



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:11 AM UTC

PDB ID : 9SD8 / pdb_00009sd8
Title : Crystal structure of C-terminally truncated human PGGHG in complex with glucose.
Authors : Casas-Florez, D.; Ortega-Garcia, R.; Sanz-Aparicio, J.; Gonzalez, B.
Deposited on : 2025-08-12
Resolution : 1.61 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

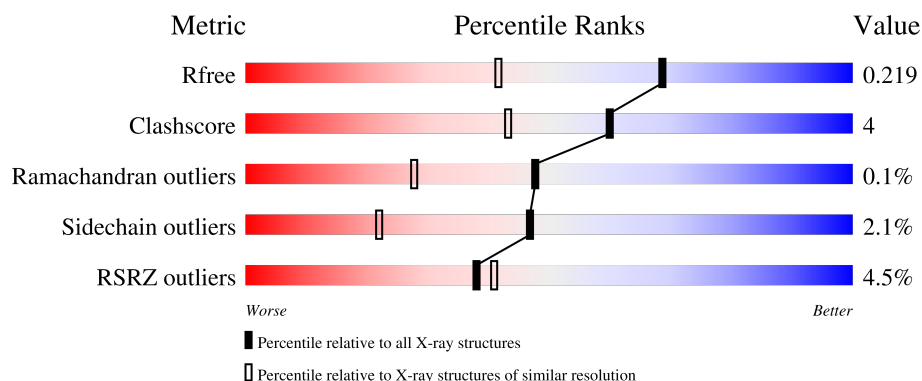
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 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	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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	693	4% 87% 10% ..
1	B	693	4% 88% 9% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11700 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 Protein-glucosylgalactosylhydroxylysine glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	685	Total	C	N	O	S	0	15	0
			5438	3461	948	1005	24			
1	B	679	Total	C	N	O	S	0	13	0
			5372	3424	931	996	21			

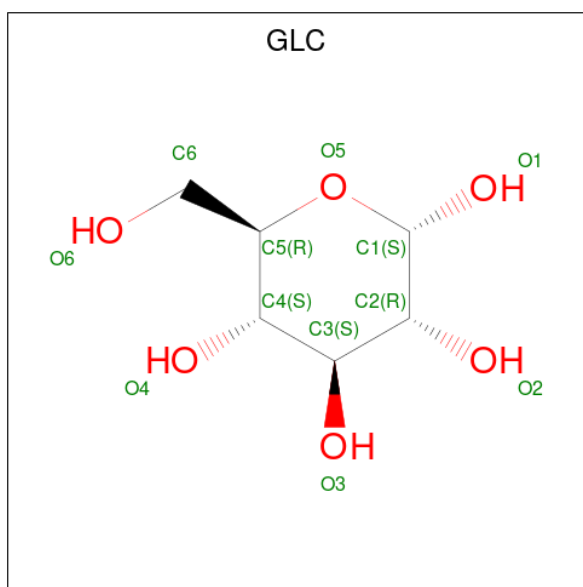
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q32M88
B	0	GLY	-	expression tag	UNP Q32M88

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

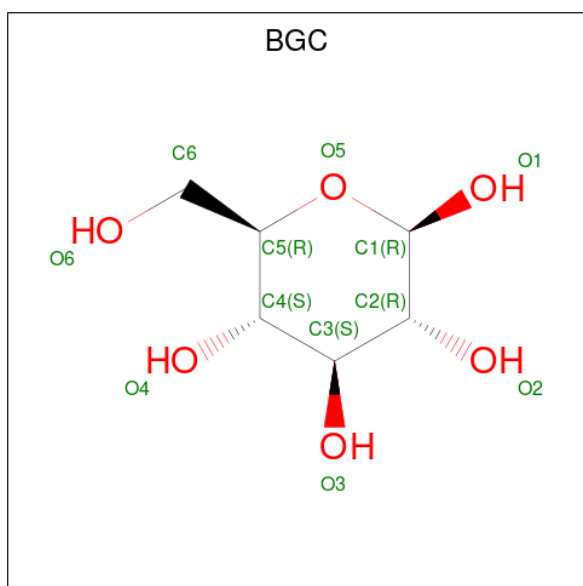
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		
2	B	1	Total	Cl	0	0
			1	1		

- 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	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



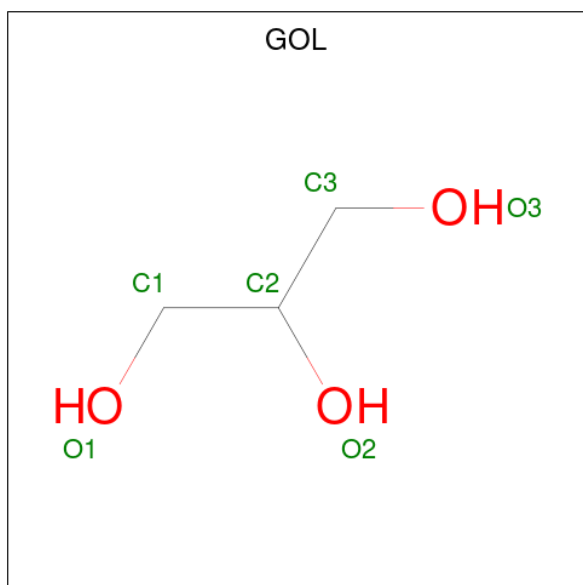
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		

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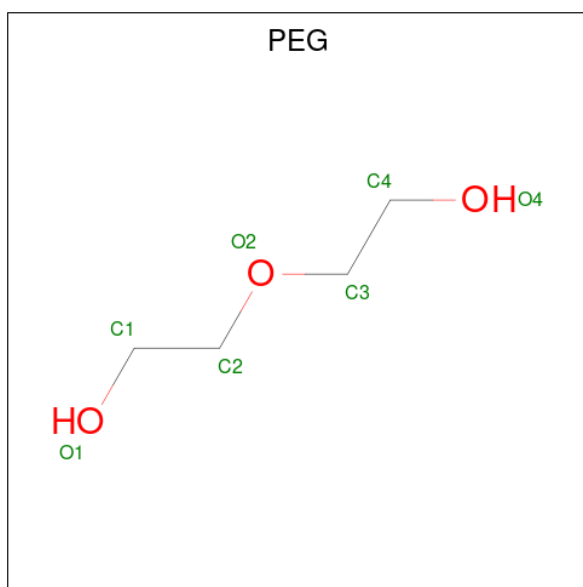
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

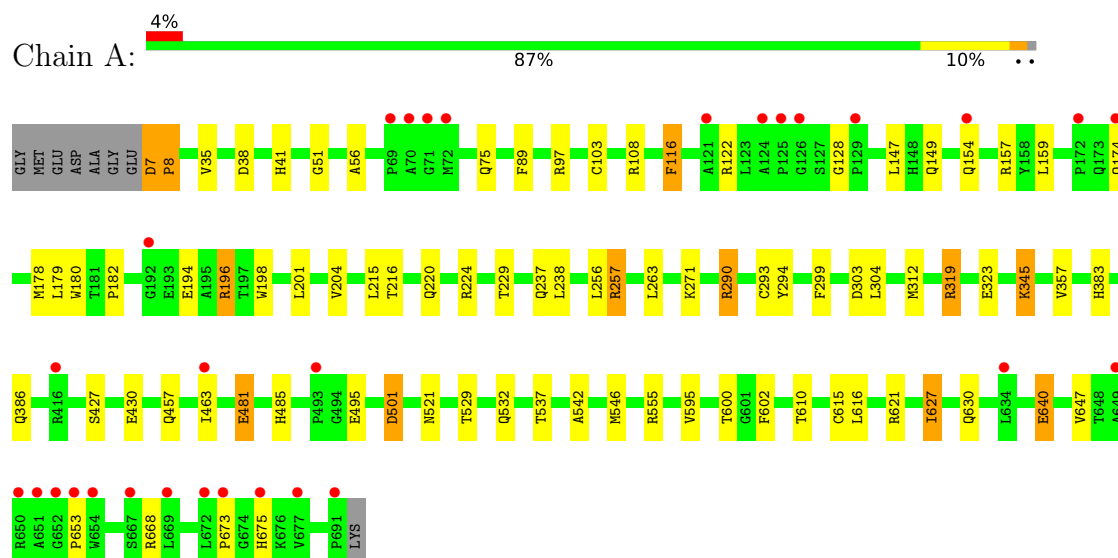
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	456	Total	O	0	1
			457	457		
7	B	338	Total	O	0	1
			339	339		

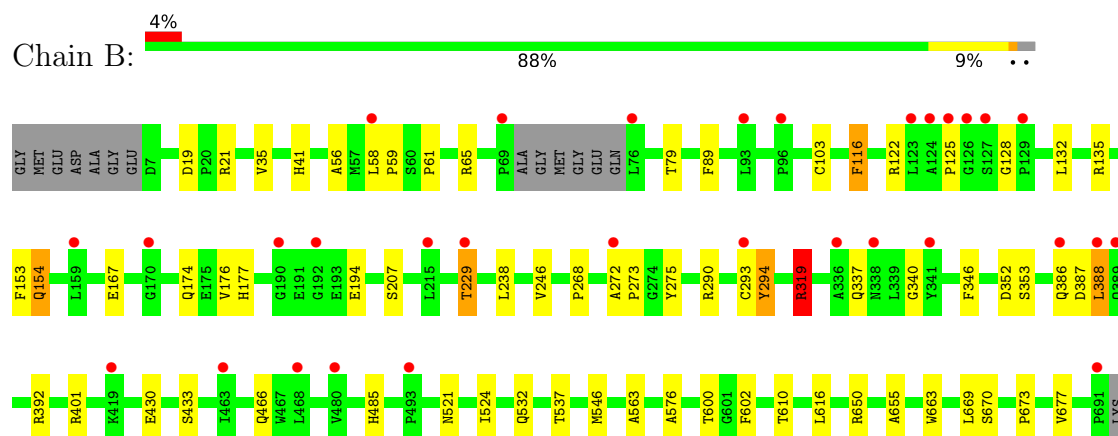
3 Residue-property plots [i](#)

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: Protein-glucosylgalactosylhydroxylysine glucosidase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.32Å 75.89Å 318.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	159.45 – 1.61 159.45 – 1.61	Depositor EDS
% Data completeness (in resolution range)	99.9 (159.45-1.61) 99.9 (159.45-1.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.174 , 0.209 0.184 , 0.219	Depositor DCC
R_{free} test set	8735 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.0	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	0.97	EDS
Total number of atoms	11700	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: CL, PEG, GOL, BGC, GLC

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	0.64	0/5595	1.09	19/7632 (0.2%)
1	B	0.62	1/5528 (0.0%)	1.05	13/7547 (0.2%)
All	All	0.63	1/11123 (0.0%)	1.07	32/15179 (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	10
1	B	0	5
All	All	0	15

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	433	SER	CA-CB	-5.13	1.45	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	TYR	CB-CA-C	9.15	128.62	110.42
1	A	257	ARG	NE-CZ-NH2	-8.04	111.96	119.20
1	B	229	THR	CA-CB-OG1	-7.31	98.64	109.60
1	B	319	ARG	CD-NE-CZ	6.82	133.94	124.40
1	A	319[A]	ARG	NE-CZ-NH2	-6.72	113.15	119.20
1	A	319[B]	ARG	NE-CZ-NH2	-6.72	113.15	119.20
1	A	319[A]	ARG	CD-NE-CZ	-6.34	115.52	124.40
1	A	319[B]	ARG	CD-NE-CZ	-6.34	115.52	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319[A]	ARG	NE-CZ-NH1	6.29	127.79	121.50
1	A	319[B]	ARG	NE-CZ-NH1	6.29	127.79	121.50
1	A	116	PHE	CA-CB-CG	6.23	120.03	113.80
1	A	294	TYR	N-CA-C	-6.20	102.78	112.77
1	A	600	THR	CA-CB-OG1	-6.03	100.55	109.60
1	A	294	TYR	N-CA-CB	5.89	124.12	111.35
1	A	8	PRO	N-CA-CB	-5.60	97.37	103.25
1	B	346	PHE	CA-CB-CG	-5.56	108.24	113.80
1	A	481	GLU	CB-CG-CD	5.54	122.02	112.60
1	A	38	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	345	LYS	CG-CD-CE	5.37	123.64	111.30
1	A	229	THR	CA-CB-OG1	-5.29	101.67	109.60
1	B	116	PHE	CA-CB-CG	5.28	119.08	113.80
1	B	600	THR	CA-CB-OG1	-5.26	101.71	109.60
1	B	294	TYR	N-CA-CB	5.26	119.37	110.49
1	A	97	ARG	N-CA-CB	-5.25	102.38	110.20
1	A	299	PHE	CA-CB-CG	5.18	118.98	113.80
1	B	19	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	293[A]	CYS	CA-C-N	5.12	131.32	121.54
1	B	293[A]	CYS	C-N-CA	5.12	131.32	121.54
1	B	293[B]	CYS	CA-C-N	5.12	131.32	121.54
1	B	293[B]	CYS	C-N-CA	5.12	131.32	121.54
1	B	537	THR	CA-CB-OG1	-5.06	102.01	109.60
1	A	501	ASP	CA-CB-CG	5.05	117.65	112.60

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain
1	A	196[A]	ARG	Sidechain
1	A	257	ARG	Sidechain
1	A	290	ARG	Sidechain
1	A	293[A]	CYS	Peptide,Mainchain
1	A	293[B]	CYS	Peptide,Mainchain
1	A	555	ARG	Sidechain
1	A	668	ARG	Sidechain
1	B	135	ARG	Sidechain
1	B	290	ARG	Sidechain
1	B	319	ARG	Sidechain
1	B	401	ARG	Sidechain
1	B	65	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	5438	0	5234	56	0
1	B	5372	0	5166	35	0
2	A	2	0	0	1	0
2	B	1	0	0	0	0
3	A	12	0	6	1	0
3	B	12	0	12	1	0
4	A	24	0	18	3	0
4	B	12	0	12	2	0
5	A	18	0	24	3	0
5	B	6	0	8	1	0
6	A	7	0	10	0	0
7	A	457	0	0	11	0
7	B	339	0	0	5	1
All	All	11700	0	10490	92	1

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 4.

All (92) 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:122[A]:ARG:NH2	1:A:128:GLY:O	1.94	1.00
1:A:615[B]:CYS:SG	7:A:1081:HOH:O	2.25	0.95
1:B:58:LEU:HD21	1:B:176:VAL:HG11	1.50	0.93
1:B:650:ARG:NH1	1:B:655:ALA:O	2.17	0.78
5:A:709:GOL:H2	1:B:532:GLN:HG2	1.65	0.77
1:A:386:GLN:HG3	1:A:630:GLN:HE22	1.55	0.71
1:A:653:PRO:HB2	1:B:563:ALA:HB1	1.74	0.69
1:A:149:GLN:HE22	1:A:157:ARG:HH11	1.40	0.68
1:A:485:HIS:HD2	1:A:521:ASN:HD21	1.39	0.68
1:B:485:HIS:HD2	1:B:521:ASN:HD21	1.41	0.67
1:A:430:GLU:OE2	4:A:704:BGC:O2	2.10	0.67
1:A:319[A]:ARG:NH1	1:A:323:GLU:OE1	2.27	0.67
1:B:79:THR:OG1	7:B:801:HOH:O	2.14	0.66
1:B:650:ARG:HG3	1:B:673:PRO:HG3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:HIS:HD2	7:A:900:HOH:O	1.79	0.65
1:A:149:GLN:NE2	1:A:157:ARG:HH11	1.96	0.62
1:A:621[A]:ARG:NH1	7:A:801:HOH:O	2.05	0.61
1:A:647:VAL:O	1:A:673:PRO:HA	2.02	0.60
1:B:21[A]:ARG:HD2	7:B:827:HOH:O	2.02	0.59
1:B:122[A]:ARG:NH2	1:B:128:GLY:O	2.35	0.58
1:B:167:GLU:OE1	1:B:353:SER:OG	2.14	0.58
1:A:319[A]:ARG:HG2	1:A:319[A]:ARG:HH11	1.67	0.58
1:A:481:GLU:HG3	7:A:1061:HOH:O	2.04	0.57
1:B:41:HIS:HE1	7:B:912:HOH:O	1.86	0.57
1:B:388:LEU:HD13	1:B:392:ARG:NH1	2.21	0.56
1:A:41:HIS:HD2	1:A:56:ALA:O	1.88	0.55
1:A:41:HIS:HE1	7:A:863:HOH:O	1.90	0.54
1:B:485:HIS:HE1	7:B:1121:HOH:O	1.91	0.53
1:A:154:GLN:NE2	1:A:216:THR:OG1	2.42	0.52
1:A:182:PRO:HA	5:A:705:GOL:H32	1.92	0.51
3:A:703:GLC:O1	4:A:704:BGC:H2	2.11	0.51
1:B:386:GLN:HA	7:B:946:HOH:O	2.09	0.51
1:B:485:HIS:CD2	1:B:521:ASN:HD21	2.26	0.51
1:A:237:GLN:NE2	7:A:811:HOH:O	2.44	0.50
1:B:546:MET:HG2	1:B:616:LEU:HD21	1.93	0.50
1:A:457:GLN:HG3	1:A:463:ILE:HD11	1.94	0.49
1:B:663:TRP:CD1	5:B:704:GOL:H2	2.47	0.49
1:A:7:ASP:N	7:A:813:HOH:O	2.45	0.48
1:A:319[B]:ARG:O	1:A:319[B]:ARG:HG2	2.11	0.48
1:A:602:PHE:HA	1:A:610:THR:O	2.13	0.48
1:A:485:HIS:CD2	1:A:521:ASN:HD21	2.26	0.48
1:A:675:HIS:O	2:A:702:CL:CL	2.68	0.48
1:B:41:HIS:HD2	1:B:56:ALA:O	1.97	0.48
1:A:180:TRP:CD1	5:A:705:GOL:H11	2.50	0.47
1:B:546:MET:HE2	1:B:616:LEU:HD11	1.96	0.47
1:A:220:GLN:HB3	1:A:224:ARG:HH21	1.80	0.47
1:A:383:HIS:HE1	7:A:1207:HOH:O	1.97	0.46
1:B:238:LEU:C	1:B:238:LEU:HD23	2.40	0.46
1:A:147:LEU:HB3	1:A:159:LEU:HD22	1.97	0.46
1:A:201:LEU:HD11	1:A:215:LEU:HD12	1.97	0.46
1:A:485:HIS:HE1	7:A:1214:HOH:O	1.97	0.46
3:B:702:GLC:O1	4:B:703:BGC:H2	2.16	0.46
1:A:35:VAL:HG11	1:A:89:PHE:CG	2.50	0.46
1:A:319[A]:ARG:NH1	1:A:319[A]:ARG:CG	2.78	0.45
1:A:178[A]:MET:HG3	1:A:204:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLN:HE22	1:A:157:ARG:NH1	2.11	0.45
1:A:319[A]:ARG:HH11	1:A:319[A]:ARG:CG	2.15	0.45
4:A:704:BGC:H2	7:A:871:HOH:O	2.15	0.45
1:A:542:ALA:O	1:A:546:MET:HG3	2.17	0.45
1:A:529:THR:HG21	1:A:537:THR:HG21	1.98	0.45
1:A:615[A]:CYS:SG	1:A:640:GLU:HA	2.57	0.45
1:A:345:LYS:HD3	1:A:345:LYS:C	2.41	0.44
1:B:430:GLU:OE2	4:B:703:BGC:O2	2.22	0.44
1:B:153:PHE:CE2	1:B:154:GLN:HG3	2.53	0.43
1:B:602:PHE:HA	1:B:610:THR:O	2.18	0.43
1:B:122[A]:ARG:HD3	1:B:125:PRO:HA	2.00	0.43
1:A:319[A]:ARG:NH1	1:A:319[A]:ARG:HG2	2.32	0.43
1:B:103:CYS:O	1:B:116:PHE:HA	2.17	0.43
1:A:103:CYS:O	1:A:116:PHE:HA	2.19	0.43
1:A:427:SER:OG	1:A:501:ASP:OD2	2.29	0.43
1:B:272:ALA:HA	1:B:273:PRO:HD3	1.94	0.42
1:A:238:LEU:C	1:A:238:LEU:HD23	2.44	0.42
1:A:178[B]:MET:HB2	1:A:178[B]:MET:HE2	1.77	0.42
1:B:268:PRO:HG3	1:B:275:TYR:CD2	2.55	0.42
1:B:177:HIS:CD2	1:B:207:SER:HA	2.54	0.42
1:A:196[A]:ARG:HD3	1:A:198:TRP:CZ2	2.55	0.41
1:A:201:LEU:CD1	1:A:215:LEU:HD12	2.50	0.41
1:B:59:PRO:O	1:B:61:PRO:HD3	2.20	0.41
1:B:669:LEU:HD13	1:B:677:VAL:HG13	2.02	0.41
1:A:303:ASP:OD2	1:A:303:ASP:N	2.52	0.41
1:A:386:GLN:HG3	1:A:630:GLN:NE2	2.27	0.41
1:B:337:GLN:O	1:B:340:GLY:N	2.52	0.41
1:A:256:LEU:HD21	1:A:595:VAL:HG21	2.02	0.41
1:A:653:PRO:HD2	1:B:576:ALA:O	2.19	0.41
1:A:157:ARG:O	1:A:179:LEU:HA	2.21	0.41
1:A:546:MET:HE2	1:A:616:LEU:HD11	2.02	0.41
1:B:319:ARG:HH21	1:B:387[A]:ASP:CG	2.29	0.41
1:B:35:VAL:HG11	1:B:89:PHE:CG	2.56	0.41
1:B:58:LEU:CD2	1:B:176:VAL:HG11	2.37	0.40
1:A:75:GLN:NE2	7:A:827:HOH:O	2.53	0.40
1:A:312:MET:HB3	1:A:627:ILE:HD12	2.04	0.40
1:A:51:GLY:HA2	1:A:357:VAL:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:864:HOH:O	7:B:955:HOH:O[1_545]	1.64	0.56

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	698/693 (101%)	682 (98%)	16 (2%)	0	100	100
1	B	688/693 (99%)	668 (97%)	19 (3%)	1 (0%)	48	28
All	All	1386/1386 (100%)	1350 (97%)	35 (2%)	1 (0%)	48	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	294	TYR

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	571/561 (102%)	558 (98%)	13 (2%)	44	20
1	B	566/561 (101%)	555 (98%)	11 (2%)	50	26
All	All	1137/1122 (101%)	1113 (98%)	24 (2%)	47	22

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	8	PRO
1	A	174[A]	GLN
1	A	174[B]	GLN
1	A	194	GLU
1	A	263	LEU
1	A	271	LYS
1	A	290	ARG
1	A	304	LEU
1	A	495	GLU
1	A	532	GLN
1	A	627	ILE
1	A	640	GLU
1	B	132	LEU
1	B	154	GLN
1	B	174	GLN
1	B	194	GLU
1	B	229	THR
1	B	246	VAL
1	B	352	ASP
1	B	388	LEU
1	B	466	GLN
1	B	524	ILE
1	B	670	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	75	GLN
1	A	149	GLN
1	A	154	GLN
1	A	222	GLN
1	A	233	GLN
1	A	237	GLN
1	A	383	HIS
1	A	386	GLN
1	A	466	GLN
1	A	485	HIS
1	A	532	GLN
1	A	630	GLN
1	B	41	HIS
1	B	102	GLN

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Mol	Chain	Res	Type
1	B	278	HIS
1	B	485	HIS
1	B	657	HIS
1	B	675	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\# Z > 2$
5	GOL	A	705	-	5,5,5	0.14	0	5,5,5	0.47	0
5	GOL	B	704	-	5,5,5	0.14	0	5,5,5	0.45	0
3	GLC	A	703	4	12,12,12	0.58	0	17,17,17	0.82	0
4	BGC	B	703	-	12,12,12	0.35	0	17,17,17	0.63	1 (5%)
5	GOL	A	706	-	5,5,5	0.12	0	5,5,5	0.32	0
4	BGC	A	708	3	12,12,12	0.58	0	17,17,17	1.15	2 (11%)
6	PEG	A	707	-	6,6,6	0.29	0	5,5,5	0.18	0
4	BGC	A	704	-	12,12,12	0.89	0	17,17,17	1.60	3 (17%)
5	GOL	A	709	-	5,5,5	0.17	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	B	702	-	12,12,12	0.70	0	17,17,17	1.27	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
5	GOL	A	705	-	-	4/4/4/4	-
5	GOL	B	704	-	-	2/4/4/4	-
3	GLC	A	703	4	-	0/2/22/22	0/1/1/1
4	BGC	B	703	-	-	0/2/22/22	0/1/1/1
5	GOL	A	706	-	-	4/4/4/4	-
4	BGC	A	708	3	-	0/2/22/22	0/1/1/1
6	PEG	A	707	-	-	1/4/4/4	-
4	BGC	A	704	-	-	0/2/22/22	0/1/1/1
5	GOL	A	709	-	-	1/4/4/4	-
3	GLC	B	702	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	704	BGC	C1-O5-C5	-3.14	107.58	113.65
4	A	708	BGC	C1-O5-C5	2.99	119.43	113.65
4	A	704	BGC	O5-C1-C2	-2.76	105.45	110.30
3	B	702	GLC	O1-C1-C2	2.68	116.76	108.98
3	B	702	GLC	O1-C1-O5	-2.59	102.72	110.41
4	A	704	BGC	O1-C1-C2	2.40	115.95	108.98
4	A	708	BGC	O5-C1-C2	2.40	114.52	110.30
3	B	702	GLC	O5-C5-C6	-2.06	101.33	106.44
4	B	703	BGC	C1-C2-C3	2.03	114.50	110.36

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	705	GOL	O1-C1-C2-C3
5	A	705	GOL	C1-C2-C3-O3
5	A	706	GOL	O1-C1-C2-C3

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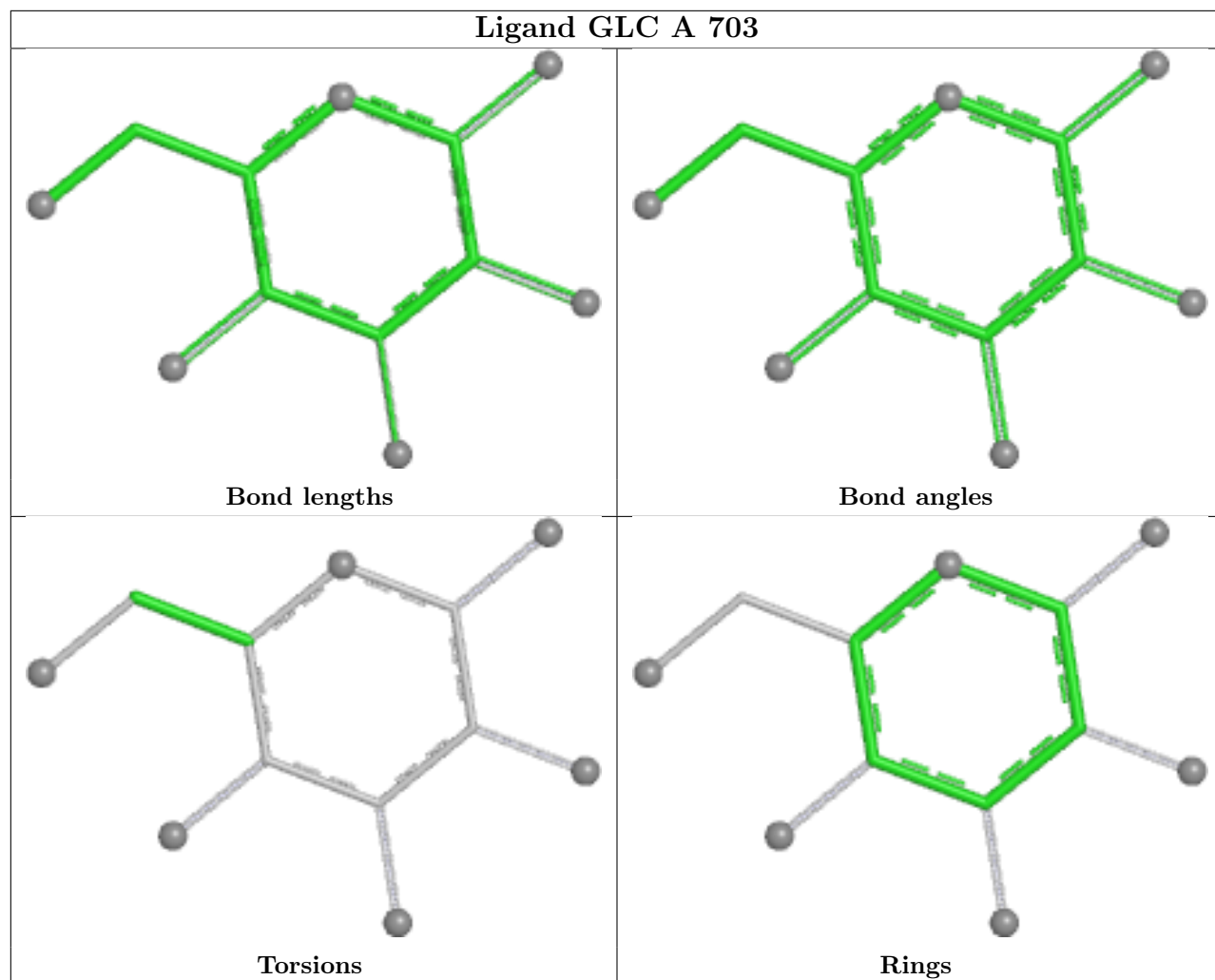
Mol	Chain	Res	Type	Atoms
5	A	706	GOL	C1-C2-C3-O3
5	B	704	GOL	C1-C2-C3-O3
5	A	706	GOL	O1-C1-C2-O2
5	A	706	GOL	O2-C2-C3-O3
5	B	704	GOL	O2-C2-C3-O3
5	A	705	GOL	O1-C1-C2-O2
5	A	709	GOL	O2-C2-C3-O3
6	A	707	PEG	C1-C2-O2-C3
5	A	705	GOL	O2-C2-C3-O3

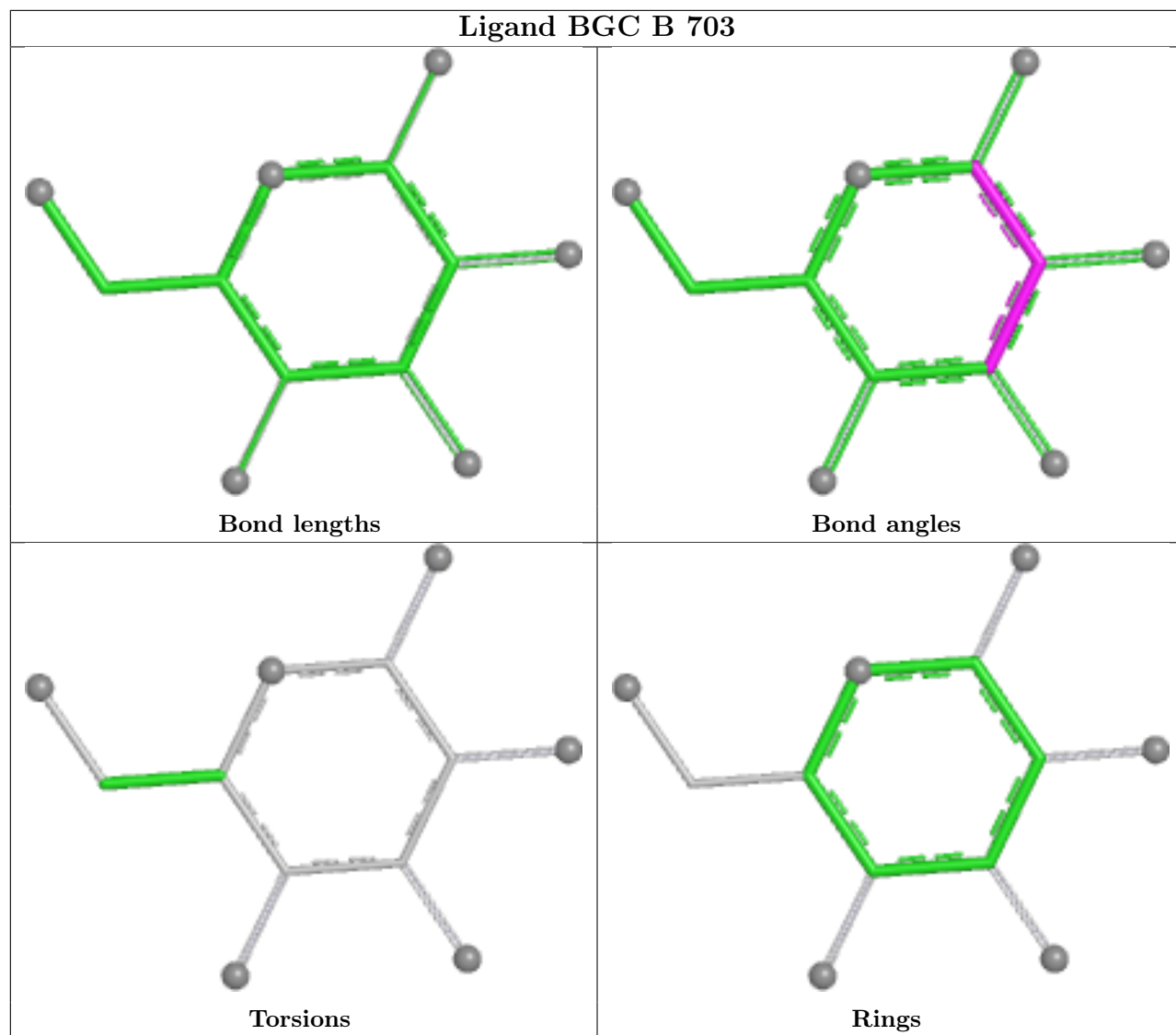
There are no ring outliers.

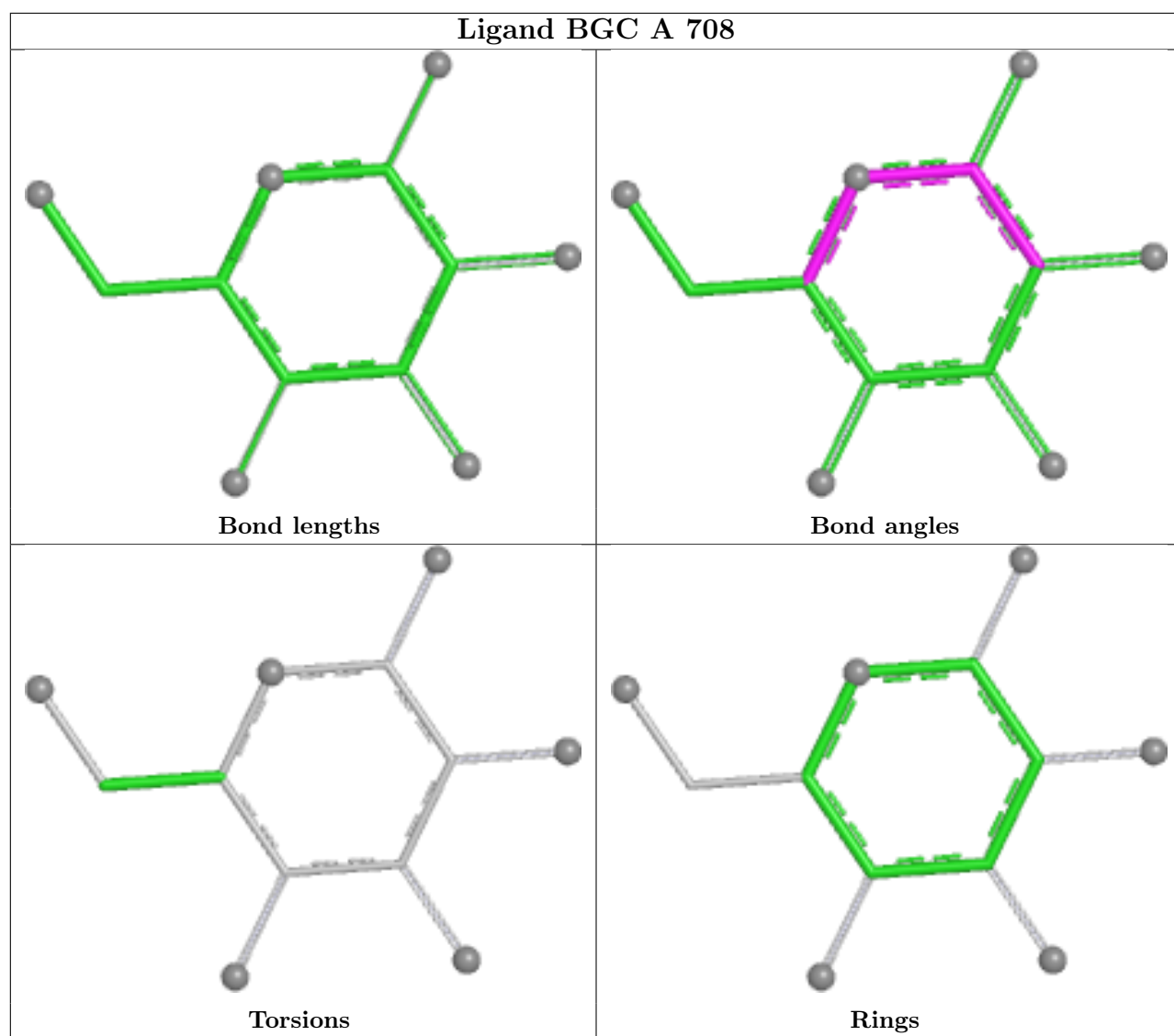
7 monomers are involved in 9 short contacts:

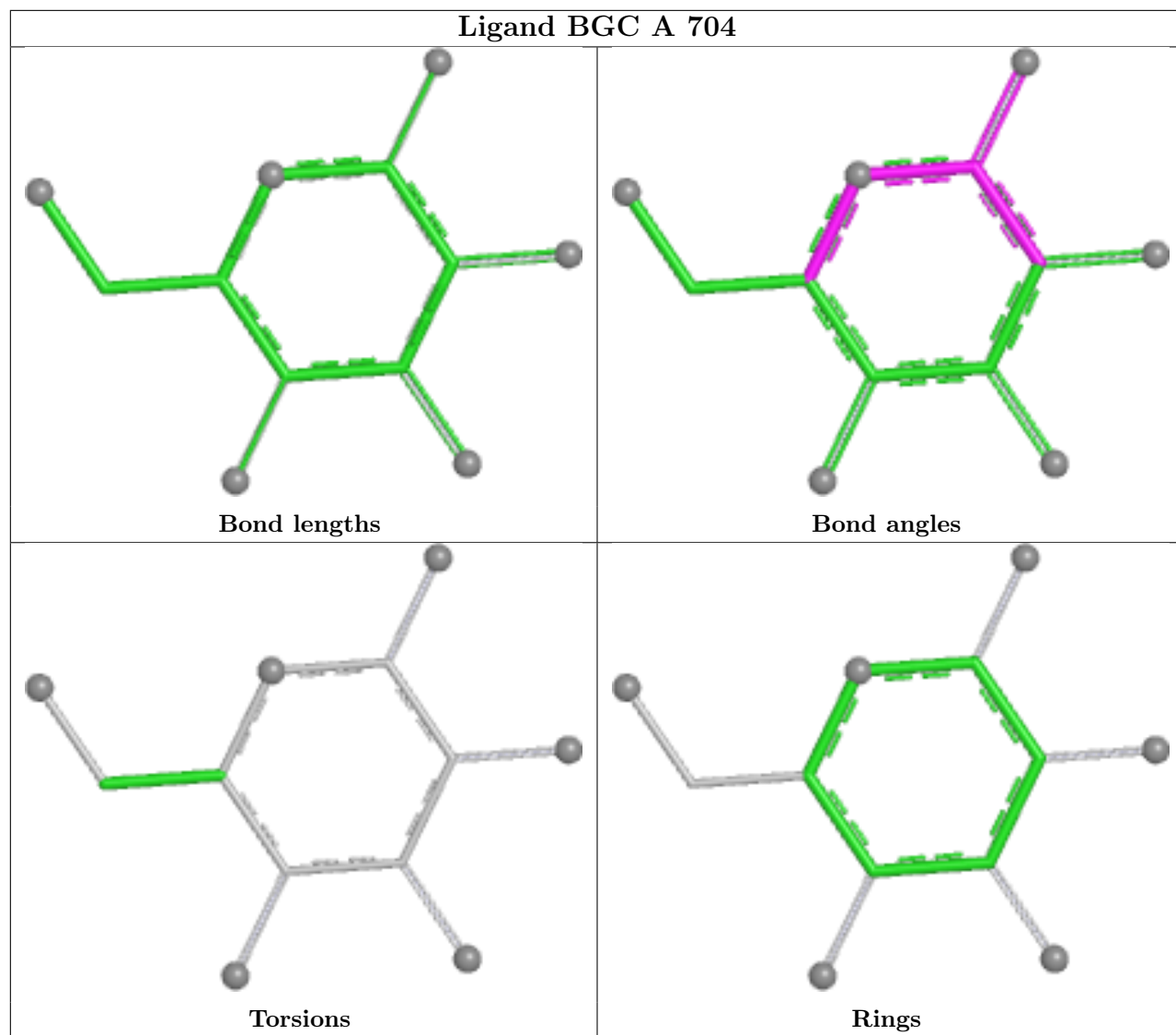
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	705	GOL	2	0
5	B	704	GOL	1	0
3	A	703	GLC	1	0
4	B	703	BGC	2	0
4	A	704	BGC	3	0
5	A	709	GOL	1	0
3	B	702	GLC	1	0

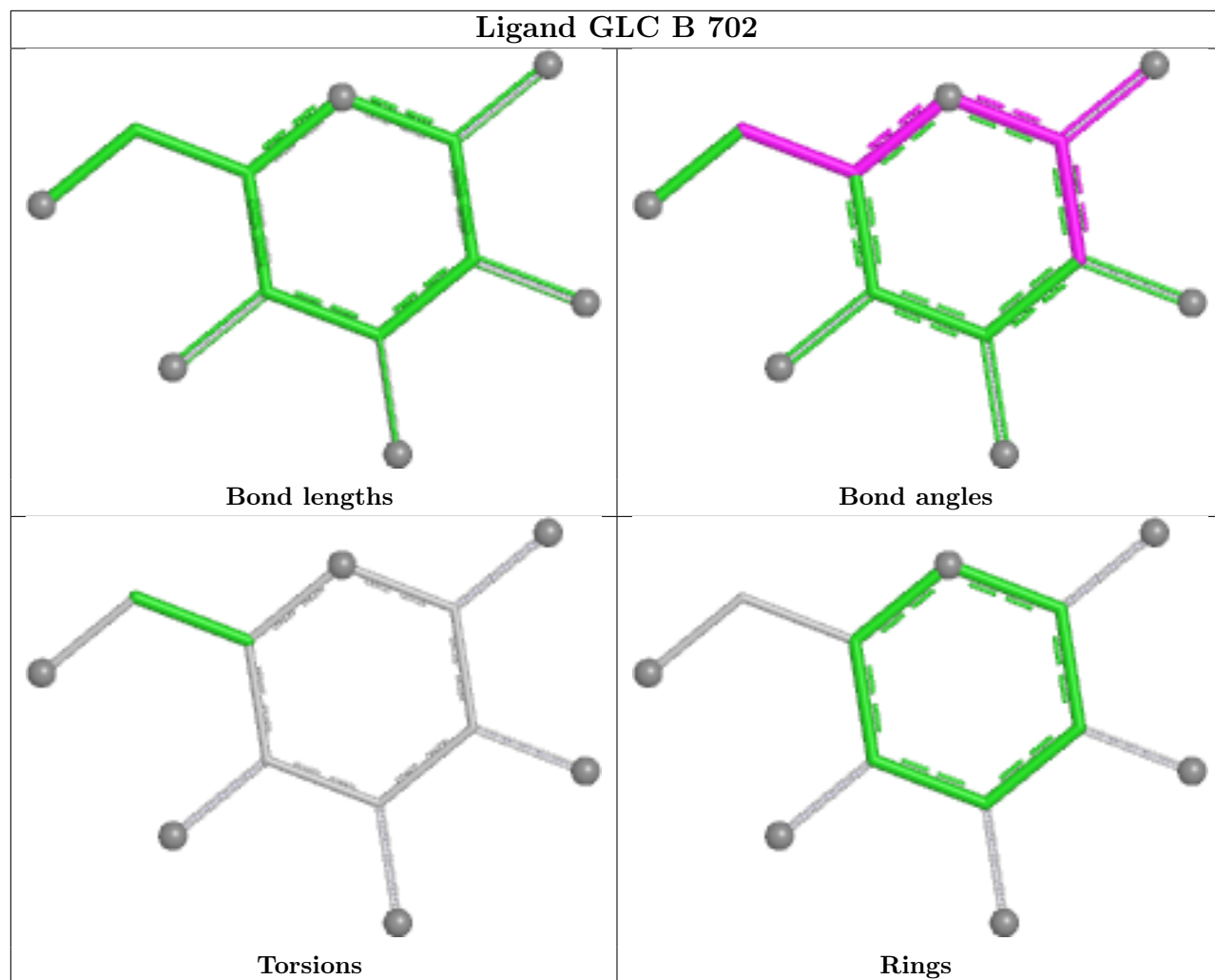
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	685/693 (98%)	0.27	30 (4%)	39 42	12, 31, 58, 98	15 (2%)
1	B	679/693 (97%)	0.48	31 (4%)	37 40	12, 36, 64, 103	13 (1%)
All	All	1364/1386 (98%)	0.38	61 (4%)	38 41	12, 33, 62, 103	28 (2%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	672	LEU	6.0
1	A	651	ALA	5.1
1	B	124	ALA	5.1
1	B	493	PRO	4.8
1	A	70	ALA	4.6
1	A	654	TRP	4.5
1	A	652	GLY	3.9
1	B	125	PRO	3.8
1	B	691	PRO	3.8
1	B	76	LEU	3.7
1	A	653	PRO	3.6
1	A	124	ALA	3.5
1	A	691	PRO	3.4
1	A	71	GLY	3.3
1	B	127	SER	3.2
1	A	172	PRO	3.1
1	A	677	VAL	3.0
1	B	170	GLY	3.0
1	B	69	PRO	2.9
1	A	650	ARG	2.9
1	B	129	PRO	2.9
1	B	192	GLY	2.7
1	B	93	LEU	2.7
1	B	159	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	126	GLY	2.7
1	B	96	PRO	2.6
1	A	125	PRO	2.6
1	A	72	MET	2.6
1	A	126	GLY	2.6
1	A	192	GLY	2.6
1	B	123	LEU	2.6
1	B	389	GLN	2.5
1	A	675	HIS	2.5
1	B	336	ALA	2.5
1	A	69	PRO	2.4
1	A	667	SER	2.4
1	B	338	ASN	2.4
1	A	174[A]	GLN	2.4
1	A	121	ALA	2.4
1	B	229	THR	2.3
1	B	463	ILE	2.3
1	A	649	ALA	2.3
1	B	419	LYS	2.3
1	A	154	GLN	2.2
1	A	669	LEU	2.2
1	B	468	LEU	2.2
1	A	463	ILE	2.2
1	A	129	PRO	2.2
1	B	272	ALA	2.2
1	B	388	LEU	2.2
1	A	416	ARG	2.1
1	B	480	VAL	2.1
1	B	293[A]	CYS	2.1
1	B	58	LEU	2.1
1	B	190	GLY	2.1
1	B	386	GLN	2.1
1	A	634	LEU	2.1
1	B	341	TYR	2.1
1	B	215	LEU	2.0
1	A	493	PRO	2.0
1	A	673	PRO	2.0

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

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](#)

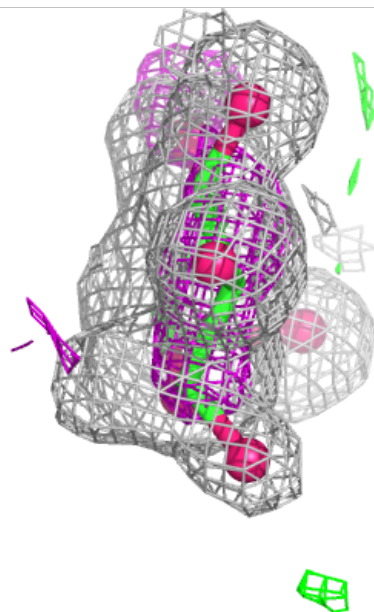
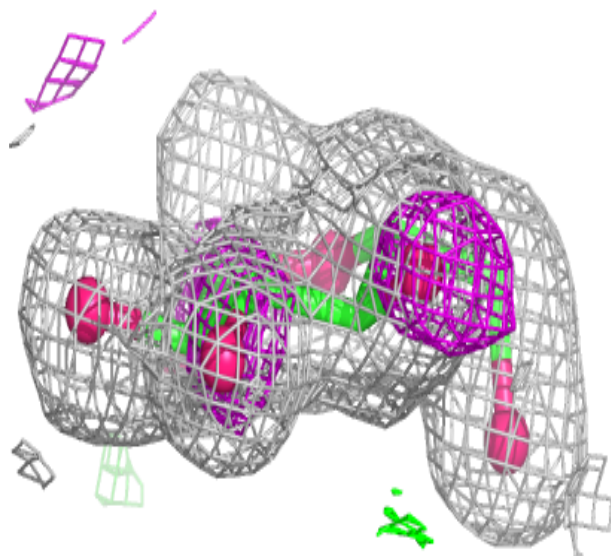
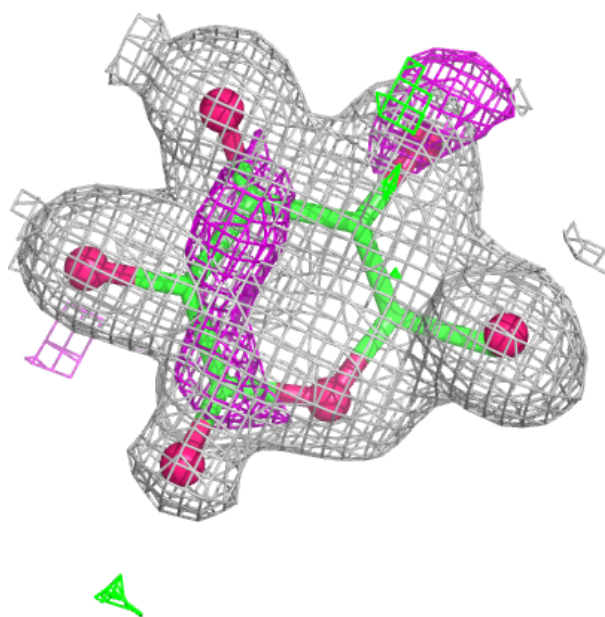
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	B	704	6/6	0.78	0.12	59,60,62,69	0
4	BGC	A	708	12/12	0.82	0.12	28,32,34,34	12
4	BGC	A	704	12/12	0.82	0.13	27,44,56,58	0
5	GOL	A	709	6/6	0.83	0.16	38,52,55,57	0
5	GOL	A	706	6/6	0.85	0.14	37,49,60,68	0
5	GOL	A	705	6/6	0.86	0.14	51,57,59,64	0
4	BGC	B	703	12/12	0.87	0.11	29,51,59,62	0
2	CL	A	702	1/1	0.89	0.34	62,62,62,62	0
3	GLC	B	702	12/12	0.90	0.10	26,34,40,45	0
6	PEG	A	707	7/7	0.90	0.13	23,44,58,61	0
3	GLC	A	703	12/12	0.92	0.08	17,21,26,27	12
2	CL	B	701	1/1	0.98	0.05	29,29,29,29	0
2	CL	A	701	1/1	0.99	0.03	22,22,22,22	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.

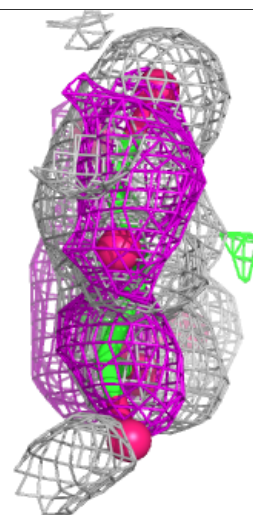
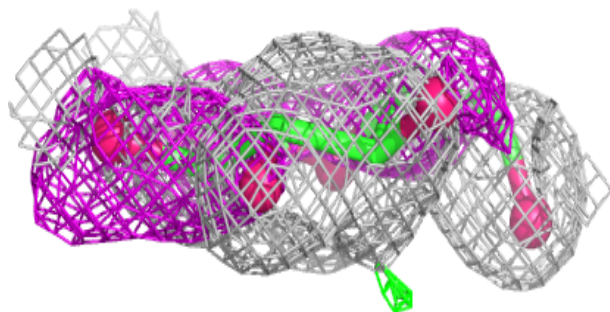
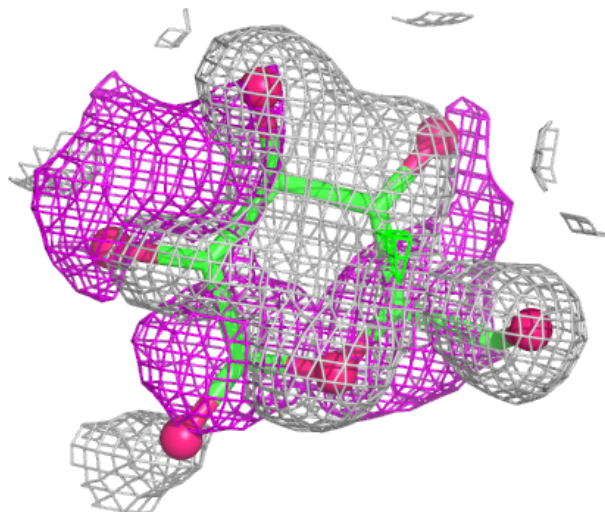
Electron density around BGC A 708:

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



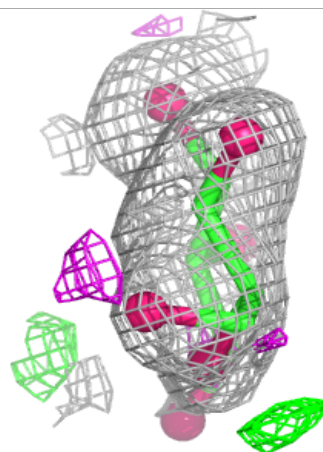
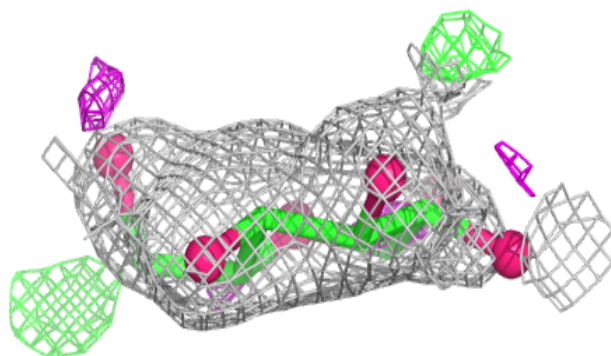
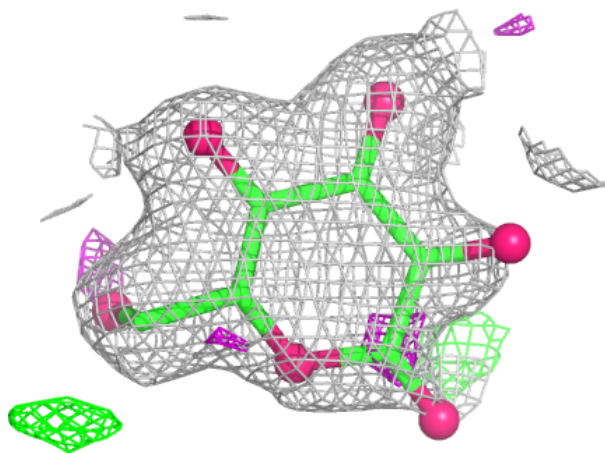
Electron density around BGC A 704:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



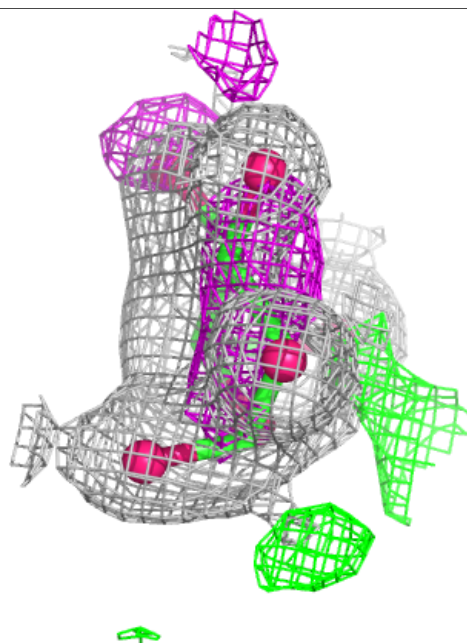
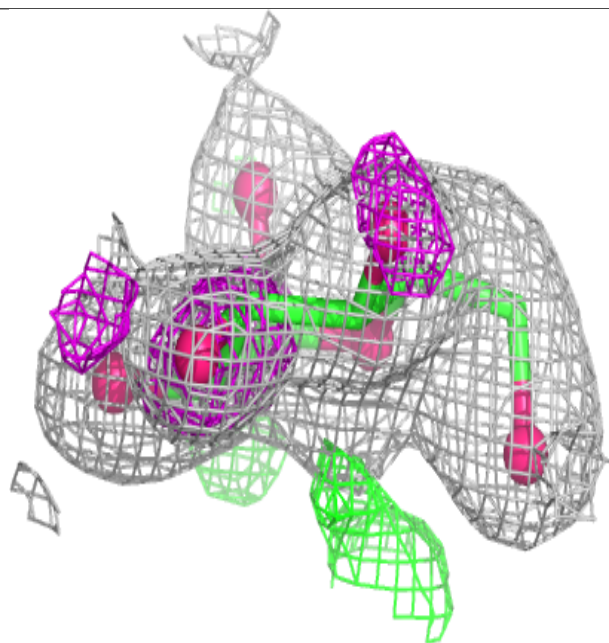
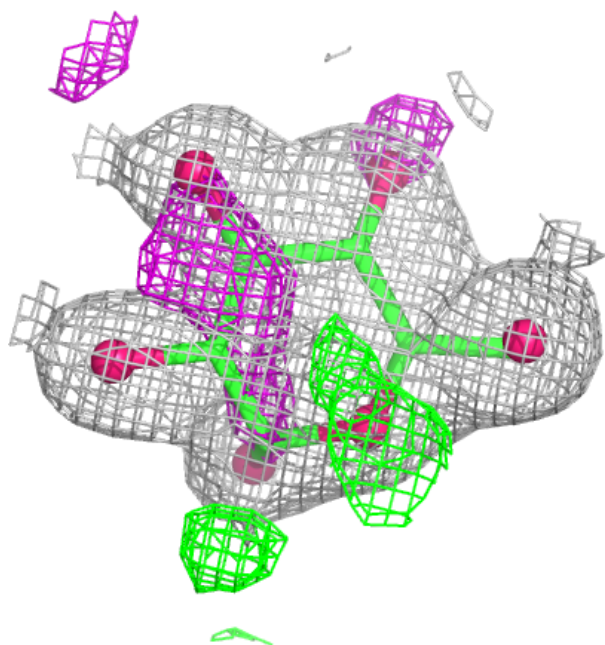
Electron density around BGC B 703:

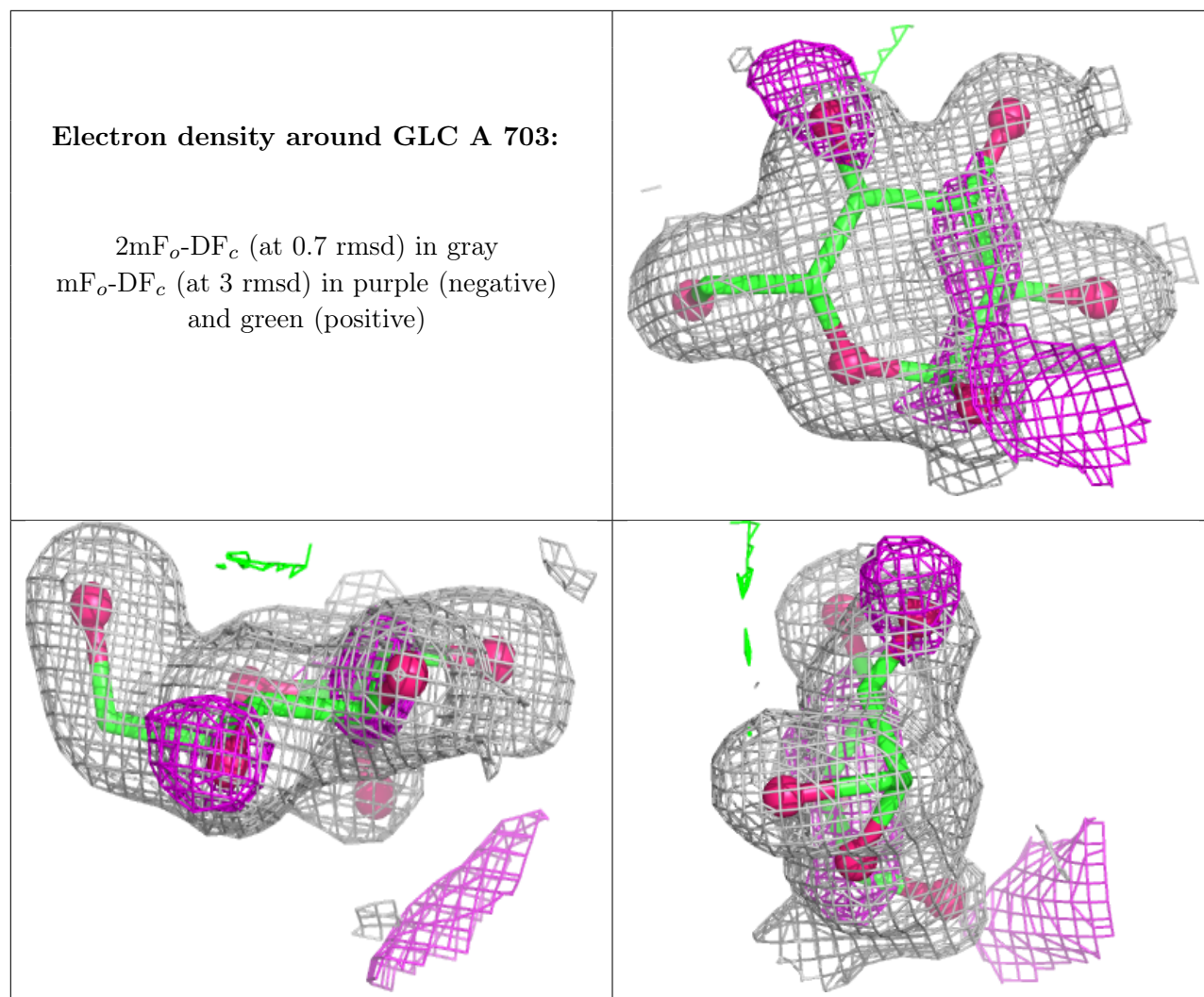
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GLC B 702:

$2mF_o-DF_c$ (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.