



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:34 PM UTC

PDB ID : 7EXF / pdb_00007exf
Title : Crystal structure of wild-type 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 : 2.17 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

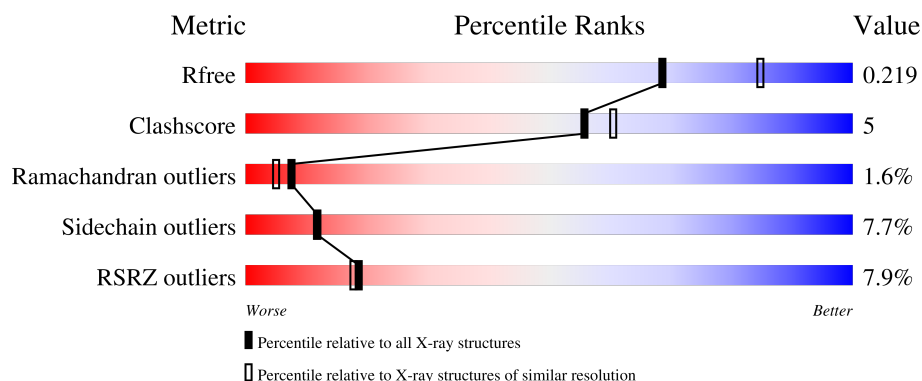
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	12% 78% 15% • •
1	B	749	3% 81% 13% • • •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11451 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.

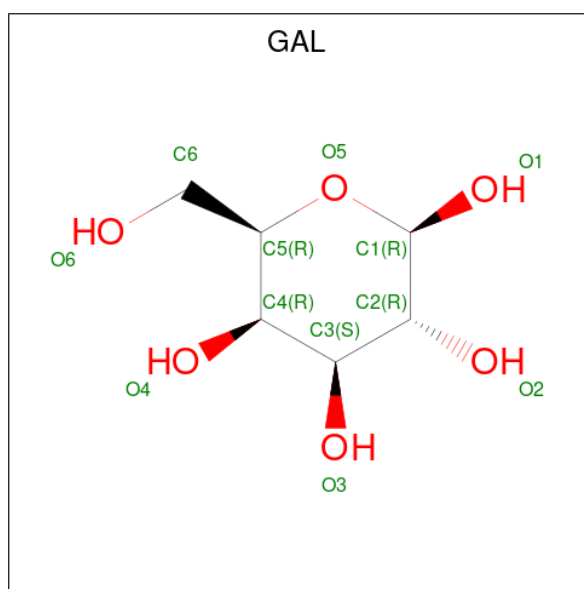
- Molecule 1 is a protein called Probable galactinol–sucrose galactosyltransferase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	719	Total	C	N	O	S	0	0	0
			5633	3579	970	1055	29			
1	A	717	Total	C	N	O	S	0	0	0
			5618	3571	968	1050	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	302	ARG	LYS	conflict	UNP Q8RX87
A	302	ARG	LYS	conflict	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
			12	6	6		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	136	Total	O	0	0
			136	136		
3	A	40	Total	O	0	0
			40	40		

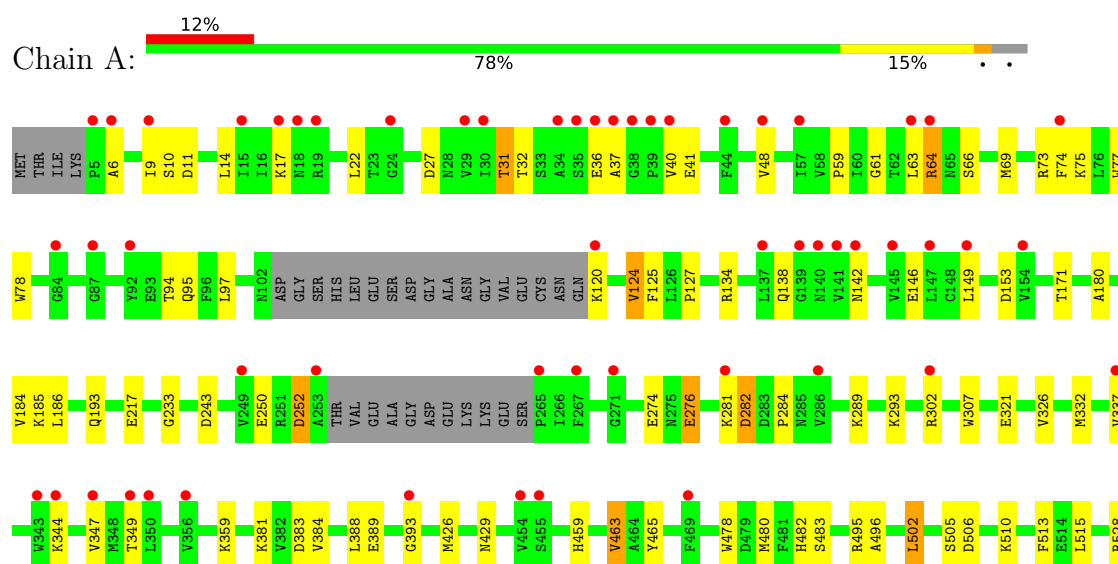
3 Residue-property plots

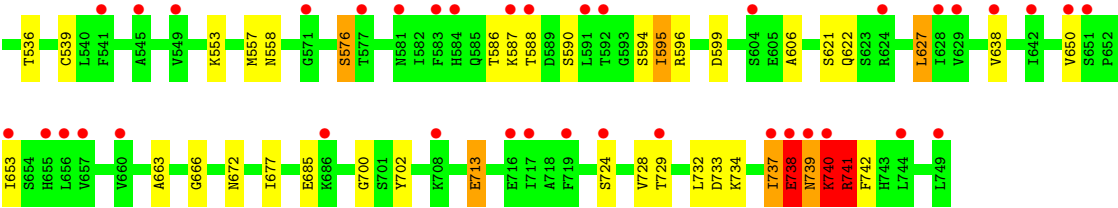
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	94.94Å 103.64Å 181.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.17 30.00 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.17) 99.6 (30.00-2.17)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.208 , 0.267 0.220 , 0.219	Depositor DCC
R_{free} test set	4731 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 24.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11451	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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	0.98	0/5752	1.07	10/7789 (0.1%)
1	B	1.13	3/5767 (0.1%)	1.11	13/7810 (0.2%)
All	All	1.06	3/11519 (0.0%)	1.09	23/15599 (0.1%)

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
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	LEU	C-N	-7.64	1.22	1.33
1	B	528	ARG	C-O	-5.33	1.17	1.24
1	B	124	VAL	CA-C	-5.15	1.46	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	VAL	CB-CA-C	-10.13	98.46	112.14
1	B	387	VAL	N-CA-CB	8.65	122.31	110.54
1	B	124	VAL	CB-CA-C	-8.23	97.69	110.95
1	A	124	VAL	CB-CA-C	-7.24	100.78	110.98
1	A	142	ASN	N-CA-C	6.93	120.62	111.75
1	B	741	ARG	N-CA-C	6.48	124.60	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	627	LEU	N-CA-C	5.97	118.25	108.52
1	B	43	VAL	N-CA-C	5.88	117.14	108.45
1	B	601	HIS	N-CA-C	5.79	118.34	111.33
1	A	252	ASP	N-CA-C	5.78	118.09	109.25
1	A	496	ALA	N-CA-C	5.72	118.29	111.71
1	B	538	ASP	N-CA-C	5.54	122.61	110.80
1	B	437	LYS	N-CA-C	5.50	119.70	112.89
1	A	127	PRO	N-CA-C	5.48	119.48	110.55
1	B	463	VAL	CG1-CB-CG2	5.41	122.69	110.80
1	B	737	ILE	N-CA-C	5.38	115.01	107.37
1	B	463	VAL	CB-CA-C	5.37	118.85	111.97
1	A	41	GLU	N-CA-C	5.34	119.50	113.15
1	B	30	ILE	N-CA-C	5.32	116.95	108.87
1	B	463	VAL	N-CA-CB	-5.21	104.45	110.55
1	A	740	LYS	N-CA-C	-5.14	99.86	110.80
1	A	738	GLU	CA-C-O	-5.05	113.29	120.51
1	A	650	VAL	N-CA-C	5.02	113.61	106.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ASP	Peptide
1	B	394	GLY	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	5618	0	5537	51	0
1	B	5633	0	5547	55	0
2	A	12	0	12	1	0
2	B	12	0	12	0	0
3	A	40	0	0	1	0
3	B	136	0	0	2	0
All	All	11451	0	11108	104	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 (104) 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:739:ASN:C	1:A:741:ARG:H	1.82	0.88
1:A:558:ASN:HD21	1:A:672:ASN:HD21	1.29	0.80
1:A:738:GLU:C	1:A:740:LYS:H	1.87	0.79
1:A:738:GLU:C	1:A:740:LYS:N	2.37	0.79
1:A:95:GLN:HE21	1:A:134:ARG:HH21	1.31	0.77
1:B:558:ASN:HD21	1:B:672:ASN:HD21	1.34	0.75
1:B:738:GLU:C	1:B:740:LYS:H	1.98	0.71
1:B:738:GLU:O	1:B:740:LYS:N	2.24	0.71
1:A:739:ASN:C	1:A:741:ARG:N	2.47	0.71
1:A:740:LYS:O	1:A:742:PHE:N	2.24	0.70
1:B:95:GLN:HE21	1:B:134:ARG:HH21	1.41	0.68
1:A:738:GLU:O	1:A:740:LYS:N	2.27	0.67
1:B:95:GLN:HE22	1:B:429:ASN:HA	1.59	0.66
1:B:7:VAL:HG13	1:B:16:ILE:CD1	2.27	0.65
1:A:737:ILE:O	1:A:738:GLU:HB2	1.98	0.62
1:A:495:ARG:HB3	1:A:502:LEU:HD22	1.83	0.61
1:A:95:GLN:HE22	1:A:429:ASN:HA	1.68	0.58
1:B:489:GLU:OE1	1:B:671:TYR:OH	2.21	0.57
1:A:738:GLU:O	1:A:739:ASN:C	2.46	0.57
1:B:135:SER:OG	1:B:149:LEU:HD13	2.06	0.56
1:B:456:HIS:HE1	3:B:936:HOH:O	1.88	0.56
1:B:738:GLU:C	1:B:740:LYS:N	2.65	0.55
1:A:22:LEU:HB3	1:A:61:GLY:HA3	1.91	0.52
1:A:653:ILE:HA	1:A:663:ALA:HB2	1.90	0.52
1:A:332:MET:HE3	1:A:349:THR:HG23	1.92	0.51
1:B:491:HIS:HD1	1:B:495:ARG:HH12	1.59	0.51
1:B:463:VAL:HG13	1:B:478:TRP:CE2	2.46	0.51
1:A:383:ASP:HB3	1:A:384:VAL:HG23	1.94	0.50
1:B:83:MET:SD	1:B:83:MET:N	2.85	0.50
1:B:699:PHE:HB2	1:B:732:LEU:HD22	1.93	0.50
1:A:463:VAL:HG13	1:A:478:TRP:CE2	2.47	0.50
1:A:627:LEU:HD21	1:A:702:TYR:HB2	1.94	0.50
1:B:384:VAL:O	1:B:387:VAL:HG22	2.12	0.49
1:A:666:GLY:CA	1:A:677:ILE:HD11	2.42	0.49
1:B:664:PRO:HB2	1:B:677:ILE:HD13	1.94	0.49
1:A:558:ASN:ND2	1:A:672:ASN:HD21	2.05	0.49
1:B:208:TRP:CH2	1:B:226:GLY:HA3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ARG:O	1:B:197:LYS:HE3	2.13	0.49
1:B:238:LYS:HD2	1:B:302:ARG:HH21	1.77	0.48
1:B:463:VAL:HG13	1:B:478:TRP:CD2	2.49	0.48
1:A:276:GLU:H	1:A:276:GLU:CD	2.21	0.48
1:B:482:HIS:HD2	3:B:999:HOH:O	1.97	0.47
1:A:95:GLN:HE21	1:A:134:ARG:NH2	2.06	0.47
1:B:738:GLU:O	1:B:738:GLU:HG2	2.15	0.47
1:B:263:GLU:O	1:B:264:SER:C	2.58	0.47
1:A:483:SER:OG	1:A:506:ASP:OD2	2.30	0.47
1:A:153:ASP:OD1	1:A:393:GLY:O	2.33	0.47
1:B:58:VAL:HG22	1:B:59:PRO:O	2.14	0.47
1:B:92:TYR:CE2	1:B:338:GLU:HG2	2.50	0.47
1:B:492:ALA:HB1	1:B:519:LEU:HD11	1.96	0.46
1:B:166:TYR:CE2	1:B:168:HIS:HB2	2.50	0.46
1:B:185:LYS:NZ	1:B:193:GLN:HE21	2.14	0.46
1:B:276:GLU:H	1:B:276:GLU:CD	2.23	0.46
1:B:194:ARG:HD3	1:B:471:GLY:O	2.16	0.46
1:B:678:GLU:HG3	1:B:742:PHE:CE1	2.52	0.45
1:A:557:MET:HE1	1:A:606:ALA:HB2	1.99	0.45
1:B:124:VAL:CG2	1:B:176:THR:HG22	2.47	0.45
1:A:9:ILE:HD12	1:A:31:THR:HG21	1.99	0.45
1:B:739:ASN:HD22	1:A:741:ARG:NH1	2.13	0.45
1:B:307:TRP:CE3	1:B:308:HIS:HA	2.52	0.45
1:B:63:LEU:CD1	1:B:66:SER:HB2	2.47	0.45
1:A:243:ASP:HA	1:A:307:TRP:HB2	1.99	0.45
1:B:739:ASN:HD22	1:A:741:ARG:HH12	1.64	0.45
1:A:63:LEU:HD11	1:A:66:SER:HB2	1.98	0.45
1:A:77:TRP:HB2	1:A:78:TRP:CD1	2.51	0.45
1:A:381:LYS:NZ	3:A:904:HOH:O	2.46	0.44
1:B:153:ASP:OD1	1:B:393:GLY:O	2.36	0.44
1:B:693:VAL:HG21	1:B:745:ILE:HD12	1.98	0.44
1:A:465:TYR:OH	1:A:539:CYS:O	2.34	0.43
1:B:332:MET:HE3	1:B:349:THR:HG23	2.00	0.43
1:A:97:LEU:HB3	1:A:125:PHE:HB2	2.00	0.43
1:A:63:LEU:HD12	1:A:64:ARG:N	2.34	0.43
1:A:138:GLN:O	1:A:146:GLU:HB2	2.18	0.43
1:B:238:LYS:HD2	1:B:302:ARG:NH2	2.33	0.43
1:B:69:MET:HE3	1:B:70:SER:N	2.33	0.43
1:A:536:THR:HG21	1:A:599:ASP:HB3	2.00	0.43
1:A:426:MET:SD	2:A:801:GAL:O1	2.77	0.43
1:A:480:MET:SD	1:A:505:SER:HB3	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:VAL:O	1:B:354:GLY:HA3	2.19	0.42
1:B:495:ARG:HB3	1:B:502:LEU:CD2	2.50	0.42
1:A:73:ARG:NH1	1:A:389:GLU:OE1	2.47	0.42
1:B:739:ASN:O	1:B:741:ARG:N	2.52	0.42
1:A:553:LYS:HD3	1:A:595:ILE:HD12	2.02	0.42
1:A:463:VAL:HG13	1:A:478:TRP:CD2	2.55	0.42
1:B:243:ASP:HA	1:B:307:TRP:HB2	2.02	0.41
1:A:233:GLY:HA3	1:A:513:PHE:CE1	2.56	0.41
1:A:740:LYS:HA	1:A:740:LYS:HD3	1.56	0.41
1:B:266:ILE:HD12	1:B:347:VAL:HG12	2.02	0.41
1:A:700:GLY:HA2	1:A:728:VAL:O	2.21	0.41
1:B:626:GLU:OE1	1:B:628:ILE:HD11	2.21	0.41
1:B:738:GLU:O	1:B:738:GLU:CG	2.69	0.41
1:B:56:HIS:C	1:B:57:ILE:HG22	2.46	0.41
1:B:442:ILE:O	1:B:442:ILE:HG23	2.21	0.41
1:A:9:ILE:HD12	1:A:31:THR:CG2	2.51	0.41
1:A:59:PRO:HA	1:A:146:GLU:HA	2.03	0.41
1:A:185:LYS:NZ	1:A:193:GLN:HE21	2.18	0.41
1:B:311:THR:O	1:B:316:GLY:HA2	2.21	0.40
1:B:741:ARG:CZ	1:B:741:ARG:HB2	2.51	0.40
1:A:74:PHE:CD1	1:A:75:LYS:HG3	2.57	0.40
1:A:459:HIS:O	1:A:463:VAL:HB	2.21	0.40
1:B:38:GLY:O	1:B:39:PRO:C	2.64	0.40
1:A:180:ALA:O	1:A:184:VAL:HG23	2.20	0.40
1:B:566:VAL:O	1:B:645:HIS:HA	2.20	0.40
1:B:130:GLU:OE1	1:B:161:PHE:HB3	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	711/749 (95%)	659 (93%)	40 (6%)	12 (2%)	7 4
1	B	713/749 (95%)	670 (94%)	32 (4%)	11 (2%)	8 5
All	All	1424/1498 (95%)	1329 (93%)	72 (5%)	23 (2%)	7 5

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	538	ASP
1	A	738	GLU
1	A	739	ASN
1	A	741	ARG
1	B	38	GLY
1	B	39	PRO
1	B	282	ASP
1	B	739	ASN
1	B	741	ARG
1	A	6	ALA
1	A	282	ASP
1	A	713	GLU
1	A	17	LYS
1	A	37	ALA
1	A	576	SER
1	B	264	SER
1	B	420	ASN
1	B	6	ALA
1	B	36	GLU
1	A	284	PRO
1	A	724	SER
1	B	393	GLY
1	A	347	VAL

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	615/641 (96%)	557 (91%)	58 (9%)	8 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	617/641 (96%)	580 (94%)	37 (6%)	17	19
All	All	1232/1282 (96%)	1137 (92%)	95 (8%)	12	12

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	36	GLU
1	B	43	VAL
1	B	48	VAL
1	B	56	HIS
1	B	57	ILE
1	B	63	LEU
1	B	69	MET
1	B	124	VAL
1	B	149	LEU
1	B	186	LEU
1	B	264	SER
1	B	280	LYS
1	B	301	LEU
1	B	330	PRO
1	B	337	VAL
1	B	359	LYS
1	B	384	VAL
1	B	387	VAL
1	B	388	LEU
1	B	460	ILE
1	B	463	VAL
1	B	538	ASP
1	B	549	VAL
1	B	587	LYS
1	B	588	THR
1	B	624	ARG
1	B	633	ASN
1	B	636	LEU
1	B	641	LYS
1	B	688	LYS
1	B	729	THR
1	B	732	LEU
1	B	733	ASP
1	B	737	ILE
1	B	738	GLU
1	B	739	ASN

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Mol	Chain	Res	Type
1	B	741	ARG
1	A	10	SER
1	A	14	LEU
1	A	27	ASP
1	A	31	THR
1	A	32	THR
1	A	36	GLU
1	A	40	VAL
1	A	48	VAL
1	A	64	ARG
1	A	69	MET
1	A	94	THR
1	A	120	LYS
1	A	124	VAL
1	A	149	LEU
1	A	171	THR
1	A	186	LEU
1	A	217	GLU
1	A	250	GLU
1	A	252	ASP
1	A	274	GLU
1	A	276	GLU
1	A	281	LYS
1	A	282	ASP
1	A	289	LYS
1	A	293	LYS
1	A	302	ARG
1	A	321	GLU
1	A	326	VAL
1	A	337	VAL
1	A	344	LYS
1	A	359	LYS
1	A	388	LEU
1	A	463	VAL
1	A	482	HIS
1	A	502	LEU
1	A	510	LYS
1	A	515	LEU
1	A	528	ARG
1	A	576	SER
1	A	586	THR
1	A	587	LYS

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Mol	Chain	Res	Type
1	A	588	THR
1	A	590	SER
1	A	594	SER
1	A	595	ILE
1	A	596	ARG
1	A	621	SER
1	A	622	GLN
1	A	638	VAL
1	A	685	GLU
1	A	713	GLU
1	A	729	THR
1	A	732	LEU
1	A	733	ASP
1	A	734	LYS
1	A	737	ILE
1	A	740	LYS
1	A	741	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	GLN
1	B	175	GLN
1	B	187	HIS
1	B	193	GLN
1	B	385	GLN
1	B	406	HIS
1	B	456	HIS
1	B	482	HIS
1	B	581	ASN
1	B	622	GLN
1	B	672	ASN
1	B	739	ASN
1	A	95	GLN
1	A	163	HIS
1	A	175	GLN
1	A	187	HIS
1	A	193	GLN
1	A	220	GLN
1	A	247	GLN
1	A	290	ASN
1	A	385	GLN

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Mol	Chain	Res	Type
1	A	456	HIS
1	A	558	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	A	801	-	12,12,12	0.82	1 (8%)	17,17,17	1.19	3 (17%)
2	GAL	B	801	-	12,12,12	0.82	0	17,17,17	1.48	3 (17%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	GAL	O1-C1	2.10	1.46	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	GAL	O5-C1-C2	-3.52	104.12	110.30
2	B	801	GAL	C4-C3-C2	-2.40	106.62	110.83
2	B	801	GAL	O3-C3-C4	2.35	115.92	110.38
2	A	801	GAL	O3-C3-C4	2.26	115.69	110.38
2	A	801	GAL	C1-O5-C5	2.22	117.96	113.65
2	A	801	GAL	C3-C4-C5	-2.04	106.54	110.23

There are no chirality outliers.

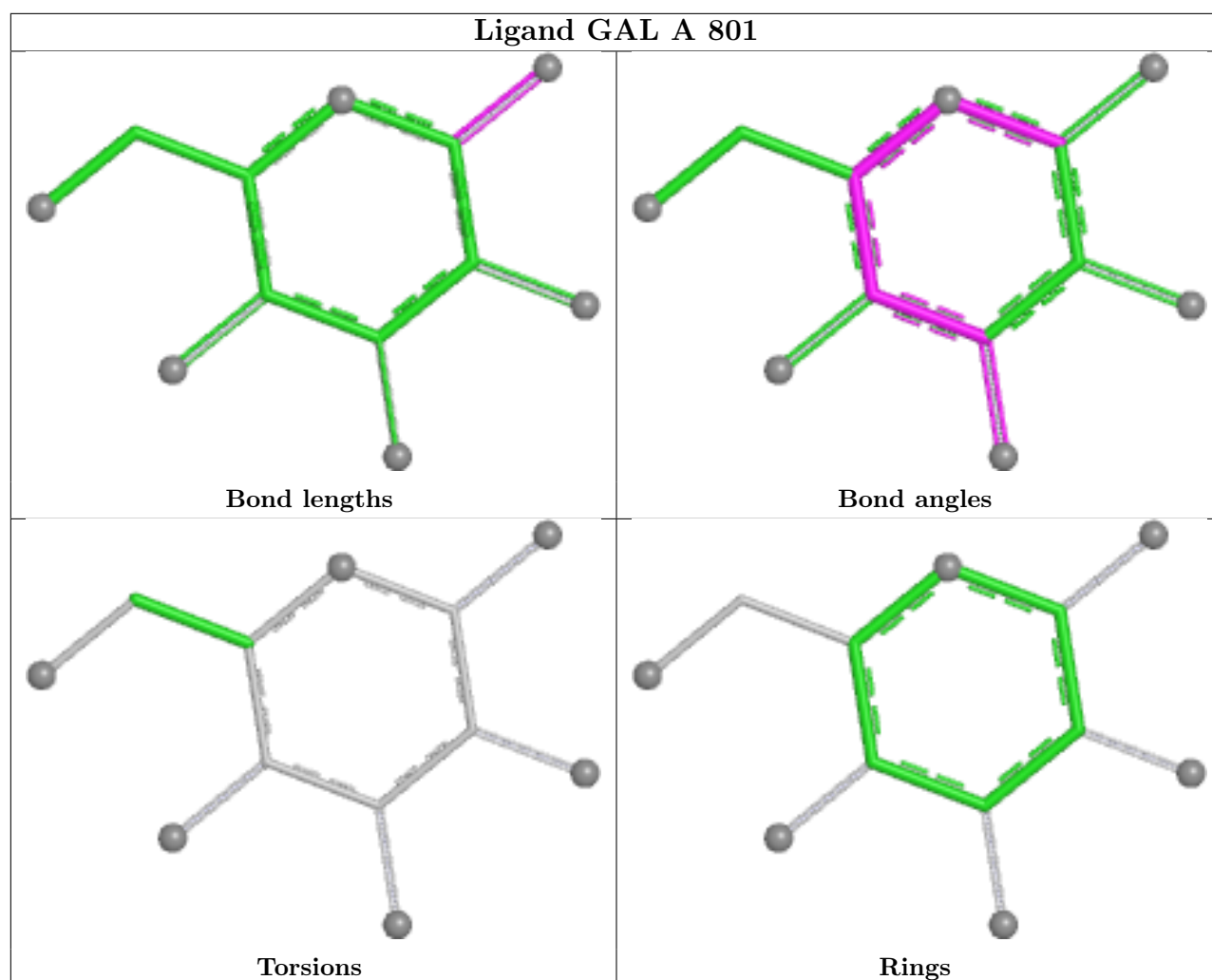
There are no torsion outliers.

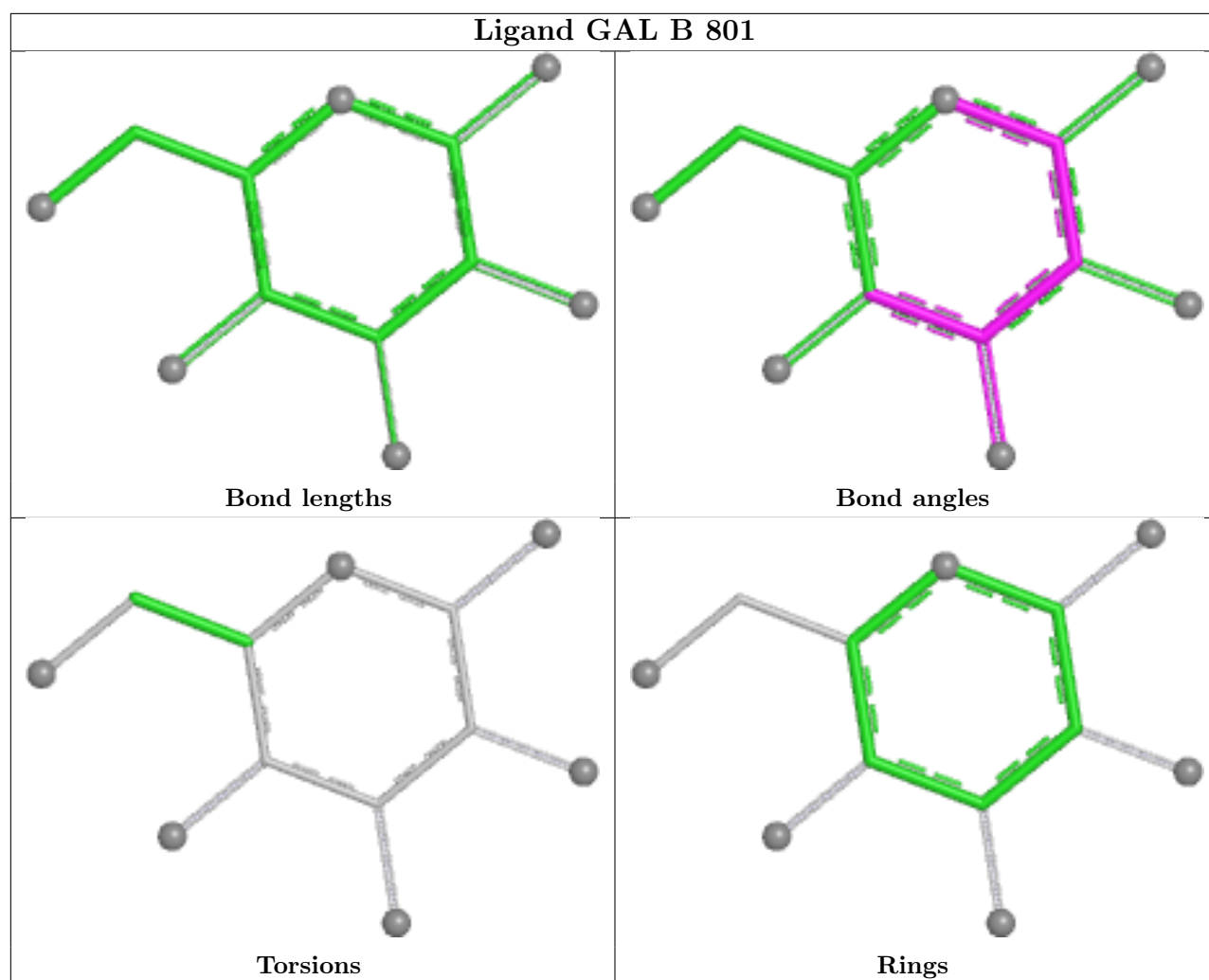
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	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	717/749 (95%)	0.92	93 (12%) 7 6	30, 67, 108, 136	0
1	B	719/749 (95%)	0.17	20 (2%) 55 54	30, 46, 82, 132	0
All	All	1436/1498 (95%)	0.55	113 (7%) 18 18	30, 57, 101, 136	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	738	GLU	6.9
1	A	37	ALA	6.8
1	B	737	ILE	6.6
1	A	737	ILE	6.6
1	A	141	VAL	6.2
1	A	139	GLY	5.2
1	B	739	ASN	5.2
1	B	39	PRO	5.1
1	B	5	PRO	4.9
1	A	739	ASN	4.6
1	A	57	ILE	4.5
1	A	154	VAL	4.1
1	A	253	ALA	4.1
1	B	263	GLU	4.0
1	A	281	LYS	3.9
1	A	15	ILE	3.7
1	B	37	ALA	3.7
1	A	271	GLY	3.6
1	B	264	SER	3.5
1	B	48	VAL	3.4
1	A	5	PRO	3.4
1	A	344	LYS	3.3
1	A	347	VAL	3.3
1	A	38	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	738	GLU	3.3
1	A	642	ILE	3.3
1	A	6	ALA	3.2
1	B	302	ARG	3.2
1	A	48	VAL	3.1
1	A	587	LYS	3.1
1	B	141	VAL	3.1
1	B	154	VAL	3.0
1	A	719	PHE	3.0
1	A	653	ILE	3.0
1	A	63	LEU	2.9
1	A	140	ASN	2.9
1	A	40	VAL	2.9
1	B	36	GLU	2.9
1	A	120	LYS	2.9
1	A	740	LYS	2.9
1	B	34	ALA	2.9
1	B	394	GLY	2.8
1	A	343	TRP	2.8
1	A	142	ASN	2.8
1	A	350	LEU	2.8
1	A	30	ILE	2.8
1	A	651	SER	2.8
1	A	34	ALA	2.8
1	B	740	LYS	2.8
1	A	265	PRO	2.8
1	A	655	HIS	2.7
1	A	583	PHE	2.7
1	A	39	PRO	2.7
1	A	267	PHE	2.7
1	A	577	THR	2.7
1	A	657	VAL	2.7
1	A	592	THR	2.6
1	A	729	THR	2.6
1	A	638	VAL	2.6
1	B	49	PHE	2.5
1	A	145	VAL	2.5
1	A	455	SER	2.5
1	A	604	SER	2.5
1	A	724	SER	2.5
1	A	35	SER	2.5
1	A	84	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	249	VAL	2.5
1	A	656	LEU	2.5
1	A	650	VAL	2.4
1	A	628	ILE	2.4
1	A	591	LEU	2.4
1	A	469	PHE	2.4
1	A	660	VAL	2.4
1	A	18	ASN	2.3
1	A	749	LEU	2.3
1	A	541	PHE	2.3
1	A	29	VAL	2.3
1	A	24	GLY	2.3
1	A	9	ILE	2.3
1	A	584	HIS	2.3
1	A	454	VAL	2.3
1	B	38	GLY	2.3
1	A	92	TYR	2.3
1	A	44	PHE	2.3
1	A	17	LYS	2.3
1	A	393	GLY	2.3
1	A	571	GLY	2.3
1	A	716	GLU	2.2
1	A	286	VAL	2.2
1	A	349	THR	2.2
1	A	137	LEU	2.2
1	A	19	ARG	2.2
1	A	337	VAL	2.2
1	A	549	VAL	2.2
1	A	87	GLY	2.2
1	A	545	ALA	2.2
1	A	686	LYS	2.2
1	A	302	ARG	2.2
1	A	581	ASN	2.2
1	A	64	ARG	2.1
1	A	147	LEU	2.1
1	A	588	THR	2.1
1	B	40	VAL	2.1
1	A	629	VAL	2.1
1	B	16	ILE	2.1
1	A	717	ILE	2.1
1	A	356	VAL	2.1
1	A	149	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	744	LEU	2.0
1	A	36	GLU	2.0
1	A	74	PHE	2.0
1	A	624	ARG	2.0
1	A	708	LYS	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](#)

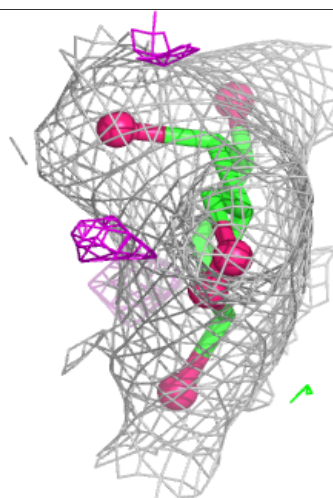
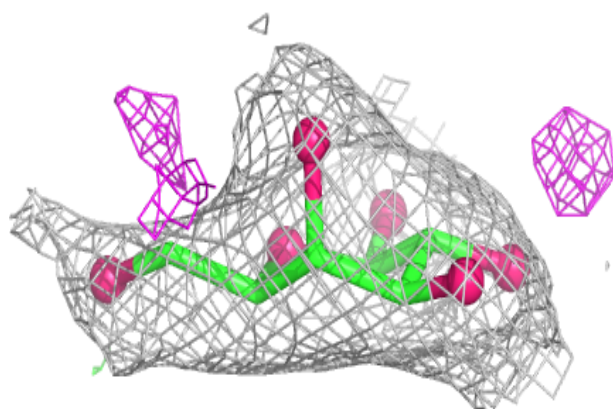
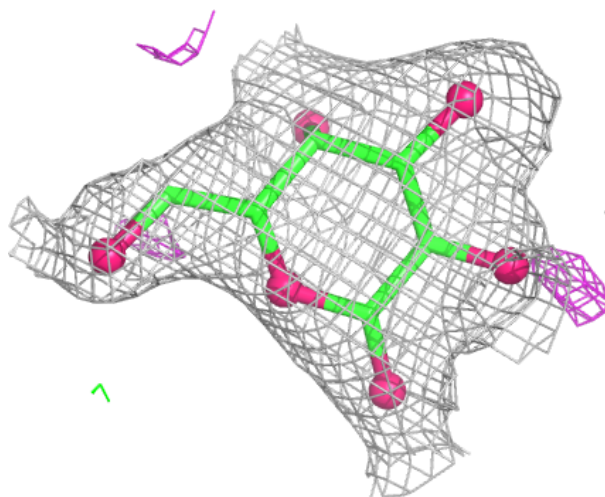
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

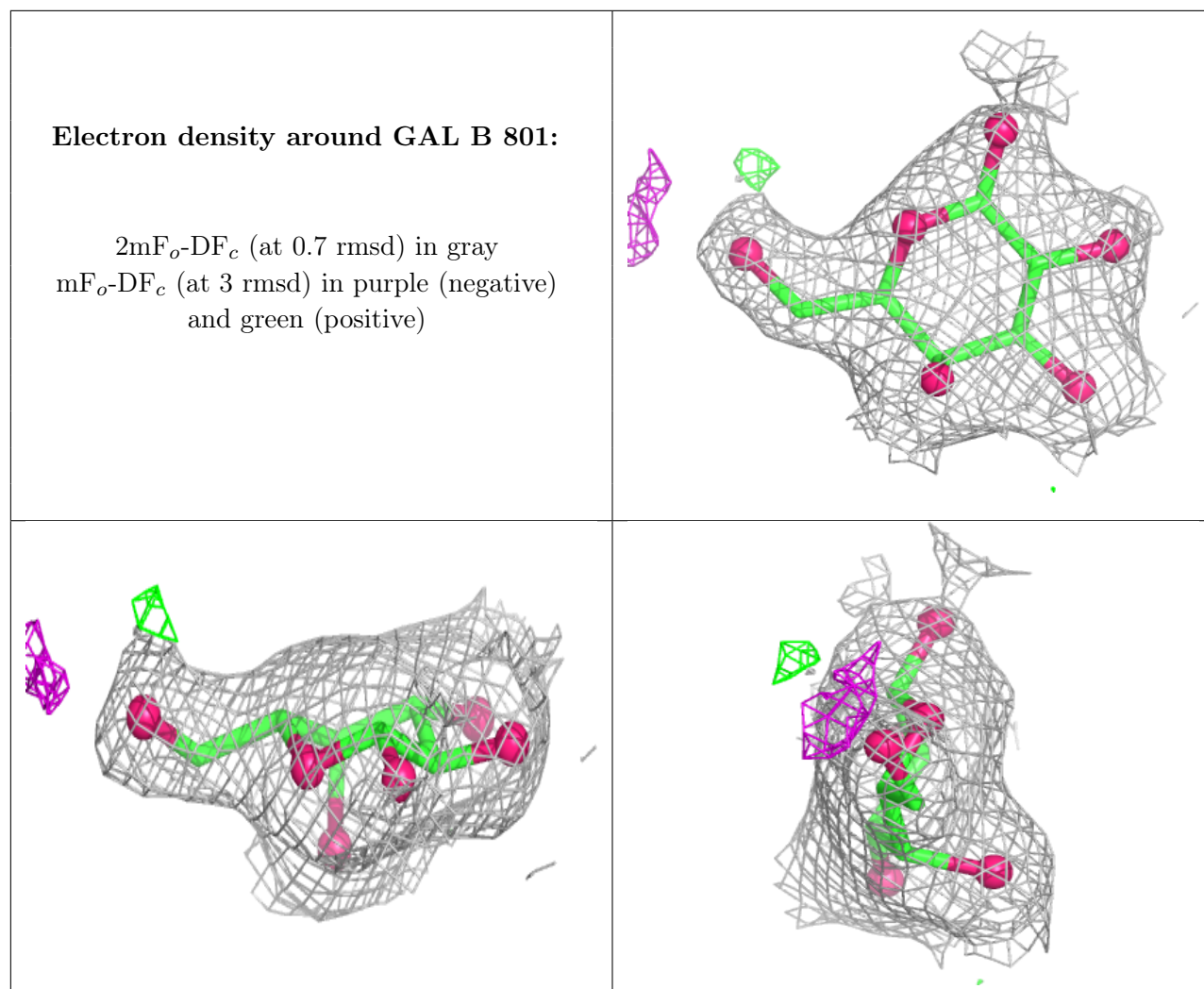
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	A	801	12/12	0.87	0.11	52,60,64,64	0
2	GAL	B	801	12/12	0.94	0.09	36,46,52,55	0

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)





6.5 Other polymers ⓘ

There are no such residues in this entry.