



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:19 AM UTC

PDB ID : 7EXG / pdb_00007exg
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

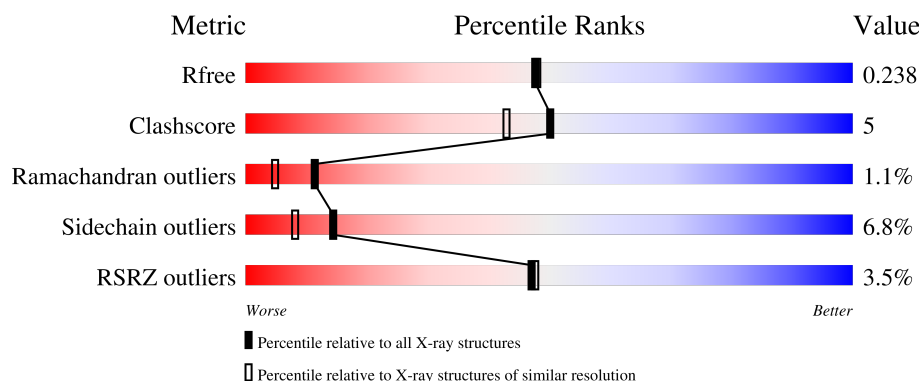
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 $\leq 5\%$. 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	749	4% 78% 15% • •
1	B	749	2% 80% 13% • •

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.

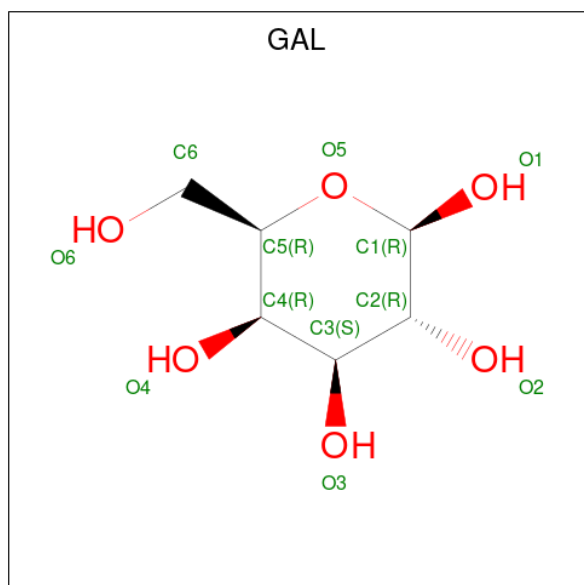
- Molecule 1 is a protein called Probable galactinol–sucrose galactosyltransferase 6.

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 (CCD ID: GAL) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			11	5	6		
2	A	1	Total	C	O	0	0
			11	6	5		

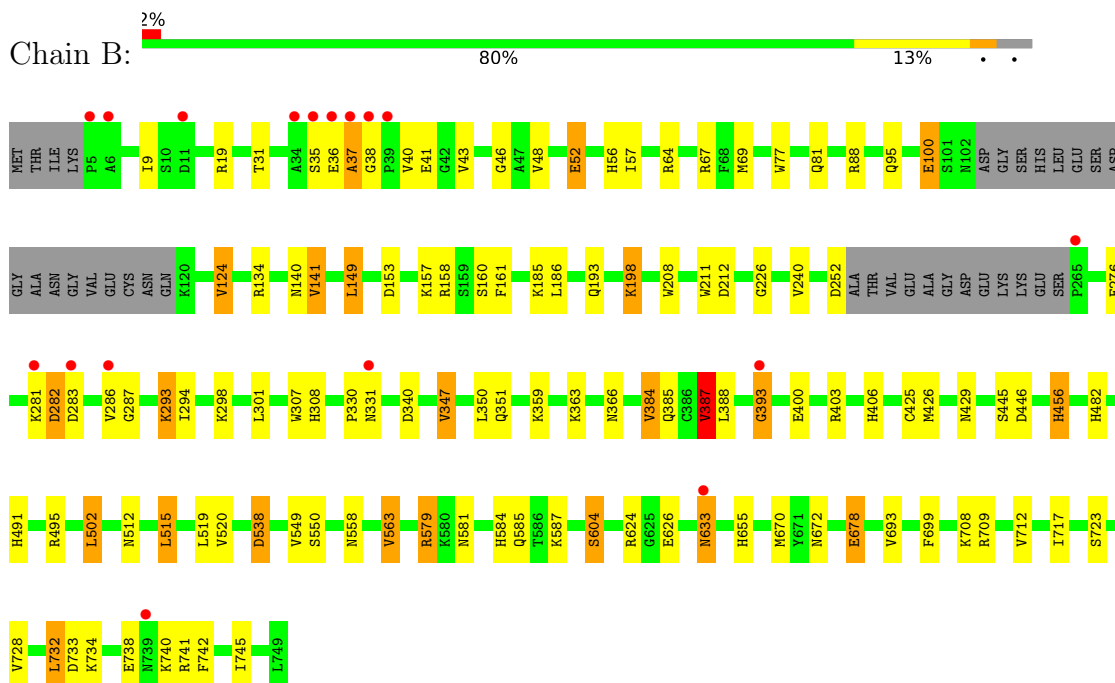
- Molecule 3 is water.

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

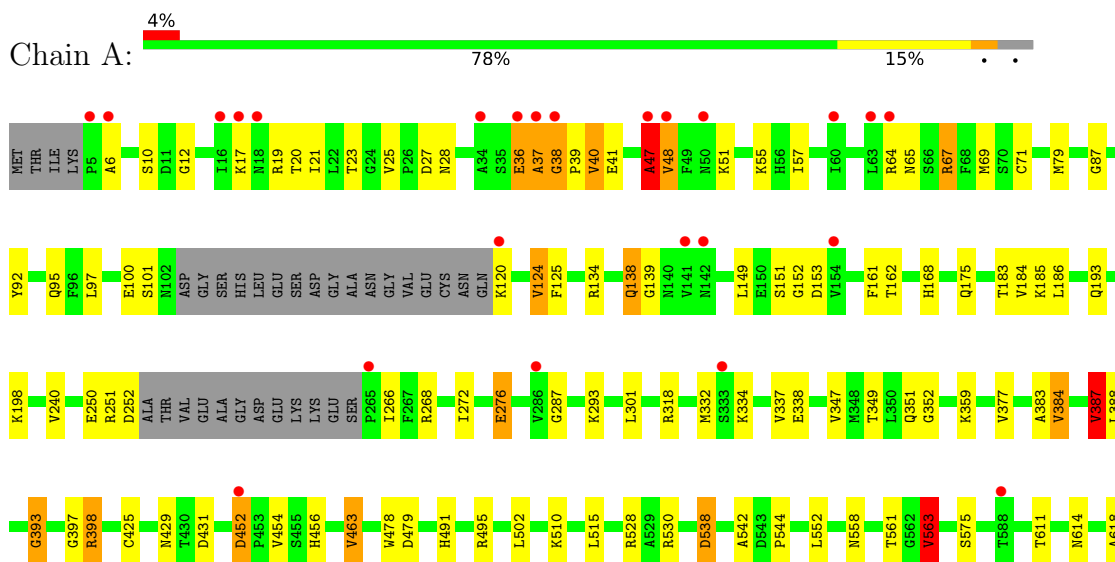
3 Residue-property plots

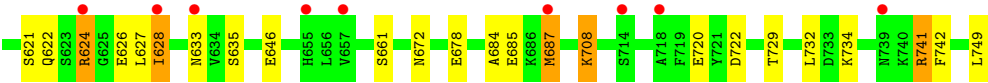
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Probable galactinol–sucrose galactosyltransferase 6



- Molecule 1: Probable galactinol–sucrose galactosyltransferase 6





4 Data and refinement statistics

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 30.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-2.05) 92.8 (30.00-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.184 , 0.235 (Not available) , 0.238	Depositor DCC
R_{free} test set	5259 reflections (4.68%)	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)	0.37 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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

5.1 Standard geometry

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	1.15	8/5744 (0.1%)	1.18	23/7778 (0.3%)
1	B	1.34	15/5744 (0.3%)	1.19	14/7778 (0.2%)
All	All	1.25	23/11488 (0.2%)	1.18	37/15556 (0.2%)

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 (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	581	ASN	N-CA	-7.06	1.37	1.46
1	B	670	MET	CA-C	-6.75	1.44	1.52
1	A	287	GLY	N-CA	5.72	1.52	1.45
1	B	294	ILE	C-O	5.68	1.30	1.24
1	B	678	GLU	C-O	-5.56	1.16	1.24
1	B	212	ASP	C-O	-5.56	1.16	1.24
1	B	520	VAL	C-O	-5.53	1.18	1.24
1	A	515	LEU	CA-C	5.46	1.59	1.52
1	B	64	ARG	CA-C	-5.42	1.46	1.52
1	B	350	LEU	C-O	-5.38	1.17	1.24
1	B	512	ASN	C-O	5.35	1.30	1.23
1	A	240	VAL	C-O	-5.35	1.18	1.24
1	B	633	ASN	CA-C	5.31	1.59	1.52
1	B	340	ASP	CA-C	5.28	1.58	1.52
1	B	445	SER	C-O	-5.28	1.17	1.23
1	A	431	ASP	CA-C	5.23	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	VAL	N-CA	-5.22	1.40	1.46
1	A	552	LEU	CA-C	-5.18	1.46	1.52
1	B	81	GLN	CA-C	5.11	1.59	1.52
1	A	528	ARG	CD-NE	-5.08	1.39	1.46
1	B	298	LYS	N-CA	-5.05	1.39	1.46
1	A	377	VAL	CA-C	5.03	1.58	1.52
1	B	240	VAL	C-O	5.01	1.29	1.24

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	VAL	CB-CA-C	-9.62	97.25	112.16
1	A	387	VAL	CB-CA-C	-9.23	98.58	112.05
1	B	124	VAL	CB-CA-C	-8.63	97.70	110.81
1	A	124	VAL	CB-CA-C	-8.13	99.04	111.31
1	B	563	VAL	CB-CA-C	-7.37	97.53	110.71
1	A	563	VAL	CB-CA-C	-7.07	98.05	110.71
1	B	387	VAL	N-CA-CB	7.03	122.67	110.65
1	A	47	ALA	CA-C-N	6.98	134.54	121.97
1	A	47	ALA	C-N-CA	6.98	134.54	121.97
1	B	633	ASN	N-CA-C	6.57	124.79	110.80
1	A	41	GLU	N-CA-C	6.54	121.10	113.18
1	A	528	ARG	NE-CZ-NH2	-6.51	113.34	119.20
1	A	334	LYS	N-CA-C	6.48	118.00	111.07
1	A	398	ARG	CB-CA-C	-6.35	100.65	110.81
1	B	141	VAL	CB-CA-C	-6.13	102.32	112.26
1	B	286	VAL	N-CA-C	6.10	119.61	111.44
1	A	387	VAL	N-CA-CB	6.04	120.02	110.54
1	B	550	SER	N-CA-C	5.97	119.78	110.17
1	A	397	GLY	CA-C-N	5.93	128.54	120.54
1	A	397	GLY	C-N-CA	5.93	128.54	120.54
1	A	614	ASN	N-CA-C	5.91	118.51	111.71
1	B	41	GLU	N-CA-C	5.91	117.72	111.28
1	A	37	ALA	N-CA-C	5.89	117.39	110.97
1	A	528	ARG	CG-CD-NE	-5.86	99.12	112.00
1	B	211	TRP	N-CA-C	5.61	117.08	110.97
1	A	452	ASP	CB-CA-C	5.31	118.83	110.71
1	B	738	GLU	CB-CA-C	-5.28	110.50	116.63
1	B	366	ASN	N-CA-C	5.26	117.01	111.28
1	A	538	ASP	CB-CA-C	-5.24	99.99	110.42
1	A	138	GLN	CB-CA-C	-5.23	98.77	109.38
1	B	728	VAL	CB-CA-C	-5.21	103.76	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	GLY	CA-C-N	5.10	126.22	119.84
1	A	38	GLY	C-N-CA	5.10	126.22	119.84
1	A	27	ASP	CB-CA-C	-5.07	102.33	110.74
1	A	538	ASP	N-CA-C	5.02	121.50	110.80
1	B	456	HIS	N-CA-C	5.02	116.44	110.97
1	A	528	ARG	CD-NE-CZ	5.01	131.41	124.40

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 ⓘ

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	56	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	13	0
All	All	11821	0	11084	118	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 (118) 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	1.26
1:A:71:CYS:HB3	1:A:79:MET:HE2	1.20	1.19
1:A:71:CYS:CB	1:A:79:MET:HE2	1.84	1.07
2:B:801:GAL:O6	2:B:801:GAL:C5	2.06	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:CB	1:A:79:MET:CE	2.64	0.74
1:B:52:GLU:HA	1:B:52:GLU:OE1	1.88	0.73
1:A:153:ASP:OD1	1:A:393:GLY:O	2.09	0.71
1:A:276:GLU:H	1:A:276:GLU:CD	1.98	0.70
1:B:331:ASN:HB3	3:B:1174:HOH:O	1.91	0.68
1:A:452:ASP:OD1	1:A:454:VAL:HG12	1.94	0.68
1:B:515:LEU:C	1:B:515:LEU:HD23	2.19	0.67
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:687:MET:HE3	1:A:749:LEU:O	2.08	0.53
1:A:67:ARG:HD3	1:A:100:GLU:OE1	2.09	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
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:251:ARG:O	1:A:252:ASP:C	2.52	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: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: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:71:CYS:O	1:A:79:MET:HE3	2.16	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: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:37:ALA:HB3	1:B:38:GLY:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:36:GLU:O	1:B:37:ALA:C	2.61	0.43
1:B:77:TRP:CD2	1:B:426:MET:HE2	2.53	0.43
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
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:A:332:MET:HE3	1:A:349:THR:HG23	2.00	0.42
1:A:708:LYS:HE3	1:A:749:LEU:C	2.45	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:A:722:ASP:OD1	1:A:722:ASP:C	2.64	0.41
1:B:733:ASP:HB3	1:B:734:LYS:HE3	2.03	0.40
1:B:140:ASN:OD1	1:B:140:ASN:C	2.63	0.40
1:B:208:TRP:CH2	1:B:226:GLY:HA3	2.56	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

5.3.1 Protein backbone

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%)	11	5
1	B	710/749 (95%)	677 (95%)	25 (4%)	8 (1%)	11	5
All	All	1420/1498 (95%)	1341 (94%)	63 (4%)	16 (1%)	11	5

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ALA
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 ⓘ

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%)	569 (93%)	45 (7%)	13	7
1	B	614/640 (96%)	576 (94%)	38 (6%)	16	9
All	All	1228/1280 (96%)	1145 (93%)	83 (7%)	14	8

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	19	ARG
1	B	40	VAL
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
1	B	141	VAL
1	B	149	LEU
1	B	157	LYS
1	B	186	LEU
1	B	198	LYS
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	363	LYS
1	B	384	VAL
1	B	387	VAL
1	B	388	LEU
1	B	502	LEU
1	B	515	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	708	LYS
1	B	723	SER
1	B	732	LEU
1	A	10	SER
1	A	17	LYS
1	A	19	ARG
1	A	36	GLU

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Mol	Chain	Res	Type
1	A	40	VAL
1	A	51	LYS
1	A	67	ARG
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
1	A	198	LYS
1	A	272	ILE
1	A	276	GLU
1	A	293	LYS
1	A	301	LEU
1	A	337	VAL
1	A	359	LYS
1	A	384	VAL
1	A	387	VAL
1	A	388	LEU
1	A	463	VAL
1	A	502	LEU
1	A	510	LYS
1	A	530	ARG
1	A	561	THR
1	A	563	VAL
1	A	575	SER
1	A	611	THR
1	A	622	GLN
1	A	624	ARG
1	A	628	ILE
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
1	A	741	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28)

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	56	HIS
1	B	95	GLN
1	B	138	GLN
1	B	175	GLN
1	B	193	GLN
1	B	247	GLN
1	B	385	GLN
1	B	404	GLN
1	B	438	GLN
1	B	456	HIS
1	B	466	ASN
1	B	482	HIS
1	B	584	HIS
1	B	585	GLN
1	B	622	GLN
1	B	645	HIS
1	B	655	HIS
1	B	672	ASN
1	A	65	ASN
1	A	95	GLN
1	A	168	HIS
1	A	193	GLN
1	A	247	GLN
1	A	385	GLN
1	A	456	HIS
1	A	466	ASN
1	A	584	HIS
1	A	672	ASN

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 oligosaccharides 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	1.20	1 (10%)	14,14,17	3.78	7 (50%)
2	GAL	A	801	-	11,11,12	1.35	2 (18%)	13,15,17	3.81	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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	GAL	C2-C1	2.65	1.58	1.51
2	A	801	GAL	C2-C3	2.39	1.57	1.52
2	B	801	GAL	O5-C5	2.23	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	GAL	C1-C2-C3	-8.87	92.26	110.36
2	A	801	GAL	C1-C2-C3	-8.53	87.01	111.23
2	A	801	GAL	C2-C3-C4	5.65	118.82	110.67
2	B	801	GAL	C5-C4-C3	5.04	116.98	109.64
2	A	801	GAL	O5-C5-C6	4.70	118.09	106.44
2	B	801	GAL	C5-O5-C1	-4.57	102.97	112.46
2	B	801	GAL	O1-C1-C2	4.56	122.22	108.98
2	B	801	GAL	O2-C2-C1	4.41	119.43	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	GAL	O5-C5-C4	-3.92	102.64	109.70
2	B	801	GAL	O1-C1-O5	3.90	119.92	109.91
2	A	801	GAL	C3-C4-C5	3.42	113.42	109.99
2	A	801	GAL	O3-C3-C2	2.82	116.88	109.86
2	B	801	GAL	C4-C3-C2	-2.81	105.92	110.86
2	A	801	GAL	O6-C6-C5	2.71	120.58	111.33
2	A	801	GAL	O1-C1-C2	2.47	122.69	111.39
2	A	801	GAL	O4-C4-C3	2.22	114.58	110.05

There are no chirality outliers.

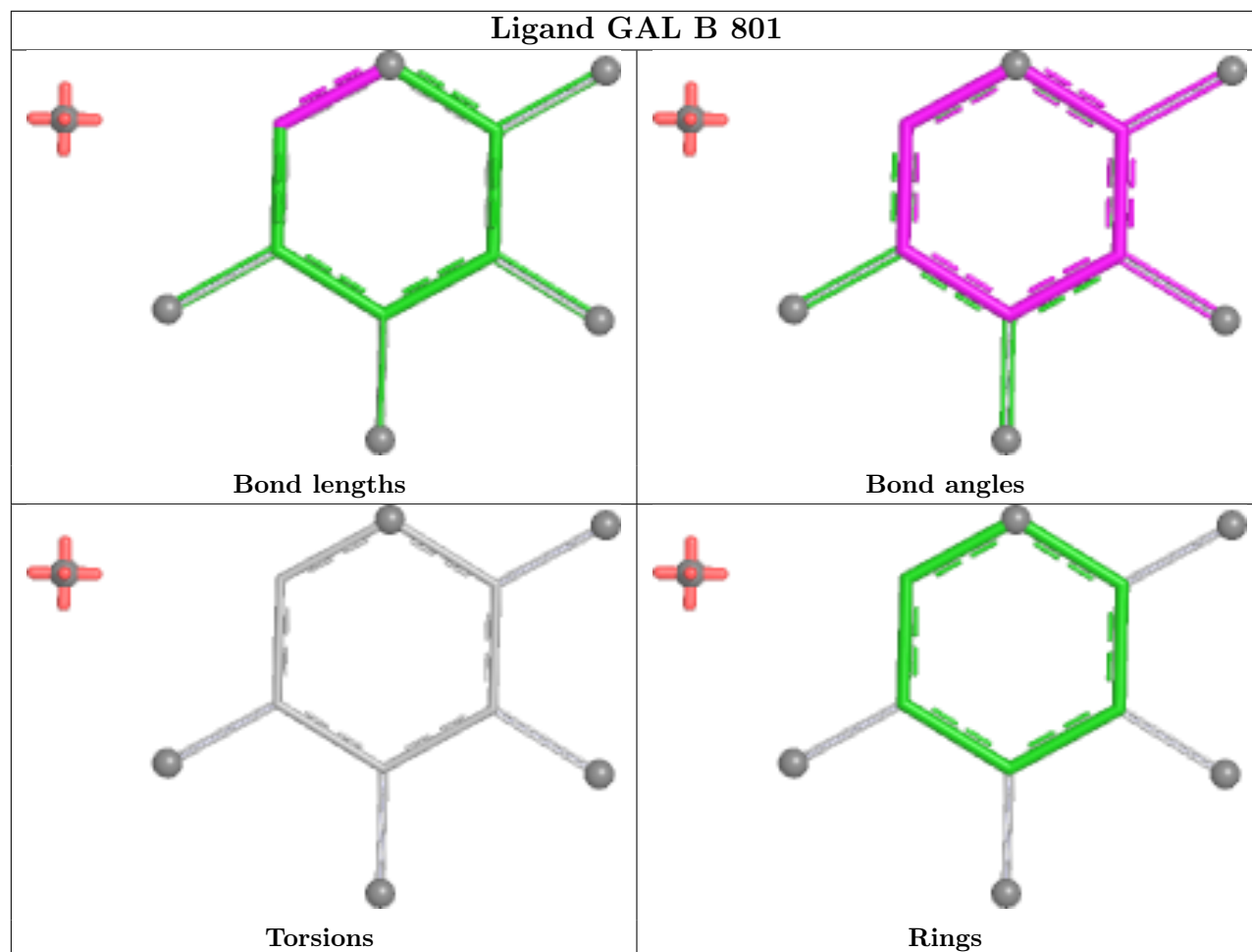
There are no torsion outliers.

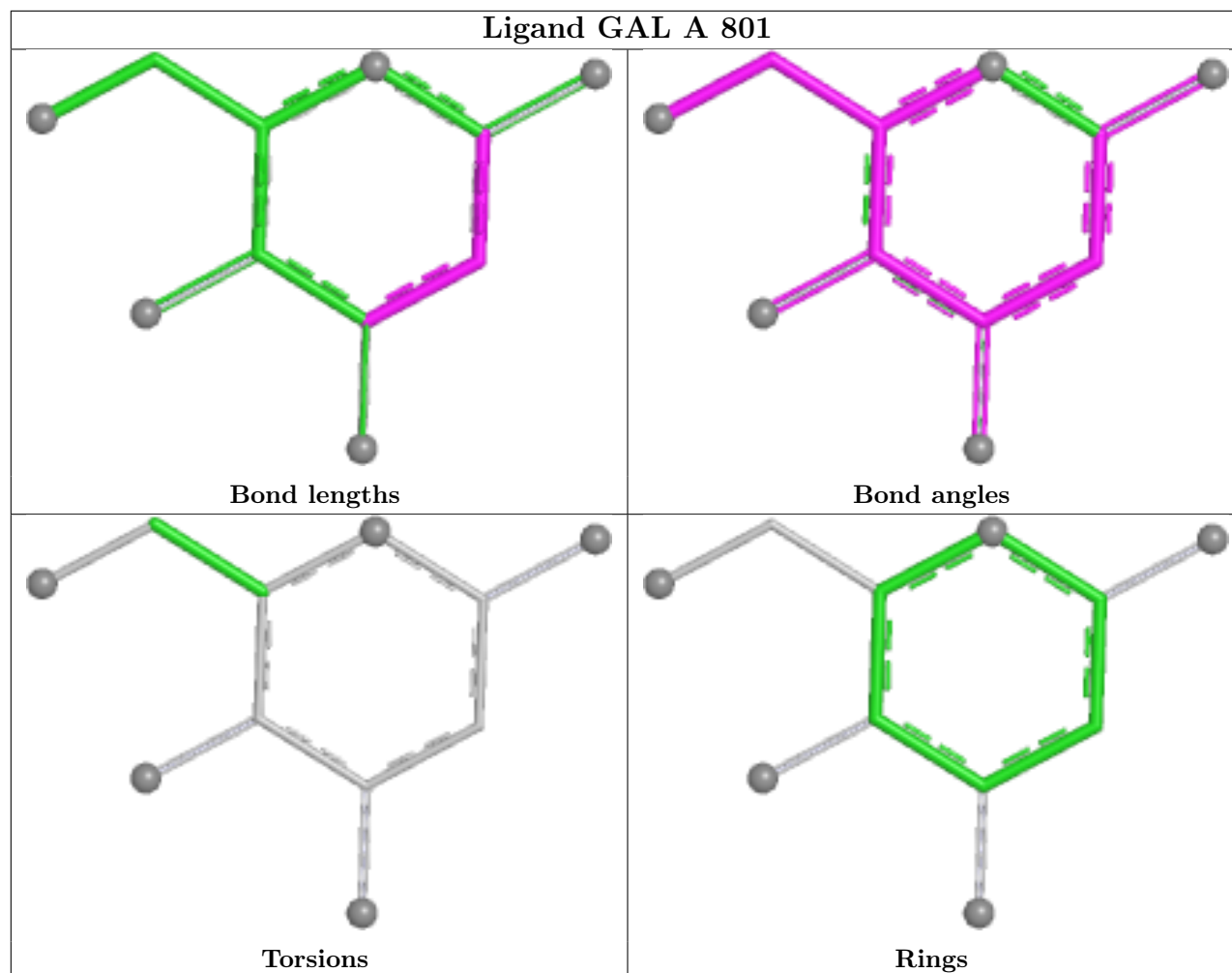
There are no ring outliers.

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 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	716/749 (95%)	0.38	33 (4%) 37 37	15, 33, 61, 88	0
1	B	716/749 (95%)	-0.15	17 (2%) 59 61	11, 22, 49, 99	0
All	All	1432/1498 (95%)	0.12	50 (3%) 47 48	11, 28, 57, 99	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	PRO	5.1
1	B	37	ALA	5.0
1	B	35	SER	4.4
1	A	37	ALA	4.4
1	A	48	VAL	4.2
1	B	739	ASN	4.1
1	A	739	ASN	4.0
1	B	11	ASP	3.7
1	A	5	PRO	3.6
1	A	38	GLY	3.5
1	B	36	GLU	3.5
1	B	38	GLY	3.5
1	A	141	VAL	3.4
1	A	657	VAL	3.3
1	A	286	VAL	3.3
1	A	17	LYS	3.2
1	B	281	LYS	3.1
1	B	331	ASN	3.0
1	B	393	GLY	3.0
1	A	6	ALA	2.9
1	B	6	ALA	2.8
1	A	687	MET	2.8
1	A	628	ILE	2.8
1	A	633	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	265	PRO	2.7
1	B	34	ALA	2.6
1	A	655	HIS	2.6
1	A	333	SER	2.6
1	A	60	ILE	2.6
1	A	142	ASN	2.5
1	A	36	GLU	2.4
1	B	39	PRO	2.4
1	A	34	ALA	2.4
1	A	47	ALA	2.4
1	A	64	ARG	2.4
1	A	63	LEU	2.4
1	A	18	ASN	2.4
1	B	286	VAL	2.3
1	A	588	THR	2.3
1	A	624	ARG	2.3
1	A	452	ASP	2.2
1	A	714	SER	2.2
1	A	154	VAL	2.1
1	A	718	ALA	2.1
1	B	633	ASN	2.1
1	A	16	ILE	2.1
1	B	283	ASP	2.1
1	A	120	LYS	2.1
1	A	50	ASN	2.0
1	A	265	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](#)

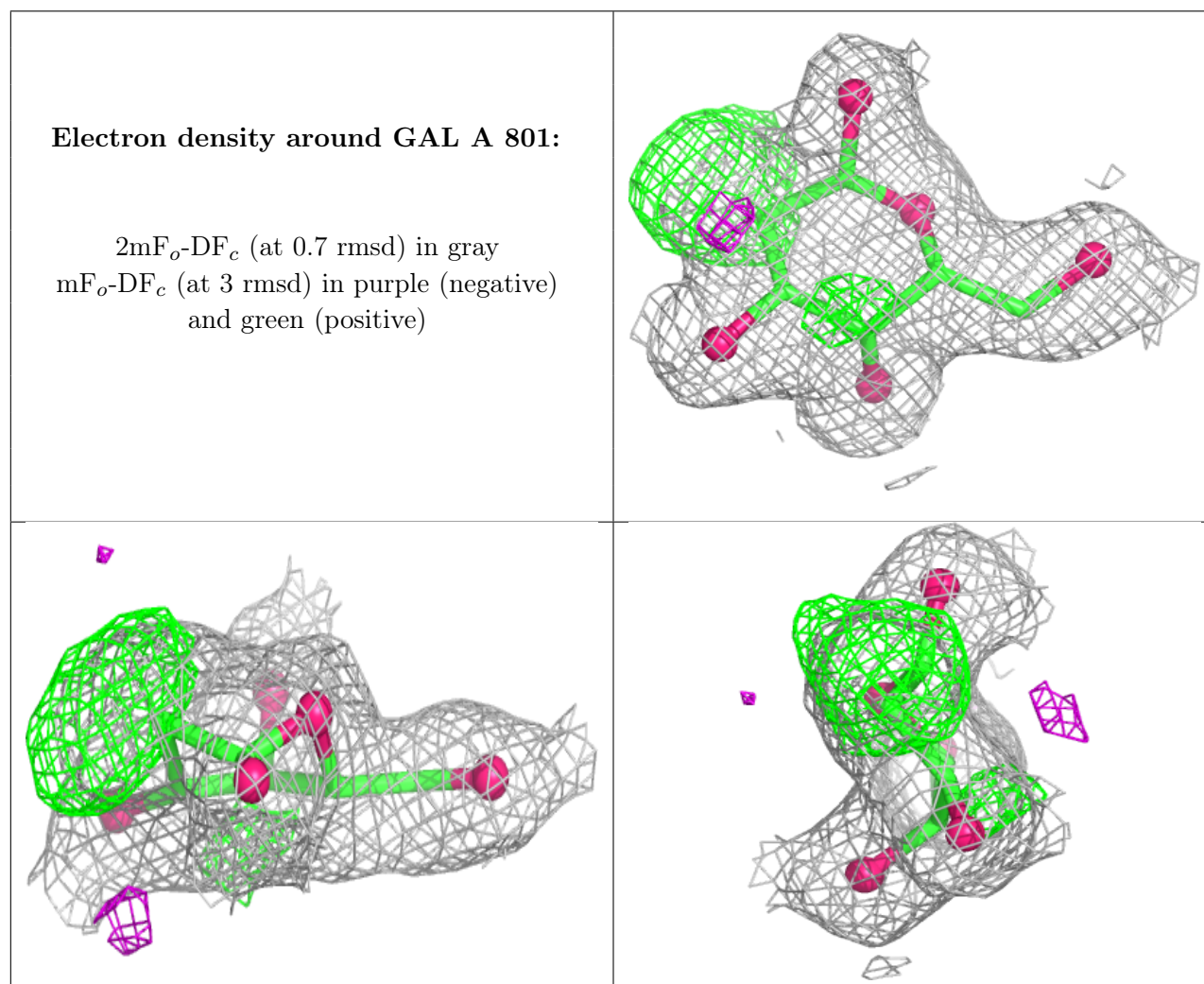
There are no oligosaccharides in this entry.

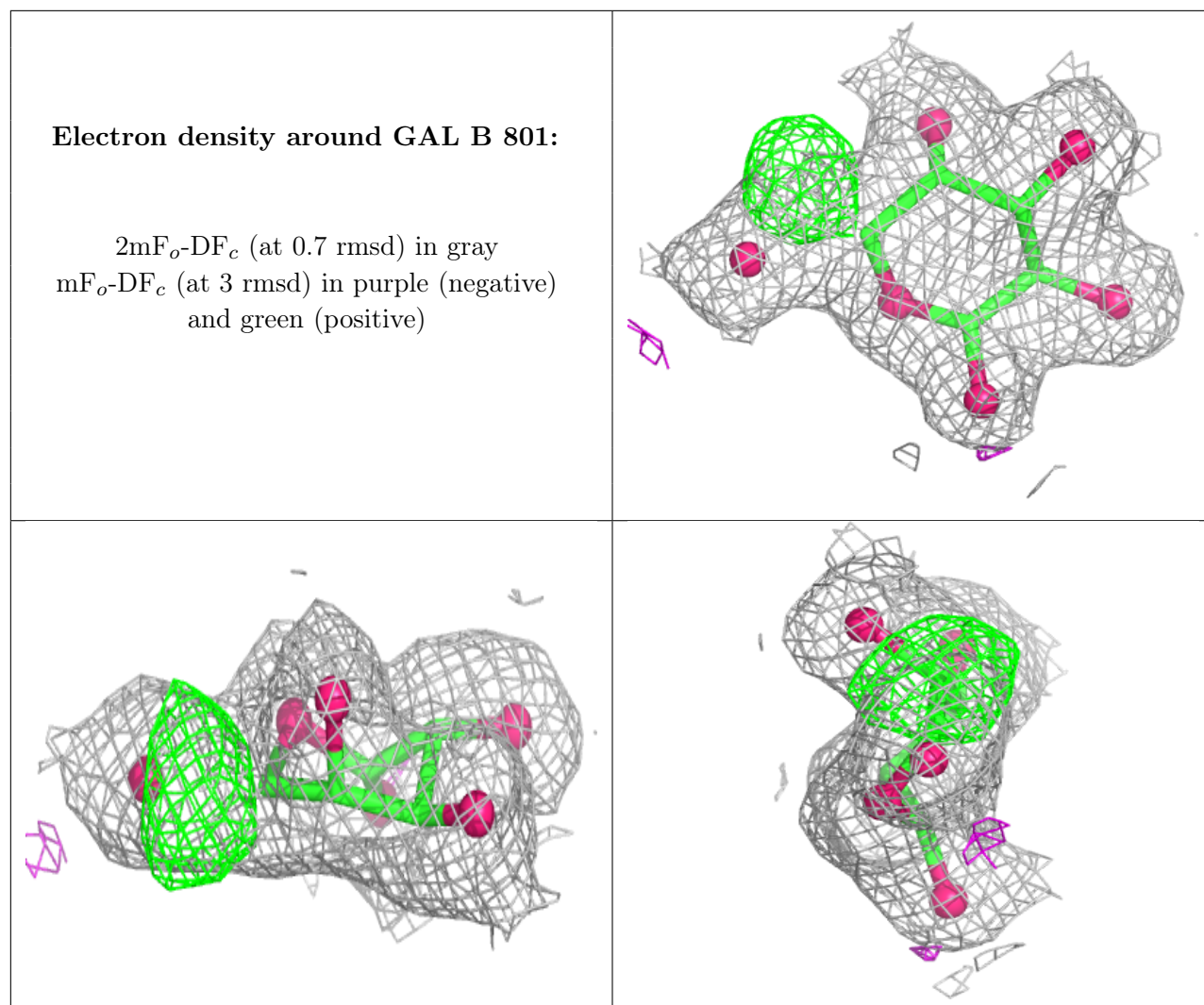
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	GAL	A	801	11/12	0.82	0.10	21,22,29,31	0
2	GAL	B	801	11/12	0.93	0.07	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.