



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:54 AM UTC

PDB ID : 7FE4 / pdb_00007fe4
Title : Crystal structure of GH65 alpha-1,2-glucosidase from *Flavobacterium johnsoniae* in complex with glucose
Authors : Nakamura, S.; Miyazaki, T.
Deposited on : 2021-07-19
Resolution : 1.40 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

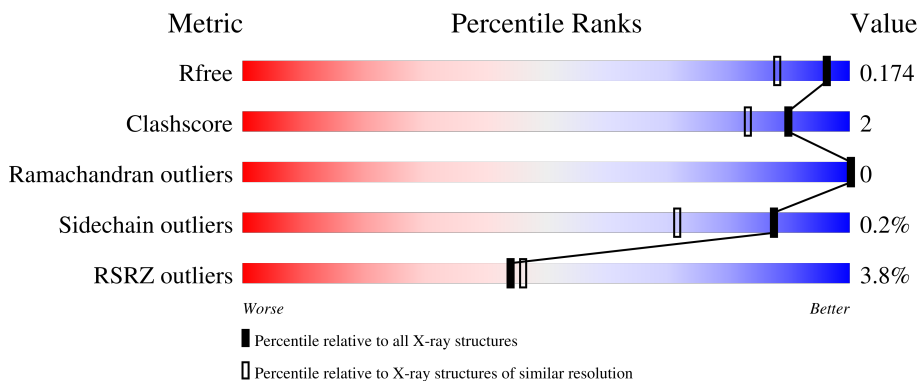
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	678	 4% 92% 5% •
1	B	678	 4% 91% 6% •
1	C	678	 3% 92% 5% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17674 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 Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	659	5300	3375	891	1013	21	0	8	0
1	B	659	5280	3363	888	1008	21	0	5	0
1	C	659	5282	3366	888	1007	21	0	5	0

There are 60 discrepancies between the modelled and reference sequences:

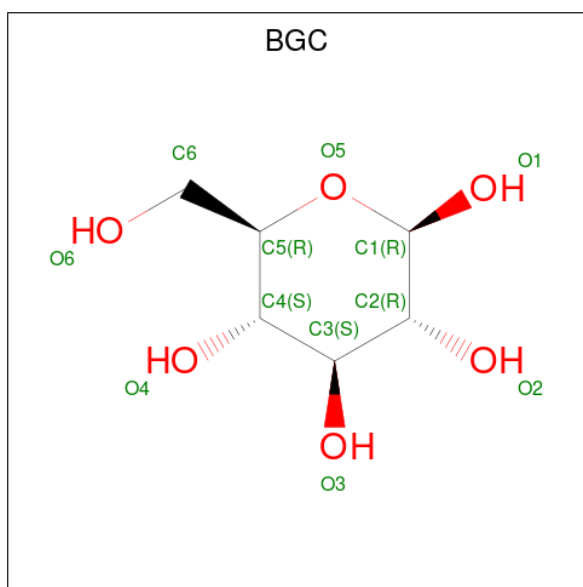
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP A5FBJ5
A	5	GLY	-	expression tag	UNP A5FBJ5
A	6	SER	-	expression tag	UNP A5FBJ5
A	7	SER	-	expression tag	UNP A5FBJ5
A	8	HIS	-	expression tag	UNP A5FBJ5
A	9	HIS	-	expression tag	UNP A5FBJ5
A	10	HIS	-	expression tag	UNP A5FBJ5
A	11	HIS	-	expression tag	UNP A5FBJ5
A	12	HIS	-	expression tag	UNP A5FBJ5
A	13	HIS	-	expression tag	UNP A5FBJ5
A	14	SER	-	expression tag	UNP A5FBJ5
A	15	SER	-	expression tag	UNP A5FBJ5
A	16	GLY	-	expression tag	UNP A5FBJ5
A	17	LEU	-	expression tag	UNP A5FBJ5
A	18	VAL	-	expression tag	UNP A5FBJ5
A	19	PRO	-	expression tag	UNP A5FBJ5
A	20	ARG	-	expression tag	UNP A5FBJ5
A	21	GLY	-	expression tag	UNP A5FBJ5
A	22	SER	-	expression tag	UNP A5FBJ5
A	23	HIS	-	expression tag	UNP A5FBJ5
B	4	MET	-	initiating methionine	UNP A5FBJ5
B	5	GLY	-	expression tag	UNP A5FBJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	SER	-	expression tag	UNP A5FBJ5
B	7	SER	-	expression tag	UNP A5FBJ5
B	8	HIS	-	expression tag	UNP A5FBJ5
B	9	HIS	-	expression tag	UNP A5FBJ5
B	10	HIS	-	expression tag	UNP A5FBJ5
B	11	HIS	-	expression tag	UNP A5FBJ5
B	12	HIS	-	expression tag	UNP A5FBJ5
B	13	HIS	-	expression tag	UNP A5FBJ5
B	14	SER	-	expression tag	UNP A5FBJ5
B	15	SER	-	expression tag	UNP A5FBJ5
B	16	GLY	-	expression tag	UNP A5FBJ5
B	17	LEU	-	expression tag	UNP A5FBJ5
B	18	VAL	-	expression tag	UNP A5FBJ5
B	19	PRO	-	expression tag	UNP A5FBJ5
B	20	ARG	-	expression tag	UNP A5FBJ5
B	21	GLY	-	expression tag	UNP A5FBJ5
B	22	SER	-	expression tag	UNP A5FBJ5
B	23	HIS	-	expression tag	UNP A5FBJ5
C	4	MET	-	initiating methionine	UNP A5FBJ5
C	5	GLY	-	expression tag	UNP A5FBJ5
C	6	SER	-	expression tag	UNP A5FBJ5
C	7	SER	-	expression tag	UNP A5FBJ5
C	8	HIS	-	expression tag	UNP A5FBJ5
C	9	HIS	-	expression tag	UNP A5FBJ5
C	10	HIS	-	expression tag	UNP A5FBJ5
C	11	HIS	-	expression tag	UNP A5FBJ5
C	12	HIS	-	expression tag	UNP A5FBJ5
C	13	HIS	-	expression tag	UNP A5FBJ5
C	14	SER	-	expression tag	UNP A5FBJ5
C	15	SER	-	expression tag	UNP A5FBJ5
C	16	GLY	-	expression tag	UNP A5FBJ5
C	17	LEU	-	expression tag	UNP A5FBJ5
C	18	VAL	-	expression tag	UNP A5FBJ5
C	19	PRO	-	expression tag	UNP A5FBJ5
C	20	ARG	-	expression tag	UNP A5FBJ5
C	21	GLY	-	expression tag	UNP A5FBJ5
C	22	SER	-	expression tag	UNP A5FBJ5
C	23	HIS	-	expression tag	UNP A5FBJ5

- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



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

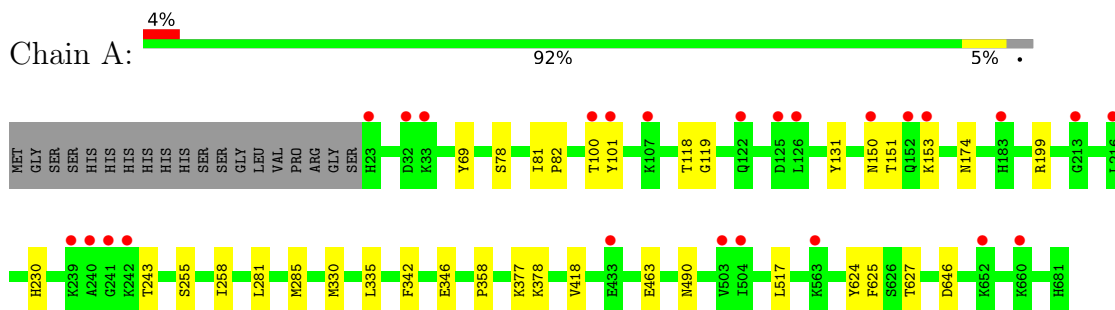
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	561	Total 561	O 561	0	0
3	B	537	Total 537	O 537	0	0
3	C	570	Total 570	O 570	0	0

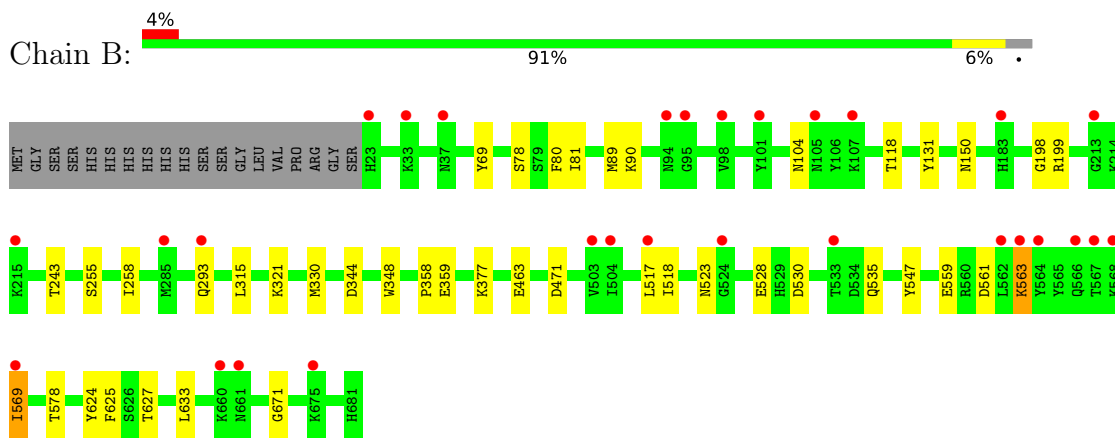
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

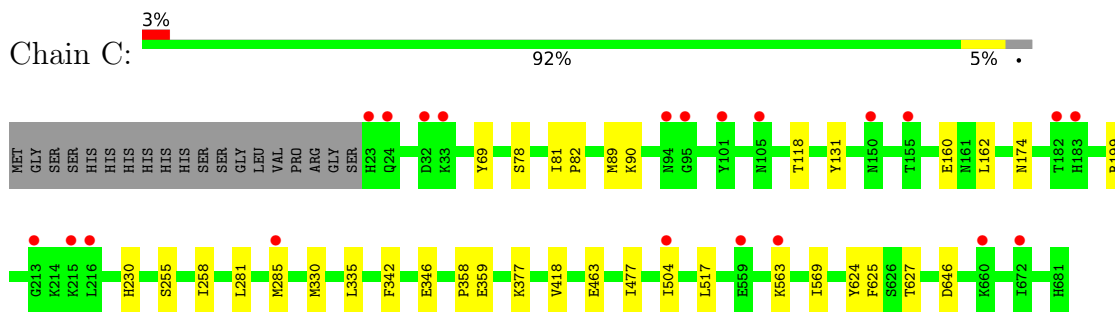
- Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65



- Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65



- Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.50Å 194.20Å 112.01Å 90.00° 116.60° 90.00°	Depositor
Resolution (Å)	44.70 – 1.40 44.70 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.0 (44.70-1.40) 98.0 (44.70-1.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.157 , 0.170 0.160 , 0.174	Depositor DCC
R_{free} test set	22421 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtrriage
Anisotropy	0.161	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17674	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: BGC

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	0.91	0/5429	1.08	4/7367 (0.1%)
1	B	0.98	7/5409 (0.1%)	1.09	6/7340 (0.1%)
1	C	0.94	1/5411 (0.0%)	1.08	4/7343 (0.1%)
All	All	0.94	8/16249 (0.0%)	1.09	14/22050 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	523	ASN	C-O	10.21	1.37	1.24
1	B	561	ASP	C-O	6.99	1.32	1.24
1	B	523	ASN	C-N	6.32	1.42	1.33
1	B	563	LYS	C-O	6.05	1.31	1.24
1	B	530	ASP	CB-CG	5.41	1.65	1.52
1	B	535	GLN	C-O	5.14	1.30	1.23
1	C	569	ILE	N-CA	5.09	1.50	1.46
1	B	569	ILE	N-CA	5.00	1.50	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	563	LYS	O-C-N	6.08	128.34	122.07
1	A	81	ILE	N-CA-CB	-5.87	106.15	112.37
1	B	359	GLU	CB-CG-CD	5.83	122.52	112.60
1	A	490	ASN	CA-CB-CG	5.80	118.40	112.60
1	C	342	PHE	CA-CB-CG	5.67	119.47	113.80
1	A	646	ASP	CA-CB-CG	5.61	118.21	112.60
1	C	81	ILE	N-CA-CB	-5.56	106.48	112.37
1	C	646	ASP	CA-CB-CG	5.41	118.01	112.60
1	C	359	GLU	CB-CG-CD	5.36	121.72	112.60
1	B	81	ILE	N-CA-CB	-5.11	106.96	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	PHE	CA-CB-CG	5.08	118.88	113.80
1	B	80	PHE	CA-CB-CG	5.05	118.85	113.80
1	B	198	GLY	CA-C-N	5.03	127.01	120.28
1	B	198	GLY	C-N-CA	5.03	127.01	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5300	0	5180	18	0
1	B	5280	0	5162	22	0
1	C	5282	0	5168	18	0
2	A	48	0	48	0	0
2	B	48	0	48	0	0
2	C	48	0	48	0	0
3	A	561	0	0	3	0
3	B	537	0	0	9	0
3	C	570	0	0	4	0
All	All	17674	0	15654	58	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 (58) 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:293:GLN:HG3	3:B:1147:HOH:O	1.84	0.76
1:A:358:PRO:HG3	3:A:1077:HOH:O	1.88	0.72
1:A:377:LYS:HD3	3:B:1010:HOH:O	1.91	0.70
1:B:559:GLU:O	1:B:563:LYS:HG2	1.96	0.64
1:B:377:LYS:HD3	3:C:1240:HOH:O	1.96	0.64
1:A:463:GLU:HG2	1:A:517:LEU:HD12	1.80	0.63
1:B:463:GLU:HG2	1:B:517:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PRO:HG3	3:B:923:HOH:O	2.01	0.59
3:A:934:HOH:O	1:C:377:LYS:HD3	2.06	0.55
1:C:199:ARG:HG2	3:C:1158:HOH:O	2.10	0.50
1:C:463:GLU:HG2	1:C:517:LEU:HD12	1.93	0.50
1:B:90:LYS:HE3	3:B:921:HOH:O	2.12	0.49
1:B:671:GLY:HA2	3:B:923:HOH:O	2.11	0.49
1:C:504:ILE:HG22	3:C:1574:HOH:O	2.12	0.49
1:A:150:ASN:OD1	1:A:243:THR:OG1	2.29	0.48
1:C:358:PRO:HG3	3:C:1200:HOH:O	2.14	0.48
1:A:151:THR:OG1	1:A:153:LYS:O	2.30	0.47
1:B:150:ASN:OD1	1:B:243:THR:OG1	2.21	0.47
1:C:82:PRO:HG3	1:C:335[B]:LEU:HD11	1.96	0.47
1:C:69:TYR:HB3	1:C:78:SER:HB2	1.98	0.46
1:A:82:PRO:HG3	1:A:335[B]:LEU:HD11	1.98	0.46
1:A:625:PHE:CZ	1:A:627:THR:HB	2.51	0.46
1:B:625:PHE:CZ	1:B:627:THR:HB	2.51	0.46
1:C:89:MET:HE3	1:C:89:MET:HB3	1.78	0.45
1:B:118:THR:HA	1:B:131:TYR:O	2.17	0.45
1:C:90:LYS:HE2	1:C:162:LEU:HD21	1.99	0.44
1:A:69:TYR:HB3	1:A:78:SER:HB2	2.00	0.44
1:C:477:ILE:C	1:C:477:ILE:HD12	2.43	0.44
1:B:199:ARG:HG2	3:B:834:HOH:O	2.17	0.43
1:B:255:SER:HA	1:B:258:ILE:O	2.18	0.43
1:C:174:ASN:HB3	1:C:230:HIS:CG	2.54	0.43
1:A:119:GLY:HA3	1:A:131:TYR:CZ	2.53	0.43
1:C:281:LEU:O	1:C:285:MET:HG2	2.18	0.43
1:B:69:TYR:HB3	1:B:78:SER:HB2	2.00	0.43
1:B:344:ASP:O	1:B:348:TRP:HB2	2.19	0.43
1:C:625:PHE:CZ	1:C:627:THR:HB	2.52	0.43
1:A:330:MET:HA	1:A:624:TYR:O	2.19	0.43
1:C:330:MET:HA	1:C:624:TYR:O	2.18	0.43
1:C:346:GLU:HG2	1:C:418:VAL:HA	2.01	0.43
1:C:255:SER:HA	1:C:258:ILE:O	2.19	0.43
1:A:346:GLU:HG2	1:A:418:VAL:HA	2.00	0.42
1:B:89:MET:HE3	1:B:89:MET:HB3	1.92	0.42
1:B:569:ILE:HG12	1:B:578:THR:HG21	2.01	0.42
1:A:199:ARG:HG2	3:A:834:HOH:O	2.18	0.42
1:A:255:SER:HA	1:A:258:ILE:O	2.20	0.42
1:A:378:LYS:HE3	3:B:1108:HOH:O	2.19	0.42
1:A:101:TYR:C	1:A:101:TYR:CD1	2.98	0.42
1:A:281:LEU:O	1:A:285:MET:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:MET:HA	1:B:624:TYR:O	2.20	0.41
1:B:321:LYS:HE3	3:B:1298:HOH:O	2.20	0.41
1:B:104:ASN:ND2	3:B:814:HOH:O	2.54	0.41
1:B:471:ASP:OD2	1:B:528:GLU:OE1	2.38	0.41
1:B:547:TYR:CD1	1:B:547:TYR:C	2.98	0.41
1:B:315:LEU:HD22	1:B:633:LEU:HD12	2.02	0.40
1:A:174:ASN:HB3	1:A:230:HIS:CG	2.56	0.40
1:C:118:THR:HA	1:C:131:TYR:O	2.22	0.40
1:A:118:THR:HA	1:A:131:TYR:O	2.22	0.40
1:C:89:MET:HA	1:C:160:GLU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	665/678 (98%)	646 (97%)	19 (3%)	0	100	100
1	B	662/678 (98%)	644 (97%)	18 (3%)	0	100	100
1	C	662/678 (98%)	643 (97%)	19 (3%)	0	100	100
All	All	1989/2034 (98%)	1933 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	573/581 (99%)	572 (100%)	1 (0%)	87	71
1	B	570/581 (98%)	569 (100%)	1 (0%)	87	71
1	C	570/581 (98%)	569 (100%)	1 (0%)	87	71
All	All	1713/1743 (98%)	1710 (100%)	3 (0%)	87	71

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	THR
1	B	518	ILE
1	C	563	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	85	ASN
1	A	108	GLN
1	A	152	GLN
1	A	171	ASN
1	A	178	ASN
1	A	185	ASN
1	A	206	ASN
1	A	259	ASN
1	A	282	ASN
1	A	286	GLN
1	A	539	GLN
1	A	571	GLN
1	A	608	ASN
1	B	24	GLN
1	B	85	ASN
1	B	108	GLN
1	B	171	ASN
1	B	178	ASN
1	B	185	ASN
1	B	286	GLN
1	B	539	GLN
1	B	566	GLN
1	B	571	GLN
1	B	608	ASN
1	C	23	HIS

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Mol	Chain	Res	Type
1	C	24	GLN
1	C	85	ASN
1	C	105	ASN
1	C	108	GLN
1	C	171	ASN
1	C	178	ASN
1	C	185	ASN
1	C	206	ASN
1	C	282	ASN
1	C	286	GLN
1	C	476	ASN
1	C	571	GLN
1	C	608	ASN
1	C	681	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](#)

12 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	BGC	A	701	-	12,12,12	0.63	0	17,17,17	0.86	1 (5%)
2	BGC	A	702	-	12,12,12	0.69	0	17,17,17	1.16	1 (5%)
2	BGC	A	704	-	12,12,12	0.51	0	17,17,17	0.76	0
2	BGC	A	703	-	12,12,12	0.43	0	17,17,17	0.86	1 (5%)
2	BGC	C	1002	-	12,12,12	0.79	0	17,17,17	1.20	2 (11%)
2	BGC	B	703	-	12,12,12	0.57	0	17,17,17	0.55	0
2	BGC	B	702	-	12,12,12	0.70	0	17,17,17	1.03	0
2	BGC	C	1004	-	12,12,12	0.59	0	17,17,17	0.74	0
2	BGC	B	704	-	12,12,12	0.58	0	17,17,17	0.72	0
2	BGC	C	1003	-	12,12,12	0.75	0	17,17,17	1.26	2 (11%)
2	BGC	C	1001	-	12,12,12	0.59	0	17,17,17	0.94	0
2	BGC	B	701	-	12,12,12	0.51	0	17,17,17	1.15	1 (5%)

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	BGC	A	701	-	-	0/2/22/22	0/1/1/1
2	BGC	A	702	-	-	0/2/22/22	0/1/1/1
2	BGC	A	704	-	-	0/2/22/22	0/1/1/1
2	BGC	A	703	-	-	0/2/22/22	0/1/1/1
2	BGC	C	1002	-	-	0/2/22/22	0/1/1/1
2	BGC	B	703	-	-	0/2/22/22	0/1/1/1
2	BGC	B	702	-	-	0/2/22/22	0/1/1/1
2	BGC	C	1004	-	-	0/2/22/22	0/1/1/1
2	BGC	B	704	-	-	0/2/22/22	0/1/1/1
2	BGC	C	1003	-	-	0/2/22/22	0/1/1/1
2	BGC	C	1001	-	-	0/2/22/22	0/1/1/1
2	BGC	B	701	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1003	BGC	C1-O5-C5	-3.47	106.94	113.65
2	B	701	BGC	O1-C1-O5	-3.07	101.30	110.41
2	C	1002	BGC	O1-C1-O5	-2.74	102.27	110.41
2	A	702	BGC	C1-O5-C5	-2.65	108.53	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1002	BGC	O5-C1-C2	2.57	114.82	110.30
2	A	701	BGC	O1-C1-O5	-2.43	103.19	110.41
2	A	703	BGC	O6-C6-C5	-2.31	103.46	111.33
2	C	1003	BGC	O1-C1-O5	-2.05	104.32	110.41

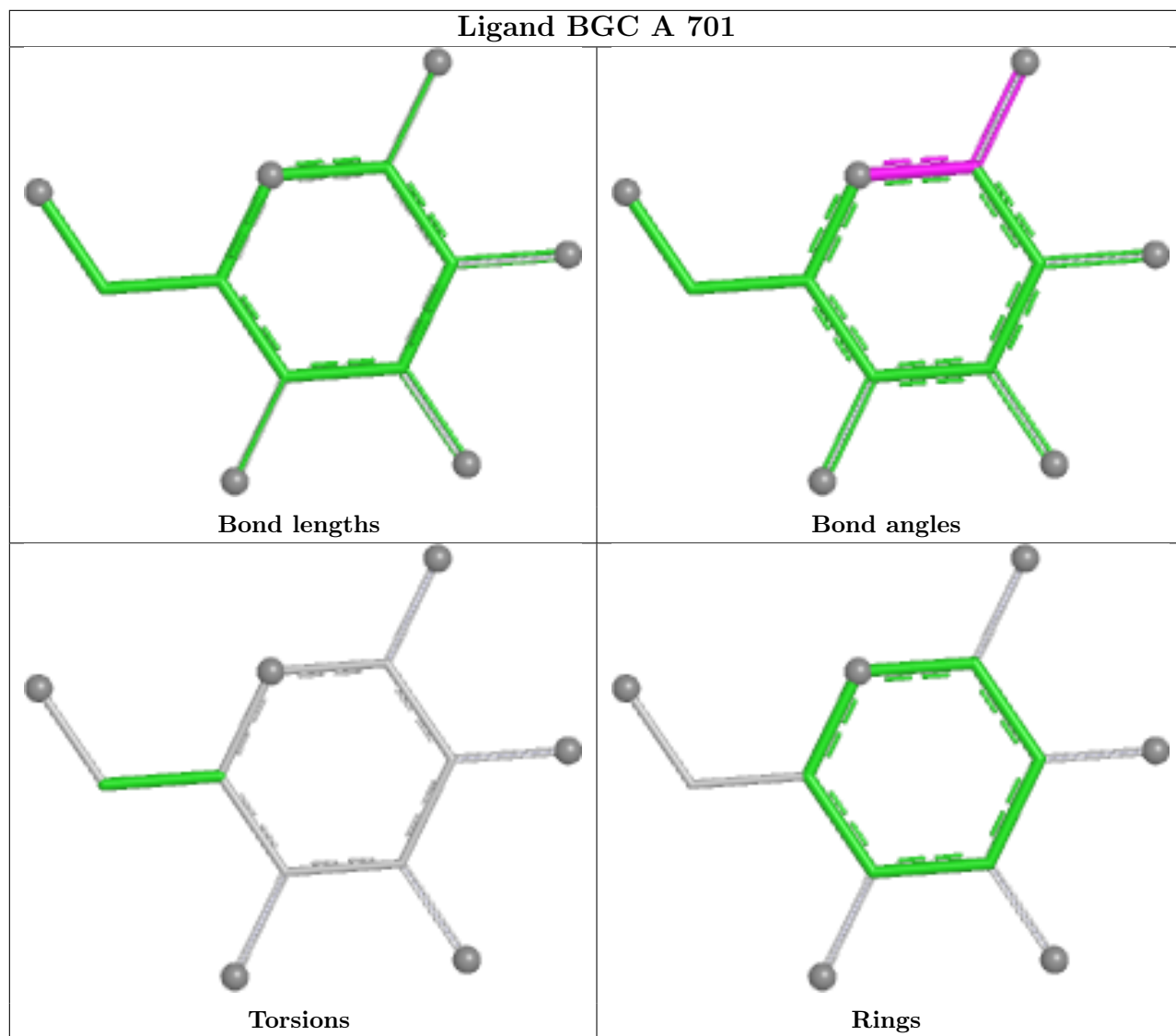
There are no chirality outliers.

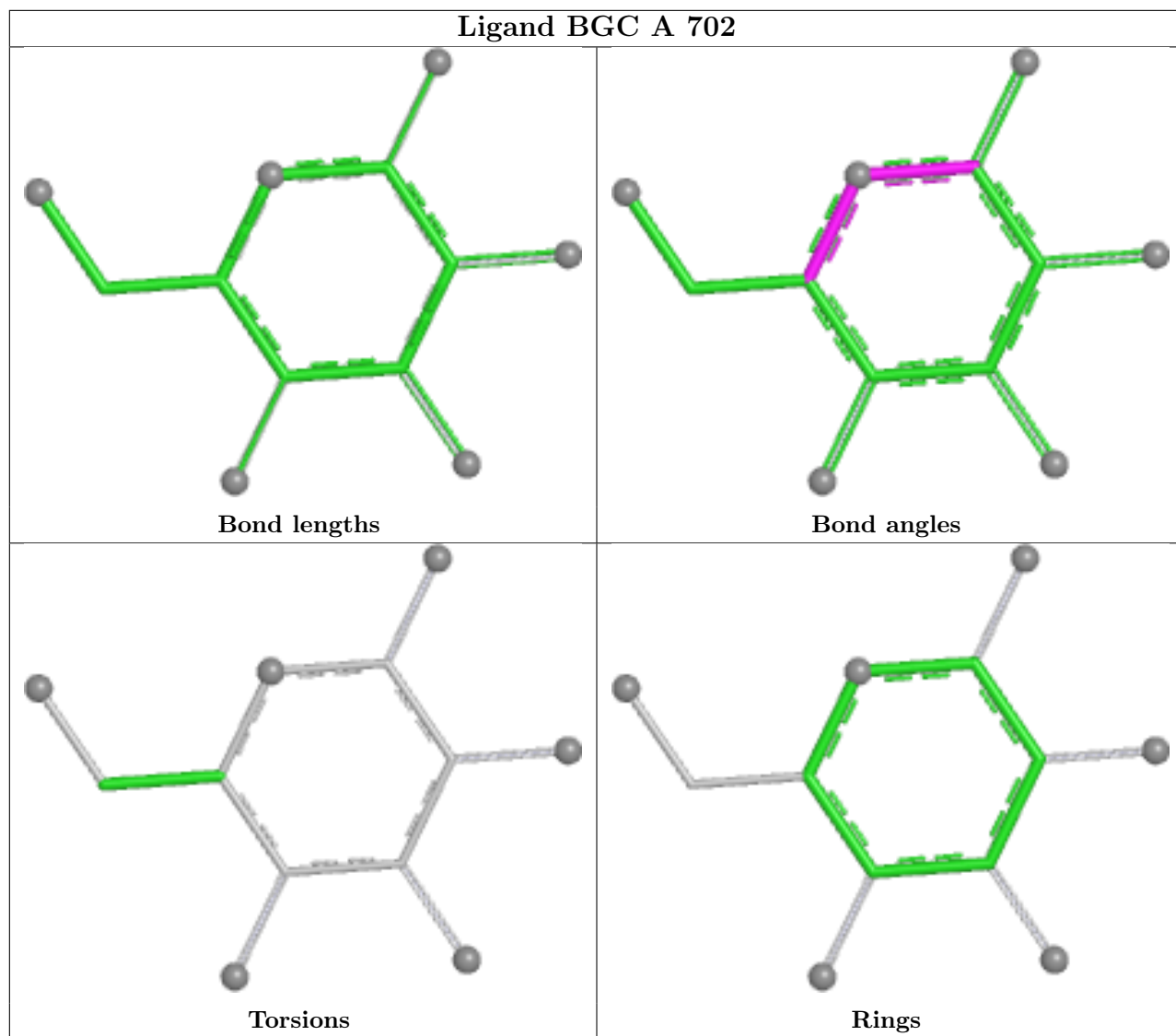
There are no torsion outliers.

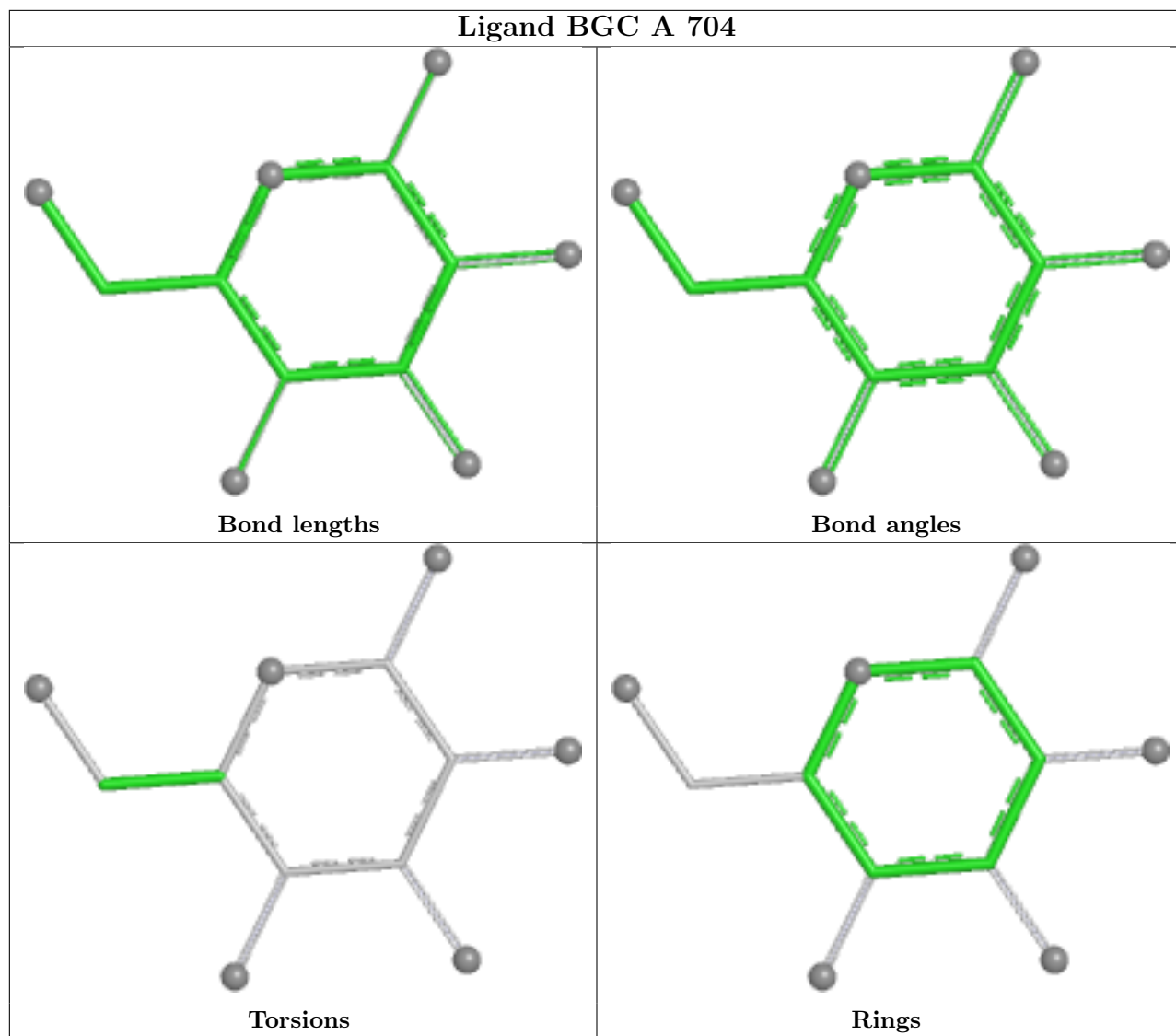
There are no ring outliers.

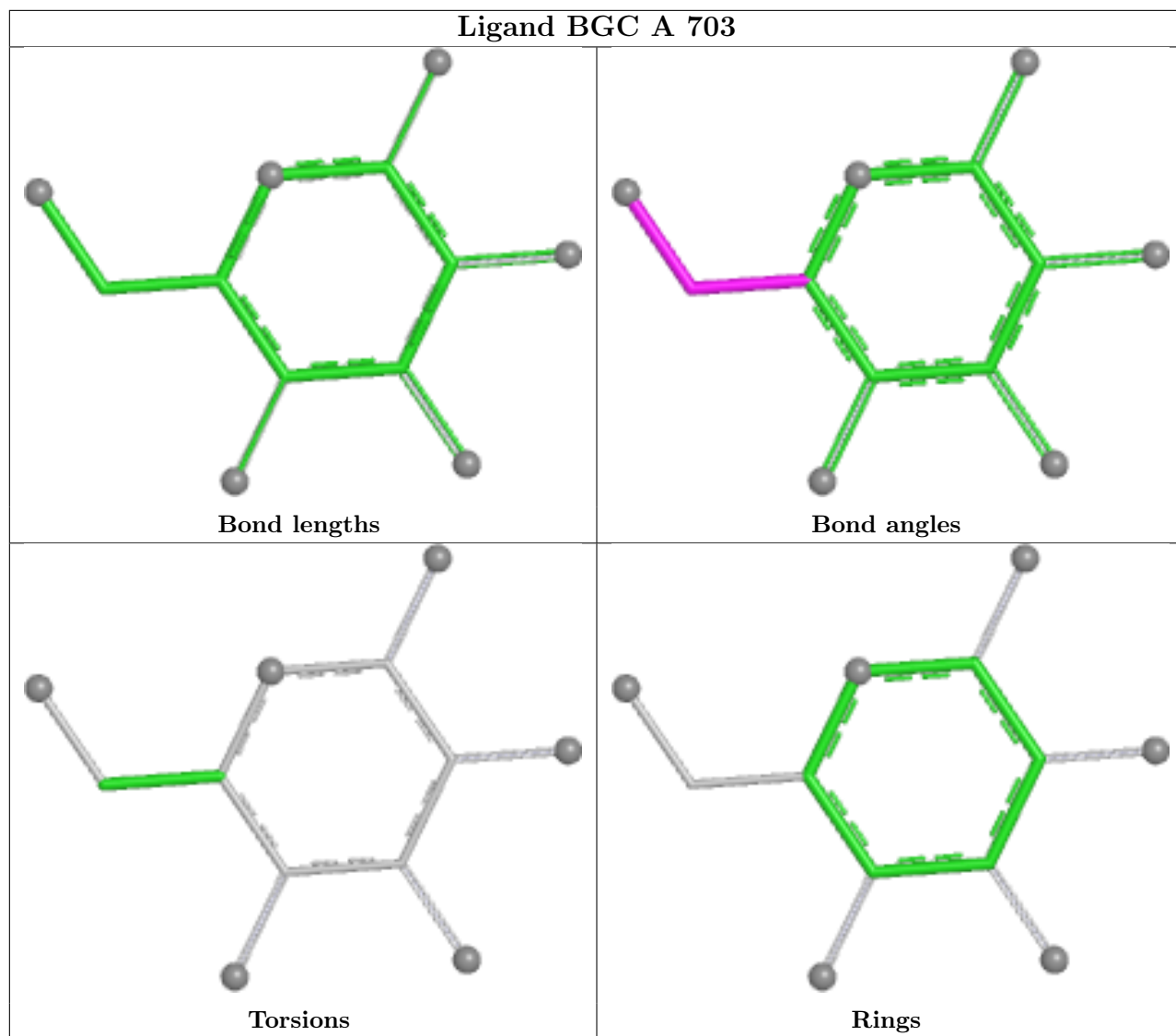
No monomer is involved in short contacts.

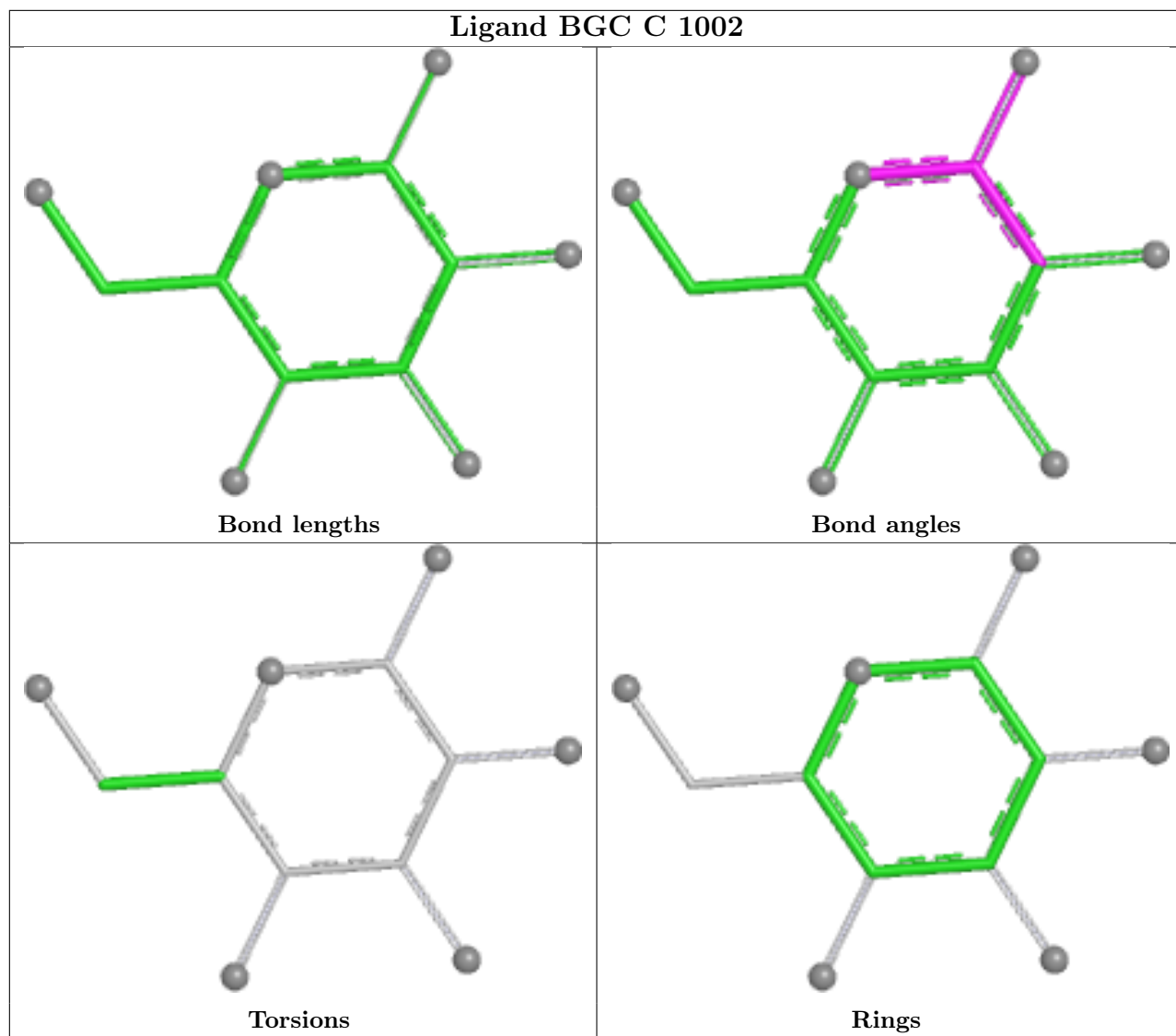
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

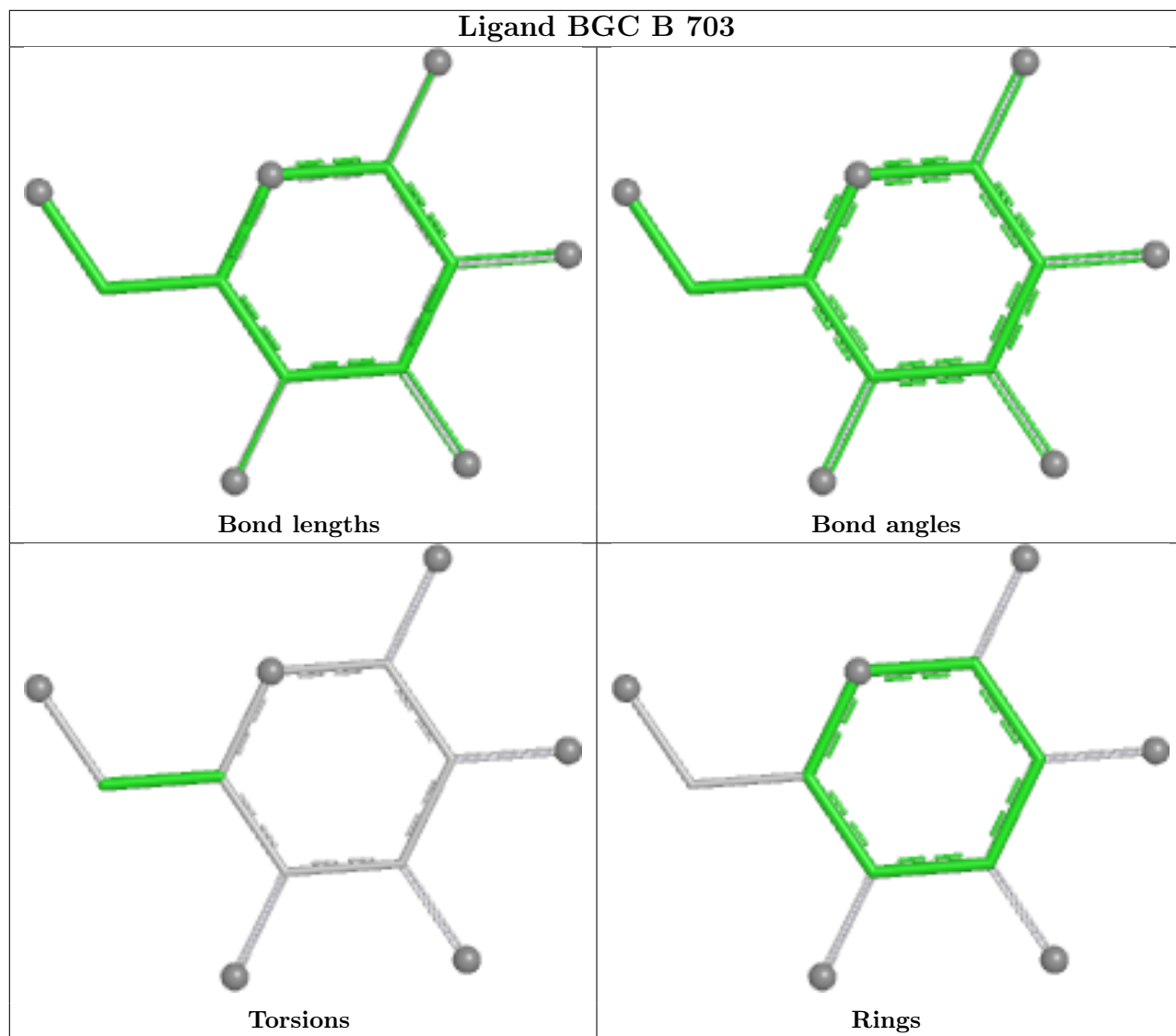


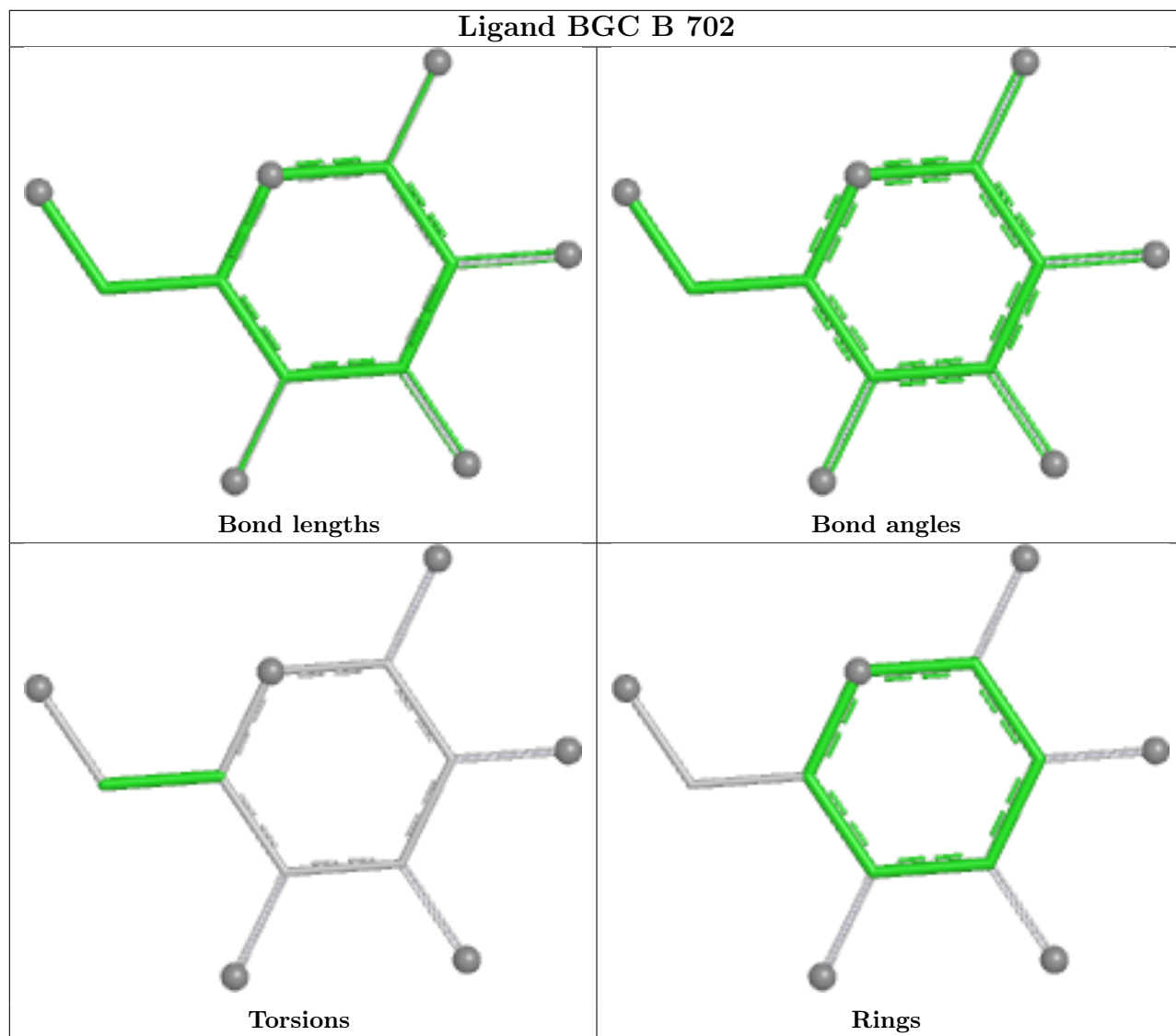


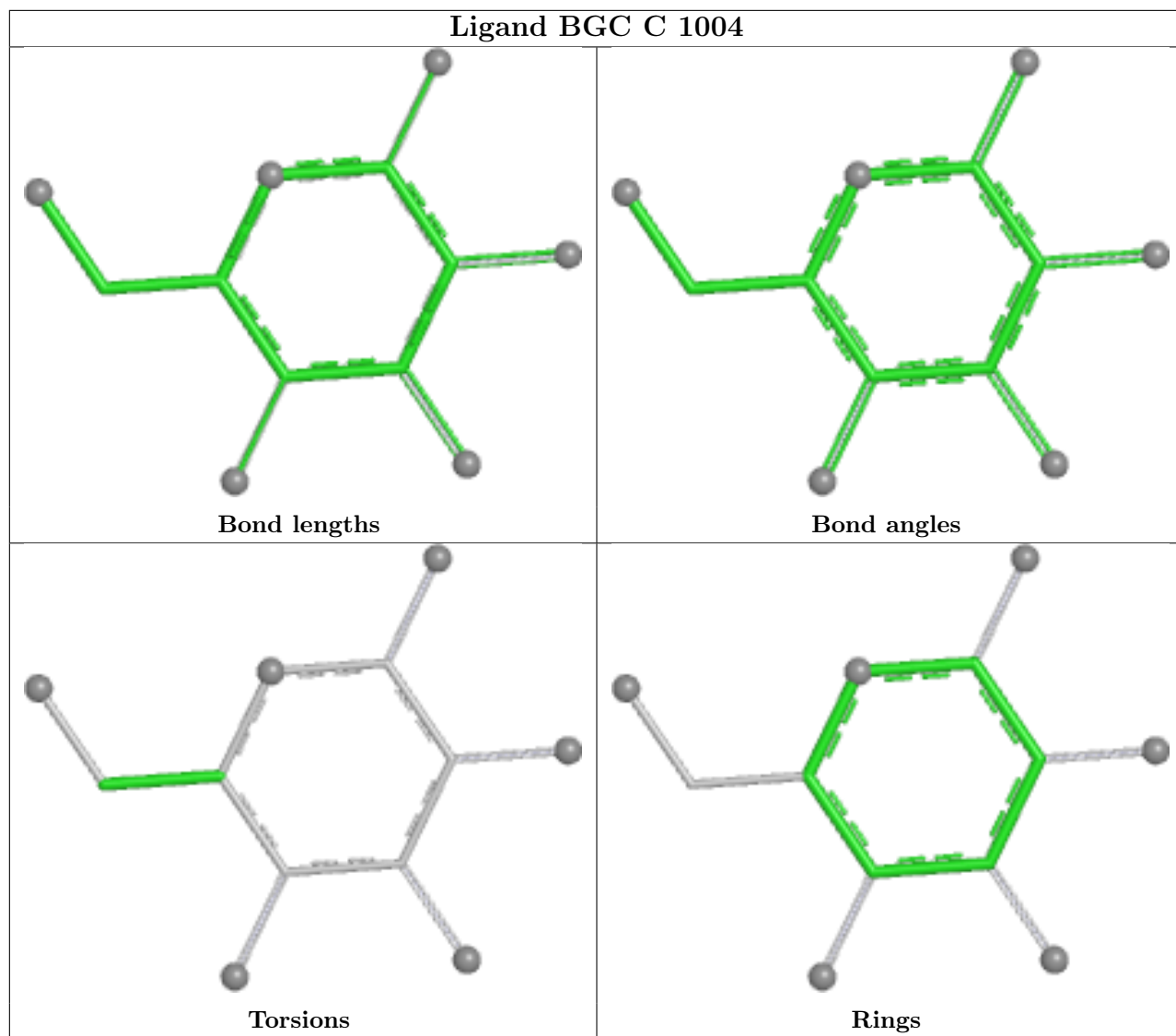


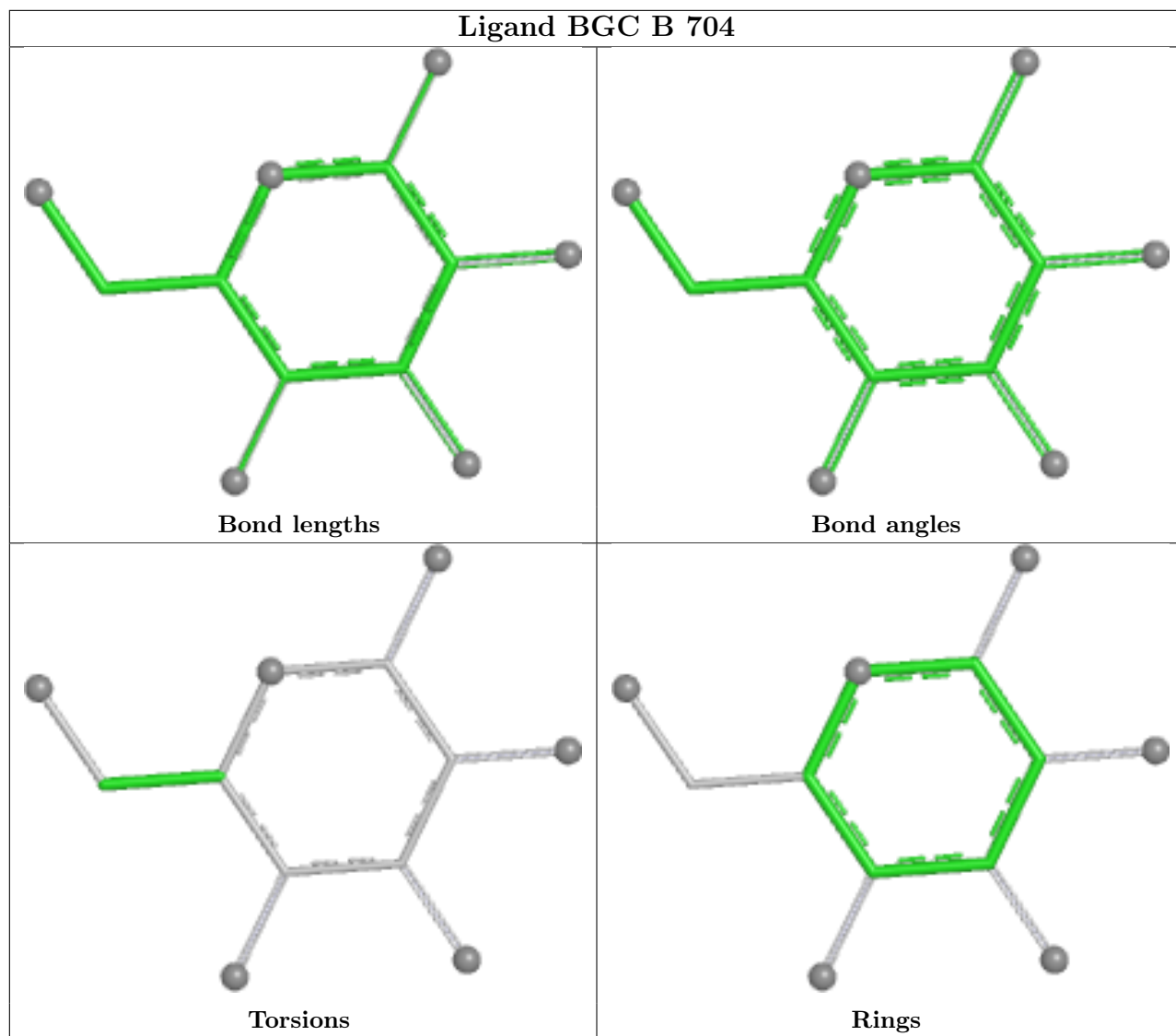


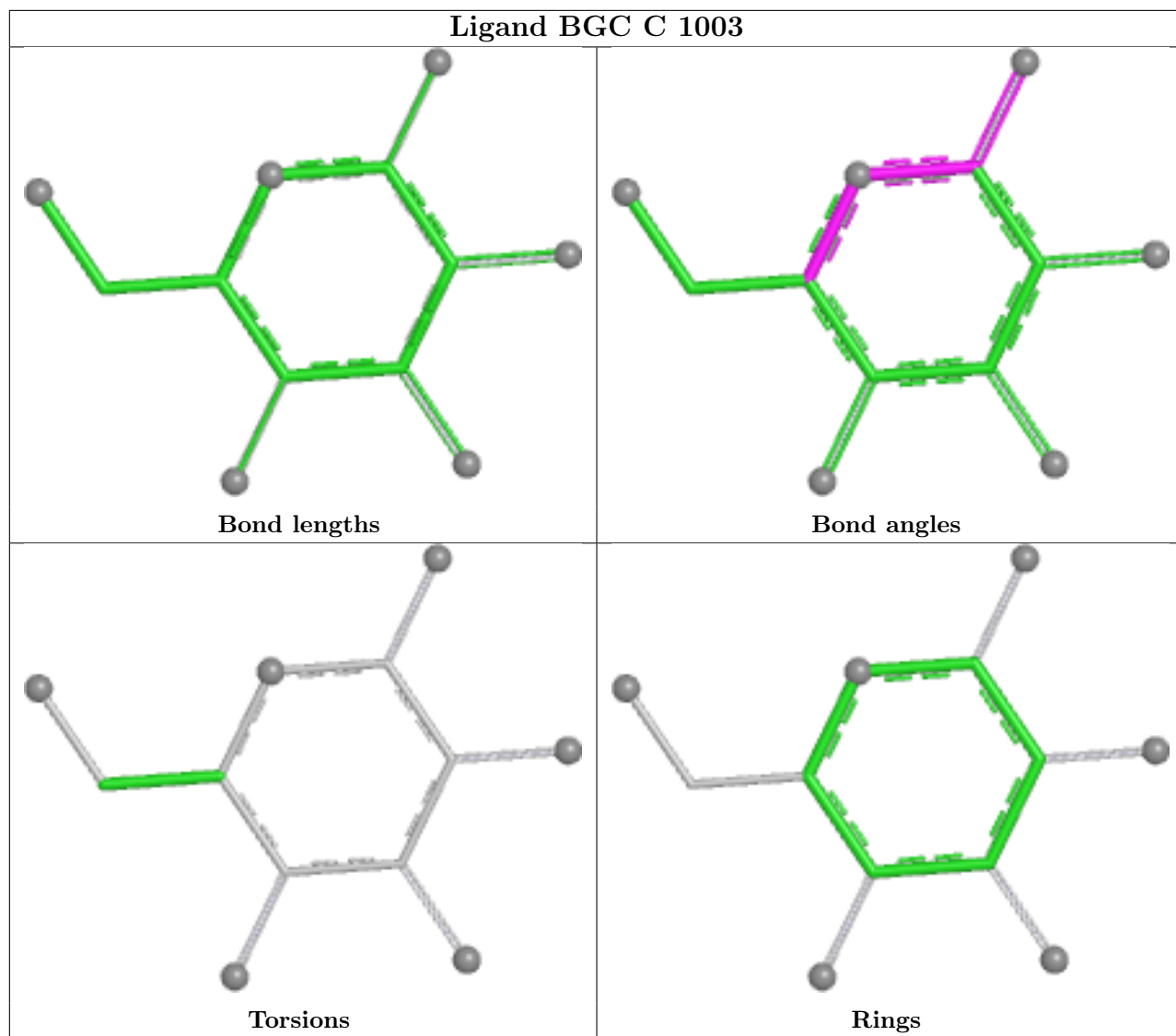


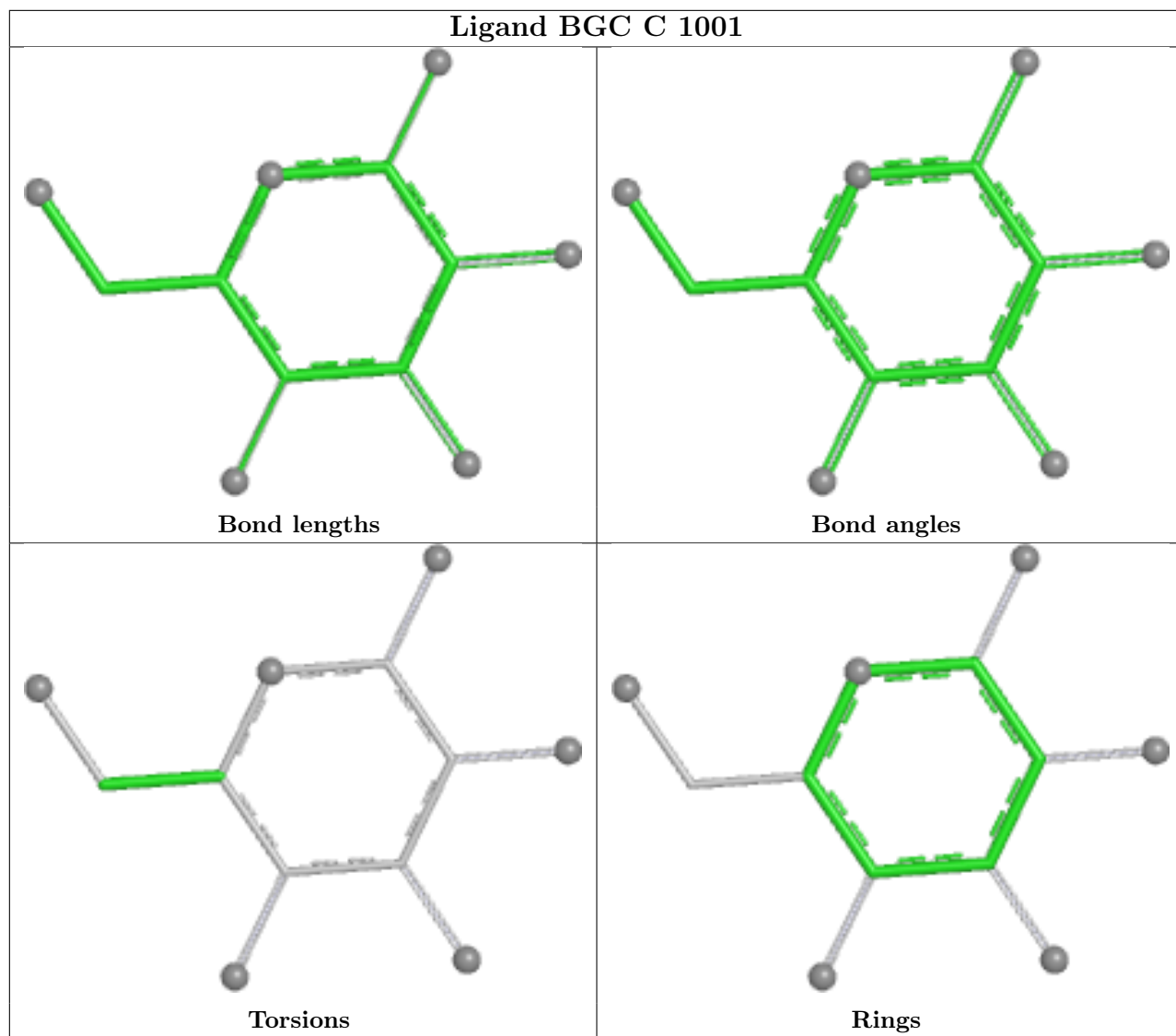


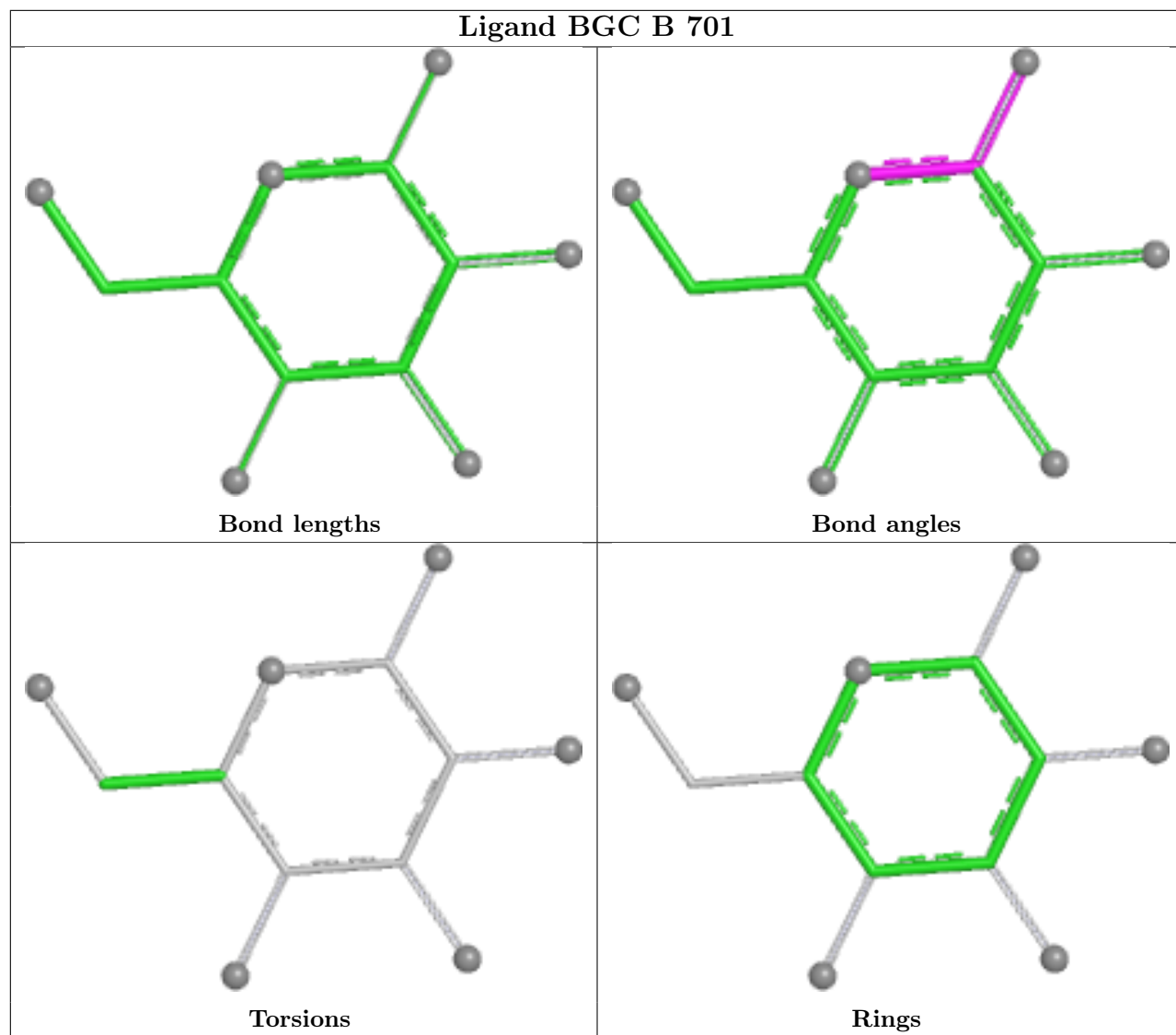












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	659/678 (97%)	0.15	25 (3%) 44 46	8, 22, 45, 65	8 (1%)
1	B	659/678 (97%)	0.25	29 (4%) 39 40	8, 25, 48, 61	5 (0%)
1	C	659/678 (97%)	0.17	21 (3%) 50 52	9, 25, 42, 54	5 (0%)
All	All	1977/2034 (97%)	0.19	75 (3%) 44 46	8, 24, 46, 65	18 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	TYR	5.0
1	C	504	ILE	5.0
1	C	101	TYR	4.9
1	B	101	TYR	4.6
1	A	152	GLN	4.2
1	A	126	LEU	3.7
1	A	23	HIS	3.7
1	A	125	ASP	3.6
1	A	150	ASN	3.5
1	A	504	ILE	3.3
1	A	100	THR	3.2
1	C	215	LYS	3.0
1	B	94	ASN	3.0
1	B	563	LYS	2.9
1	C	23	HIS	2.8
1	A	107	LYS	2.8
1	B	285	MET	2.7
1	B	33	LYS	2.7
1	C	285	MET	2.7
1	A	240	ALA	2.6
1	B	215	LYS	2.6
1	C	33	LYS	2.6
1	A	563	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	105	ASN	2.5
1	A	122	GLN	2.5
1	A	213	GLY	2.5
1	A	33	LYS	2.5
1	C	182	THR	2.5
1	B	569	ILE	2.5
1	A	239	LYS	2.5
1	C	94	ASN	2.5
1	A	153	LYS	2.4
1	B	660	LYS	2.4
1	C	660	LYS	2.4
1	B	213	GLY	2.4
1	A	32	ASP	2.4
1	B	23	HIS	2.4
1	C	183	HIS	2.4
1	B	533	THR	2.4
1	B	567	THR	2.4
1	B	37	ASN	2.4
1	C	95	GLY	2.4
1	B	504	ILE	2.3
1	A	241	GLY	2.3
1	C	24	GLN	2.3
1	B	105	ASN	2.3
1	C	563	LYS	2.3
1	B	566	GLN	2.2
1	B	183	HIS	2.2
1	C	213	GLY	2.2
1	B	107	LYS	2.2
1	C	150	ASN	2.2
1	A	503	VAL	2.2
1	B	98	VAL	2.2
1	B	568	LYS	2.2
1	B	95	GLY	2.2
1	C	155	THR	2.2
1	B	661	ASN	2.2
1	A	433	GLU	2.2
1	C	559	GLU	2.2
1	A	660	LYS	2.2
1	B	675	LYS	2.2
1	A	183	HIS	2.2
1	B	562	LEU	2.1
1	B	524	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	503	VAL	2.1
1	B	564	TYR	2.1
1	C	32	ASP	2.1
1	C	672	ILE	2.1
1	A	216	LEU	2.1
1	A	242	LYS	2.1
1	A	652	LYS	2.1
1	B	293	GLN	2.1
1	B	517	LEU	2.0
1	C	216	LEU	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](#)

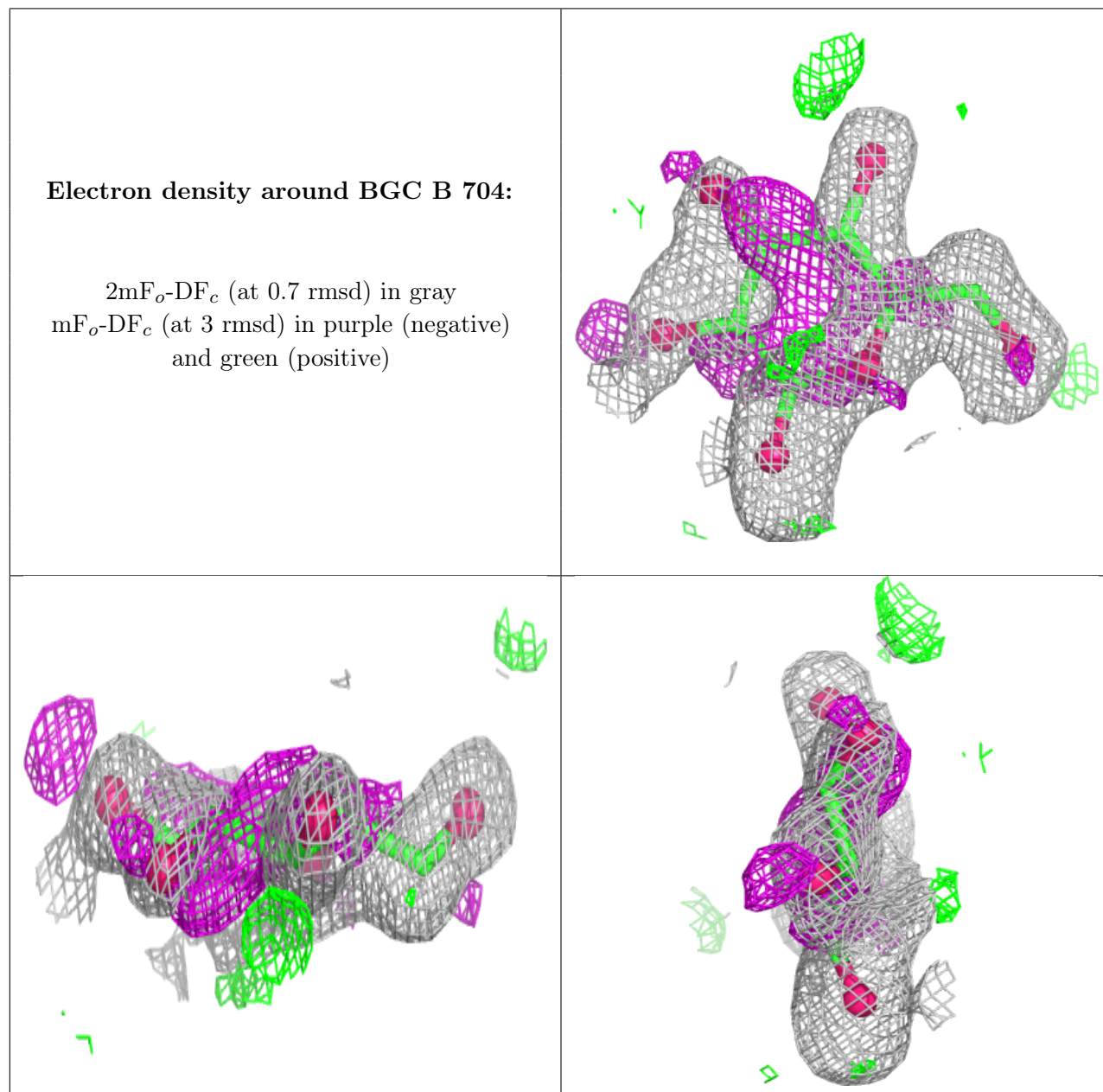
There are no oligosaccharides in this entry.

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.

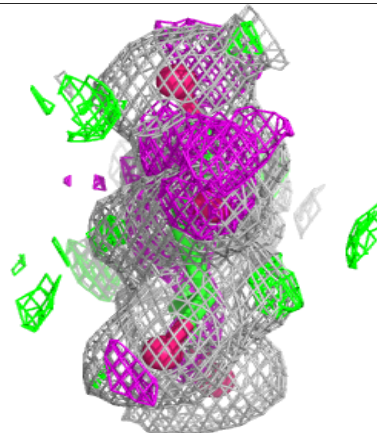
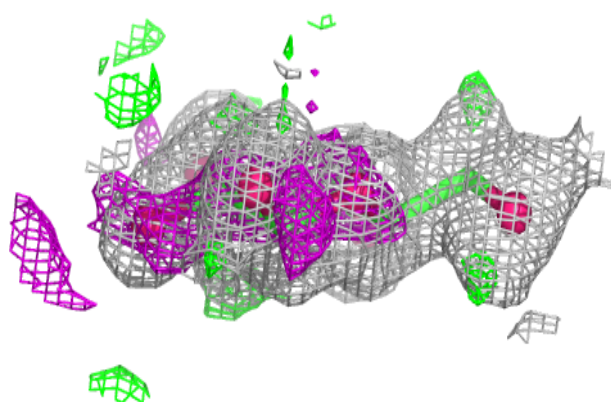
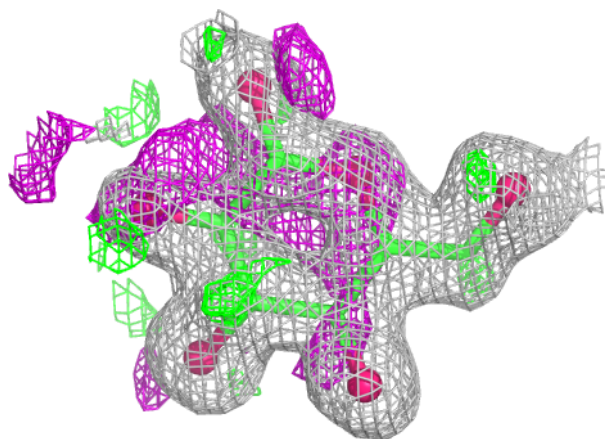
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	B	704	12/12	0.76	0.15	36,42,42,44	0
2	BGC	C	1004	12/12	0.86	0.13	24,28,29,30	0
2	BGC	C	1001	12/12	0.88	0.12	31,33,34,35	0
2	BGC	A	704	12/12	0.90	0.11	26,29,30,31	0
2	BGC	B	703	12/12	0.91	0.11	27,30,33,34	0
2	BGC	A	703	12/12	0.94	0.09	19,23,25,25	0
2	BGC	C	1003	12/12	0.94	0.09	16,17,19,20	0
2	BGC	B	701	12/12	0.94	0.09	17,19,21,22	0
2	BGC	C	1002	12/12	0.95	0.08	17,18,18,20	0
2	BGC	B	702	12/12	0.96	0.07	17,18,20,21	0
2	BGC	A	702	12/12	0.97	0.06	13,14,15,17	0
2	BGC	A	701	12/12	0.98	0.05	14,15,16,17	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.



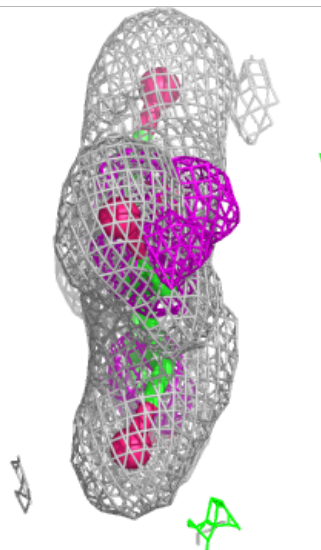
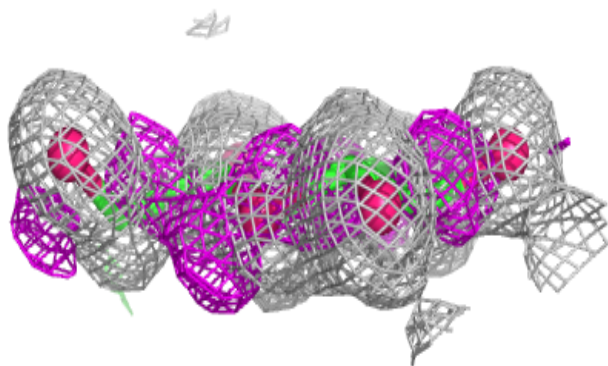
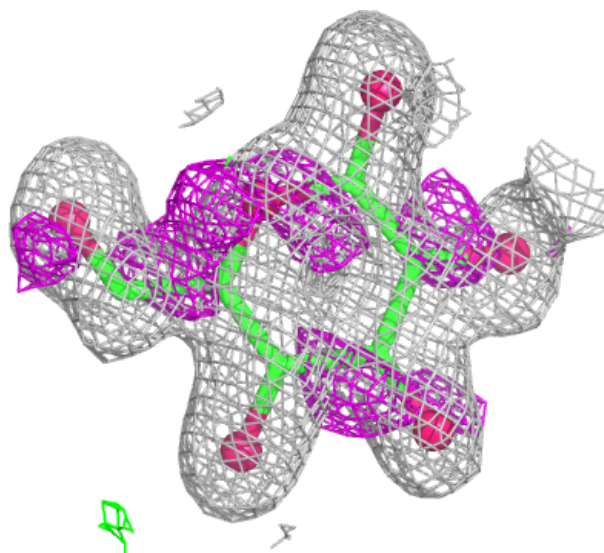
Electron density around BGC C 1004:

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



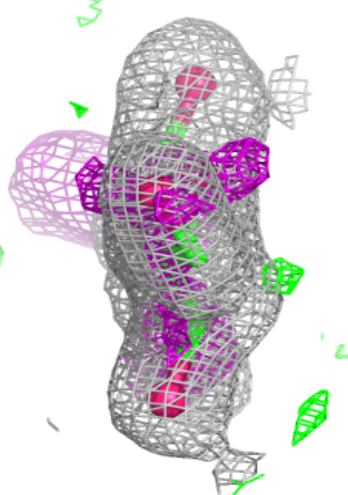
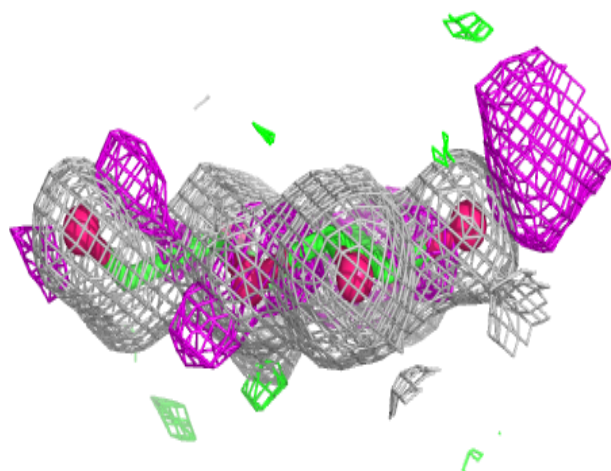
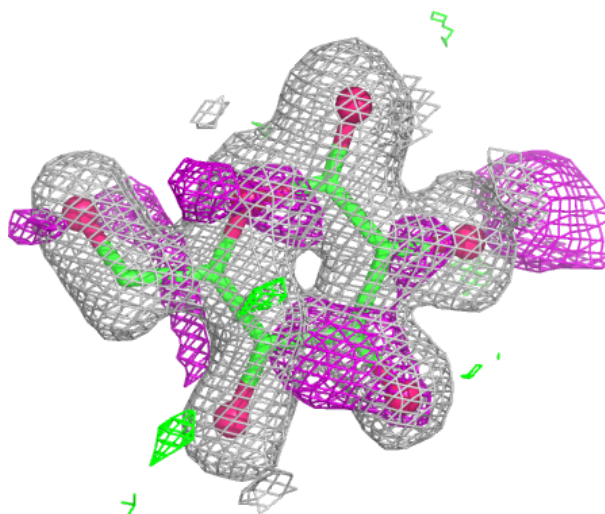
Electron density around BGC C 1001:

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



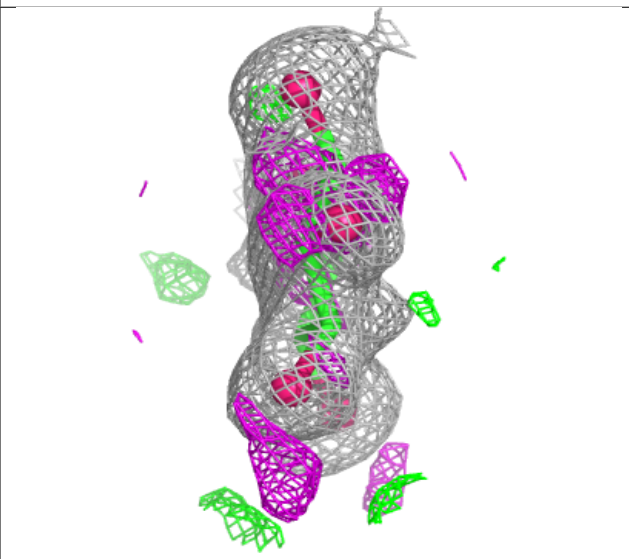
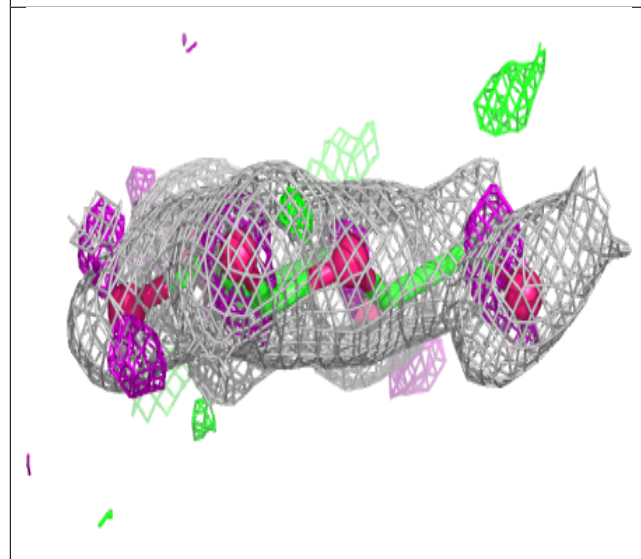
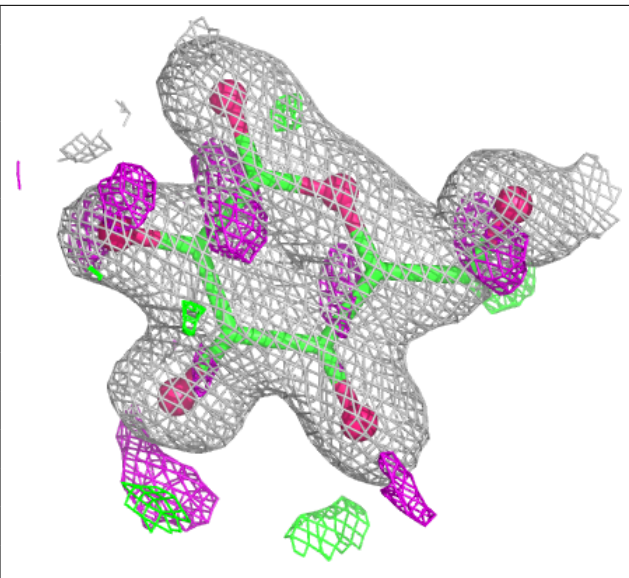
Electron density around BGC A 704:

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



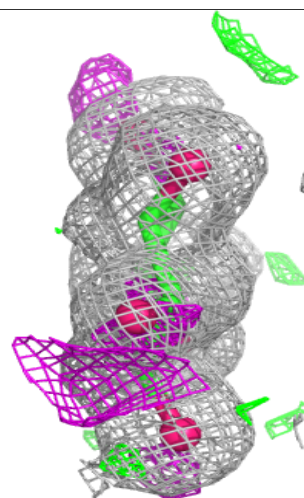
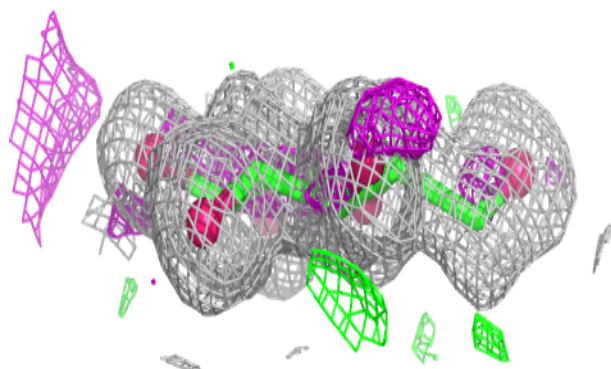
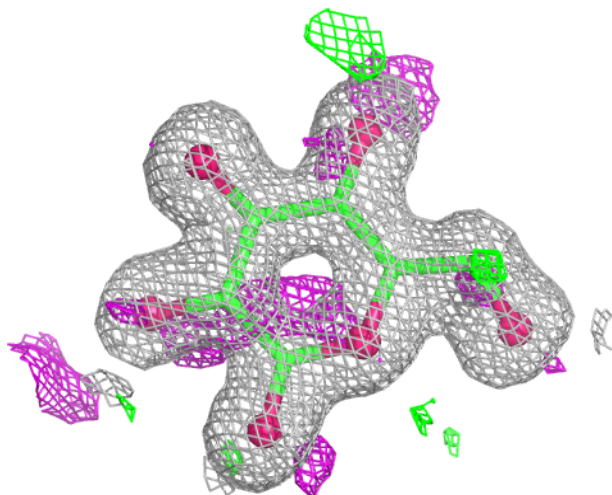
Electron density around BGC B 703:

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



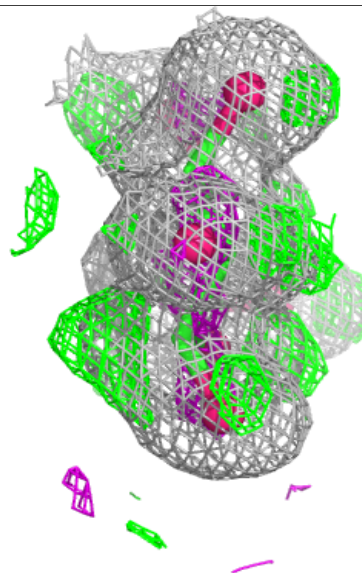
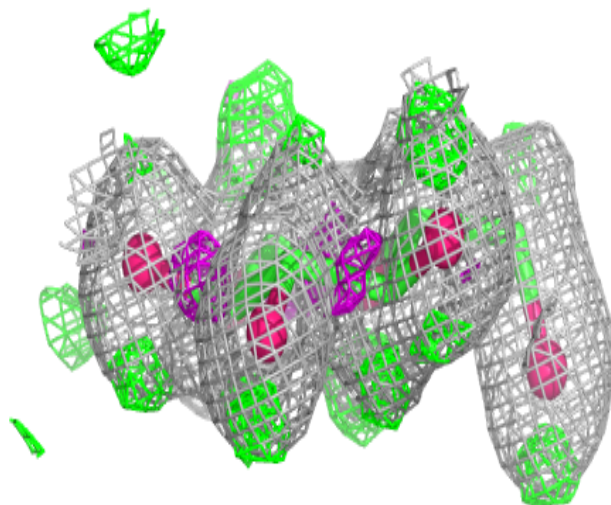
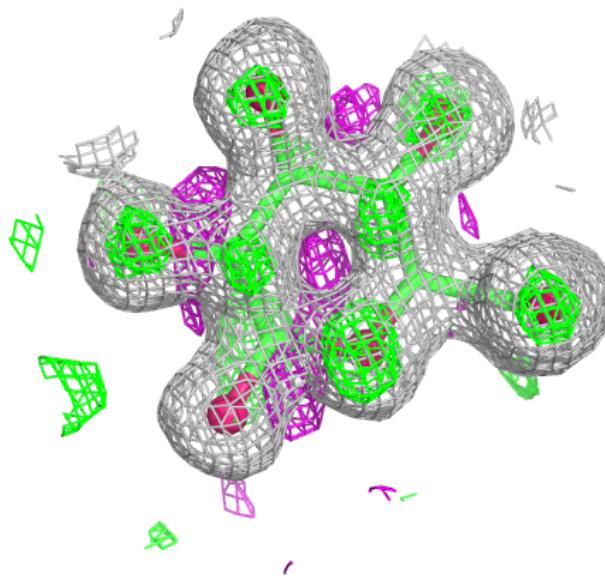
Electron density around BGC A 703:

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and green (positive)



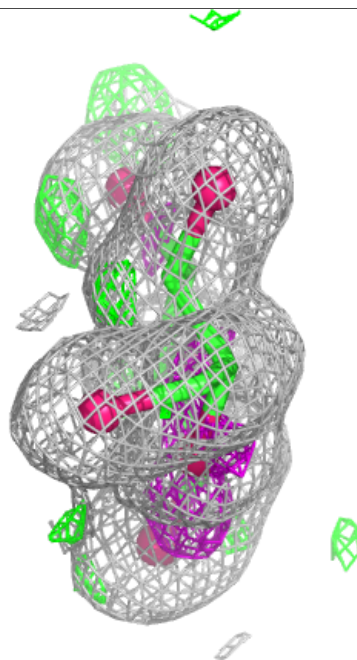
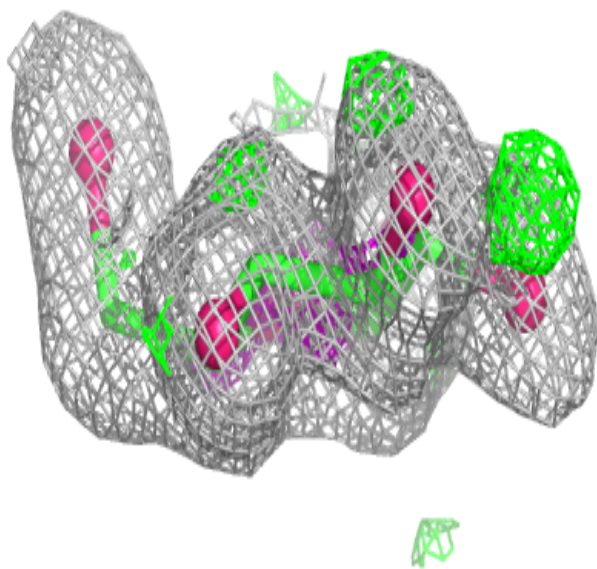
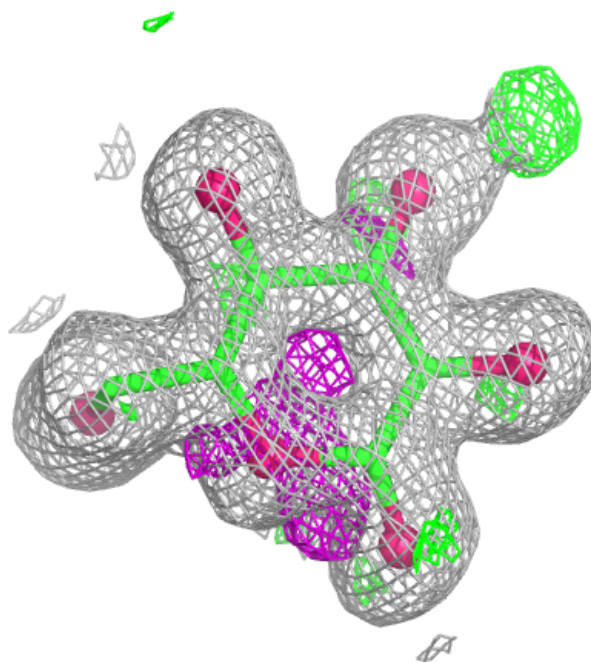
Electron density around BGC C 1003:

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



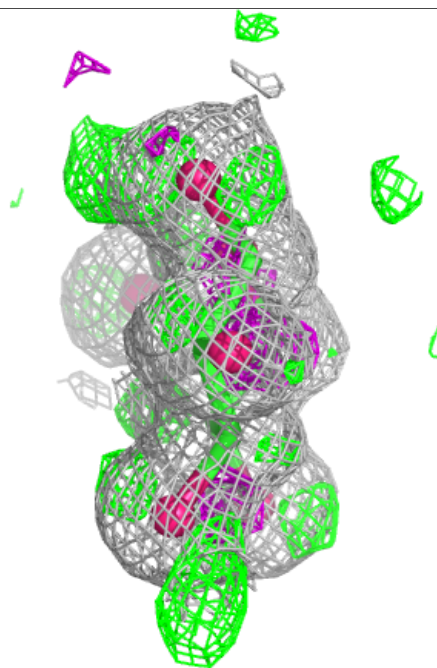
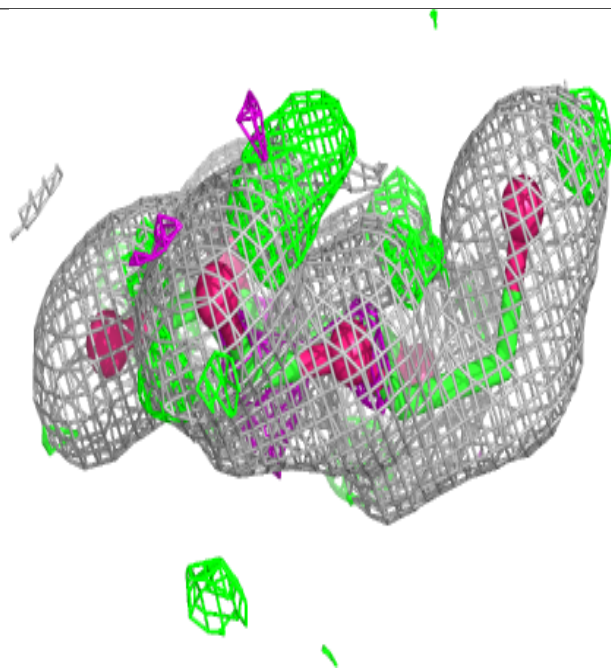
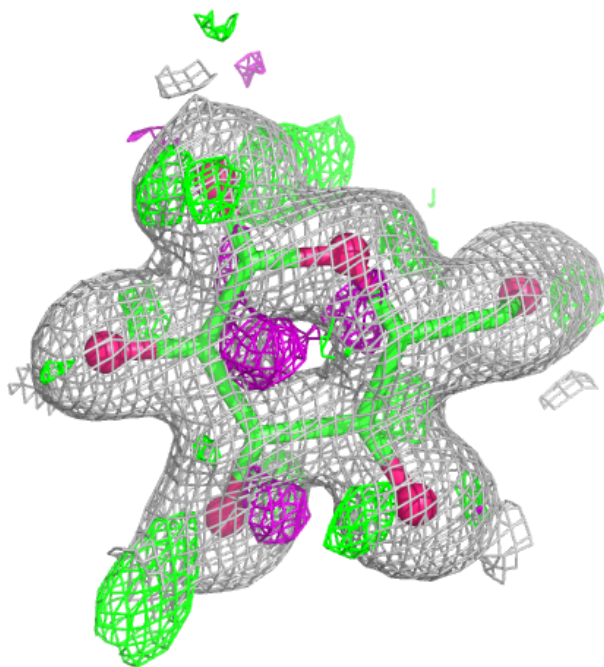
Electron density around BGC B 701:

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



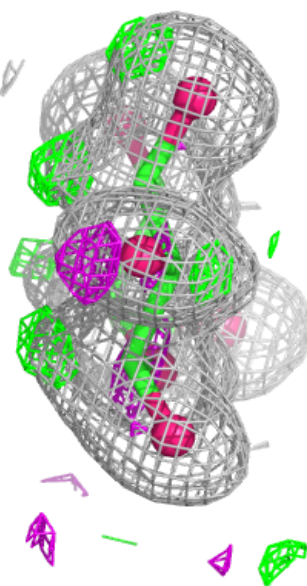
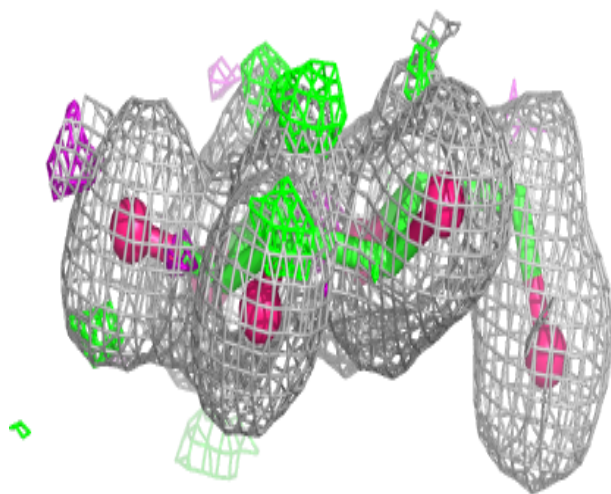
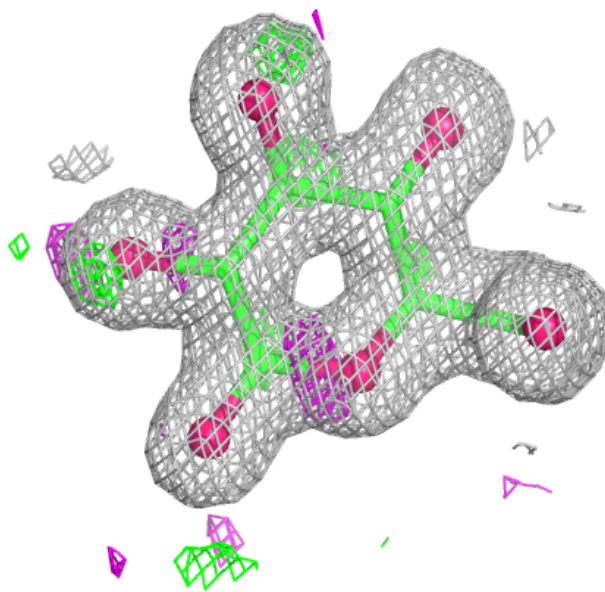
Electron density around BGC C 1002:

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



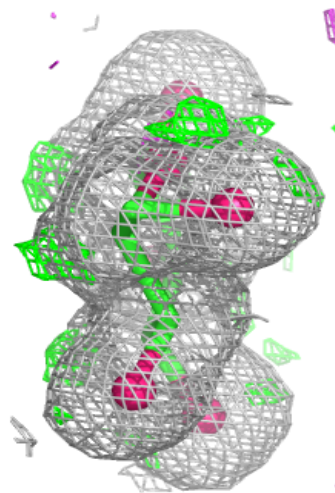
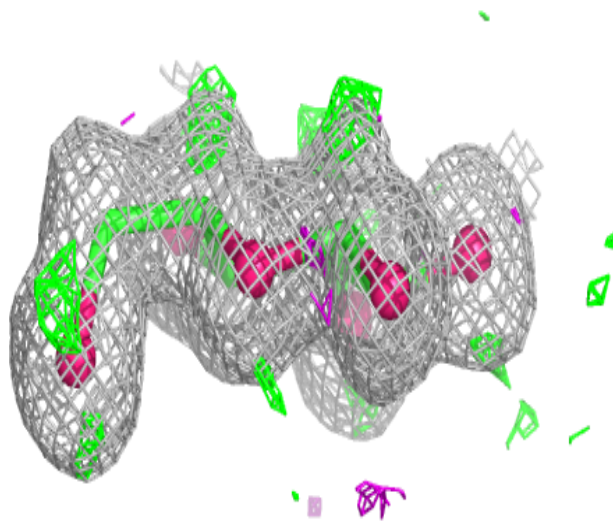
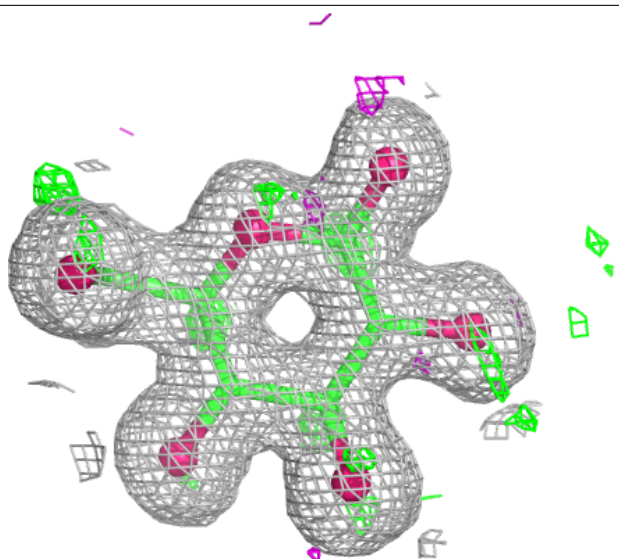
Electron density around BGC B 702:

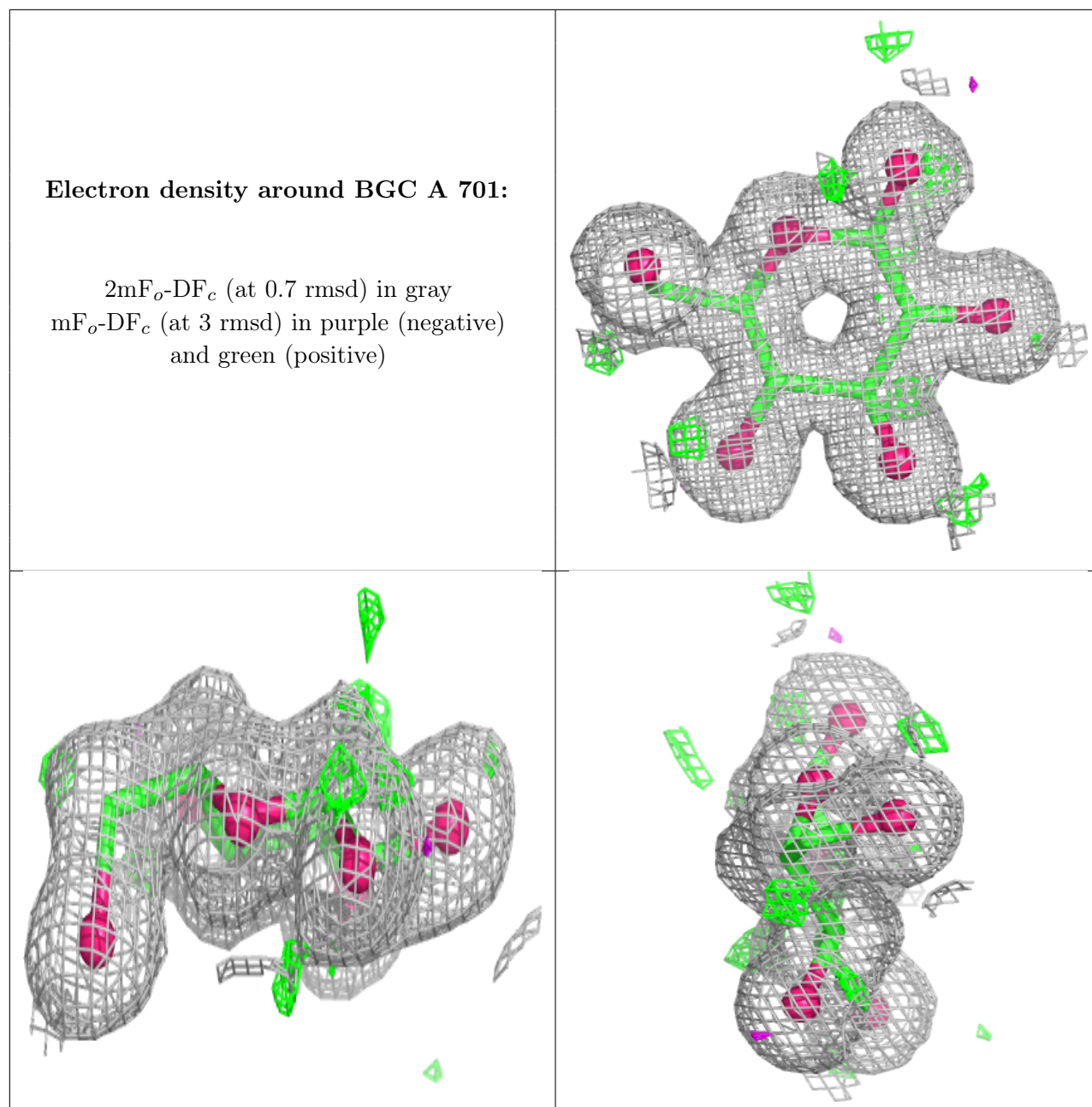
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BGC A 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 [i](#)

There are no such residues in this entry.