:732:LEU:HD22	1.97	0.47
1:B:48:VAL:HG12	1:B:160:SER:HB3	1.96	0.46
1:B:742:PHE:CE2	1:A:741:ARG:NH2	2.84	0.46
1:B:149:LEU:N	1:B:149:LEU:CD2	2.78	0.46
1:A:97:LEU:HB3	1:A:125:PHE:HB2	1.98	0.46
1:A:383:ALA:HA	1:A:425:CYS:HB3	1.96	0.46
1:A:71:CYS:HB3	1:A:79:MET:HE1	1.93	0.45
1:A:92:TYR:CE1	1:A:338:GLU:HG2	2.51	0.45
1:B:153:ASP:OD1	1:B:393:GLY:O	2.34	0.45
1:A:95:GLN:NE2	1:A:134:ARG:HH21	2.03	0.45
1:B:384:VAL:O	1:B:387:VAL:HG22	2.16	0.44
1:B:604:SER:HB3	3:B:1231:HOH:O	2.17	0.44
1:A:250:GLU:OE1	1:A:318:ARG:HD2	2.17	0.44
1:B:67:ARG:HD3	1:B:100:GLU:OE1	2.18	0.44
1:A:266:ILE:HD12	1:A:347:VAL:HG13	1.99	0.44
1:B:584:HIS:HD2	3:B:1116:HOH:O	2.01	0.44
1:A:152:GLY:HA3	1:A:398:ARG:HG3	1.99	0.44
1:B:48:VAL:HG12	1:B:160:SER:HB2	1.99	0.44
1:A:47:ALA:CA	1:A:48:VAL:HG12	2.44	0.44
1:A:268:ARG:NH2	1:A:352:GLY:O	2.52	0.43
1:B:185:LYS:NZ	1:B:193:GLN:HE21	2.17	0.42
1:B:385:GLN:HE22	1:B:406:HIS:HE1	1.67	0.42
1:A:40:VAL:HG21	1:A:183:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:HB3	1:A:65:ASN:ND2	2.35	0.42
1:B:655:HIS:HD2	3:B:1173:HOH:O	2.01	0.42
1:B:293:LYS:NZ	3:B:908:HOH:O	2.46	0.42
1:A:185:LYS:NZ	1:A:193:GLN:HE21	2.17	0.42
1:A:64:ARG:HB3	1:A:65:ASN:HD22	1.85	0.42
1:B:307:TRP:CE3	1:B:308:HIS:HA	2.55	0.41
1:B:712:VAL:HG21	1:B:717:ILE:HD13	2.02	0.41
1:A:542:ALA:O	1:A:544:PRO:HD3	2.20	0.41
1:A:558:ASN:HD21	1:A:672:ASN:ND2	1.96	0.41
1:B:456:HIS:HD2	1:B:491:HIS:NE2	2.17	0.41
1:B:579:ARG:HH11	1:B:579:ARG:HG3	1.84	0.41
1:A:347:VAL:HG23	1:A:351:GLN:NE2	2.35	0.41
1:A:28:ASN:HB2	1:A:48:VAL:HG13	2.03	0.41
1:B:733:ASP:HB3	1:B:734:LYS:HE3	2.03	0.40
1:B:208:TRP:CH2	1:B:226:GLY:HA3	2.56	0.40
1:B:37:ALA:HB3	1:B:38:GLY:C	2.42	0.40
1:B:46:GLY:HA3	1:B:161:PHE:O	2.21	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	710/749 (95%)	664 (94%)	38 (5%)	8 (1%)	14 5
1	B	710/749 (95%)	677 (95%)	25 (4%)	8 (1%)	14 5
All	All	1420/1498 (95%)	1341 (94%)	63 (4%)	16 (1%)	14 5

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ALA

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Mol	Chain	Res	Type
1	A	39	PRO
1	A	48	VAL
1	B	37	ALA
1	B	282	ASP
1	B	393	GLY
1	A	538	ASP
1	A	36	GLU
1	B	538	ASP
1	B	35	SER
1	B	633	ASN
1	A	479	ASP
1	A	684	ALA
1	B	446	ASP
1	B	283	ASP
1	A	393	GLY

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	614/640 (96%)	571 (93%)	43 (7%)	15 7
1	B	614/640 (96%)	578 (94%)	36 (6%)	19 11
All	All	1228/1280 (96%)	1149 (94%)	79 (6%)	17 9

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	19	ARG
1	B	43	VAL
1	B	52	GLU
1	B	57	ILE
1	B	69	MET
1	B	88	ARG
1	B	100	GLU
1	B	124	VAL

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Mol	Chain	Res	Type
1	B	141	VAL
1	B	149	LEU
1	B	157	LYS
1	B	186	LEU
1	B	198	LYS
1	B	243	ASP
1	B	276	GLU
1	B	281	LYS
1	B	282	ASP
1	B	293	LYS
1	B	301	LEU
1	B	330	PRO
1	B	347	VAL
1	B	359	LYS
1	B	387	VAL
1	B	388	LEU
1	B	431	ASP
1	B	502	LEU
1	B	538	ASP
1	B	549	VAL
1	B	563	VAL
1	B	579	ARG
1	B	585	GLN
1	B	587	LYS
1	B	604	SER
1	B	622	GLN
1	B	723	SER
1	B	732	LEU
1	A	10	SER
1	A	17	LYS
1	A	19	ARG
1	A	36	GLU
1	A	40	VAL
1	A	51	LYS
1	A	69	MET
1	A	120	LYS
1	A	124	VAL
1	A	149	LEU
1	A	151	SER
1	A	162	THR
1	A	175	GLN
1	A	186	LEU

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Mol	Chain	Res	Type
1	A	198	LYS
1	A	243	ASP
1	A	272	ILE
1	A	276	GLU
1	A	289	LYS
1	A	293	LYS
1	A	301	LEU
1	A	337	VAL
1	A	359	LYS
1	A	387	VAL
1	A	388	LEU
1	A	463	VAL
1	A	502	LEU
1	A	538	ASP
1	A	561	THR
1	A	563	VAL
1	A	575	SER
1	A	596	ARG
1	A	598	ARG
1	A	622	GLN
1	A	624	ARG
1	A	633	ASN
1	A	635	SER
1	A	661	SER
1	A	685	GLU
1	A	687	MET
1	A	708	LYS
1	A	732	LEU
1	A	734	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	56	HIS
1	B	95	GLN
1	B	138	GLN
1	B	168	HIS
1	B	175	GLN
1	B	193	GLN
1	B	385	GLN
1	B	456	HIS
1	B	482	HIS

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Mol	Chain	Res	Type
1	B	558	ASN
1	B	584	HIS
1	B	585	GLN
1	B	622	GLN
1	B	645	HIS
1	A	65	ASN
1	A	95	GLN
1	A	168	HIS
1	A	193	GLN
1	A	385	GLN
1	A	456	HIS
1	A	558	ASN
1	A	584	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	B	801	-	10,10,12	1.26	2 (20%)	14,14,17	4.01	10 (71%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GAL	A	801	-	11,11,12	1.36	3 (27%)	13,15,17	4.14	9 (69%)

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	B	801	-	-	-	0/1/1/1
2	GAL	A	801	-	-	0/2/18/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	GAL	C2-C3	2.58	1.57	1.52
2	A	801	GAL	C2-C1	2.42	1.58	1.51
2	B	801	GAL	O5-C5	2.33	1.47	1.43
2	A	801	GAL	C3-C4	2.01	1.55	1.52
2	B	801	GAL	O3-C3	-2.00	1.38	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	GAL	C1-C2-C3	-10.38	87.01	110.91
2	B	801	GAL	C1-C2-C3	-8.70	92.26	110.31
2	B	801	GAL	C5-C4-C3	5.95	116.98	109.67
2	B	801	GAL	C5-O5-C1	-5.79	102.97	112.71
2	A	801	GAL	C2-C3-C4	5.60	118.82	110.69
2	A	801	GAL	O5-C5-C6	4.69	118.09	106.44
2	B	801	GAL	O1-C1-C2	4.68	122.22	109.03
2	B	801	GAL	O2-C2-C1	4.43	119.43	109.16
2	B	801	GAL	O1-C1-O5	3.91	119.92	109.72
2	A	801	GAL	O5-C5-C4	-3.88	102.64	109.69
2	A	801	GAL	C3-C4-C5	3.46	113.42	109.97
2	B	801	GAL	C4-C3-C2	-2.88	105.92	110.89
2	A	801	GAL	O3-C3-C2	2.80	116.88	109.94
2	A	801	GAL	O6-C6-C5	2.71	120.58	111.29
2	A	801	GAL	O4-C4-C3	2.40	114.58	109.99
2	A	801	GAL	O1-C1-C2	2.31	122.69	111.42
2	B	801	GAL	O5-C5-C4	-2.15	107.45	110.77
2	B	801	GAL	O2-C2-C3	2.02	115.01	110.35
2	B	801	GAL	O4-C4-C3	2.01	114.16	110.14

There are no chirality outliers.

There are no torsion outliers.

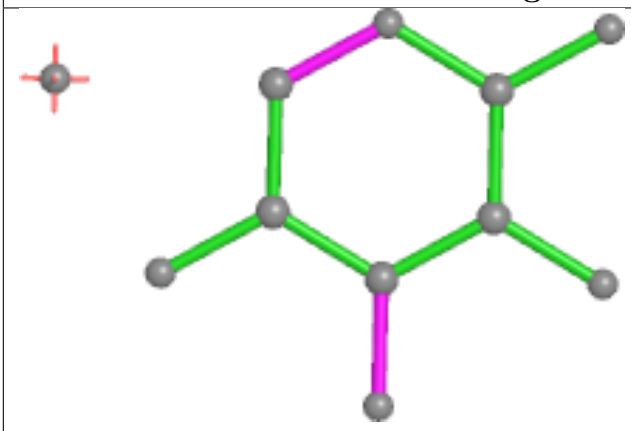
There are no ring outliers.

1 monomer is involved in 1 short contact:

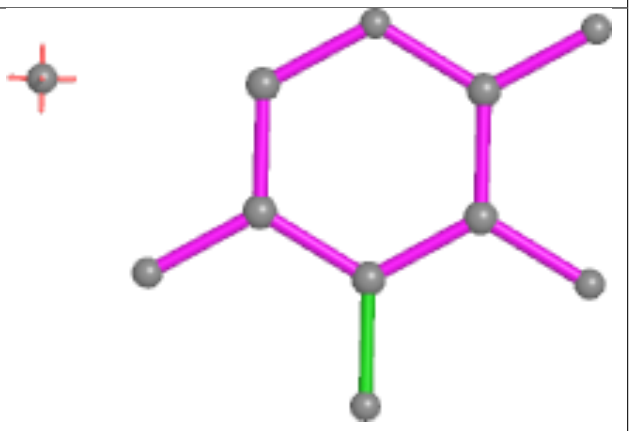
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	GAL	1	0

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 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.

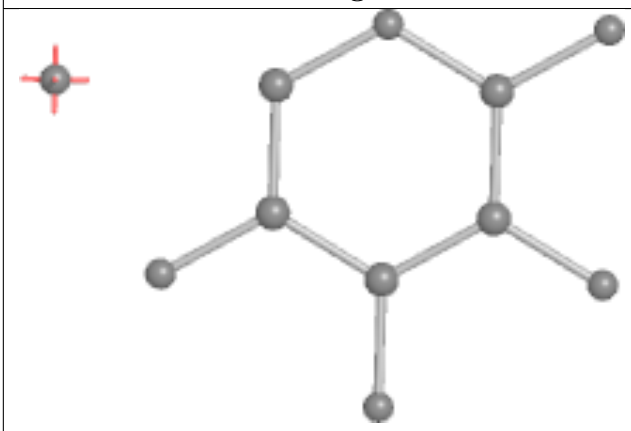
Ligand GAL B 801



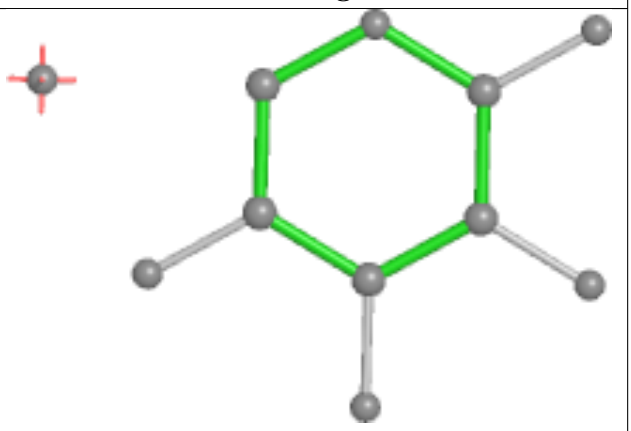
Bond lengths



Bond angles

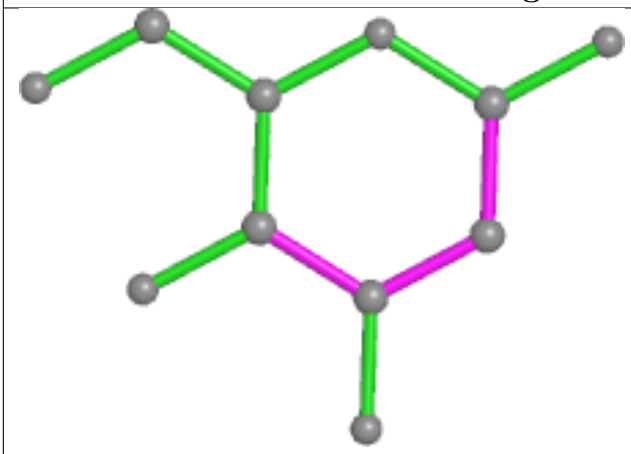


Torsions

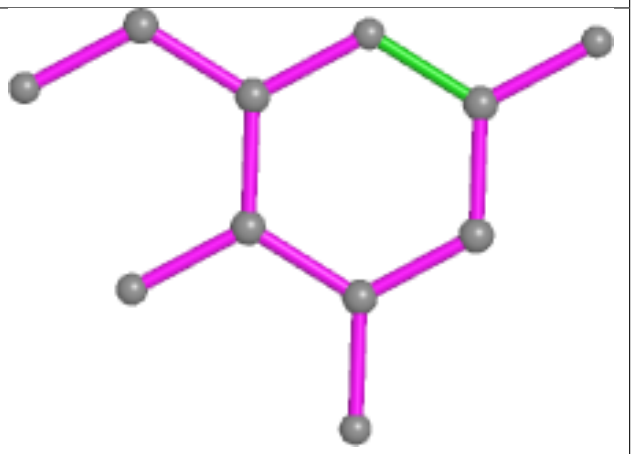


Rings

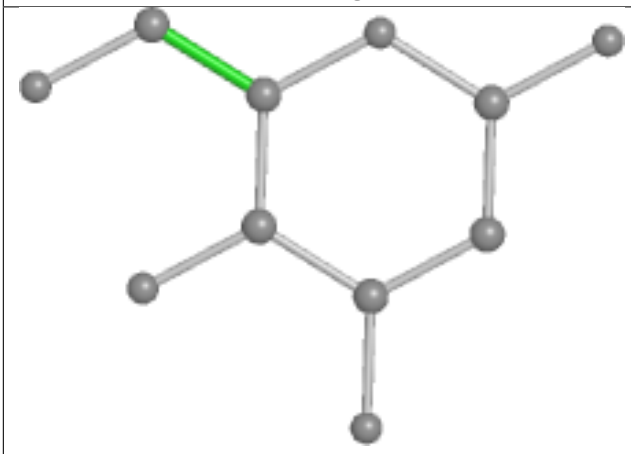
Ligand GAL A 801



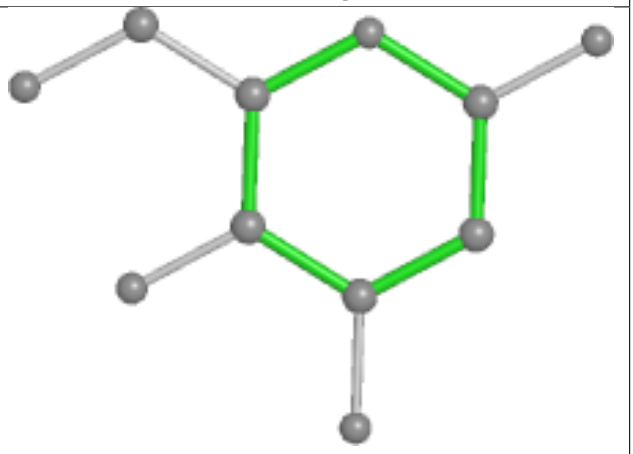
Bond lengths



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

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	716/749 (95%)	0.29	49 (6%)	17	18	15, 33, 61, 88	0
1	B	716/749 (95%)	-0.03	23 (3%)	47	52	11, 22, 49, 99	0
All	All	1432/1498 (95%)	0.13	72 (5%)	28	31	11, 28, 57, 99	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	ALA	6.4
1	B	587	LYS	4.8
1	B	281	LYS	4.4
1	A	685	GLU	4.4
1	A	18	ASN	4.3
1	A	36	GLU	4.2
1	B	739	ASN	4.1
1	A	657	VAL	4.1
1	A	50	ASN	4.0
1	B	36	GLU	3.9
1	A	154	VAL	3.9
1	A	51	LYS	3.8
1	A	5	PRO	3.8
1	B	35	SER	3.7
1	A	37	ALA	3.6
1	B	284	PRO	3.6
1	B	282	ASP	3.5
1	A	11	ASP	3.2
1	A	587	LYS	3.2
1	A	739	ASN	3.2
1	A	52	GLU	3.2
1	A	658	ASP	3.2
1	B	141	VAL	3.2
1	A	286	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	5	PRO	3.0
1	A	684	ALA	3.0
1	A	27	ASP	3.0
1	A	35	SER	2.9
1	A	632	TYR	2.9
1	B	321	GLU	2.9
1	B	633	ASN	2.8
1	A	715	ASN	2.8
1	A	38	GLY	2.7
1	A	714	SER	2.7
1	B	588	THR	2.7
1	A	141	VAL	2.5
1	B	11	ASP	2.5
1	A	12	GLY	2.5
1	B	285	ASN	2.5
1	A	39	PRO	2.4
1	A	585	GLN	2.4
1	B	741	ARG	2.4
1	A	738	GLU	2.4
1	A	614	ASN	2.4
1	A	155	ASP	2.4
1	A	612	THR	2.4
1	B	585	GLN	2.4
1	A	17	LYS	2.3
1	A	137	LEU	2.3
1	A	733	ASP	2.3
1	A	737	ILE	2.3
1	A	741	ARG	2.3
1	B	589	ASP	2.3
1	B	251	ARG	2.3
1	A	588	THR	2.3
1	B	27	ASP	2.2
1	A	577	THR	2.2
1	A	48	VAL	2.2
1	A	65	ASN	2.2
1	A	687	MET	2.2
1	A	633	ASN	2.2
1	A	611	THR	2.2
1	B	737	ILE	2.2
1	A	321	GLU	2.2
1	A	345	THR	2.2
1	A	40	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	2.1
1	B	380	VAL	2.1
1	B	382	VAL	2.1
1	A	659	GLY	2.1
1	A	251	ARG	2.0
1	A	285	ASN	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)

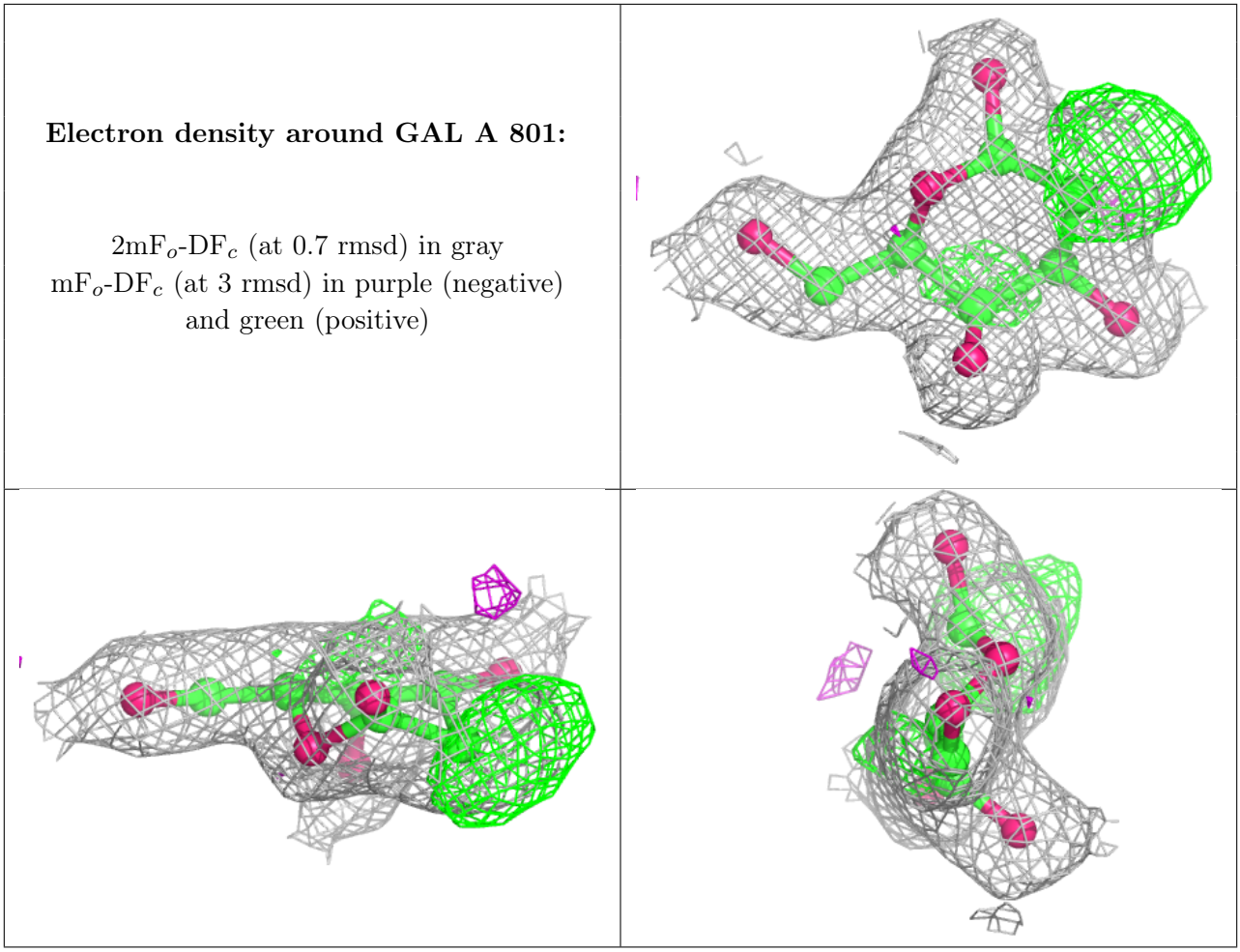
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	GAL	A	801	11/12	0.83	0.19	21,22,29,31	0
2	GAL	B	801	11/12	0.94	0.14	13,14,19,20	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.

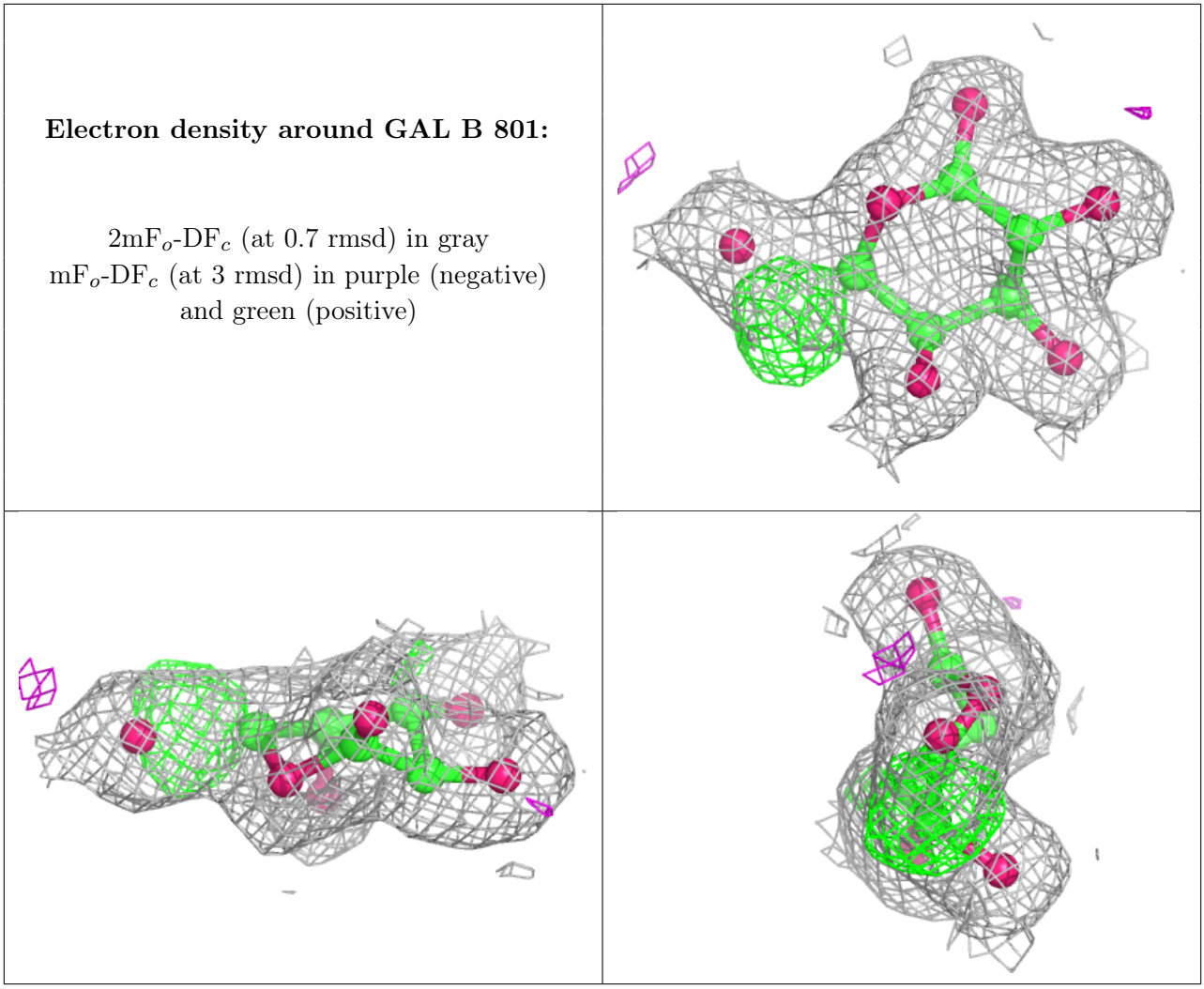
Electron density around GAL A 801:

$2mF_o$-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 B 801:

$2mF_o$-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.