



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:58 PM UTC

PDB ID : 6M20 / pdb_00006m20
Title : Crystal structure of Plasmodium falciparum hexose transporter PfHT1 bound with glucose
Authors : Jiang, X.; Yuan, Y.Y.; Zhang, S.; Wang, N.; Yan, C.Y.; Yan, N.
Deposited on : 2020-02-26
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

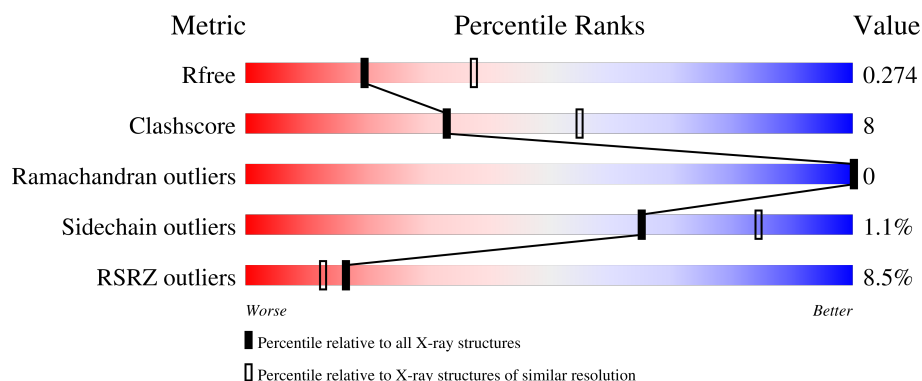
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	504	6% 78% 16% 6%
1	B	504	3% 78% 17% 5%
1	C	504	13% 78% 16% 6%
1	D	504	9% 81% 13% • 5%

2 Entry composition [i](#)

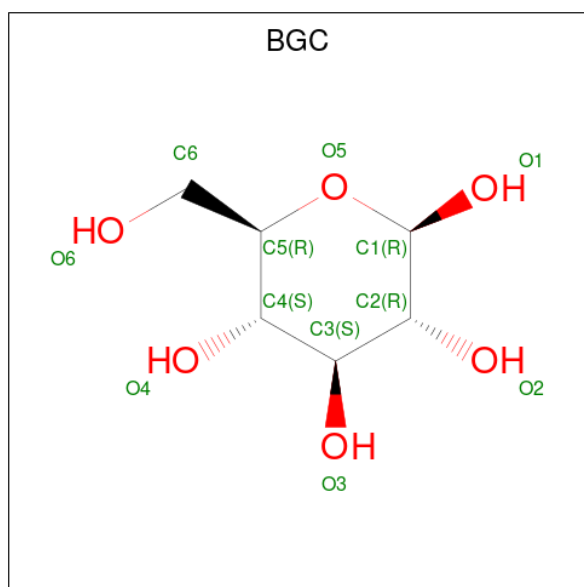
There are 4 unique types of molecules in this entry. The entry contains 15304 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hexose transporter 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3749	2496	578	656	19			
1	B	478	Total	C	N	O	S	0	0	0
			3759	2506	582	651	20			
1	C	476	Total	C	N	O	S	0	0	0
			3696	2467	569	641	19			
1	D	478	Total	C	N	O	S	0	0	0
			3733	2491	580	642	20			

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



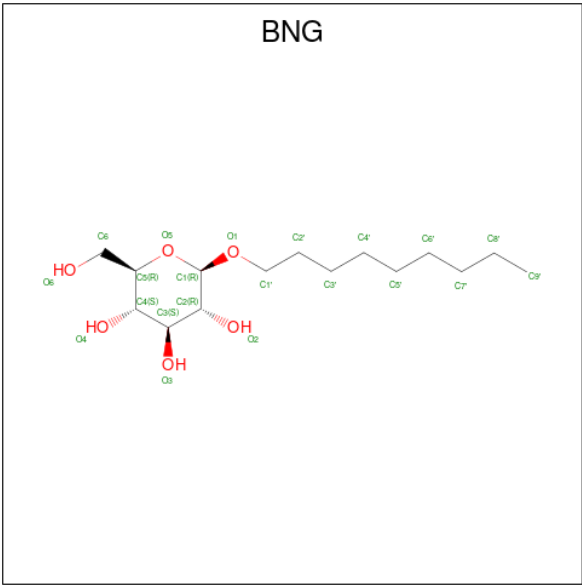
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			12	6	6		
2	B	1	Total	C	O	0	1
			12	6	6		

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

- Molecule 3 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: C₁₅H₃₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	15	6		
3	A	1	Total	C	O	0	0
			21	15	6		
3	A	1	Total	C	O	0	0
			21	15	6		
3	A	1	Total	C	O	0	0
			21	15	6		
3	B	1	Total	C	O	0	0
			21	15	6		
3	B	1	Total	C	O	0	0
			21	15	6		
3	C	1	Total	C	O	0	0
			21	15	6		
3	C	1	Total	C	O	0	0
			21	15	6		
3	C	1	Total	C	O	0	0
			21	15	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			21	15	6		
3	D	1	Total	C	O	0	0
			21	15	6		
3	D	1	Total	C	O	0	0
			21	15	6		
3	D	1	Total	C	O	0	0
			21	15	6		

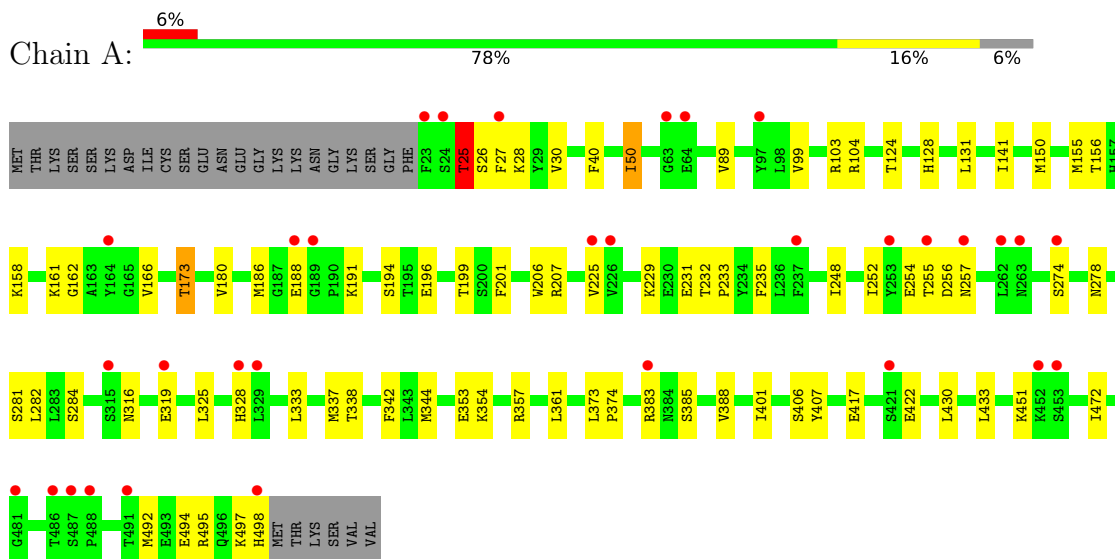
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	20	Total	O	0	0
			20	20		
4	C	8	Total	O	0	0
			8	8		
4	D	9	Total	O	0	0
			9	9		

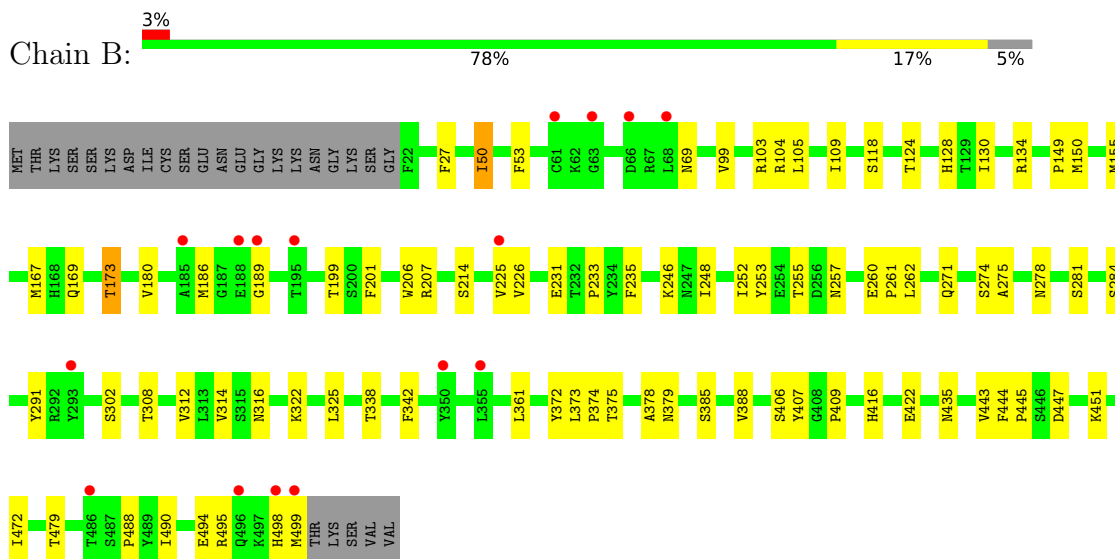
3 Residue-property plots [i](#)

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.

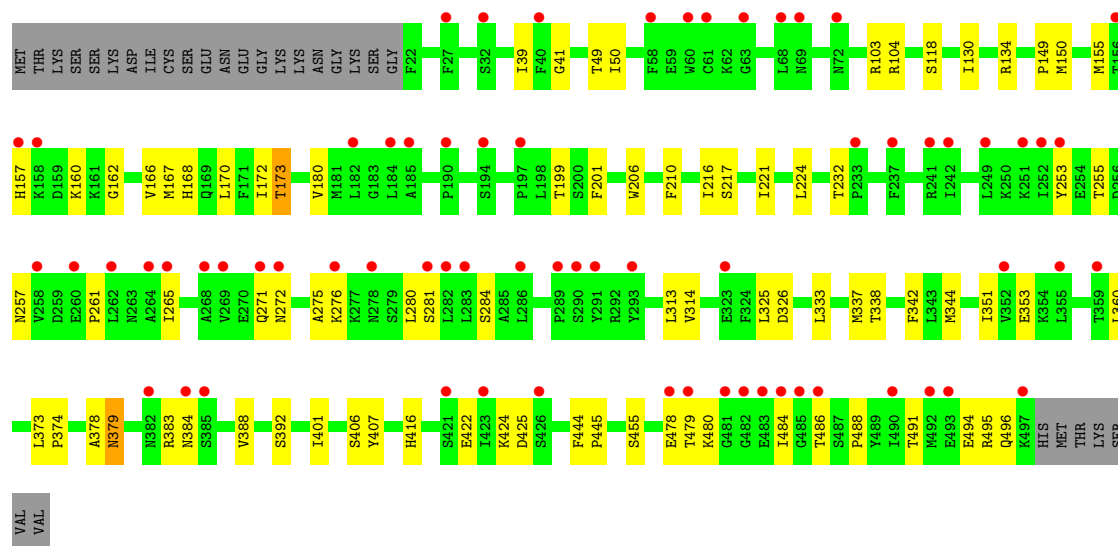
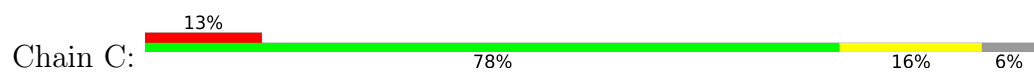
- Molecule 1: Hexose transporter 1



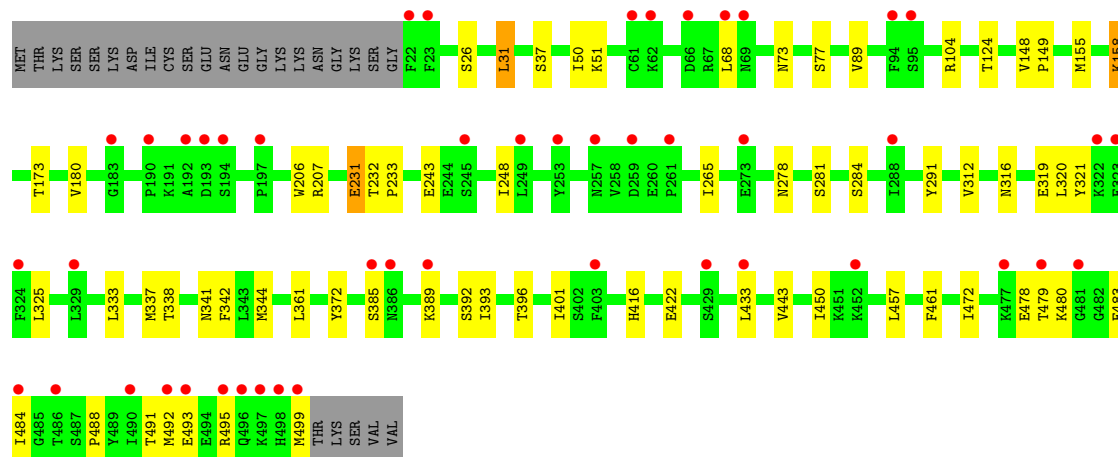
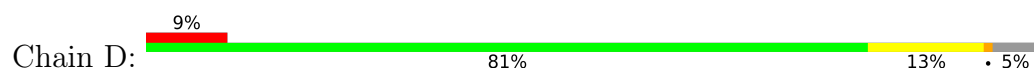
- Molecule 1: Hexose transporter 1



- Molecule 1: Hexose transporter 1



• Molecule 1: Hexose transporter 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.00Å 68.30Å 175.30Å 90.00° 103.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.60) 98.3 (20.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.3_1479	Depositor
R, R_{free}	0.245 , 0.266 0.256 , 0.274	Depositor DCC
R_{free} test set	4222 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15304	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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: BNG, 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	0.37	0/3841	0.74	2/5213 (0.0%)
1	B	0.31	0/3852	0.73	0/5227
1	C	0.34	0/3788	0.74	0/5152
1	D	0.35	0/3826	0.73	0/5195
All	All	0.34	0/15307	0.73	2/20787 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	THR	N-CA-C	-7.45	103.09	111.14
1	A	28	LYS	N-CA-C	-6.30	104.29	112.23

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	3749	0	3834	66	0
1	B	3759	0	3851	67	0
1	C	3696	0	3740	59	0
1	D	3733	0	3811	51	0
2	A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
3	A	84	0	120	6	0
3	B	42	0	60	1	0
3	C	84	0	120	7	0
3	D	63	0	90	4	0
4	A	9	0	0	0	0
4	B	20	0	0	0	0
4	C	8	0	0	0	0
4	D	9	0	0	0	0
All	All	15304	0	15674	242	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 8.

All (242) 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:173:THR:CG2	1:B:342:PHE:HA	1.56	1.32
1:A:173:THR:CG2	1:A:342:PHE:HA	1.62	1.29
1:D:173:THR:HG21	1:D:342:PHE:HA	1.22	1.19
1:C:173:THR:HG21	1:C:342:PHE:CA	1.73	1.18
1:C:173:THR:CG2	1:C:342:PHE:HA	1.71	1.18
1:B:27:PHE:HE1	1:B:167:MET:HE1	1.02	1.09
1:D:173:THR:CG2	1:D:342:PHE:HA	1.86	1.06
1:B:173:THR:HG21	1:B:342:PHE:HA	1.07	1.04
1:B:27:PHE:CE1	1:B:167:MET:HE1	1.94	1.01
1:B:173:THR:CG2	1:B:342:PHE:CA	2.41	0.99
1:A:173:THR:HG21	1:A:342:PHE:HA	0.99	0.98
1:B:27:PHE:HE1	1:B:167:MET:CE	1.77	0.97
1:A:173:THR:CG2	1:A:342:PHE:CA	2.43	0.95
1:A:173:THR:HG21	1:A:342:PHE:CA	1.95	0.95
1:C:103:ARG:NH1	1:C:150:MET:SD	2.39	0.95
1:C:173:THR:CG2	1:C:342:PHE:CA	2.41	0.89
1:D:51:LYS:HE3	1:D:77:SER:OG	1.71	0.89
1:D:491:THR:O	1:D:495:ARG:HG3	1.74	0.87
1:A:383:ARG:HG3	1:A:383:ARG:HH11	1.41	0.85
1:C:173:THR:HG22	1:C:342:PHE:HB2	1.61	0.83
1:C:173:THR:CG2	1:C:342:PHE:HB2	2.10	0.82
1:D:173:THR:HG21	1:D:342:PHE:CA	2.08	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:THR:CG2	1:C:342:PHE:CB	2.61	0.79
1:C:353:GLU:OE1	1:C:480:LYS:HE2	1.82	0.79
1:B:118:SER:HB2	1:B:214:SER:OG	1.82	0.79
1:C:173:THR:HG21	1:C:342:PHE:HA	0.84	0.77
1:D:173:THR:CG2	1:D:342:PHE:CA	2.62	0.77
1:C:265:ILE:HG12	1:C:484:ILE:HD11	1.66	0.77
1:B:27:PHE:CE1	1:B:167:MET:CE	2.60	0.77
1:C:272:ASN:O	1:C:276:LYS:HG3	1.86	0.76
1:C:104:ARG:HH12	3:C:604:BNG:H4'2	1.51	0.74
1:D:392:SER:HB3	3:D:602:BNG:H2'1	1.69	0.74
1:A:357:ARG:NH1	1:A:417:GLU:OE1	2.22	0.73
1:B:281:SER:H	1:B:284:SER:HB3	1.55	0.71
1:B:173:THR:HG23	1:B:342:PHE:HA	1.66	0.70
1:B:173:THR:HG21	1:B:342:PHE:CA	2.03	0.70
1:A:124:THR:O	1:A:207:ARG:NH2	2.25	0.69
1:A:497:LYS:O	1:A:497:LYS:HG2	1.91	0.68
1:A:357:ARG:NE	1:A:417:GLU:OE2	2.25	0.68
1:D:278:ASN:HD22	1:D:499:MET:HB2	1.58	0.68
1:C:173:THR:HG22	1:C:342:PHE:CB	2.22	0.66
1:B:255:THR:HG22	1:B:257:ASN:H	1.61	0.66
1:B:104:ARG:N	1:B:231:GLU:OE2	2.30	0.65
1:D:124:THR:O	1:D:207:ARG:NH2	2.29	0.65
1:B:494:GLU:O	1:B:498:HIS:ND1	2.30	0.65
1:C:180:VAL:HG21	1:C:338:THR:HG21	1.79	0.65
1:B:378:ALA:HB1	1:B:388:VAL:HG22	1.78	0.65
1:C:424:LYS:HG3	1:C:425:ASP:N	2.12	0.65
1:B:186:MET:HE1	1:B:206:TRP:HB3	1.79	0.65
1:D:51:LYS:CE	1:D:77:SER:OG	2.43	0.64
1:A:256:ASP:OD1	1:C:383:ARG:HD2	1.98	0.63
1:B:124:THR:O	1:B:207:ARG:NH2	2.29	0.63
1:C:491:THR:OG1	1:C:494:GLU:CB	2.47	0.63
1:D:173:THR:HG22	1:D:342:PHE:HB2	1.81	0.62
1:A:422:GLU:H	1:A:422:GLU:CD	2.09	0.61
1:A:188:GLU:O	1:A:188:GLU:HG2	1.99	0.61
1:A:357:ARG:HH11	1:A:417:GLU:CD	2.09	0.61
1:B:173:THR:HG22	1:B:342:PHE:HD1	1.65	0.60
3:A:604:BNG:H1	1:B:128:HIS:HE1	1.67	0.60
1:A:361:LEU:HB3	1:A:472:ILE:HD13	1.82	0.60
1:B:322:LYS:O	1:B:322:LYS:HG2	2.02	0.59
1:D:491:THR:C	1:D:495:ARG:HG3	2.26	0.59
1:C:424:LYS:HE3	1:C:425:ASP:OD1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:VAL:HG12	1:B:103:ARG:NH1	2.18	0.59
1:A:27:PHE:HA	1:A:30:VAL:HG22	1.86	0.58
1:A:173:THR:HG22	1:A:342:PHE:HB2	1.84	0.58
1:A:274:SER:O	1:A:278:ASN:ND2	2.33	0.58
1:B:173:THR:HG22	1:B:342:PHE:CD1	2.39	0.58
1:D:173:THR:HG22	1:D:342:PHE:CA	2.34	0.58
1:D:173:THR:HG22	1:D:342:PHE:HA	1.83	0.57
1:B:385:SER:HB3	1:B:388:VAL:HG23	1.87	0.57
1:D:31:LEU:HD12	1:D:31:LEU:O	2.05	0.57
1:A:383:ARG:HG3	1:A:383:ARG:NH1	2.16	0.57
1:A:173:THR:CG2	1:A:342:PHE:CB	2.82	0.57
1:B:180:VAL:HG21	1:B:338:THR:HG21	1.88	0.56
1:B:173:THR:HG23	1:B:342:PHE:CA	2.29	0.56
1:B:173:THR:CG2	1:B:342:PHE:CB	2.83	0.56
1:C:271:GLN:HG3	1:C:422:GLU:CG	2.35	0.56
1:A:281:SER:H	1:A:284:SER:HB3	1.70	0.56
1:C:180:VAL:HG13	3:C:603:BNG:H61	1.88	0.56
1:B:99:VAL:HG11	1:B:150:MET:SD	2.46	0.55
1:D:104:ARG:N	1:D:231:GLU:OE2	2.39	0.55
1:A:173:THR:HG22	1:A:342:PHE:CB	2.36	0.55
1:B:199:THR:HG22	1:B:201:PHE:H	1.71	0.55
1:D:180:VAL:HG21	1:D:338:THR:HG21	1.88	0.55
1:B:361:LEU:HB3	1:B:472:ILE:HD13	1.87	0.55
1:C:50:ILE:HD13	1:C:206:TRP:HB2	1.88	0.55
1:D:26:SER:OG	1:D:155:MET:O	2.25	0.55
1:C:275:ALA:HB1	1:C:280:LEU:HB3	1.89	0.54
1:C:314:VAL:HA	3:C:603:BNG:H6'1	1.88	0.54
1:A:27:PHE:CD1	1:A:27:PHE:C	2.85	0.54
1:A:180:VAL:HG21	1:A:338:THR:HG21	1.90	0.54
1:B:271:GLN:O	1:B:499:MET:HE1	2.08	0.54
1:D:265:ILE:HD13	1:D:484:ILE:HG21	1.89	0.54
1:D:372:TYR:HE1	3:D:602:BNG:H5'1	1.73	0.54
1:A:344:MET:HG3	1:A:401:ILE:HG12	1.90	0.53
1:B:406:SER:OG	1:B:407:TYR:N	2.41	0.53
1:D:50:ILE:HD13	1:D:206:TRP:HB2	1.90	0.53
1:C:406:SER:OG	1:C:407:TYR:N	2.41	0.53
1:D:158:LYS:HZ2	1:D:484:ILE:HB	1.73	0.53
1:A:494:GLU:O	1:A:498:HIS:ND1	2.40	0.53
1:A:103:ARG:N	1:A:231:GLU:OE2	2.42	0.53
1:A:191:LYS:HB2	1:A:194:SER:HB3	1.91	0.52
1:D:478:GLU:HG3	1:D:480:LYS:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:SER:OG	1:A:407:TYR:N	2.41	0.52
1:A:188:GLU:OE2	1:A:328:HIS:HA	2.09	0.52
1:B:50:ILE:HD13	1:B:206:TRP:HB2	1.92	0.52
1:B:375:THR:O	1:B:379:ASN:ND2	2.35	0.52
1:A:131:LEU:HD23	3:A:605:BNG:H8'1	1.92	0.51
1:A:99:VAL:HG11	1:A:150:MET:SD	2.50	0.51
1:D:479:THR:HG22	1:D:488:PRO:HG3	1.92	0.51
1:D:291:TYR:OH	1:D:422:GLU:OE1	2.20	0.51
1:A:199:THR:HG22	1:A:201:PHE:H	1.76	0.51
1:A:383:ARG:NH1	1:A:383:ARG:CG	2.73	0.51
1:D:173:THR:HG21	1:D:341:ASN:O	2.09	0.51
1:C:199:THR:HG22	1:C:201:PHE:H	1.75	0.50
1:C:271:GLN:HG3	1:C:422:GLU:HG3	1.93	0.50
1:B:314:VAL:HG22	3:B:603:BNG:H8'1	1.93	0.50
1:B:479:THR:HG22	1:B:488:PRO:HG3	1.93	0.50
1:C:149:PRO:HB2	1:C:416:HIS:CE1	2.46	0.50
1:D:68:LEU:O	1:D:73:ASN:ND2	2.44	0.50
1:A:173:THR:CG2	1:A:342:PHE:HB2	2.41	0.50
1:C:313:LEU:HG	3:C:603:BNG:H8'2	1.94	0.50
1:D:158:LYS:HE3	1:D:483:GLU:HA	1.93	0.49
1:D:173:THR:HG22	1:D:342:PHE:CB	2.41	0.49
1:D:180:VAL:HG13	3:D:603:BNG:H61	1.93	0.49
1:A:316:ASN:HB3	1:A:319:GLU:HB3	1.94	0.49
1:A:385:SER:HB3	1:A:388:VAL:HG23	1.95	0.49
1:C:49:THR:HA	3:C:603:BNG:H1	1.95	0.49
1:A:50:ILE:HD13	1:A:206:TRP:HB2	1.93	0.49
1:A:422:GLU:OE1	1:A:422:GLU:N	2.25	0.49
1:B:275:ALA:N	1:B:499:MET:HE3	2.28	0.48
1:C:118:SER:OG	1:C:210:PHE:O	2.27	0.48
1:D:312:VAL:HG22	1:D:443:VAL:HA	1.94	0.48
1:A:25:THR:C	1:A:27:PHE:N	2.72	0.48
1:A:158:LYS:HA	1:A:161:LYS:HG3	1.96	0.48
1:B:173:THR:HG22	1:B:342:PHE:CB	2.44	0.48
1:C:157:HIS:HB3	1:C:160:LYS:HB2	1.96	0.48
1:C:253:TYR:HE2	1:C:261:PRO:HG2	1.79	0.48
1:D:149:PRO:HB2	1:D:416:HIS:CE1	2.49	0.48
1:B:275:ALA:HB2	1:B:499:MET:HE1	1.96	0.47
1:A:255:THR:HG22	1:A:257:ASN:H	1.79	0.47
1:B:69:ASN:OD1	1:B:322:LYS:NZ	2.43	0.47
1:B:231:GLU:HG2	1:B:235:PHE:CD2	2.50	0.47
1:A:492:MET:HA	1:A:495:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:PRO:HG3	1:D:248:ILE:HG23	1.97	0.47
1:A:282:LEU:HD21	1:A:430:LEU:HD22	1.97	0.47
1:A:155:MET:HE1	1:A:248:ILE:HD11	1.96	0.46
1:C:486:THR:HA	1:C:495:ARG:NH2	2.29	0.46
1:D:361:LEU:HB3	1:D:472:ILE:HD13	1.97	0.46
1:A:89:VAL:HG13	1:A:433:LEU:HG	1.98	0.46
1:A:104:ARG:N	1:A:231:GLU:OE2	2.45	0.46
1:C:478:GLU:HG3	1:C:480:LYS:H	1.81	0.45
1:B:260:GLU:HB3	1:B:261:PRO:HD3	1.98	0.45
1:C:392:SER:HB3	3:C:602:BNG:H2'1	1.98	0.45
1:D:461:PHE:HE2	3:D:602:BNG:H9'1	1.80	0.45
1:D:393:ILE:O	1:D:396:THR:OG1	2.33	0.45
1:B:169:GLN:HG2	1:B:409:PRO:HG3	1.99	0.45
1:B:316:ASN:ND2	1:B:447:ASP:OD1	2.49	0.45
1:C:272:ASN:HA	1:C:275:ALA:HB3	1.97	0.45
1:C:379:ASN:HB3	1:C:455:SER:OG	2.16	0.45
1:D:385:SER:O	1:D:389:LYS:HG2	2.16	0.45
1:A:27:PHE:CD1	1:A:27:PHE:O	2.70	0.45
1:A:233:PRO:HG3	1:A:248:ILE:HG23	1.97	0.45
3:A:604:BNG:H1	1:B:128:HIS:CE1	2.49	0.45
1:B:274:SER:O	1:B:278:ASN:ND2	2.47	0.45
1:B:27:PHE:CE1	1:B:167:MET:HE3	2.50	0.45
1:D:319:GLU:O	1:D:319:GLU:HG3	2.15	0.45
1:A:248:ILE:O	1:A:252:ILE:HG12	2.17	0.45
1:C:162:GLY:O	1:C:166:VAL:HG23	2.16	0.44
1:D:281:SER:H	1:D:284:SER:HG	1.57	0.44
1:A:26:SER:OG	1:A:156:THR:HG22	2.17	0.44
1:C:39:ILE:HD11	1:C:216:ILE:HB	1.98	0.44
1:B:312:VAL:HG22	1:B:443:VAL:HA	2.00	0.44
1:B:373:LEU:HB3	1:B:374:PRO:HD3	2.00	0.44
1:C:167:MET:HA	1:C:170:LEU:HB3	1.99	0.44
1:A:40:PHE:CE2	1:A:141:ILE:HG23	2.53	0.44
1:A:231:GLU:HG2	1:A:235:PHE:CD2	2.53	0.44
1:D:316:ASN:O	1:D:320:LEU:HG	2.17	0.44
1:A:128:HIS:NE2	3:A:605:BNG:H1	2.33	0.43
1:B:155:MET:HE1	1:B:248:ILE:HD11	2.00	0.43
3:A:603:BNG:H9'3	3:A:603:BNG:H6'1	1.89	0.43
1:C:378:ALA:HB1	1:C:388:VAL:HG22	2.00	0.43
1:B:149:PRO:HB2	1:B:416:HIS:CE1	2.54	0.43
1:C:130:ILE:O	1:C:134:ARG:HG2	2.19	0.43
1:B:105:LEU:O	1:B:109:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:SER:C	1:B:499:MET:HE3	2.44	0.43
1:A:373:LEU:HB3	1:A:374:PRO:HD3	2.01	0.43
1:C:255:THR:HG22	1:C:257:ASN:H	1.83	0.43
1:C:479:THR:HG22	1:C:488:PRO:HG3	2.00	0.43
1:B:246:LYS:HE2	1:B:262:LEU:HD21	2.01	0.42
1:A:231:GLU:HG3	1:A:232:THR:H	1.84	0.42
1:B:173:THR:CG2	1:B:342:PHE:HB2	2.49	0.42
1:C:444:PHE:HB2	1:C:445:PRO:HD3	2.01	0.42
1:A:25:THR:C	1:A:27:PHE:H	2.28	0.42
1:B:275:ALA:HB2	1:B:499:MET:SD	2.59	0.42
1:C:49:THR:HG23	3:C:603:BNG:H5	2.00	0.42
1:B:490:ILE:HG22	1:B:495:ARG:HG3	2.02	0.42
1:C:173:THR:HG22	1:C:342:PHE:CD1	2.55	0.42
1:D:321:TYR:OH	1:D:396:THR:HG21	2.19	0.42
1:A:494:GLU:O	1:A:498:HIS:CE1	2.73	0.42
1:A:26:SER:O	1:A:30:VAL:HG13	2.20	0.41
1:A:254:GLU:HG2	1:C:384:ASN:ND2	2.35	0.41
3:A:604:BNG:H5'2	1:B:128:HIS:CD2	2.55	0.41
1:D:243:GLU:OE2	1:D:243:GLU:HA	2.19	0.41
1:B:225:VAL:HG23	1:B:226:VAL:HG23	2.02	0.41
1:C:373:LEU:HB3	1:C:374:PRO:HD3	2.02	0.41
1:B:233:PRO:HG3	1:B:248:ILE:HG23	2.02	0.41
1:C:41:GLY:HA3	1:C:172:ILE:O	2.20	0.41
1:B:130:ILE:O	1:B:134:ARG:HG2	2.20	0.41
1:D:50:ILE:H	1:D:50:ILE:HG13	1.80	0.41
1:D:344:MET:HG3	1:D:401:ILE:HG12	2.01	0.41
1:A:186:MET:C	1:A:188:GLU:H	2.29	0.41
1:A:354:LYS:HD2	1:A:354:LYS:HA	1.92	0.41
1:C:344:MET:HE2	1:C:401:ILE:HG23	2.03	0.41
1:B:302:SER:OG	1:B:435:ASN:HB2	2.20	0.41
1:B:308:THR:O	1:B:372:TYR:OH	2.30	0.41
1:C:149:PRO:HG3	1:C:168:HIS:CD2	2.56	0.41
1:C:326:ASP:OD1	1:C:326:ASP:N	2.47	0.41
1:C:333:LEU:HG	1:C:337:MET:HE2	2.03	0.41
1:C:351:ILE:HG21	1:C:360:LEU:HD13	2.03	0.41
1:B:53:PHE:CZ	1:B:189:GLY:HA2	2.56	0.41
1:C:261:PRO:O	1:C:265:ILE:HG13	2.21	0.41
1:D:37:SER:OG	1:D:148:VAL:HG11	2.20	0.41
1:D:333:LEU:HG	1:D:337:MET:HE2	2.02	0.41
1:A:225:VAL:O	1:A:229:LYS:NZ	2.54	0.41
1:A:353:GLU:OE2	1:A:353:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:MET:O	1:D:493:GLU:C	2.62	0.41
1:A:333:LEU:HG	1:A:337:MET:HE2	2.04	0.40
1:D:89:VAL:HG13	1:D:433:LEU:HG	2.02	0.40
1:D:450:ILE:HD13	1:D:457:LEU:HD23	2.02	0.40
1:B:252:ILE:HG13	1:B:253:TYR:CD1	2.57	0.40
1:C:155:MET:SD	1:C:232:THR:HA	2.61	0.40
1:D:155:MET:SD	1:D:232:THR:HA	2.62	0.40
1:A:162:GLY:O	1:A:166:VAL:HG23	2.22	0.40
1:B:275:ALA:N	1:B:499:MET:CE	2.85	0.40
1:B:291:TYR:OH	1:B:422:GLU:OE2	2.34	0.40
1:B:444:PHE:HB2	1:B:445:PRO:HD3	2.02	0.40
1:C:217:SER:O	1:C:221:ILE:HG13	2.20	0.40
1:A:319:GLU:OE2	1:A:451:LYS:HE2	2.22	0.40
1:C:281:SER:N	1:C:284:SER:OG	2.52	0.40
1:D:155:MET:HG2	1:D:232:THR:HG22	2.03	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	474/504 (94%)	465 (98%)	9 (2%)	0	100	100
1	B	476/504 (94%)	470 (99%)	6 (1%)	0	100	100
1	C	474/504 (94%)	463 (98%)	11 (2%)	0	100	100
1	D	476/504 (94%)	465 (98%)	11 (2%)	0	100	100
All	All	1900/2016 (94%)	1863 (98%)	37 (2%)	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	416/447 (93%)	411 (99%)	5 (1%)	63	83
1	B	416/447 (93%)	412 (99%)	4 (1%)	68	86
1	C	402/447 (90%)	397 (99%)	5 (1%)	63	83
1	D	409/447 (92%)	405 (99%)	4 (1%)	68	86
All	All	1643/1788 (92%)	1625 (99%)	18 (1%)	65	84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	THR
1	A	50	ILE
1	A	173	THR
1	A	196	GLU
1	A	325	LEU
1	B	50	ILE
1	B	173	THR
1	B	325	LEU
1	B	451	LYS
1	C	173	THR
1	C	224	LEU
1	C	325	LEU
1	C	379	ASN
1	C	496	GLN
1	D	31	LEU
1	D	158	LYS
1	D	231	GLU
1	D	325	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	GLN

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Mol	Chain	Res	Type
1	A	416	HIS
1	A	435	ASN
1	B	73	ASN
1	B	271	GLN
1	C	73	ASN
1	D	73	ASN
1	D	76	GLN
1	D	278	ASN
1	D	382	ASN
1	D	416	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

17 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	$\# Z > 2$
3	BNG	A	604	-	21,21,21	0.47	0	26,26,26	0.88	1 (3%)
3	BNG	A	605	-	21,21,21	0.51	0	26,26,26	1.10	1 (3%)
3	BNG	C	602	-	21,21,21	0.47	0	26,26,26	0.92	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	C	601[B]	-	12,12,12	1.04	0	17,17,17	1.64	5 (29%)
3	BNG	C	603	-	21,21,21	0.46	0	26,26,26	0.87	1 (3%)
3	BNG	A	602	-	21,21,21	0.46	0	26,26,26	0.88	1 (3%)
3	BNG	D	604	-	21,21,21	0.48	0	26,26,26	0.84	1 (3%)
3	BNG	C	605	-	21,21,21	0.47	0	26,26,26	0.81	1 (3%)
3	BNG	A	603	-	21,21,21	0.47	0	26,26,26	0.87	1 (3%)
3	BNG	D	603	-	21,21,21	0.47	0	26,26,26	0.85	1 (3%)
2	BGC	A	601[B]	-	12,12,12	1.07	0	17,17,17	1.65	4 (23%)
2	BGC	B	601[B]	-	12,12,12	1.06	0	17,17,17	1.66	4 (23%)
3	BNG	D	602	-	21,21,21	0.49	0	26,26,26	0.91	1 (3%)
3	BNG	C	604	-	21,21,21	0.46	0	26,26,26	0.83	1 (3%)
2	BGC	D	601[B]	-	12,12,12	1.06	0	17,17,17	1.65	4 (23%)
3	BNG	B	602	-	21,21,21	0.47	0	26,26,26	0.91	1 (3%)
3	BNG	B	603	-	21,21,21	0.50	0	26,26,26	0.89	1 (3%)

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	BNG	A	604	-	-	7/12/32/32	0/1/1/1
3	BNG	A	605	-	-	2/12/32/32	0/1/1/1
3	BNG	C	602	-	-	7/12/32/32	0/1/1/1
2	BGC	C	601[B]	-	-	0/2/22/22	0/1/1/1
3	BNG	C	603	-	-	3/12/32/32	0/1/1/1
3	BNG	A	602	-	-	6/12/32/32	0/1/1/1
3	BNG	D	604	-	-	3/12/32/32	0/1/1/1
3	BNG	C	605	-	-	1/12/32/32	0/1/1/1
3	BNG	A	603	-	-	5/12/32/32	0/1/1/1
3	BNG	D	603	-	-	4/12/32/32	0/1/1/1
2	BGC	A	601[B]	-	-	0/2/22/22	0/1/1/1
2	BGC	B	601[B]	-	-	0/2/22/22	0/1/1/1
3	BNG	D	602	-	-	8/12/32/32	0/1/1/1
3	BNG	C	604	-	-	5/12/32/32	0/1/1/1
2	BGC	D	601[B]	-	-	0/2/22/22	0/1/1/1
3	BNG	B	602	-	-	4/12/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BNG	B	603	-	-	4/12/32/32	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	605	BNG	C1-O5-C5	-3.55	106.79	113.72
2	C	601[B]	BGC	C6-C5-C4	-3.17	105.23	113.02
3	D	602	BNG	C1-O5-C5	-3.15	107.58	113.72
2	A	601[B]	BGC	C1-C2-C3	-3.10	104.03	110.36
2	D	601[B]	BGC	C6-C5-C4	-3.06	105.50	113.02
2	B	601[B]	BGC	C6-C5-C4	-3.04	105.55	113.02
2	A	601[B]	BGC	C6-C5-C4	-3.03	105.57	113.02
3	A	602	BNG	C1-O5-C5	-3.02	107.82	113.72
2	B	601[B]	BGC	C1-C2-C3	-3.01	104.23	110.36
2	D	601[B]	BGC	C1-C2-C3	-2.98	104.28	110.36
3	C	603	BNG	C1-O5-C5	-2.88	108.09	113.72
3	C	602	BNG	C1-O5-C5	-2.85	108.15	113.72
3	A	603	BNG	C1-O5-C5	-2.84	108.17	113.72
3	D	603	BNG	C1-O5-C5	-2.81	108.23	113.72
3	B	602	BNG	C1-O5-C5	-2.81	108.23	113.72
2	C	601[B]	BGC	C1-C2-C3	-2.74	104.76	110.36
3	D	604	BNG	C1-O5-C5	-2.59	108.66	113.72
3	C	604	BNG	C1-O5-C5	-2.56	108.72	113.72
2	C	601[B]	BGC	O1-C1-C2	-2.46	101.86	108.98
2	A	601[B]	BGC	C4-C3-C2	-2.42	106.58	110.83
3	A	604	BNG	C1-O5-C5	-2.42	109.00	113.72
2	A	601[B]	BGC	O1-C1-C2	-2.37	102.10	108.98
2	D	601[B]	BGC	O1-C1-C2	-2.37	102.11	108.98
3	C	605	BNG	C1-O5-C5	-2.37	109.10	113.72
2	B	601[B]	BGC	O1-C1-C2	-2.35	102.17	108.98
2	D	601[B]	BGC	C4-C3-C2	-2.29	106.81	110.83
2	B	601[B]	BGC	C4-C3-C2	-2.29	106.81	110.83
2	C	601[B]	BGC	C4-C3-C2	-2.12	107.11	110.83
3	B	603	BNG	C1-O5-C5	-2.07	109.67	113.72
2	C	601[B]	BGC	O3-C3-C4	-2.01	105.65	110.38

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	BNG	C2-C1-O1-C1'
3	A	604	BNG	O5-C1-O1-C1'
3	A	604	BNG	C2'-C1'-O1-C1
3	B	603	BNG	C2-C1-O1-C1'
3	B	603	BNG	O5-C1-O1-C1'
3	C	604	BNG	C2'-C1'-O1-C1
3	A	603	BNG	O5-C5-C6-O6
3	C	602	BNG	O5-C5-C6-O6
3	D	603	BNG	O5-C5-C6-O6
3	A	605	BNG	O5-C5-C6-O6
3	C	603	BNG	O5-C5-C6-O6
3	A	605	BNG	C4-C5-C6-O6
3	C	603	BNG	C4-C5-C6-O6
3	C	604	BNG	O1-C1'-C2'-C3'
3	A	603	BNG	C4-C5-C6-O6
3	C	602	BNG	C4-C5-C6-O6
3	D	602	BNG	O1-C1'-C2'-C3'
3	D	603	BNG	C4-C5-C6-O6
3	D	603	BNG	O1-C1'-C2'-C3'
3	A	604	BNG	O1-C1'-C2'-C3'
3	C	602	BNG	O1-C1'-C2'-C3'
3	A	602	BNG	C5'-C6'-C7'-C8'
3	A	602	BNG	O1-C1'-C2'-C3'
3	B	602	BNG	C4'-C5'-C6'-C7'
3	A	603	BNG	C3'-C4'-C5'-C6'
3	A	603	BNG	C1'-C2'-C3'-C4'
3	D	602	BNG	C2'-C3'-C4'-C5'
3	A	604	BNG	O5-C5-C6-O6
3	D	604	BNG	C1'-C2'-C3'-C4'
3	B	602	BNG	O5-C5-C6-O6
3	A	602	BNG	C4'-C5'-C6'-C7'
3	C	604	BNG	O5-C5-C6-O6
3	A	604	BNG	C5'-C6'-C7'-C8'
3	B	603	BNG	C3'-C4'-C5'-C6'
3	A	603	BNG	O1-C1'-C2'-C3'
3	C	602	BNG	C2'-C3'-C4'-C5'
3	D	602	BNG	C3'-C4'-C5'-C6'
3	A	602	BNG	C3'-C4'-C5'-C6'
3	D	602	BNG	O5-C5-C6-O6
3	C	605	BNG	C2'-C1'-O1-C1
3	D	604	BNG	C3'-C4'-C5'-C6'
3	C	602	BNG	C3'-C4'-C5'-C6'
3	C	602	BNG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
3	C	604	BNG	C2-C1-O1-C1'
3	C	603	BNG	C4'-C5'-C6'-C7'
3	D	602	BNG	O5-C1-O1-C1'
3	D	603	BNG	C1'-C2'-C3'-C4'
3	B	602	BNG	O1-C1'-C2'-C3'
3	D	604	BNG	C2'-C3'-C4'-C5'
3	D	602	BNG	C6'-C7'-C8'-C9'
3	C	604	BNG	C2'-C3'-C4'-C5'
3	B	602	BNG	C6'-C7'-C8'-C9'
3	B	603	BNG	O1-C1'-C2'-C3'
3	D	602	BNG	C2-C1-O1-C1'
3	A	604	BNG	C1'-C2'-C3'-C4'
3	C	602	BNG	C1'-C2'-C3'-C4'
3	D	602	BNG	C4'-C5'-C6'-C7'
3	A	602	BNG	C2'-C3'-C4'-C5'
3	A	602	BNG	C4-C5-C6-O6

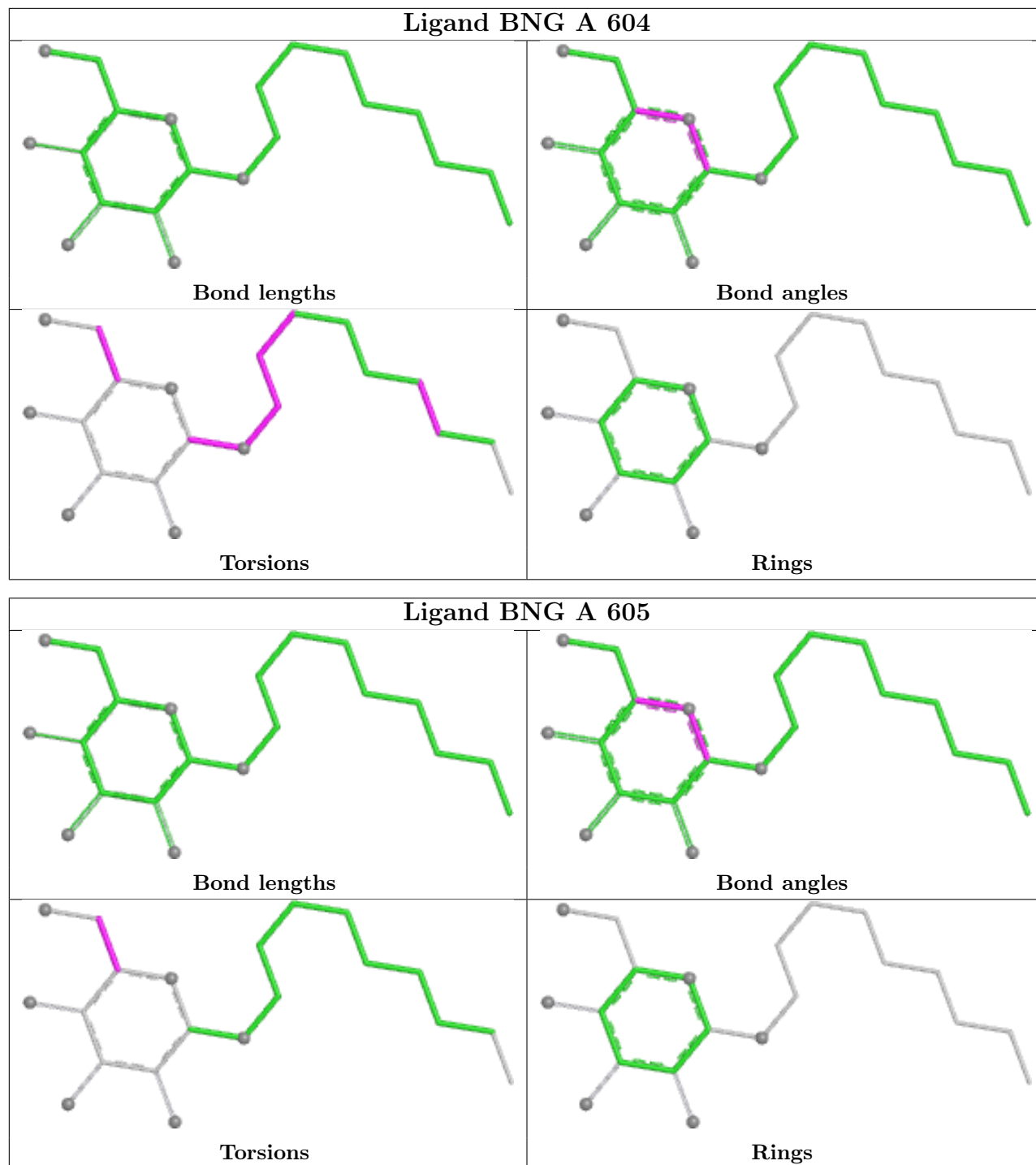
There are no ring outliers.

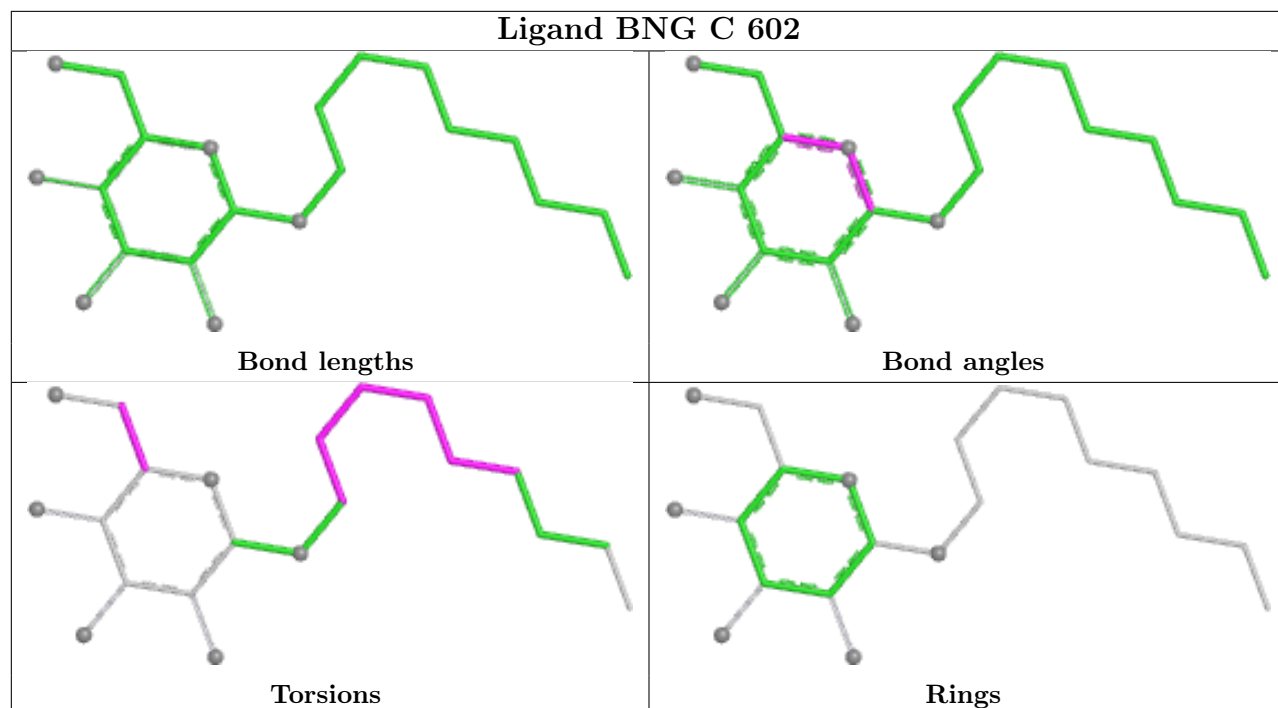
9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	BNG	3	0
3	A	605	BNG	2	0
3	C	602	BNG	1	0
3	C	603	BNG	5	0
3	A	603	BNG	1	0
3	D	603	BNG	1	0
3	D	602	BNG	3	0
3	C	604	BNG	1	0
3	B	603	BNG	1	0

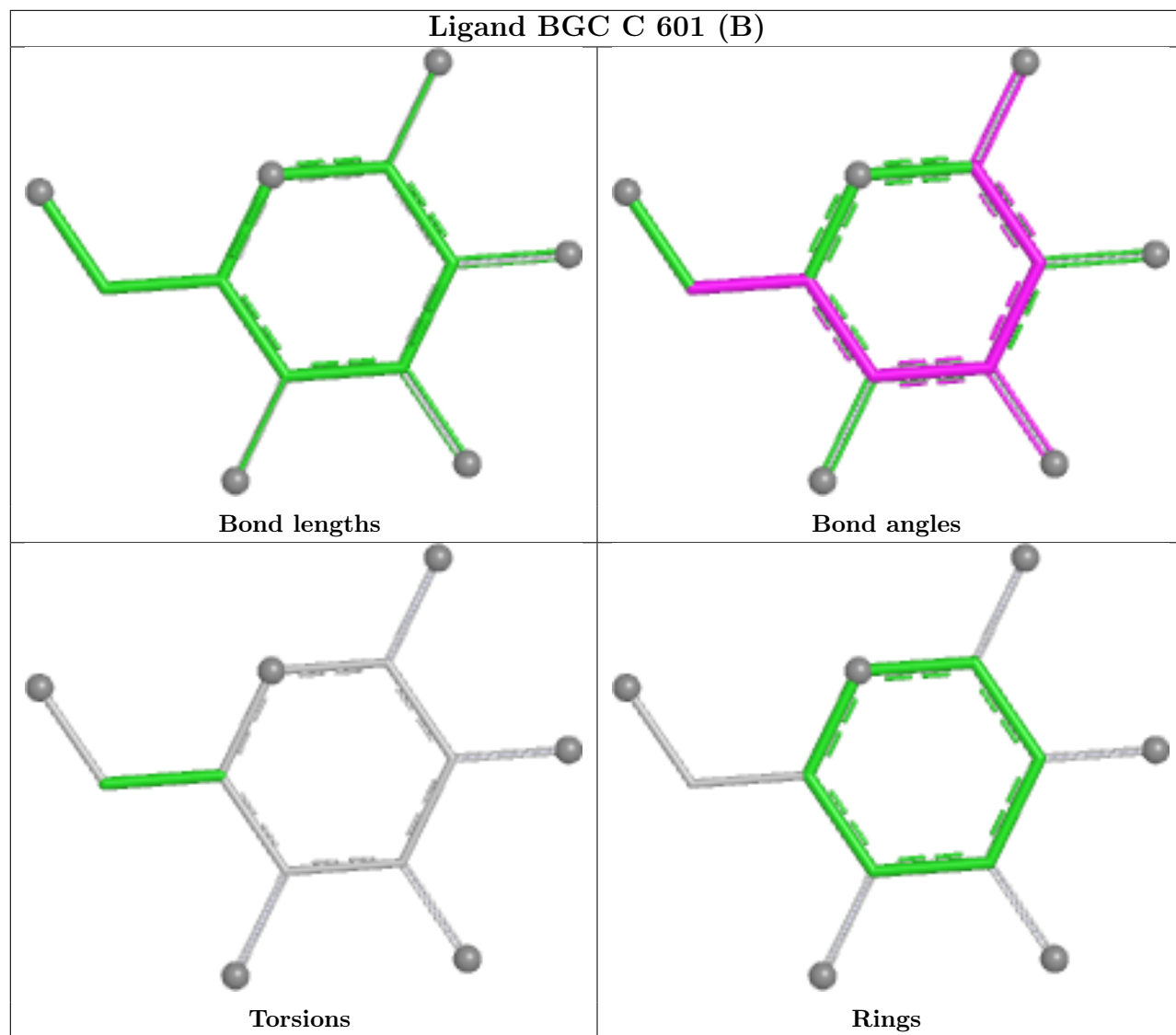
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

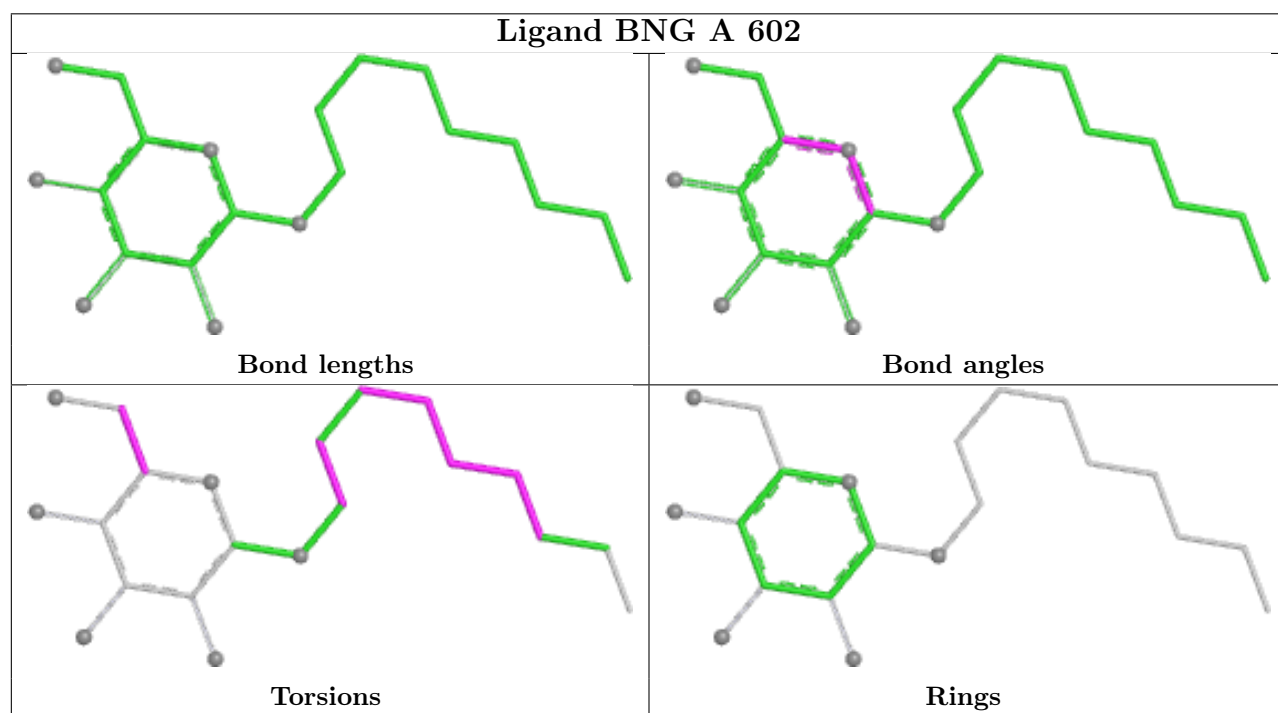
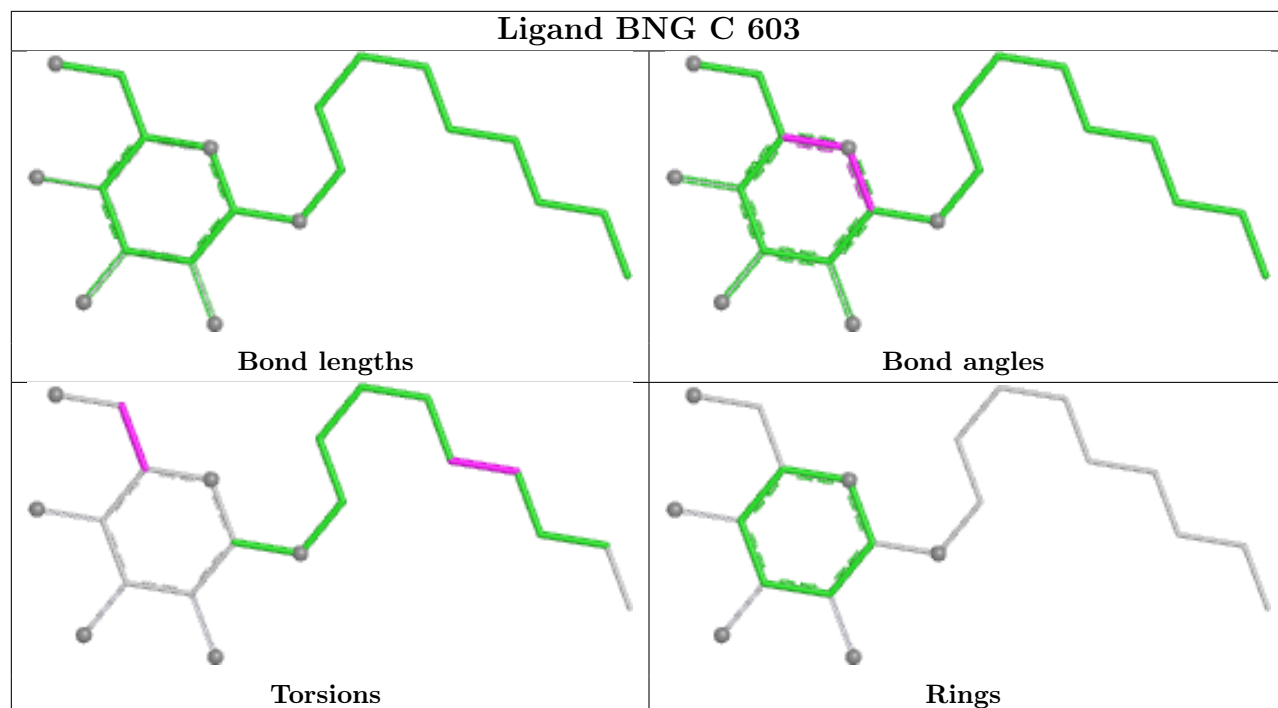
equivalents in the CSD to analyse the geometry.

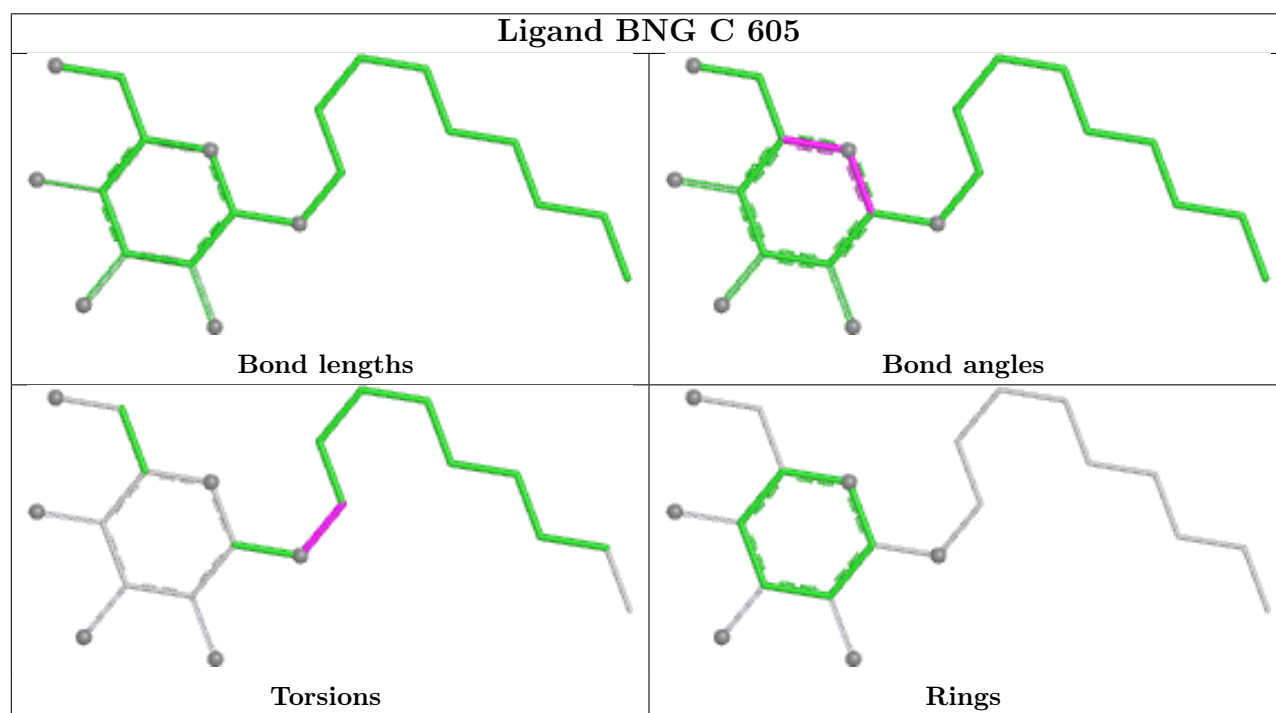
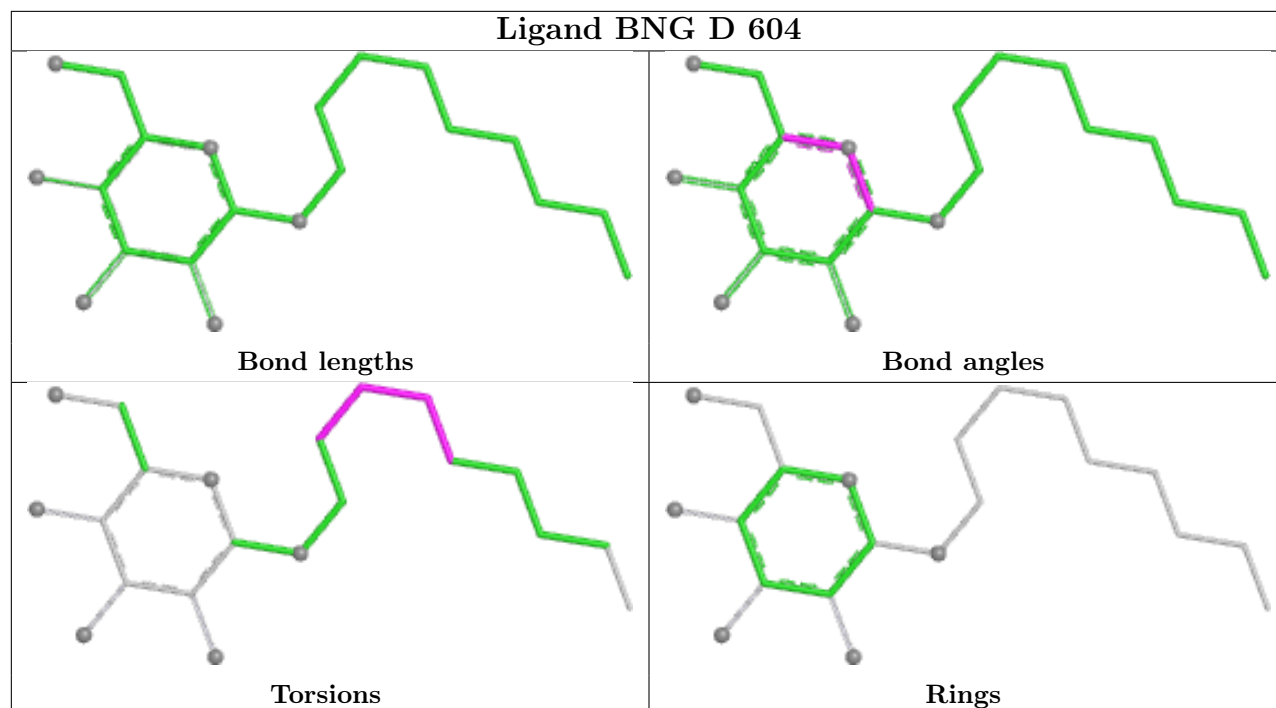


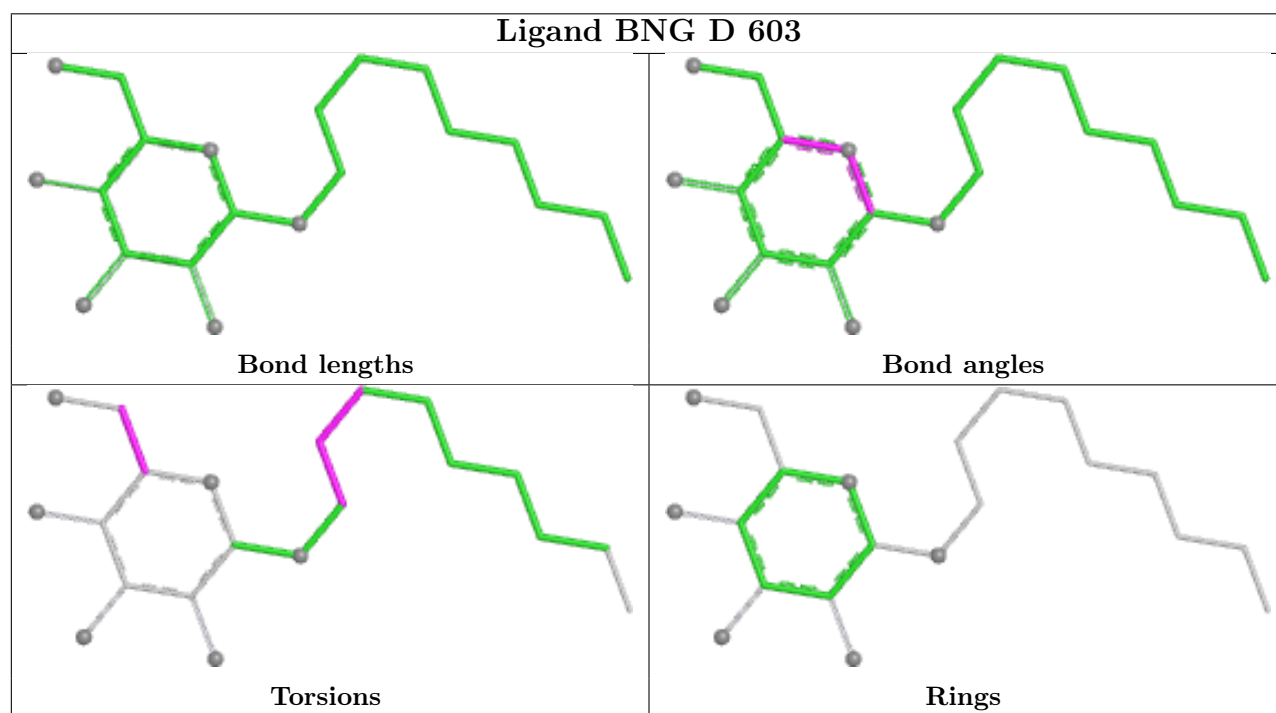
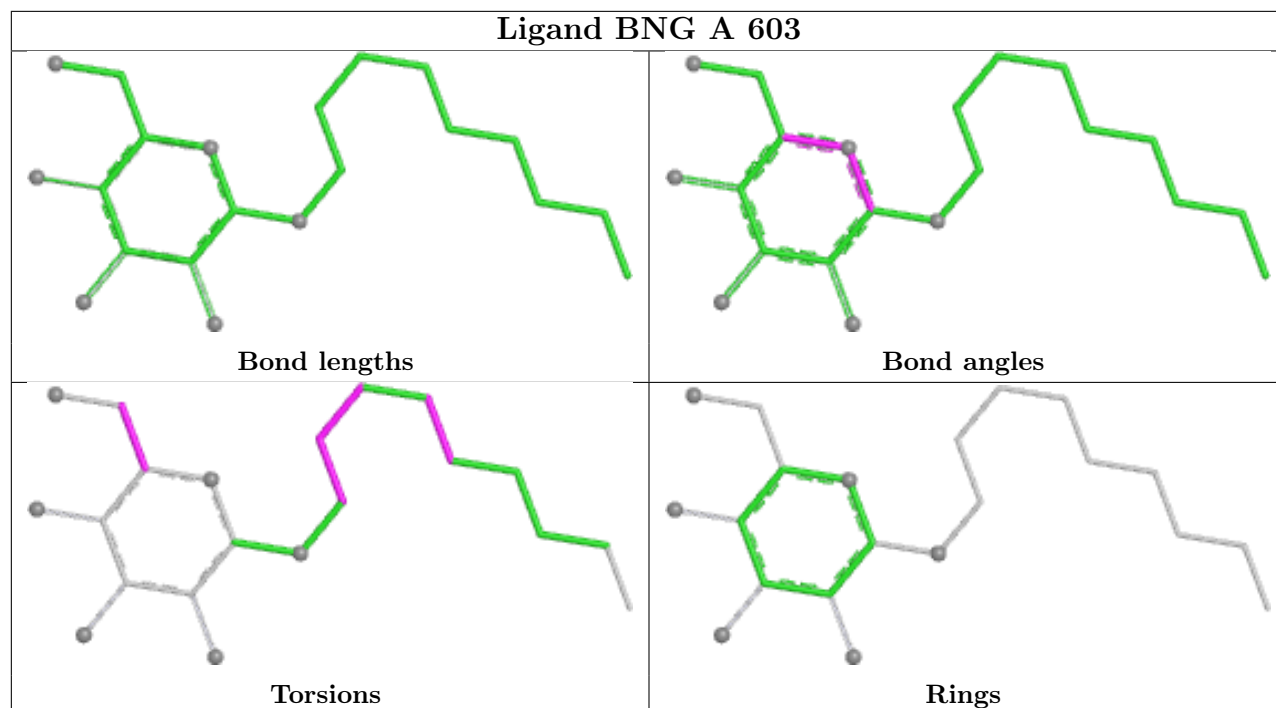


Ligand BGC C 601 (B)

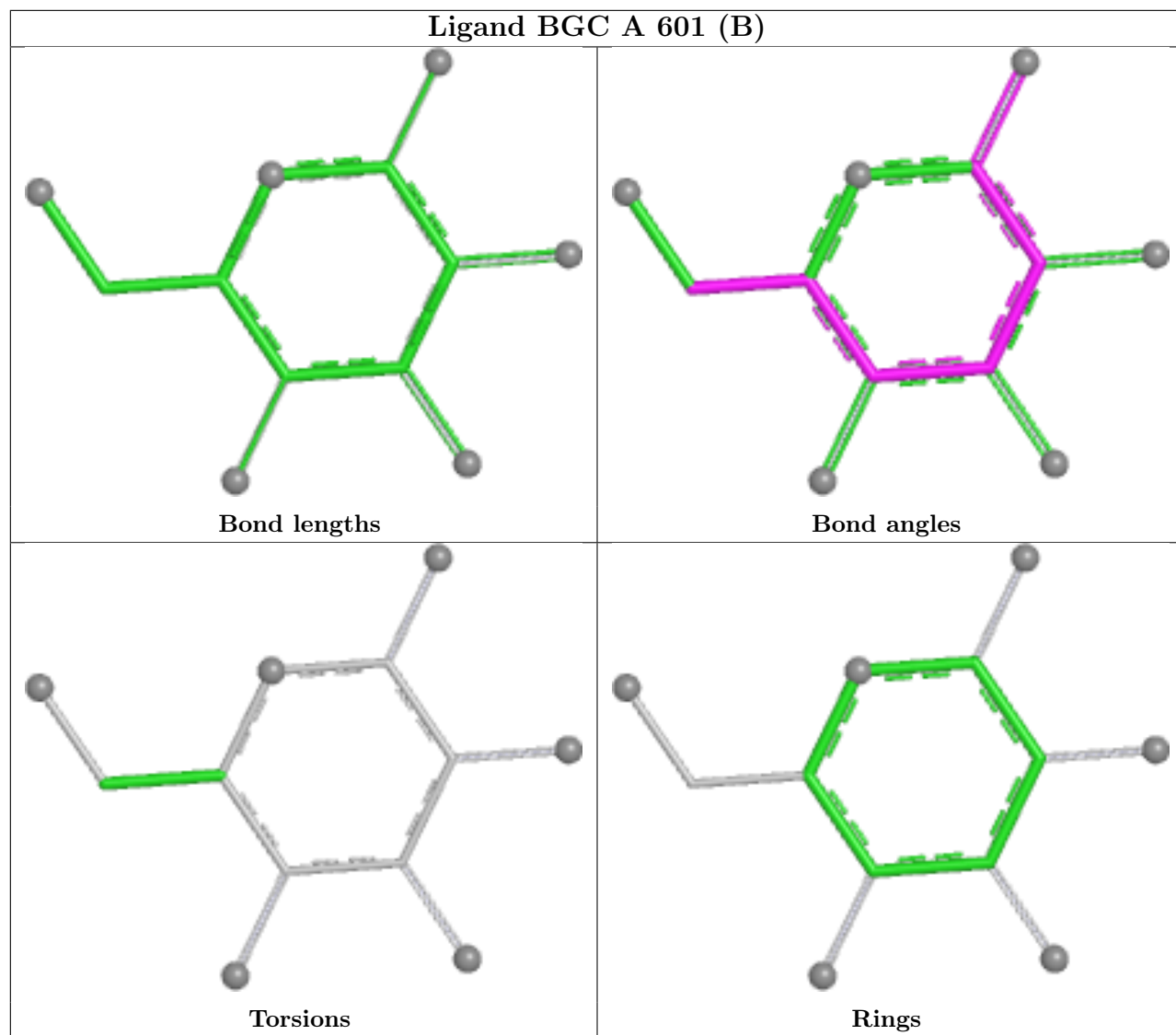




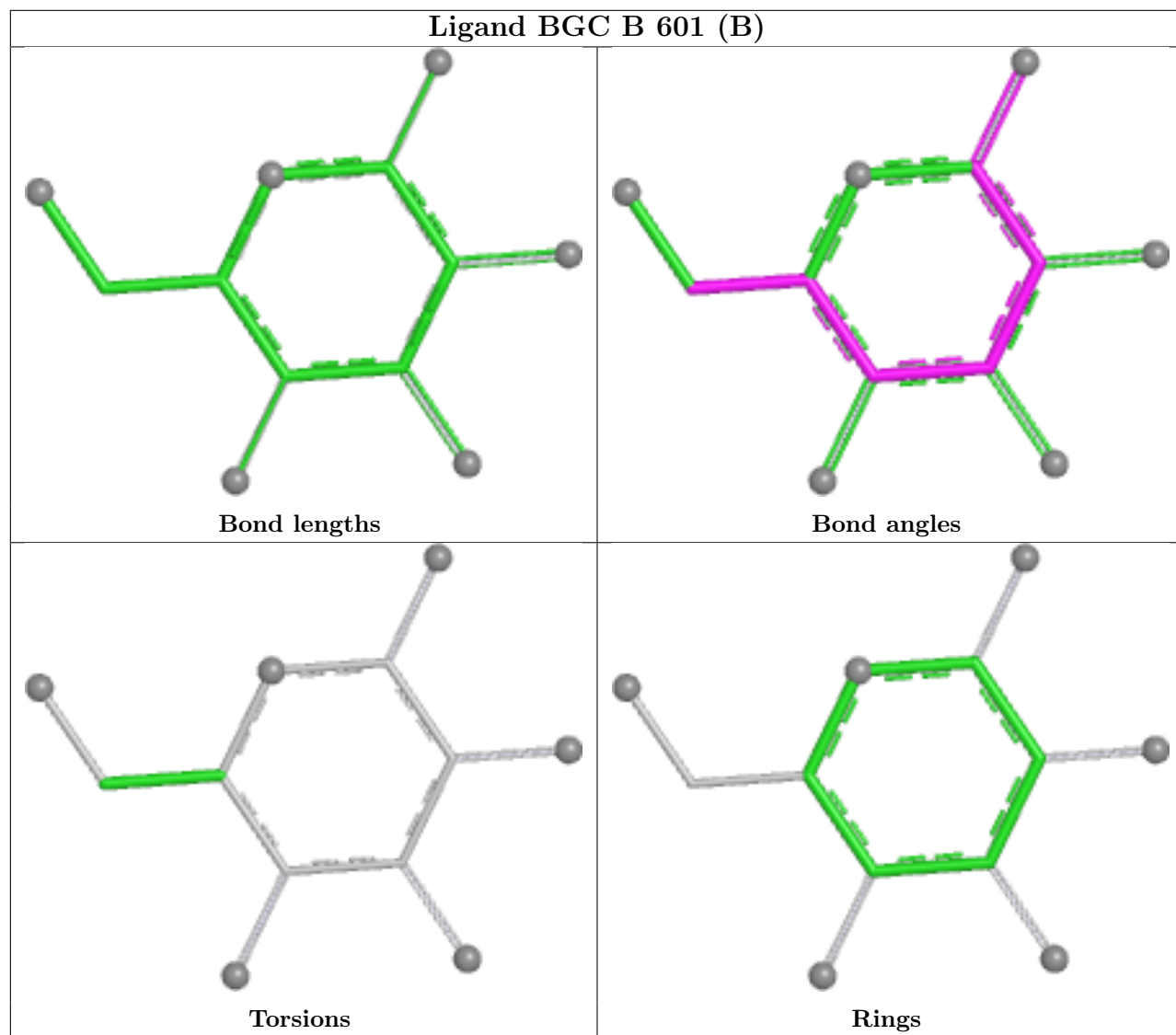


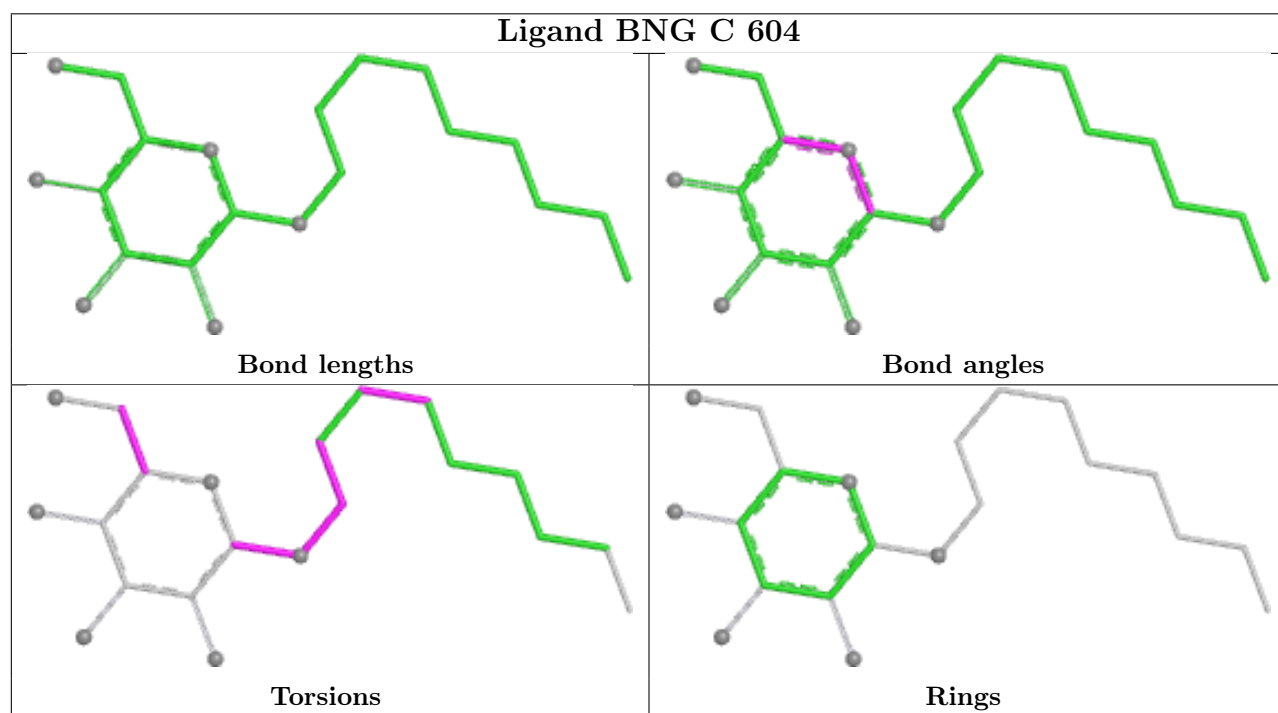
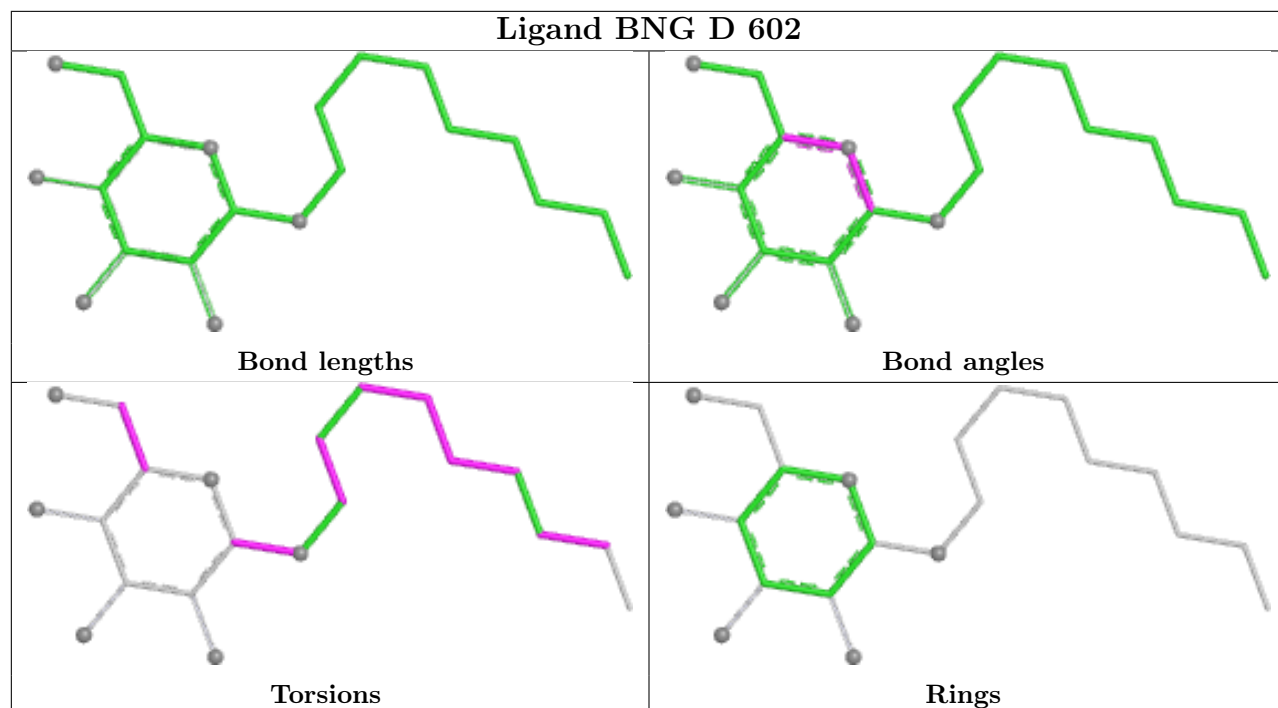


Ligand BGC A 601 (B)

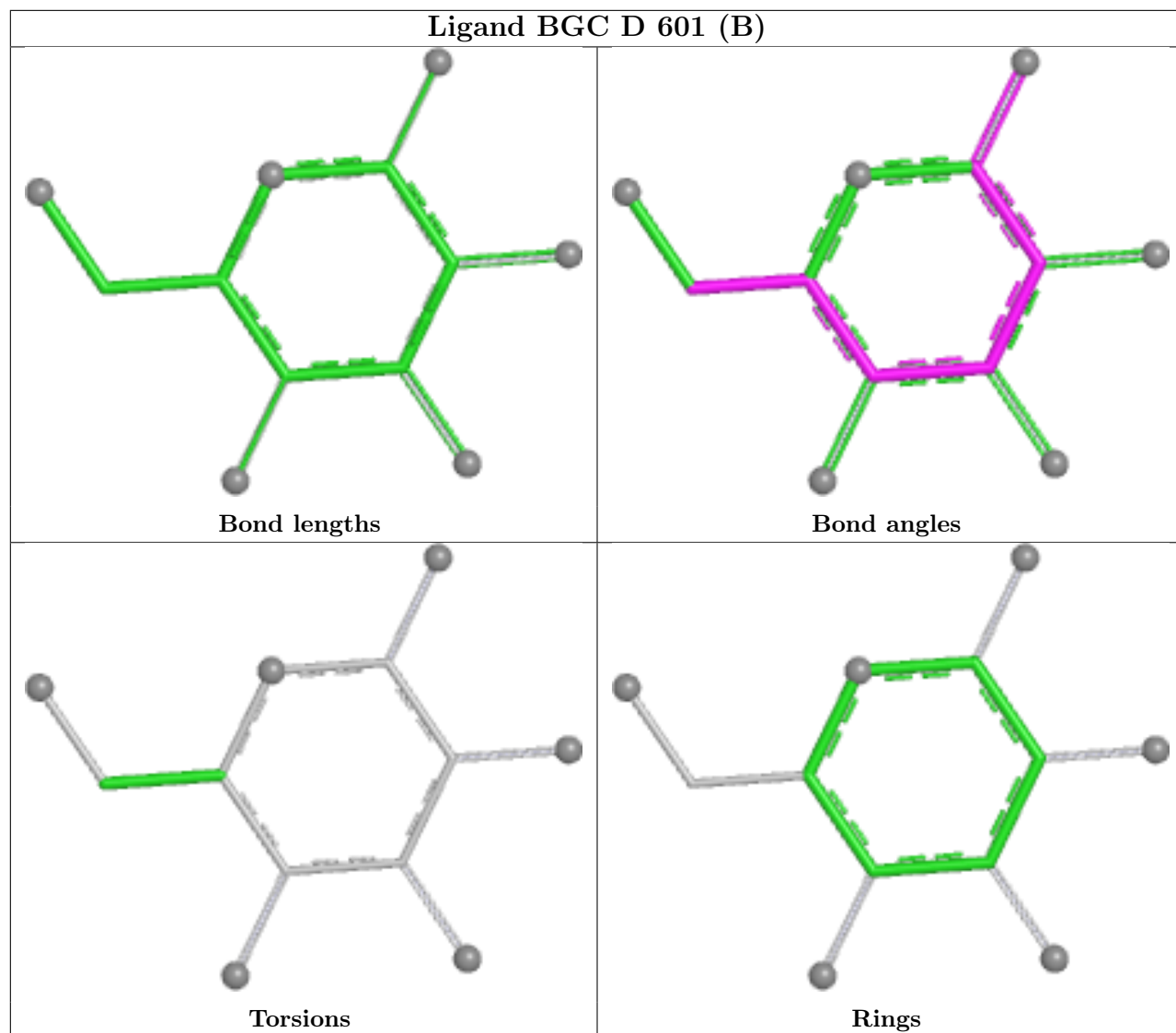


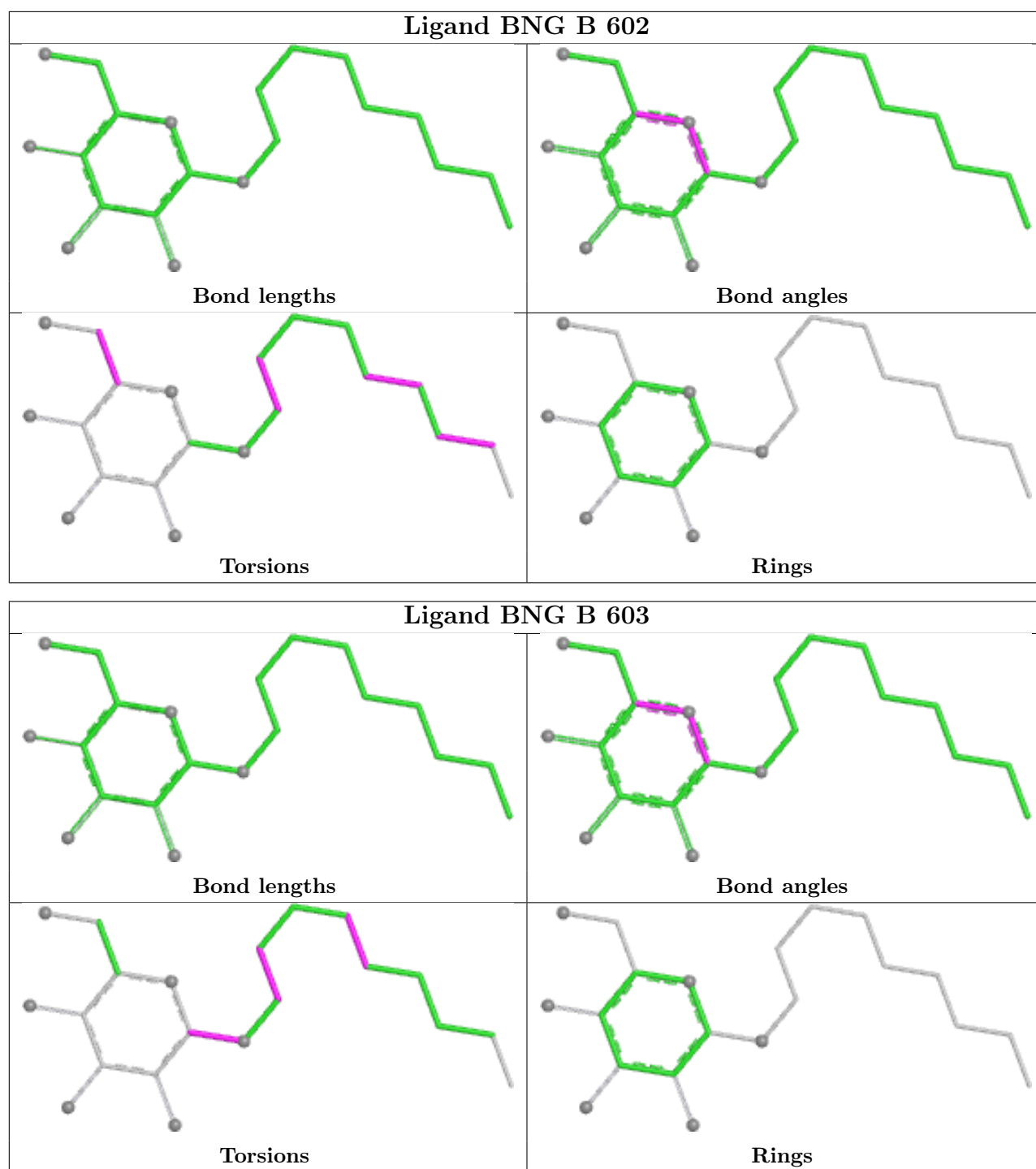
Ligand BGC B 601 (B)





Ligand BGC D 601 (B)





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	476/504 (94%)	0.60	32 (6%) 24 19	52, 71, 100, 127	0
1	B	478/504 (94%)	0.45	16 (3%) 49 43	49, 68, 100, 119	0
1	C	476/504 (94%)	1.05	68 (14%) 6 5	63, 94, 139, 161	0
1	D	478/504 (94%)	0.85	47 (9%) 13 10	62, 85, 132, 164	0
All	All	1908/2016 (94%)	0.74	163 (8%) 16 13	49, 79, 127, 164	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	272	ASN	6.1
1	D	192	ALA	5.6
1	D	193	ASP	4.9
1	D	68	LEU	4.7
1	B	499	MET	4.2
1	C	264	ALA	4.0
1	C	385	SER	3.7
1	C	484	ILE	3.7
1	C	157	HIS	3.6
1	C	482	GLY	3.6
1	C	355	LEU	3.6
1	C	423	ILE	3.5
1	B	63	GLY	3.5
1	C	158	LYS	3.5
1	D	486	THR	3.5
1	A	498	HIS	3.5
1	C	282	LEU	3.4
1	A	453	SER	3.4
1	A	383	ARG	3.4
1	C	253	TYR	3.4
1	D	322	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	63	GLY	3.3
1	C	241	ARG	3.3
1	B	66	ASP	3.3
1	C	323	GLU	3.3
1	C	481	GLY	3.2
1	C	61	CYS	3.2
1	D	257	ASN	3.2
1	C	251	LYS	3.2
1	C	289	PRO	3.1
1	C	237	PHE	3.1
1	D	253	TYR	3.1
1	D	323	GLU	3.1
1	C	486	THR	3.0
1	C	269	VAL	3.0
1	B	486	THR	3.0
1	D	194	SER	3.0
1	C	291	TYR	2.9
1	C	249	LEU	2.9
1	C	190	PRO	2.9
1	A	329	LEU	2.9
1	C	290	SER	2.9
1	C	252	ILE	2.9
1	A	486	THR	2.9
1	C	69	ASN	2.8
1	A	237	PHE	2.8
1	D	403	PHE	2.8
1	D	499	MET	2.8
1	D	386	ASN	2.8
1	C	384	ASN	2.8
1	B	498	HIS	2.8
1	D	259	ASP	2.8
1	D	479	THR	2.7
1	D	490	ILE	2.7
1	A	328	HIS	2.7
1	A	225	VAL	2.7
1	A	24	SER	2.7
1	C	68	LEU	2.7
1	A	421	SER	2.7
1	C	483	GLU	2.7
1	C	265	ILE	2.6
1	B	185	ALA	2.6
1	C	27	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	268	ALA	2.6
1	C	352	VAL	2.6
1	A	226	VAL	2.6
1	A	23	PHE	2.6
1	D	22	PHE	2.6
1	C	72	ASN	2.6
1	D	497	LYS	2.5
1	A	97	TYR	2.5
1	A	64	GLU	2.5
1	D	324	PHE	2.5
1	D	452	LYS	2.5
1	C	271	GLN	2.5
1	C	242	ILE	2.5
1	D	190	PRO	2.5
1	C	479	THR	2.5
1	A	253	TYR	2.5
1	D	481	GLY	2.5
1	C	40	PHE	2.5
1	D	69	ASN	2.4
1	C	490	ILE	2.4
1	A	487	SER	2.4
1	A	188	GLU	2.4
1	B	188	GLU	2.4
1	D	273	GLU	2.4
1	C	283	LEU	2.4
1	C	497	LYS	2.4
1	C	185	ALA	2.4
1	D	197	PRO	2.4
1	A	262	LEU	2.3
1	C	184	LEU	2.3
1	D	493	GLU	2.3
1	A	274	SER	2.3
1	C	258	VAL	2.3
1	A	452	LYS	2.3
1	D	385	SER	2.3
1	C	63	GLY	2.3
1	C	262	LEU	2.3
1	B	195	THR	2.3
1	C	359	THR	2.3
1	D	62	LYS	2.3
1	D	429	SER	2.3
1	D	484	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	233	PRO	2.2
1	C	281	SER	2.2
1	D	66	ASP	2.2
1	C	60	TRP	2.2
1	D	94	PHE	2.2
1	C	197	PRO	2.2
1	D	496	GLN	2.2
1	D	245	SER	2.2
1	C	421	SER	2.2
1	D	329	LEU	2.2
1	C	493	GLU	2.2
1	A	491	THR	2.2
1	D	61	CYS	2.2
1	A	164	TYR	2.2
1	A	488	PRO	2.2
1	D	261	PRO	2.2
1	B	189	GLY	2.2
1	A	315	SER	2.2
1	C	32	SER	2.2
1	C	426	SER	2.2
1	C	58	PHE	2.2
1	B	61	CYS	2.1
1	C	182	LEU	2.1
1	D	495	ARG	2.1
1	D	477	LYS	2.1
1	B	68	LEU	2.1
1	D	249	LEU	2.1
1	A	481	GLY	2.1
1	C	485	GLY	2.1
1	C	260	GLU	2.1
1	C	156	THR	2.1
1	D	492	MET	2.1
1	D	433	LEU	2.1
1	A	257	ASN	2.1
1	B	293	TYR	2.1
1	D	183	GLY	2.1
1	D	23	PHE	2.1
1	C	194	SER	2.1
1	D	95	SER	2.1
1	A	255	THR	2.1
1	B	496	GLN	2.1
1	B	350	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	293	TYR	2.1
1	C	478	GLU	2.0
1	C	276	LYS	2.0
1	D	389	LYS	2.0
1	B	355	LEU	2.0
1	C	286	LEU	2.0
1	C	278	ASN	2.0
1	C	382	ASN	2.0
1	D	498	HIS	2.0
1	A	189	GLY	2.0
1	A	27	PHE	2.0
1	A	319	GLU	2.0
1	C	492	MET	2.0
1	A	263	ASN	2.0
1	D	288	ILE	2.0
1	B	225	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BNG	C	604	21/21	0.57	0.21	83,94,108,114	0
3	BNG	D	604	21/21	0.75	0.15	77,91,102,106	0
3	BNG	A	604	21/21	0.77	0.15	62,77,86,92	0
3	BNG	A	605	21/21	0.80	0.15	75,85,110,127	0
3	BNG	C	603	21/21	0.83	0.16	86,97,106,109	0
3	BNG	C	605	21/21	0.86	0.11	73,84,91,98	0
3	BNG	A	603	21/21	0.86	0.17	61,78,93,102	0

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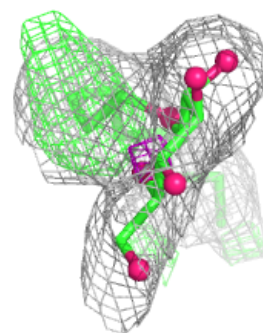
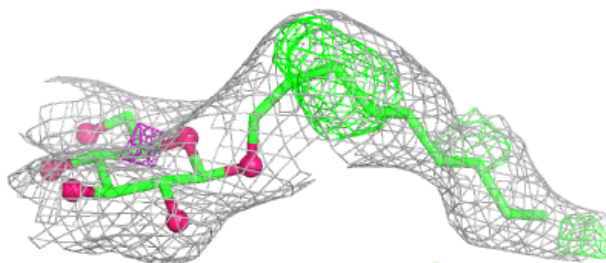
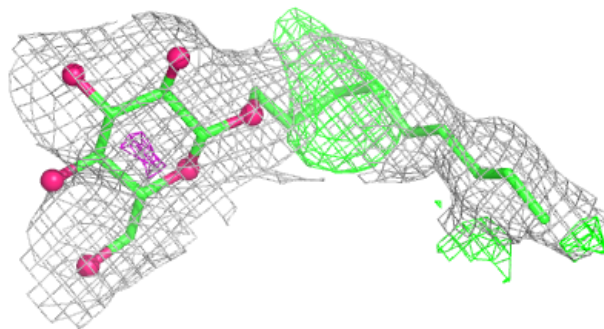
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	C	601[B]	12/12	0.87	0.12	69,75,80,80	0
3	BNG	B	603	21/21	0.87	0.13	67,79,83,86	0
3	BNG	A	602	21/21	0.87	0.13	65,76,94,101	0
3	BNG	D	602	21/21	0.88	0.15	78,99,102,104	0
3	BNG	B	602	21/21	0.88	0.14	69,82,90,103	0
2	BGC	D	601[B]	12/12	0.89	0.11	60,64,73,76	0
3	BNG	C	602	21/21	0.90	0.15	96,103,111,118	0
2	BGC	A	601[B]	12/12	0.90	0.13	58,65,72,77	0
3	BNG	D	603	21/21	0.92	0.11	77,94,106,107	0
2	BGC	B	601[B]	12/12	0.94	0.10	57,62,71,74	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.

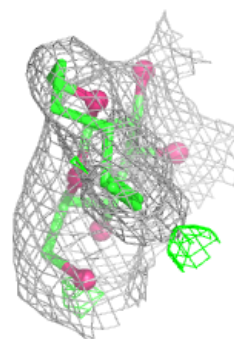
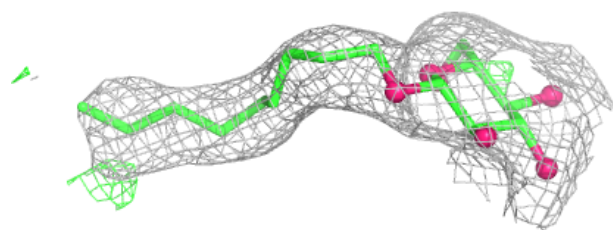
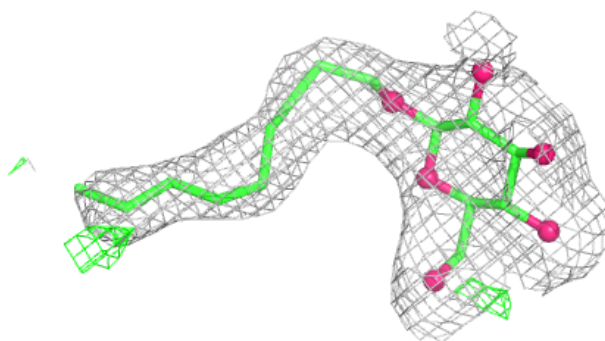
Electron density around BNG C 604:

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

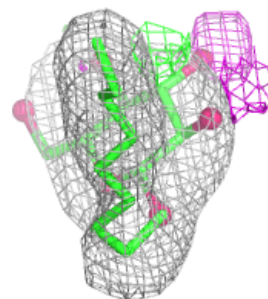
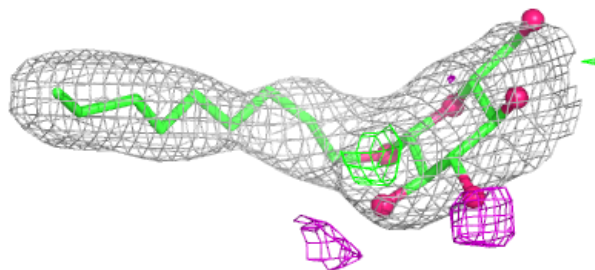
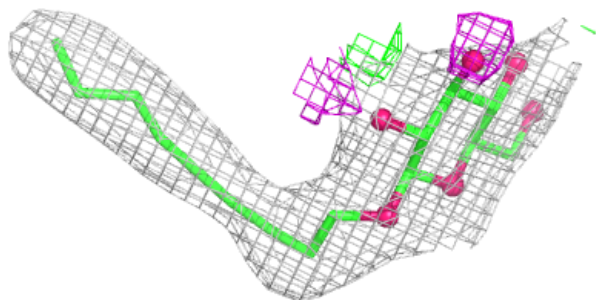


Electron density around BNG D 604:

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

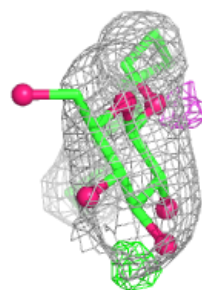
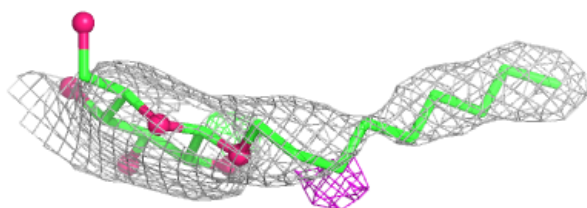
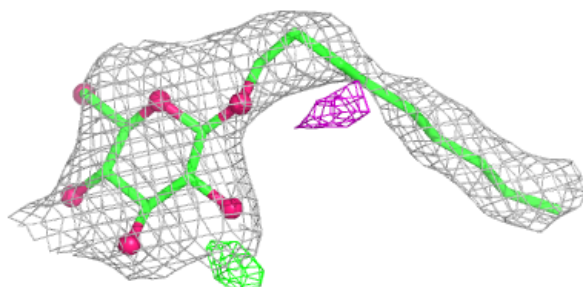
**Electron density around BNG A 604:**

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

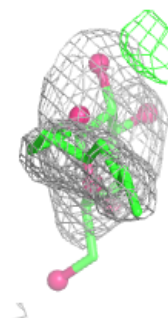
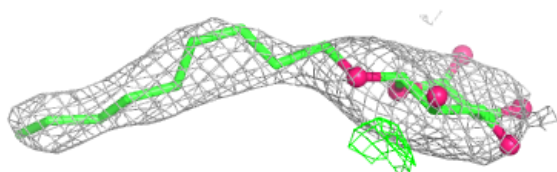
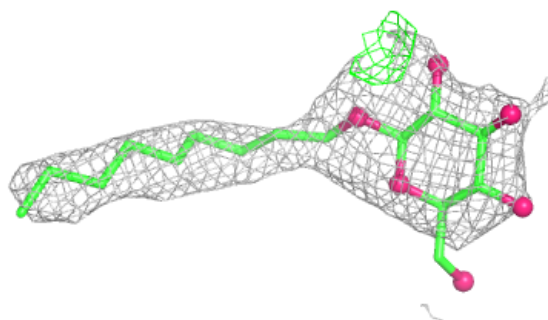


Electron density around BNG A 605:

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

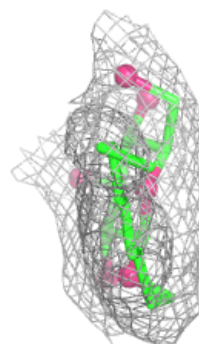
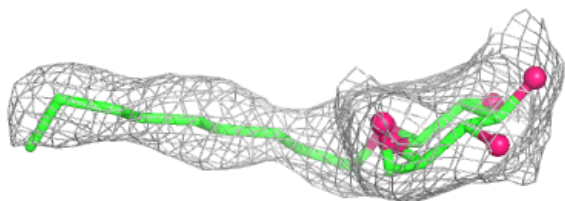
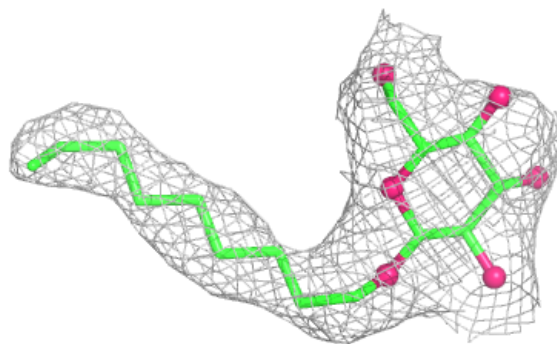
**Electron density around BNG C 603:**

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

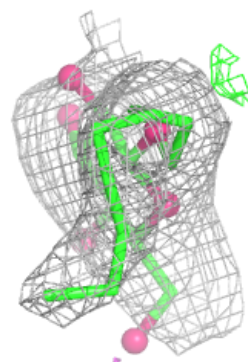
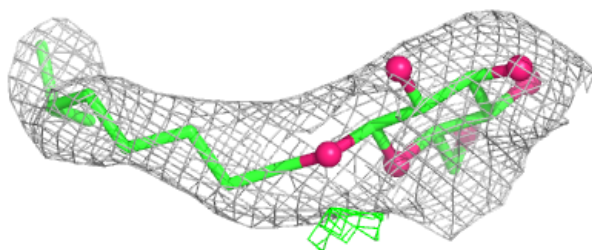
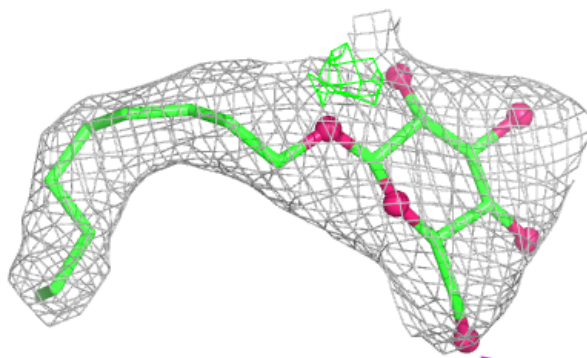


Electron density around BNG C 605:

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

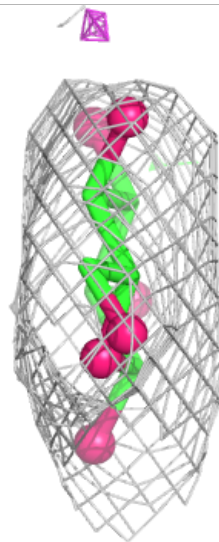
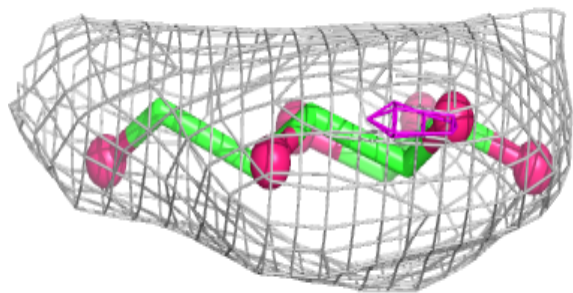
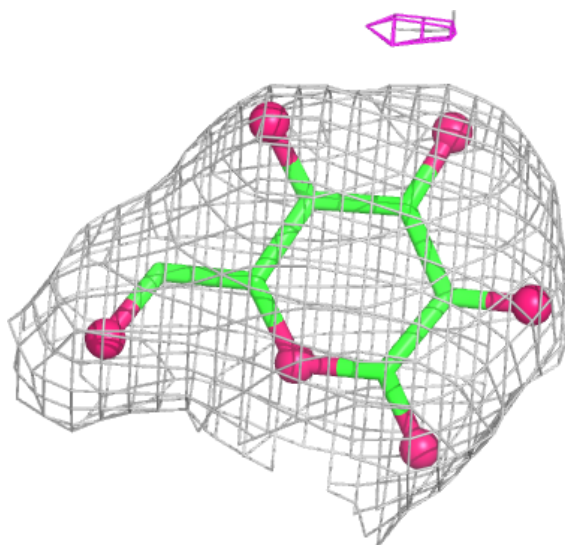
**Electron density around BNG A 603:**

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



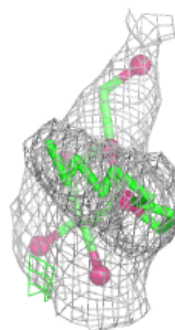
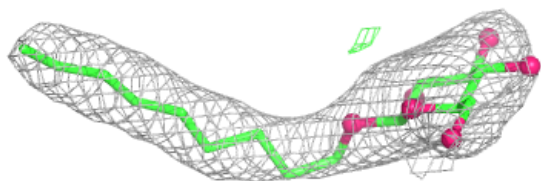
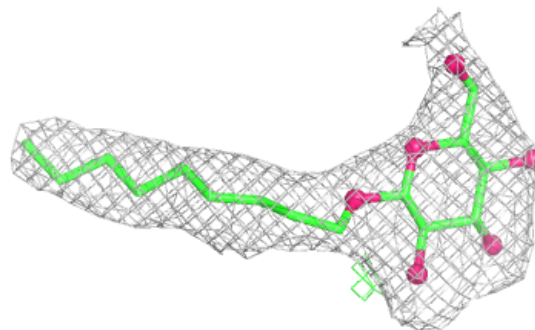
Electron density around BGC C 601 (B):

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

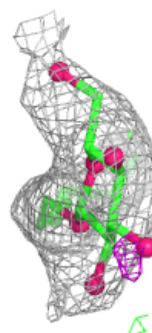
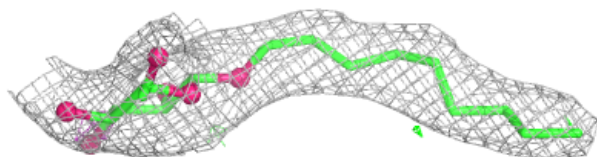
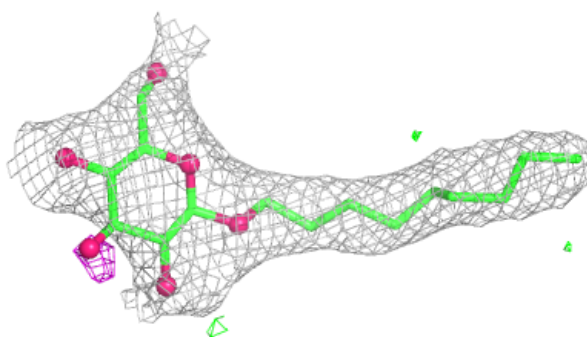


Electron density around BNG B 603:

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

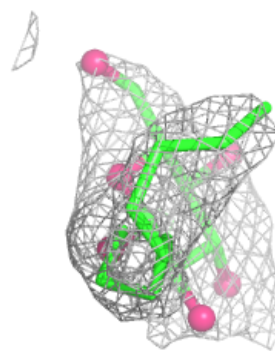
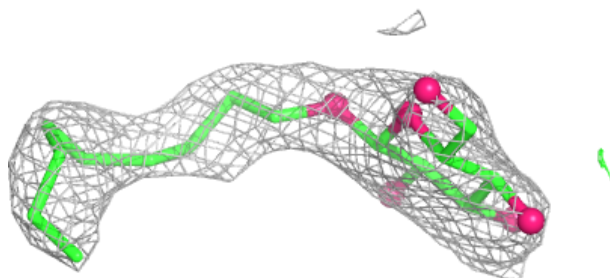
**Electron density around BNG A 602:**

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

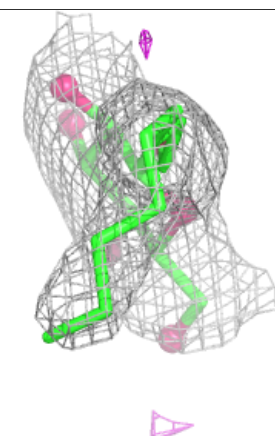
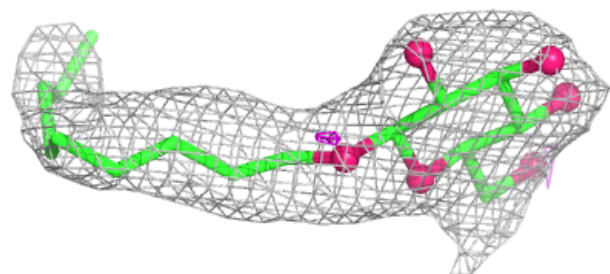


Electron density around BNG D 602:

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

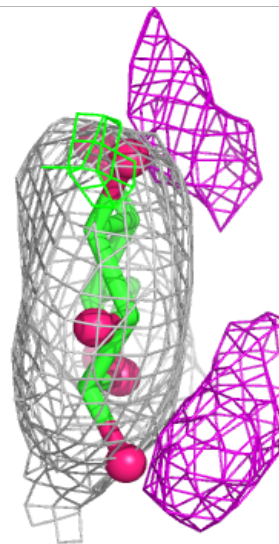
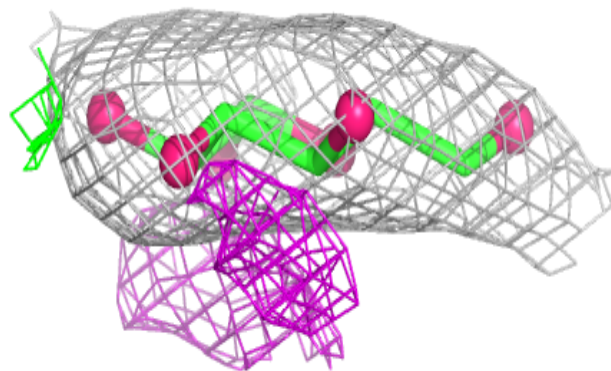
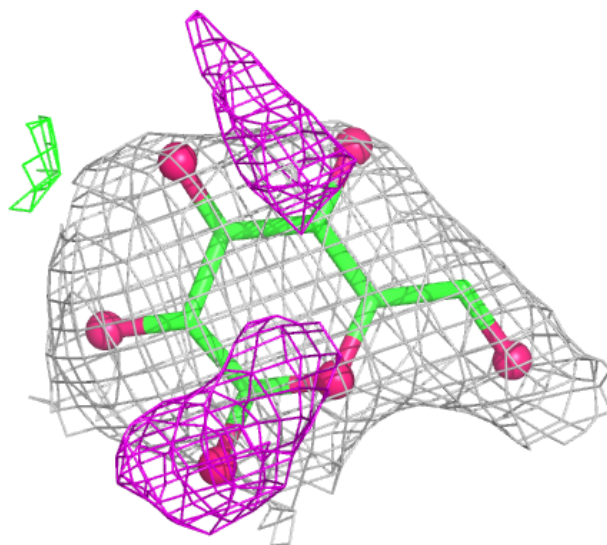
**Electron density around BNG B 602:**

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



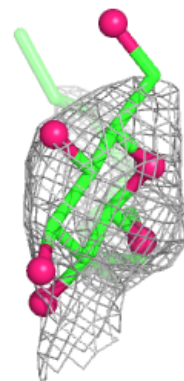
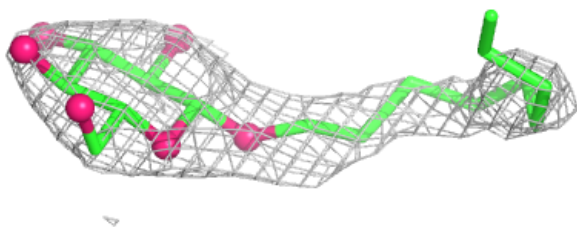
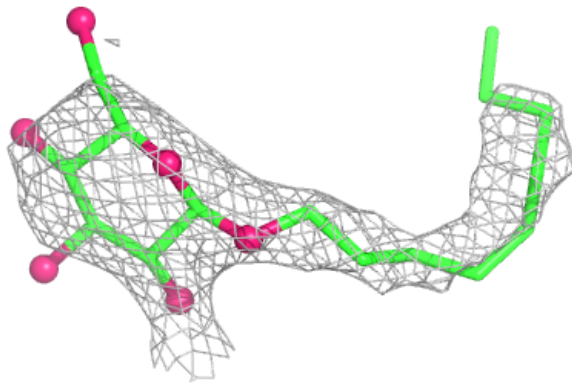
Electron density around BGC D 601 (B):

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



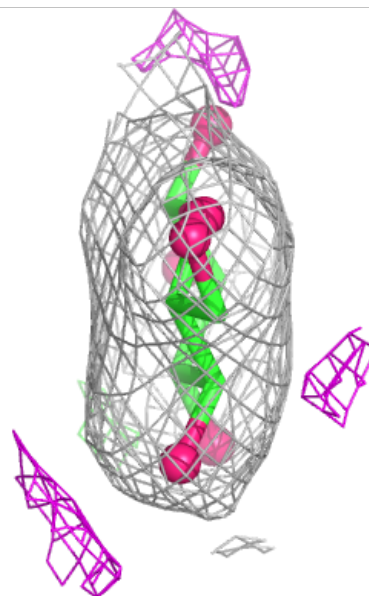
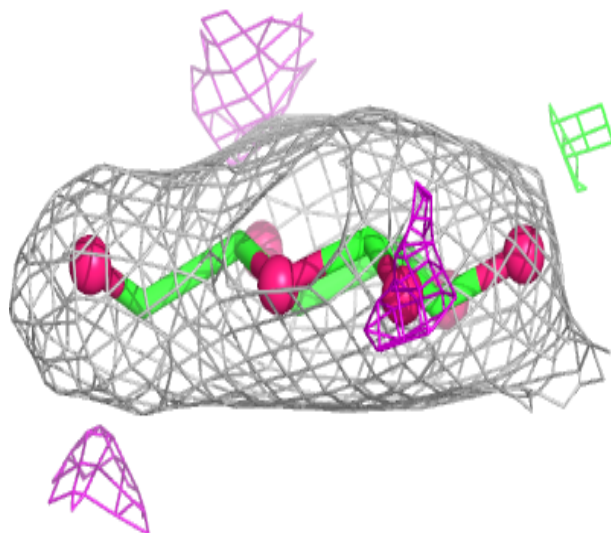
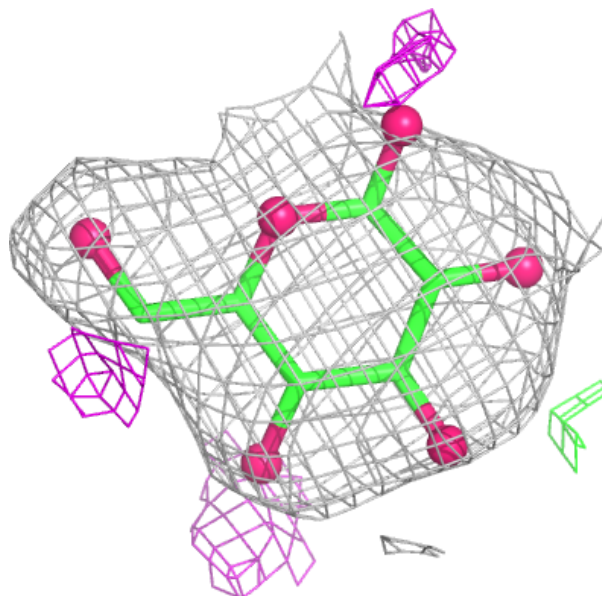
Electron density around BNG C 602:

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



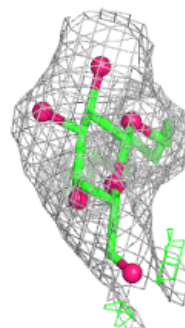
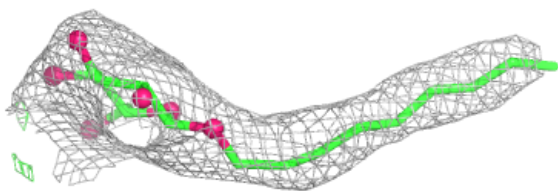
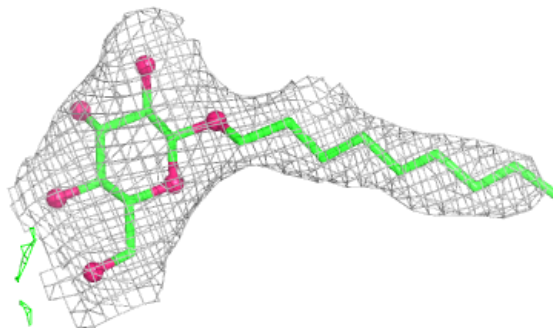
Electron density around BGC A 601 (B):

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



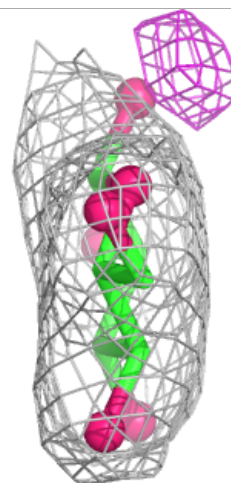
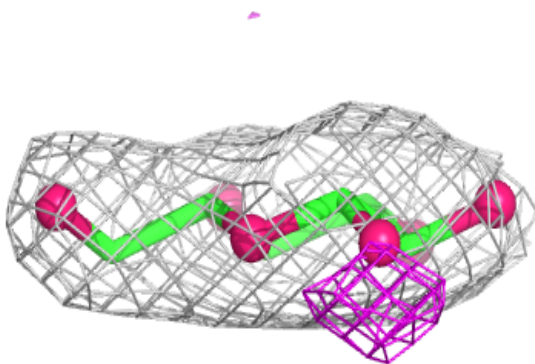
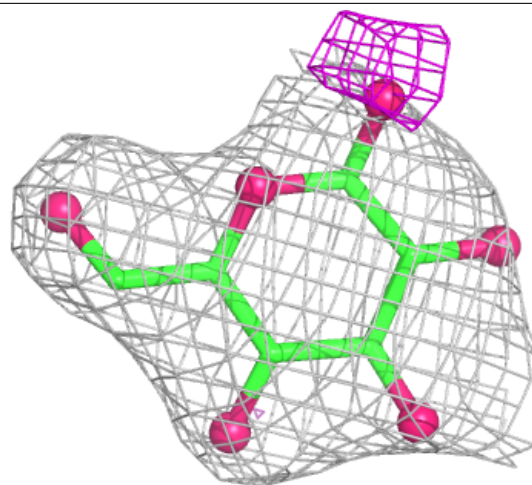
Electron density around BNG D 603:

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



Electron density around BGC B 601 (B):

$2mF_o-DF_c$ (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.