



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:52 PM UTC

PDB ID : 8WG0 / pdb_00008wg0
Title : Crystal structure of GH97 glucodextranase from *Flavobacterium johnsoniae* in complex with glucose
Authors : Kurata, R.; Nakamura, S.; Miyazaki, T.
Deposited on : 2023-09-20
Resolution : 1.95 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

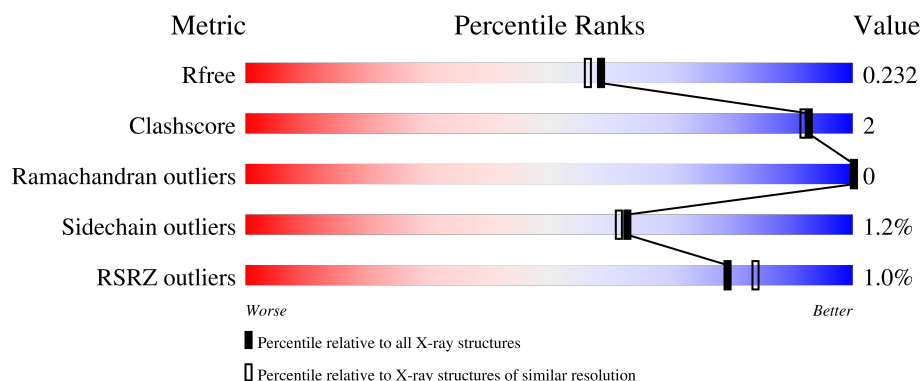
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	710	% 91% 5% .
1	B	710	2% 89% 6% 5%
1	C	710	90% 5% .
1	D	710	% 89% 6% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 43981 atoms, of which 21162 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 Candidate alpha-glucosidase Glycoside hydrolase family 97.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	682	Total	C	H	N	O	S	165	1	0
			10749	3490	5273	918	1049	19			
1	B	678	Total	C	H	N	O	S	168	1	0
			10700	3477	5248	913	1043	19			
1	C	682	Total	C	H	N	O	S	166	1	0
			10759	3492	5280	920	1048	19			
1	D	684	Total	C	H	N	O	S	166	0	0
			10761	3494	5277	919	1052	19			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP A5FBI0
A	-1	GLY	-	expression tag	UNP A5FBI0
A	0	SER	-	expression tag	UNP A5FBI0
A	1	SER	-	expression tag	UNP A5FBI0
A	2	HIS	-	expression tag	UNP A5FBI0
A	3	HIS	-	expression tag	UNP A5FBI0
A	4	HIS	-	expression tag	UNP A5FBI0
A	5	HIS	-	expression tag	UNP A5FBI0
A	6	HIS	-	expression tag	UNP A5FBI0
A	7	HIS	-	expression tag	UNP A5FBI0
A	8	SER	-	expression tag	UNP A5FBI0
A	9	SER	-	expression tag	UNP A5FBI0
A	10	GLY	-	expression tag	UNP A5FBI0
A	11	LEU	-	expression tag	UNP A5FBI0
A	12	VAL	-	expression tag	UNP A5FBI0
A	13	PRO	-	expression tag	UNP A5FBI0
A	14	ARG	-	expression tag	UNP A5FBI0
A	15	GLY	-	expression tag	UNP A5FBI0
A	16	SER	-	expression tag	UNP A5FBI0
A	17	HIS	-	expression tag	UNP A5FBI0
A	18	MET	-	expression tag	UNP A5FBI0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	-	expression tag	UNP A5FBI0
A	20	SER	-	expression tag	UNP A5FBI0
B	-2	MET	-	initiating methionine	UNP A5FBI0
B	-1	GLY	-	expression tag	UNP A5FBI0
B	0	SER	-	expression tag	UNP A5FBI0
B	1	SER	-	expression tag	UNP A5FBI0
B	2	HIS	-	expression tag	UNP A5FBI0
B	3	HIS	-	expression tag	UNP A5FBI0
B	4	HIS	-	expression tag	UNP A5FBI0
B	5	HIS	-	expression tag	UNP A5FBI0
B	6	HIS	-	expression tag	UNP A5FBI0
B	7	HIS	-	expression tag	UNP A5FBI0
B	8	SER	-	expression tag	UNP A5FBI0
B	9	SER	-	expression tag	UNP A5FBI0
B	10	GLY	-	expression tag	UNP A5FBI0
B	11	LEU	-	expression tag	UNP A5FBI0
B	12	VAL	-	expression tag	UNP A5FBI0
B	13	PRO	-	expression tag	UNP A5FBI0
B	14	ARG	-	expression tag	UNP A5FBI0
B	15	GLY	-	expression tag	UNP A5FBI0
B	16	SER	-	expression tag	UNP A5FBI0
B	17	HIS	-	expression tag	UNP A5FBI0
B	18	MET	-	expression tag	UNP A5FBI0
B	19	ALA	-	expression tag	UNP A5FBI0
B	20	SER	-	expression tag	UNP A5FBI0
C	-2	MET	-	initiating methionine	UNP A5FBI0
C	-1	GLY	-	expression tag	UNP A5FBI0
C	0	SER	-	expression tag	UNP A5FBI0
C	1	SER	-	expression tag	UNP A5FBI0
C	2	HIS	-	expression tag	UNP A5FBI0
C	3	HIS	-	expression tag	UNP A5FBI0
C	4	HIS	-	expression tag	UNP A5FBI0
C	5	HIS	-	expression tag	UNP A5FBI0
C	6	HIS	-	expression tag	UNP A5FBI0
C	7	HIS	-	expression tag	UNP A5FBI0
C	8	SER	-	expression tag	UNP A5FBI0
C	9	SER	-	expression tag	UNP A5FBI0
C	10	GLY	-	expression tag	UNP A5FBI0
C	11	LEU	-	expression tag	UNP A5FBI0
C	12	VAL	-	expression tag	UNP A5FBI0
C	13	PRO	-	expression tag	UNP A5FBI0
C	14	ARG	-	expression tag	UNP A5FBI0

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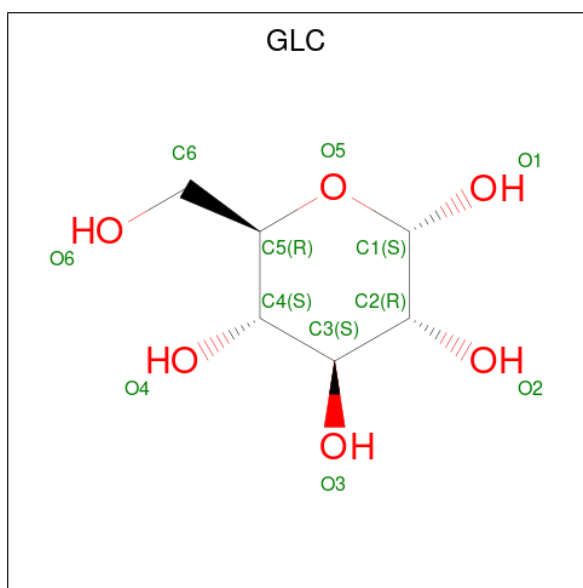
Chain	Residue	Modelled	Actual	Comment	Reference
C	15	GLY	-	expression tag	UNP A5FBI0
C	16	SER	-	expression tag	UNP A5FBI0
C	17	HIS	-	expression tag	UNP A5FBI0
C	18	MET	-	expression tag	UNP A5FBI0
C	19	ALA	-	expression tag	UNP A5FBI0
C	20	SER	-	expression tag	UNP A5FBI0
D	-2	MET	-	initiating methionine	UNP A5FBI0
D	-1	GLY	-	expression tag	UNP A5FBI0
D	0	SER	-	expression tag	UNP A5FBI0
D	1	SER	-	expression tag	UNP A5FBI0
D	2	HIS	-	expression tag	UNP A5FBI0
D	3	HIS	-	expression tag	UNP A5FBI0
D	4	HIS	-	expression tag	UNP A5FBI0
D	5	HIS	-	expression tag	UNP A5FBI0
D	6	HIS	-	expression tag	UNP A5FBI0
D	7	HIS	-	expression tag	UNP A5FBI0
D	8	SER	-	expression tag	UNP A5FBI0
D	9	SER	-	expression tag	UNP A5FBI0
D	10	GLY	-	expression tag	UNP A5FBI0
D	11	LEU	-	expression tag	UNP A5FBI0
D	12	VAL	-	expression tag	UNP A5FBI0
D	13	PRO	-	expression tag	UNP A5FBI0
D	14	ARG	-	expression tag	UNP A5FBI0
D	15	GLY	-	expression tag	UNP A5FBI0
D	16	SER	-	expression tag	UNP A5FBI0
D	17	HIS	-	expression tag	UNP A5FBI0
D	18	MET	-	expression tag	UNP A5FBI0
D	19	ALA	-	expression tag	UNP A5FBI0
D	20	SER	-	expression tag	UNP A5FBI0

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	3	0
			24	6	12	6		
3	B	1	Total	C	H	O	3	0
			24	6	12	6		
3	C	1	Total	C	H	O	3	0
			24	6	12	6		
3	C	1	Total	C	H	O	4	0
			24	6	12	6		
3	D	1	Total	C	H	O	3	0
			24	6	12	6		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

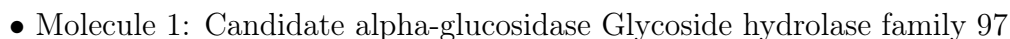


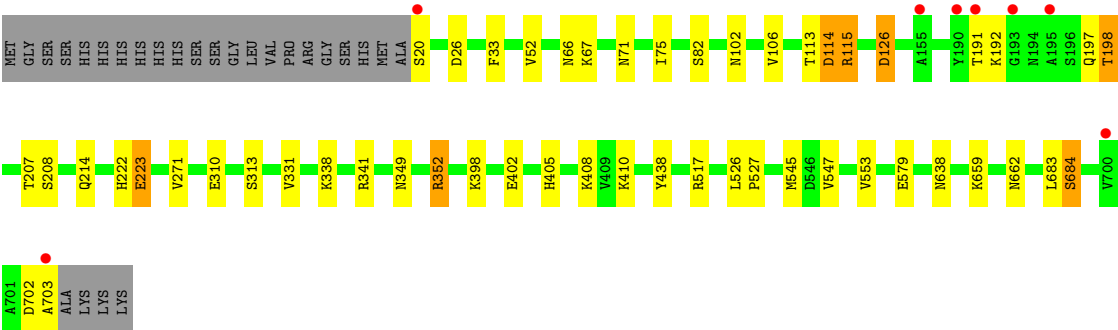
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	1	0
			10	2	6	2		
4	A	1	Total	C	H	O	1	0
			10	2	6	2		
4	C	1	Total	C	H	O	1	0
			10	2	6	2		
4	D	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	250	Total	O	0	0
			250	250		
5	B	165	Total	O	0	0
			165	165		
5	C	277	Total	O	0	0
			277	277		
5	D	156	Total	O	0	0
			156	156		

- Molecule 1: Candidate alpha-glucosidase Glycoside hydrolase family 97





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	307.93Å 103.69Å 95.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.13 – 1.95 49.13 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.13-1.95) 100.0 (49.13-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.189 , 0.229 0.193 , 0.232	Depositor DCC
R_{free} test set	10922 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	43981	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.88% 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: CA, GLC, EDO

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	0.95	1/5623 (0.0%)	1.19	9/7626 (0.1%)
1	B	0.86	0/5599	1.17	7/7593 (0.1%)
1	C	0.93	2/5626 (0.0%)	1.17	12/7629 (0.2%)
1	D	0.88	1/5628 (0.0%)	1.17	16/7633 (0.2%)
All	All	0.91	4/22476 (0.0%)	1.17	44/30481 (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	3
1	B	0	2
1	C	0	4
1	D	0	2
All	All	0	11

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	383	ASP	CG-OD1	6.24	1.37	1.25
1	C	405	HIS	CE1-NE2	6.04	1.38	1.32
1	A	75	ILE	C-O	-5.41	1.18	1.24
1	D	75	ILE	C-O	-5.07	1.18	1.24

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	579	GLU	CB-CA-C	-12.40	90.97	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	579	GLU	CB-CA-C	-10.79	93.54	110.81
1	A	32	HIS	CA-CB-CG	9.97	123.77	113.80
1	C	579	GLU	CB-CA-C	-9.62	94.82	110.79
1	D	703	ALA	CA-C-O	-8.89	105.68	120.80
1	C	341	ARG	CG-CD-NE	-8.24	93.86	112.00
1	A	331	VAL	N-CA-C	-8.17	105.17	111.62
1	B	640	ASP	CB-CA-C	7.96	122.89	109.75
1	A	138	ASN	CA-CB-CG	-7.39	105.21	112.60
1	C	88	LYS	CB-CA-C	-6.88	103.36	110.17
1	D	331	VAL	N-CA-C	-6.37	106.58	111.62
1	A	638	ASN	CA-C-N	6.33	131.00	122.01
1	A	638	ASN	C-N-CA	6.33	131.00	122.01
1	D	341	ARG	CG-CD-NE	-6.21	98.35	112.00
1	D	198	THR	CA-C-N	5.98	131.60	120.95
1	D	198	THR	C-N-CA	5.98	131.60	120.95
1	B	51	ASP	CA-CB-CG	5.95	118.55	112.60
1	D	310	GLU	CB-CA-C	-5.90	101.37	110.81
1	C	331	VAL	N-CA-C	-5.88	106.51	111.56
1	C	310	GLU	CB-CA-C	-5.85	101.45	110.81
1	D	115	ARG	CG-CD-NE	-5.83	99.18	112.00
1	D	26	ASP	CA-CB-CG	5.82	118.42	112.60
1	D	331	VAL	N-CA-CB	5.82	116.41	111.64
1	B	252	HIS	CA-CB-CG	5.72	119.52	113.80
1	C	689	SER	CB-CA-C	5.71	118.38	110.16
1	C	26	ASP	CA-CB-CG	5.69	118.29	112.60
1	C	191	THR	CA-CB-OG1	-5.62	101.17	109.60
1	C	662	ASN	CA-CB-CG	-5.60	107.00	112.60
1	D	702	ASP	CA-C-N	5.58	131.75	121.70
1	D	702	ASP	C-N-CA	5.58	131.75	121.70
1	C	579	GLU	N-CA-CB	5.55	118.28	110.12
1	D	352	ARG	CB-CA-C	-5.55	101.93	110.81
1	A	331	VAL	N-CA-CB	5.53	116.17	111.64
1	B	662	ASN	CA-CB-CG	-5.48	107.12	112.60
1	A	640	ASP	N-CA-CB	-5.29	100.92	109.60
1	C	579	GLU	CB-CG-CD	5.28	121.57	112.60
1	C	639	ILE	N-CA-C	5.26	115.54	108.17
1	B	115	ARG	CB-CG-CD	-5.26	99.20	111.30
1	A	191	THR	CB-CA-C	5.20	118.53	109.65
1	D	223	GLU	CA-C-O	-5.18	115.71	121.51
1	D	662	ASN	CA-CB-CG	-5.12	107.48	112.60
1	A	517	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	D	191	THR	CB-CA-C	5.05	118.28	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	633	THR	CA-CB-OG1	-5.02	102.07	109.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	352	ARG	Sidechain
1	A	583	ARG	Sidechain
1	A	602	ARG	Sidechain
1	B	190	TYR	Peptide
1	B	352	ARG	Sidechain
1	C	341	ARG	Sidechain
1	C	352[A]	ARG	Sidechain
1	C	352[B]	ARG	Sidechain
1	C	583	ARG	Sidechain
1	D	115	ARG	Sidechain
1	D	517	ARG	Sidechain

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	5476	5273	5257	12	0
1	B	5452	5248	5230	17	0
1	C	5479	5280	5264	18	0
1	D	5484	5277	5260	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	12	11	0	0
3	B	12	12	10	0	0
3	C	24	24	23	3	0
3	D	12	12	10	0	0
4	A	8	12	12	0	0
4	C	4	6	6	0	0
4	D	4	6	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	250	0	0	1	0
5	B	165	0	0	2	0
5	C	277	0	0	2	0
5	D	156	0	0	1	0
All	All	22819	21162	21089	65	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 (65) 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:639:ILE:HD12	1:A:683:LEU:HB3	1.51	0.90
1:B:190:TYR:CE2	1:B:199:SER:HB3	2.21	0.75
1:B:52:VAL:HG11	1:B:271:VAL:HG21	1.75	0.68
1:B:600:ASP:OD2	1:B:602:ARG:NH1	2.29	0.64
1:B:65:ASP:OD2	1:B:115:ARG:NH2	2.34	0.60
1:D:192:LYS:HA	1:D:197:GLN:HE22	1.68	0.59
1:A:65:ASP:OD2	1:A:115:ARG:NH2	2.34	0.59
1:B:114:ASP:O	1:B:116:LYS:HE2	2.03	0.59
1:C:65:ASP:OD2	1:C:115:ARG:NH2	2.35	0.58
1:A:74:LYS:HE3	5:A:1102:HOH:O	2.07	0.55
1:C:192:LYS:HA	1:C:197:GLN:HE22	1.72	0.55
1:B:397:ILE:HG22	5:B:1037:HOH:O	2.04	0.55
1:C:597:ASP:OD2	3:C:804:GLC:H62	2.06	0.55
1:C:52:VAL:HG11	1:C:271:VAL:HG21	1.88	0.54
1:B:190:TYR:CE1	1:B:197:GLN:OE1	2.61	0.54
1:C:545:MET:HG3	1:C:553:VAL:HB	1.90	0.54
1:D:82:SER:OG	1:D:102:ASN:OD1	2.26	0.53
1:D:52:VAL:HG11	1:D:271:VAL:HG21	1.90	0.53
1:C:544:GLU:OE2	1:C:583:ARG:NH2	2.42	0.52
1:B:640:ASP:OD1	1:B:682:LYS:HE2	2.09	0.52
1:A:192:LYS:HA	1:A:197:GLN:HE22	1.75	0.51
1:A:398:LYS:HE3	1:A:402:GLU:OE1	2.11	0.50
1:A:545:MET:HG3	1:A:553:VAL:HB	1.95	0.49
1:B:190:TYR:CZ	1:B:197:GLN:OE1	2.67	0.48
1:D:405:HIS:HE1	1:D:438:TYR:O	1.95	0.48
1:C:299:ILE:O	3:C:804:GLC:H3	2.14	0.48
1:A:52:VAL:HG11	1:A:271:VAL:HG21	1.96	0.47
1:B:645:GLU:OE2	1:B:648:LYS:HD2	2.16	0.46
1:C:46:ILE:HG22	5:C:1100:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:PRO:HD2	3:C:804:GLC:H5	1.97	0.46
1:D:126:ASP:N	1:D:126:ASP:OD1	2.49	0.46
1:D:349:ASN:O	1:D:352:ARG:HB2	2.16	0.46
1:C:683:LEU:HD23	1:C:683:LEU:HA	1.84	0.44
1:C:71:ASN:OD1	1:C:71:ASN:C	2.61	0.44
1:A:222:HIS:CG	1:A:223:GLU:H	2.36	0.44
1:D:545:MET:HG3	1:D:553:VAL:HB	2.00	0.44
1:D:398:LYS:HE3	1:D:402:GLU:OE1	2.18	0.43
1:B:310:GLU:HG3	5:B:1025:HOH:O	2.18	0.43
1:C:222:HIS:CG	1:C:223:GLU:H	2.36	0.43
1:C:207:THR:HA	1:C:208:SER:C	2.44	0.43
1:C:422:ARG:O	1:C:426:ARG:HG3	2.19	0.43
1:A:207:THR:HA	1:A:208:SER:C	2.43	0.42
1:A:71:ASN:C	1:A:71:ASN:OD1	2.62	0.42
1:B:71:ASN:OD1	1:B:71:ASN:C	2.62	0.42
1:D:71:ASN:OD1	1:D:71:ASN:C	2.62	0.42
1:A:652:ALA:HA	1:A:696:SER:O	2.20	0.42
1:B:405:HIS:HE1	1:B:438:TYR:O	2.03	0.42
1:C:444:LYS:HE3	1:C:484:HIS:CE1	2.55	0.42
1:D:33:PHE:CE2	1:D:106:VAL:HG11	2.55	0.42
1:D:66:ASN:OD1	1:D:67:LYS:N	2.53	0.41
1:B:545:MET:HG3	1:B:553:VAL:HB	2.01	0.41
1:D:113:THR:O	1:D:114:ASP:HB2	2.20	0.41
1:B:222:HIS:CG	1:B:223:GLU:H	2.37	0.41
1:B:652:ALA:HA	1:B:696:SER:O	2.20	0.41
1:C:88:LYS:HE3	1:C:95:SER:O	2.20	0.41
1:B:207:THR:HA	1:B:208:SER:C	2.46	0.41
1:A:405:HIS:HE1	1:A:438:TYR:O	2.04	0.41
1:D:638:ASN:OD1	1:D:684:SER:HB2	2.21	0.41
1:D:207:THR:HA	1:D:208:SER:C	2.46	0.40
1:D:526:LEU:N	1:D:527:PRO:CD	2.84	0.40
1:D:313:SER:HB2	1:D:547:VAL:HB	2.04	0.40
1:D:410:LYS:HE3	5:D:918:HOH:O	2.21	0.40
1:C:652:ALA:HA	1:C:696:SER:O	2.22	0.40
1:C:310:GLU:HG3	5:C:1044:HOH:O	2.20	0.40
1:D:222:HIS:CG	1:D:223:GLU:H	2.39	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	681/710 (96%)	652 (96%)	29 (4%)	0	100	100
1	B	675/710 (95%)	647 (96%)	28 (4%)	0	100	100
1	C	681/710 (96%)	646 (95%)	35 (5%)	0	100	100
1	D	682/710 (96%)	648 (95%)	34 (5%)	0	100	100
All	All	2719/2840 (96%)	2593 (95%)	126 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	582/603 (96%)	579 (100%)	3 (0%)	81	82
1	B	580/603 (96%)	568 (98%)	12 (2%)	47	41
1	C	582/603 (96%)	578 (99%)	4 (1%)	76	76
1	D	582/603 (96%)	572 (98%)	10 (2%)	53	49
All	All	2326/2412 (96%)	2297 (99%)	29 (1%)	63	61

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LYS
1	A	138	ASN

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Mol	Chain	Res	Type
1	A	408	LYS
1	B	79	LYS
1	B	191	THR
1	B	198	THR
1	B	214	GLN
1	B	239	LYS
1	B	436	LYS
1	B	578	PRO
1	B	646	LYS
1	B	659	LYS
1	B	673	ARG
1	B	674	LYS
1	B	683	LEU
1	C	79	LYS
1	C	237	ASP
1	C	579	GLU
1	C	682	LYS
1	D	20	SER
1	D	114	ASP
1	D	126	ASP
1	D	198	THR
1	D	214	GLN
1	D	338	LYS
1	D	408	LYS
1	D	659	LYS
1	D	683	LEU
1	D	684	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	100	ASN
1	A	197	GLN
1	A	405	HIS
1	A	423	ASN
1	A	685	GLN
1	B	66	ASN
1	B	86	ASN
1	B	99	ASN
1	B	100	ASN
1	B	197	GLN

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Mol	Chain	Res	Type
1	B	220	ASN
1	B	380	HIS
1	B	405	HIS
1	B	468	GLN
1	B	685	GLN
1	C	99	ASN
1	C	100	ASN
1	C	197	GLN
1	D	86	ASN
1	D	99	ASN
1	D	100	ASN
1	D	197	GLN
1	D	220	ASN
1	D	360	ASN
1	D	502	ASN
1	D	630	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	C	804	-	12,12,12	2.23	6 (50%)	17,17,17	1.67	4 (23%)
4	EDO	A	803	-	3,3,3	0.74	0	2,2,2	0.30	0
4	EDO	C	803	-	3,3,3	0.25	0	2,2,2	0.34	0
3	GLC	C	802	2	12,12,12	2.00	2 (16%)	17,17,17	2.20	4 (23%)
3	GLC	D	802	2	12,12,12	1.64	2 (16%)	17,17,17	1.80	5 (29%)
4	EDO	D	803	-	3,3,3	0.46	0	2,2,2	0.76	0
4	EDO	A	804	-	3,3,3	0.62	0	2,2,2	0.59	0
3	GLC	A	802	2	12,12,12	1.84	2 (16%)	17,17,17	2.18	6 (35%)
3	GLC	B	802	2	12,12,12	1.29	1 (8%)	17,17,17	1.84	5 (29%)

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
3	GLC	C	804	-	-	0/2/22/22	0/1/1/1
4	EDO	A	803	-	-	0/1/1/1	-
4	EDO	C	803	-	-	0/1/1/1	-
3	GLC	C	802	2	-	0/2/22/22	0/1/1/1
3	GLC	D	802	2	-	0/2/22/22	0/1/1/1
4	EDO	D	803	-	-	0/1/1/1	-
4	EDO	A	804	-	-	0/1/1/1	-
3	GLC	A	802	2	-	0/2/22/22	0/1/1/1
3	GLC	B	802	2	-	0/2/22/22	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802	GLC	O1-C1	6.19	1.59	1.39
3	A	802	GLC	O1-C1	5.16	1.55	1.39
3	C	804	GLC	C3-C2	3.66	1.61	1.52
3	D	802	GLC	O1-C1	3.51	1.50	1.39
3	C	804	GLC	C1-C2	3.34	1.60	1.52
3	C	804	GLC	O5-C5	3.26	1.52	1.44
3	A	802	GLC	O5-C1	2.73	1.49	1.42
3	B	802	GLC	O5-C1	2.43	1.48	1.42
3	C	804	GLC	O5-C1	2.38	1.48	1.42
3	C	804	GLC	C4-C5	2.35	1.58	1.53
3	C	802	GLC	O5-C1	2.30	1.48	1.42
3	C	804	GLC	C4-C3	2.28	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	GLC	O5-C1	2.06	1.47	1.42

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	GLC	O1-C1-O5	6.62	130.08	110.41
3	A	802	GLC	O1-C1-O5	5.90	127.94	110.41
3	B	802	GLC	O1-C1-O5	4.91	125.00	110.41
3	C	802	GLC	O5-C1-C2	-4.41	102.55	110.30
3	D	802	GLC	O1-C1-O5	4.22	122.94	110.41
3	A	802	GLC	O5-C1-C2	-4.13	103.03	110.30
3	C	804	GLC	O2-C2-C3	3.43	118.45	110.38
3	D	802	GLC	C4-C3-C2	-3.35	104.95	110.83
3	A	802	GLC	C1-O5-C5	3.18	119.80	113.65
3	D	802	GLC	O2-C2-C3	3.15	117.80	110.38
3	B	802	GLC	O5-C1-C2	-3.02	105.00	110.30
3	C	804	GLC	O4-C4-C3	2.86	117.12	110.38
3	B	802	GLC	O2-C2-C3	2.76	116.89	110.38
3	C	804	GLC	O3-C3-C2	2.75	116.86	110.38
3	C	804	GLC	O1-C1-C2	2.59	116.49	108.98
3	C	802	GLC	O2-C2-C3	2.46	116.18	110.38
3	B	802	GLC	C1-O5-C5	2.41	118.31	113.65
3	D	802	GLC	C1-O5-C5	2.40	118.29	113.65
3	A	802	GLC	O4-C4-C5	-2.17	103.97	109.32
3	A	802	GLC	C4-C3-C2	-2.17	107.02	110.83
3	C	802	GLC	C1-O5-C5	2.05	117.62	113.65
3	A	802	GLC	O3-C3-C4	2.04	115.18	110.38
3	D	802	GLC	O4-C4-C5	-2.03	104.32	109.32
3	B	802	GLC	O2-C2-C1	2.02	113.90	109.25

There are no chirality outliers.

There are no torsion outliers.

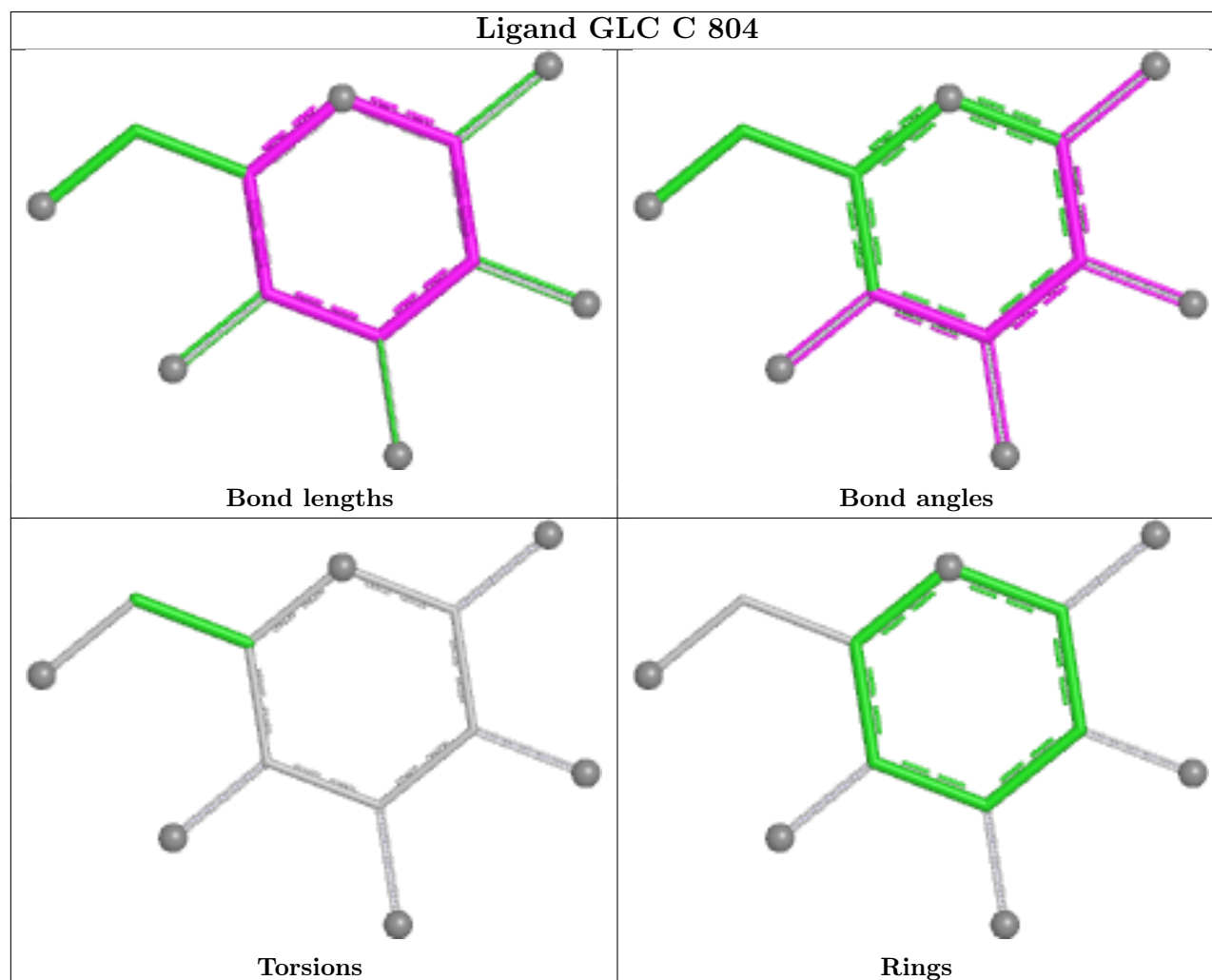
There are no ring outliers.

1 monomer is involved in 3 short contacts:

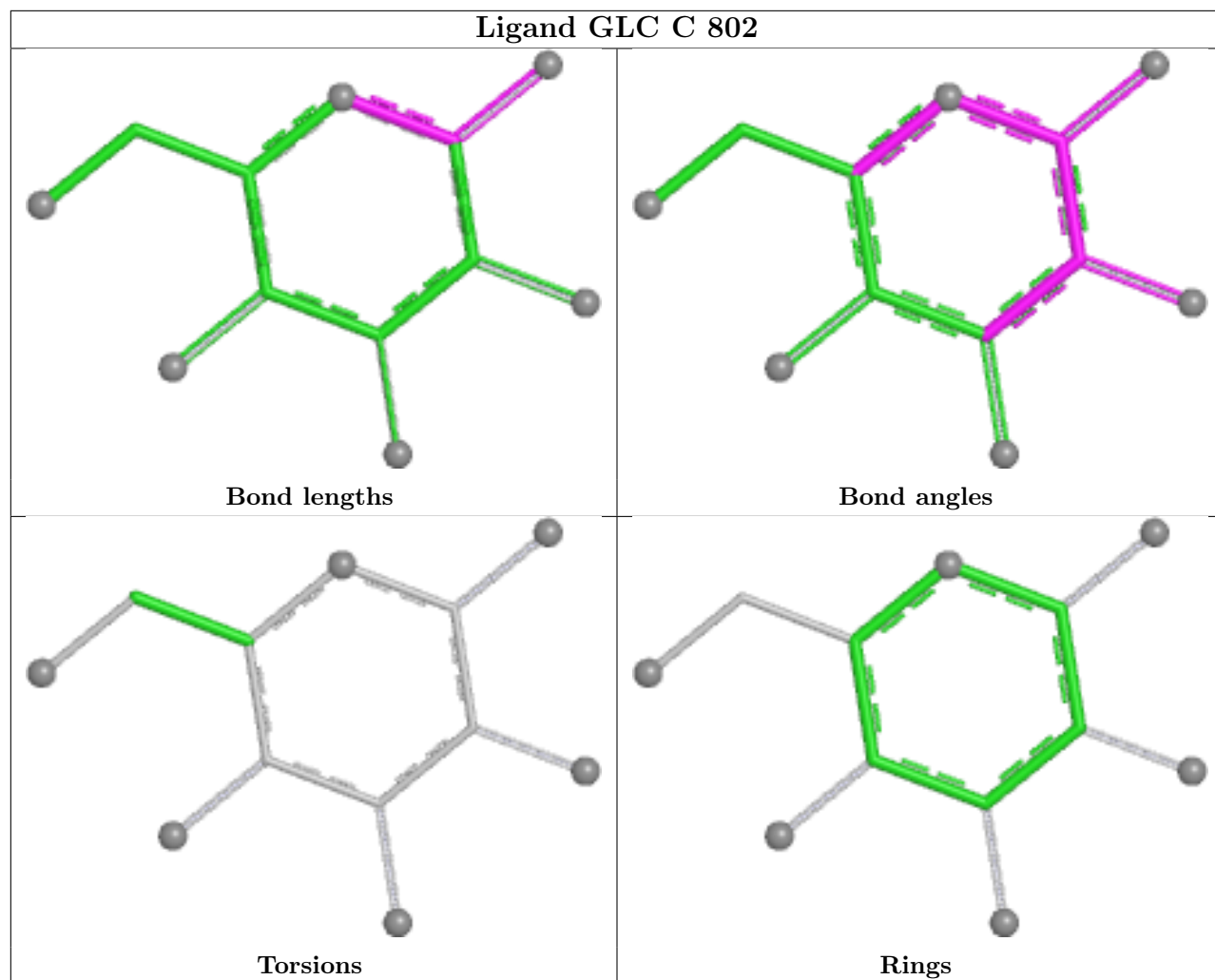
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	804	GLC	3	0

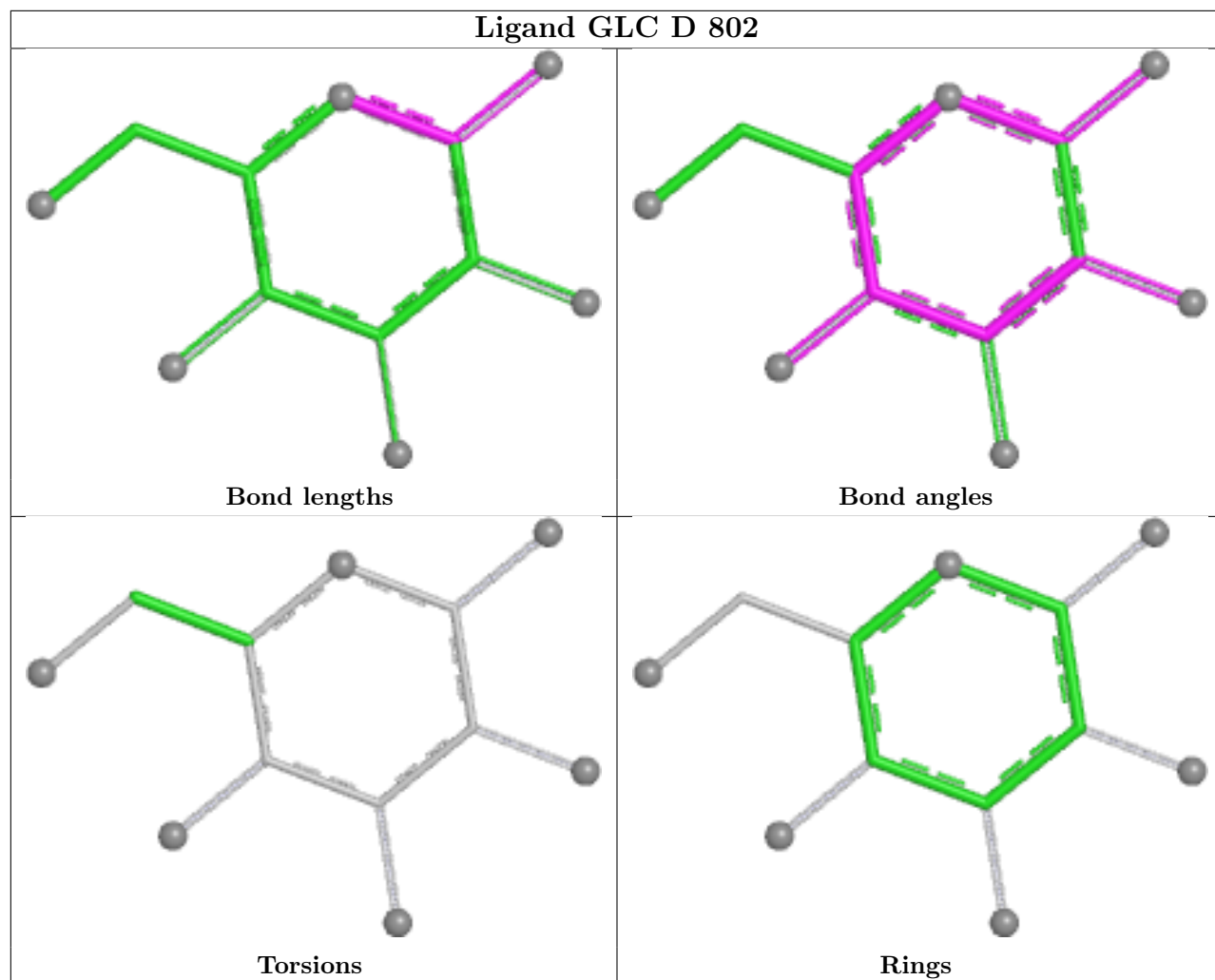
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

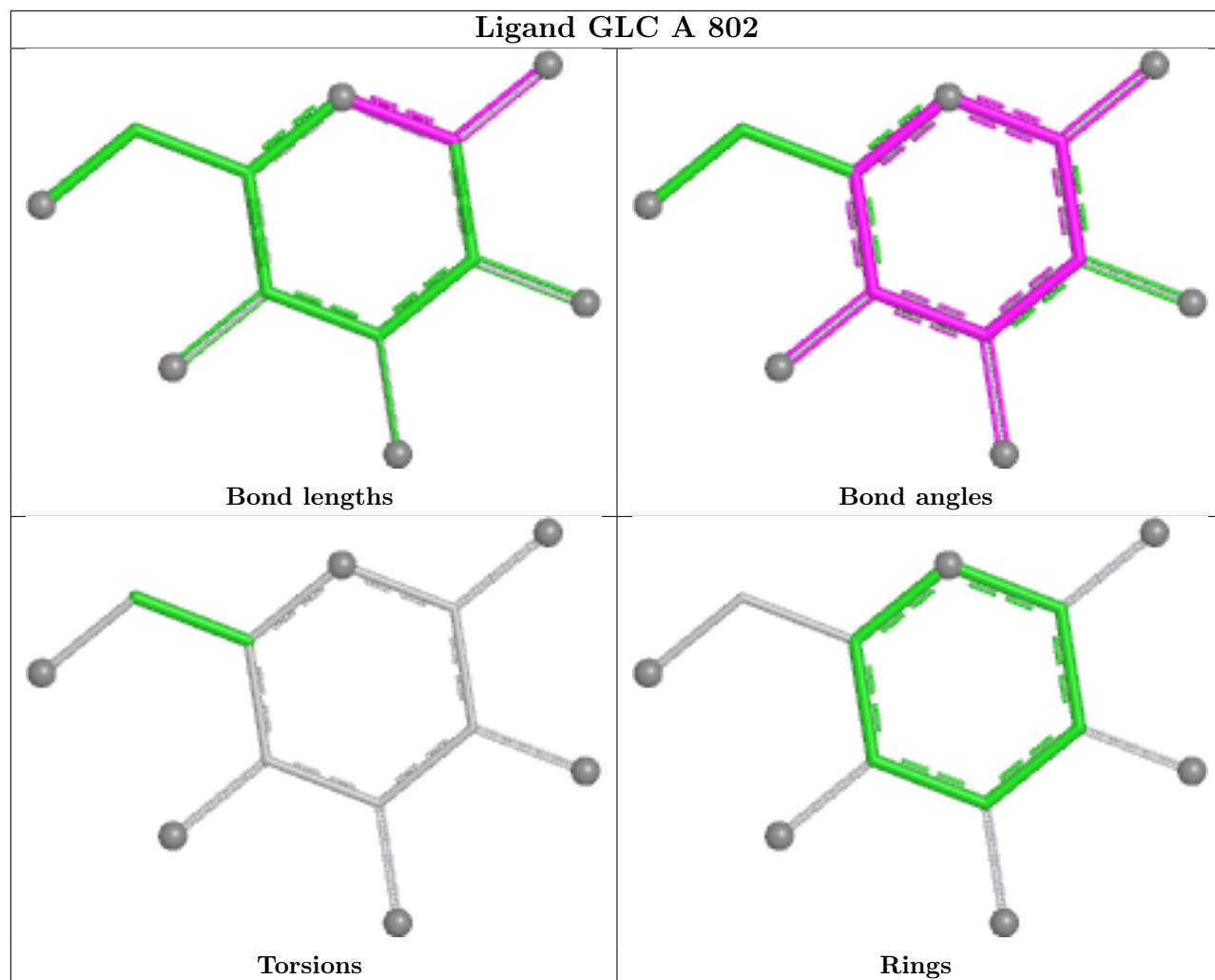
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

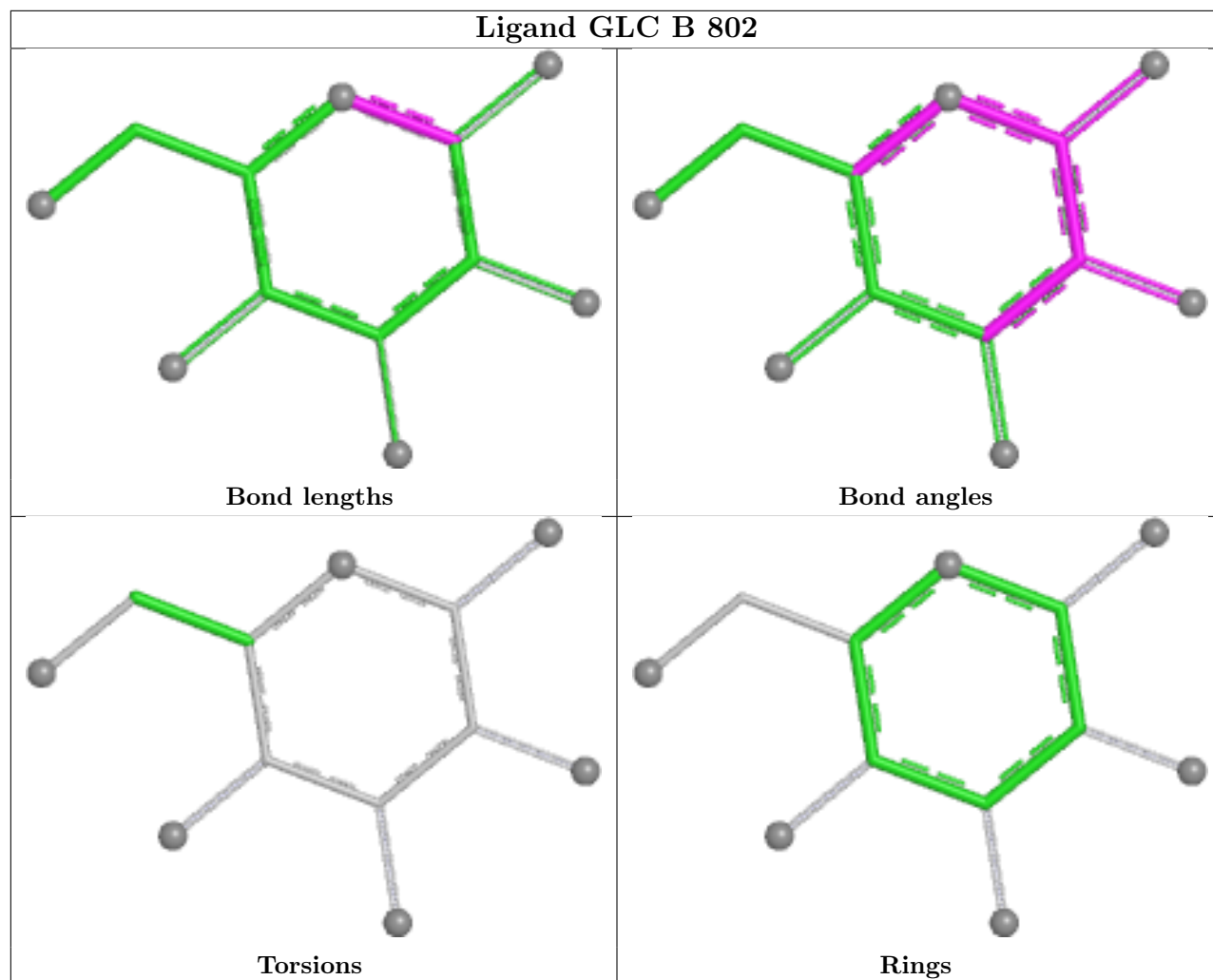


Ligand GLC C 802









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	682/710 (96%)	-0.50	6 (0%) 81 85	21, 34, 62, 85	1 (0%)
1	B	678/710 (95%)	0.09	13 (1%) 66 74	26, 46, 73, 103	1 (0%)
1	C	682/710 (96%)	-0.56	0 100 100	19, 34, 59, 90	1 (0%)
1	D	684/710 (96%)	-0.02	8 (1%) 76 82	24, 46, 73, 109	0
All	All	2726/2840 (95%)	-0.25	27 (0%) 79 84	19, 40, 69, 109	3 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	703	ALA	5.2
1	B	191	THR	5.1
1	A	195	ALA	4.6
1	B	700	VAL	4.5
1	D	195	ALA	3.7
1	B	189	ALA	3.7
1	B	195	ALA	3.6
1	D	190	TYR	3.3
1	B	190	TYR	3.3
1	B	32[A]	HIS	3.2
1	B	196	SER	3.1
1	A	20	SER	2.9
1	B	188	LYS	2.9
1	A	701	ALA	2.8
1	B	20	SER	2.8
1	D	193	GLY	2.7
1	B	187	GLU	2.6
1	B	354	ILE	2.6
1	A	682	LYS	2.6
1	B	338	LYS	2.4
1	B	198	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	155	ALA	2.3
1	A	193	GLY	2.2
1	D	20	SER	2.2
1	A	194	ASN	2.0
1	D	700	VAL	2.0
1	D	191	THR	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](#)

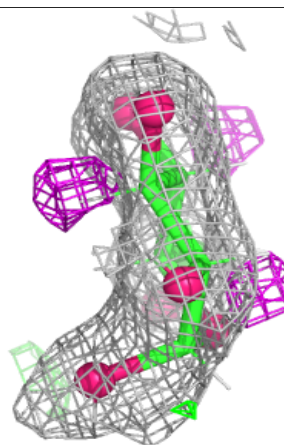
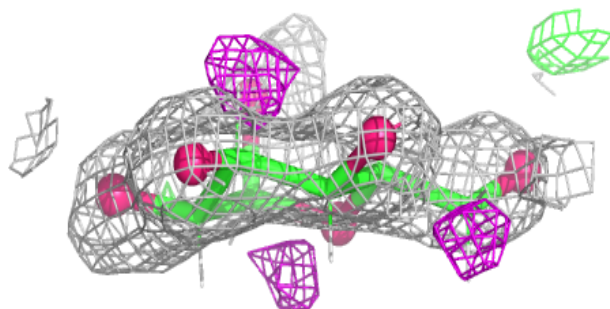
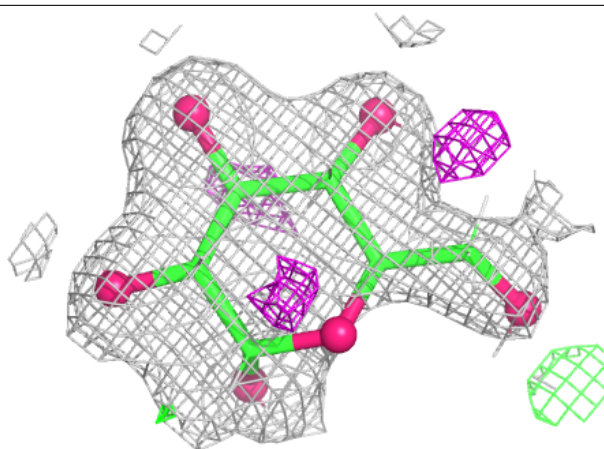
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	C	804	12/12	0.88	0.11	30,60,75,91	4
3	GLC	B	802	12/12	0.95	0.06	30,39,41,43	3
3	GLC	D	802	12/12	0.95	0.06	30,39,47,48	3
4	EDO	D	803	4/4	0.96	0.07	30,38,42,43	1
4	EDO	A	803	4/4	0.97	0.08	29,35,39,40	1
4	EDO	A	804	4/4	0.97	0.07	30,39,44,45	1
3	GLC	A	802	12/12	0.97	0.05	25,30,33,37	3
4	EDO	C	803	4/4	0.98	0.04	28,30,32,34	1
3	GLC	C	802	12/12	0.98	0.04	27,30,35,41	3
2	CA	D	801	1/1	0.99	0.04	41,41,41,41	0
2	CA	B	801	1/1	0.99	0.04	39,39,39,39	0
2	CA	A	801	1/1	1.00	0.03	26,26,26,26	0
2	CA	C	801	1/1	1.00	0.01	30,30,30,30	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.

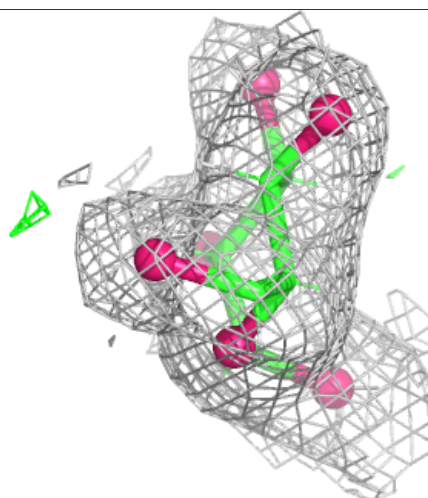
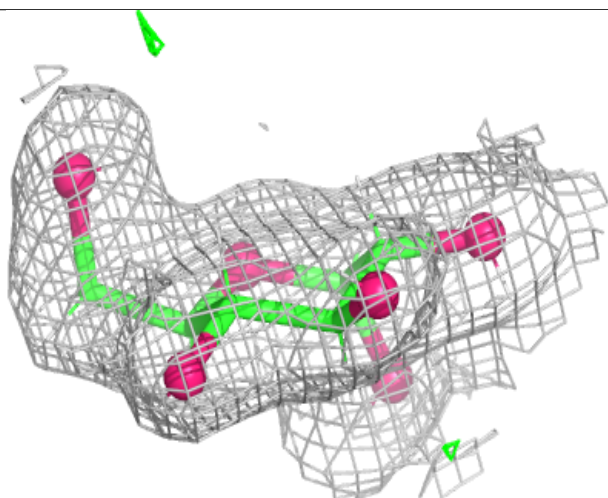
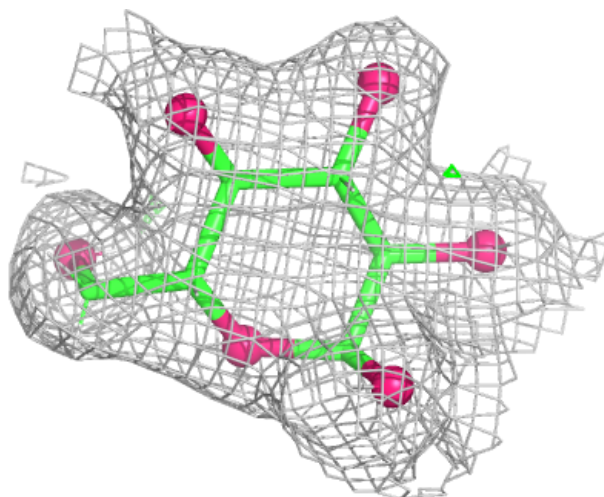
Electron density around GLC C 804:

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



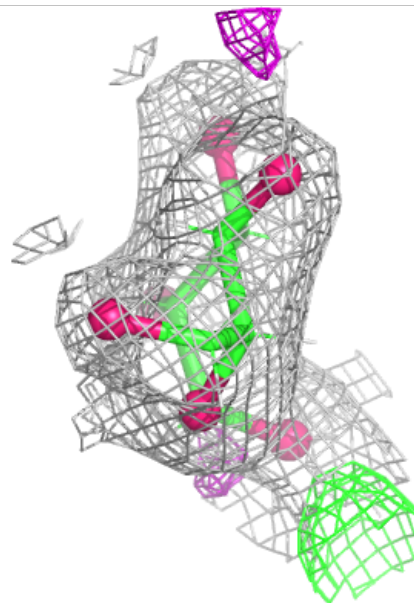
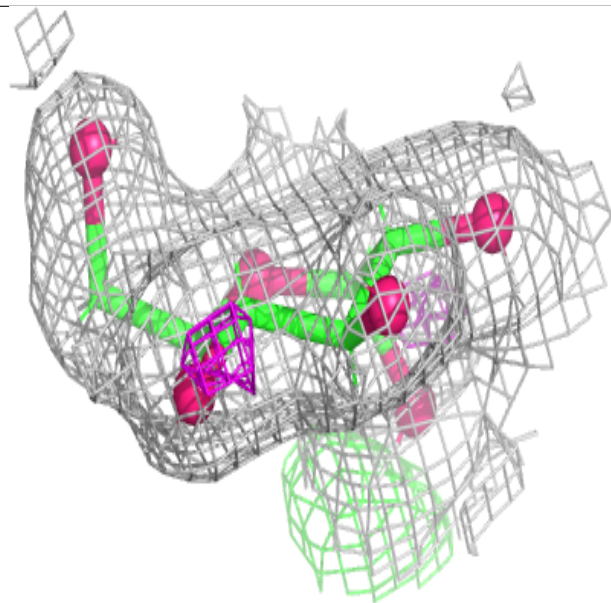
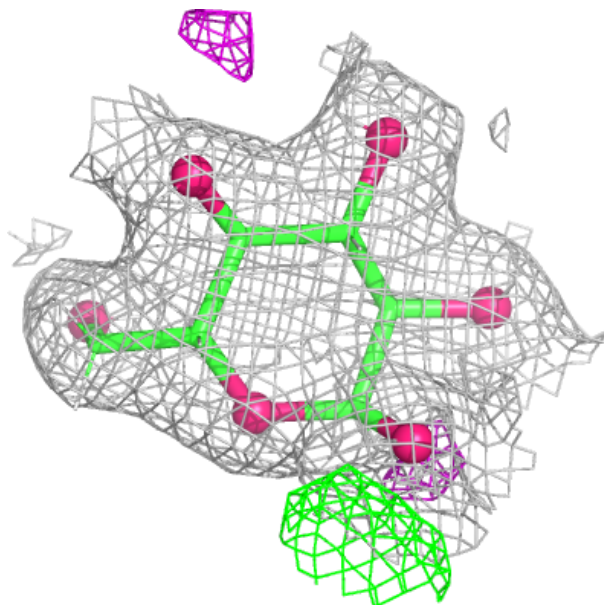
Electron density around GLC B 802:

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



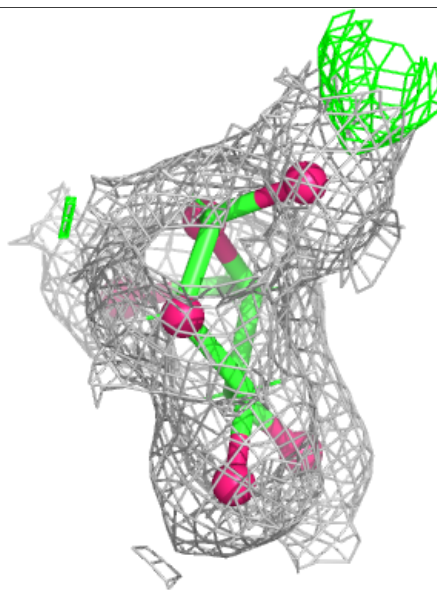
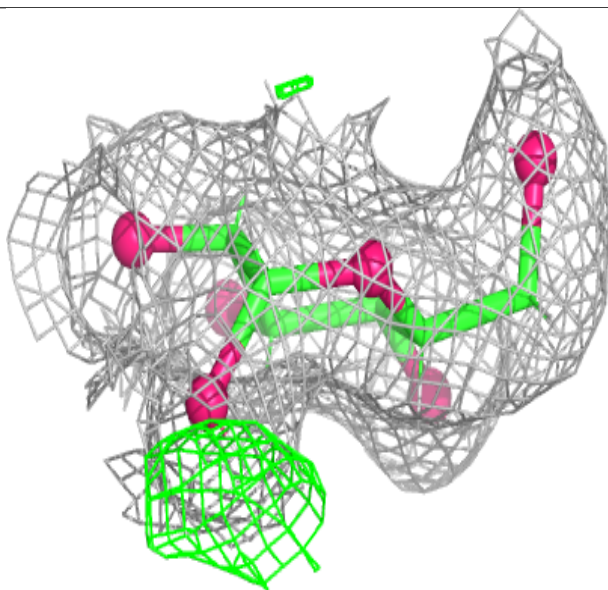
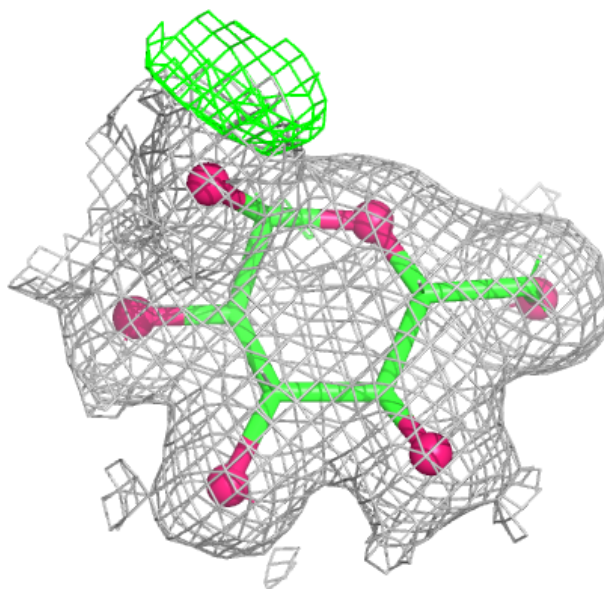
Electron density around GLC D 802:

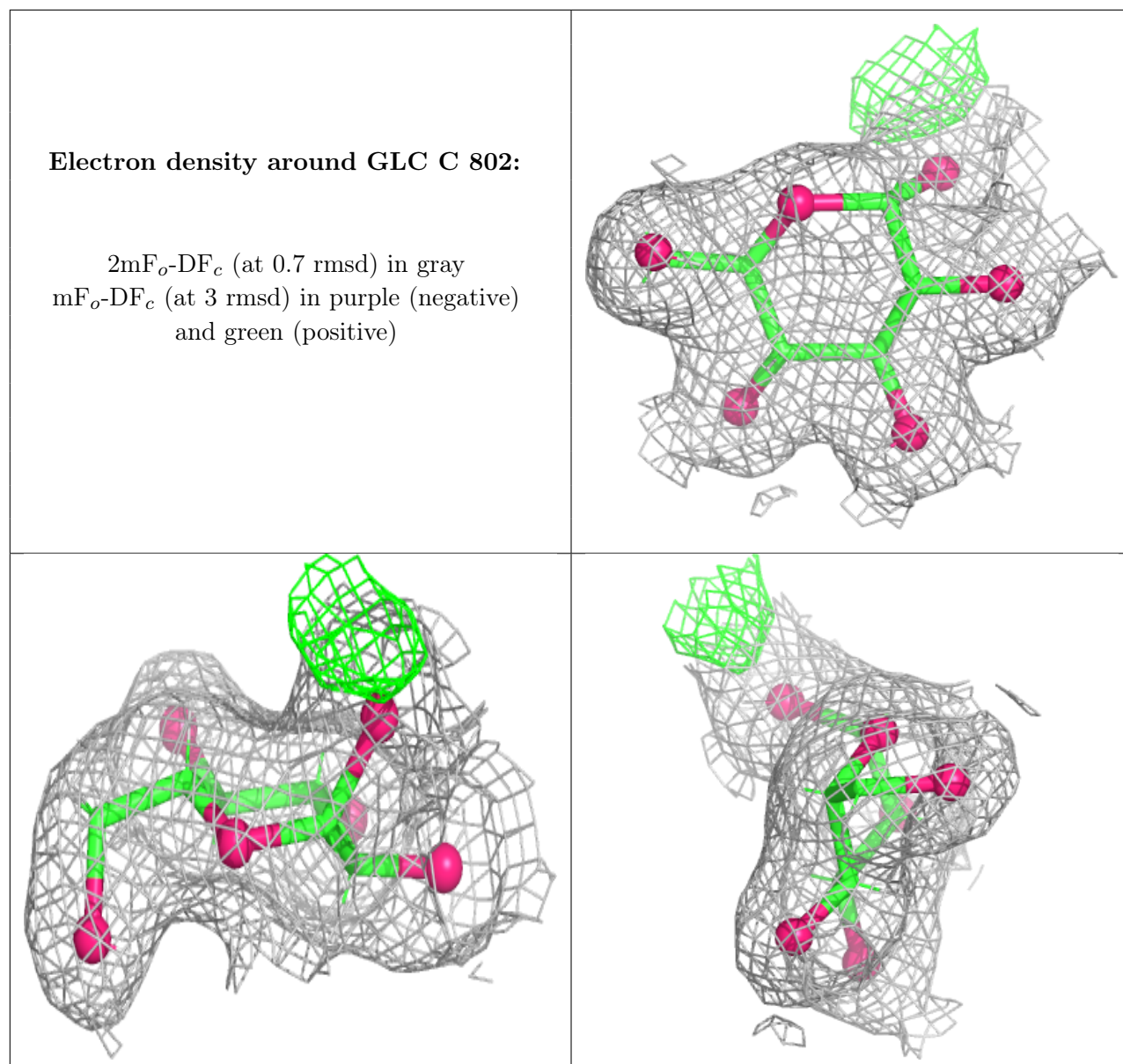
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GLC A 802:

$2mF_o-DF_c$ (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.