



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:42 PM BST

PDB ID : 6M20
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.2

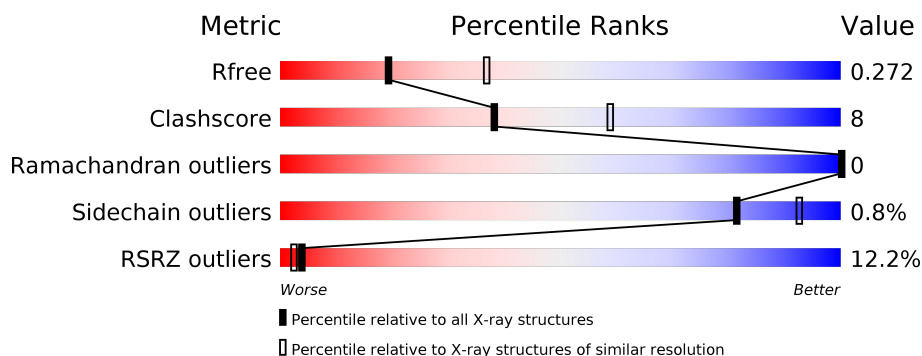
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on 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	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• 6%</div> </div> </div>
1	B	504	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>5%</div> </div> </div>
1	C	504	<div> <div>18%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>6%</div> </div> </div>
1	D	504	<div> <div>17%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>

2 Entry composition [i](#)

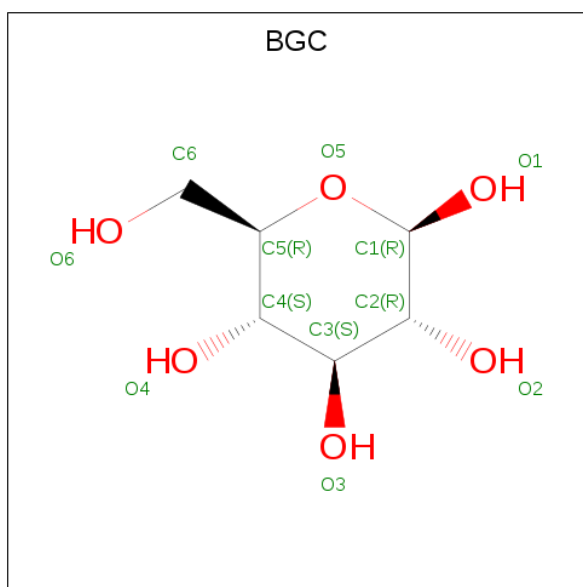
There are 4 unique types of molecules in this entry. The entry contains 15304 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: BGC) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by author).



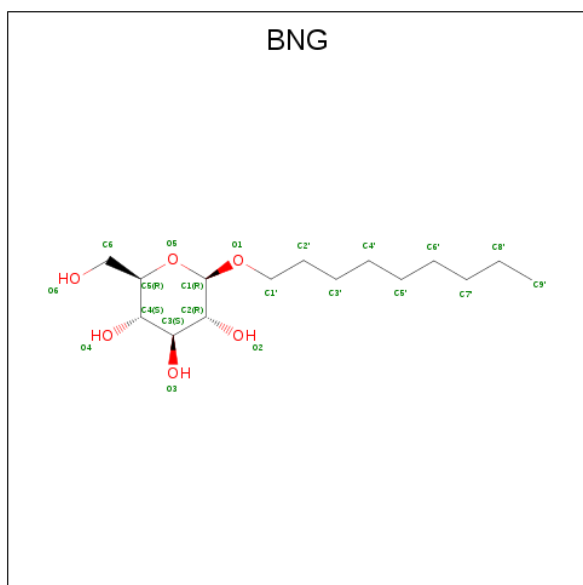
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			12	6	6		
2	B	1	Total	C	O	0	1
			12	6	6		

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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 (three-letter code: 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		

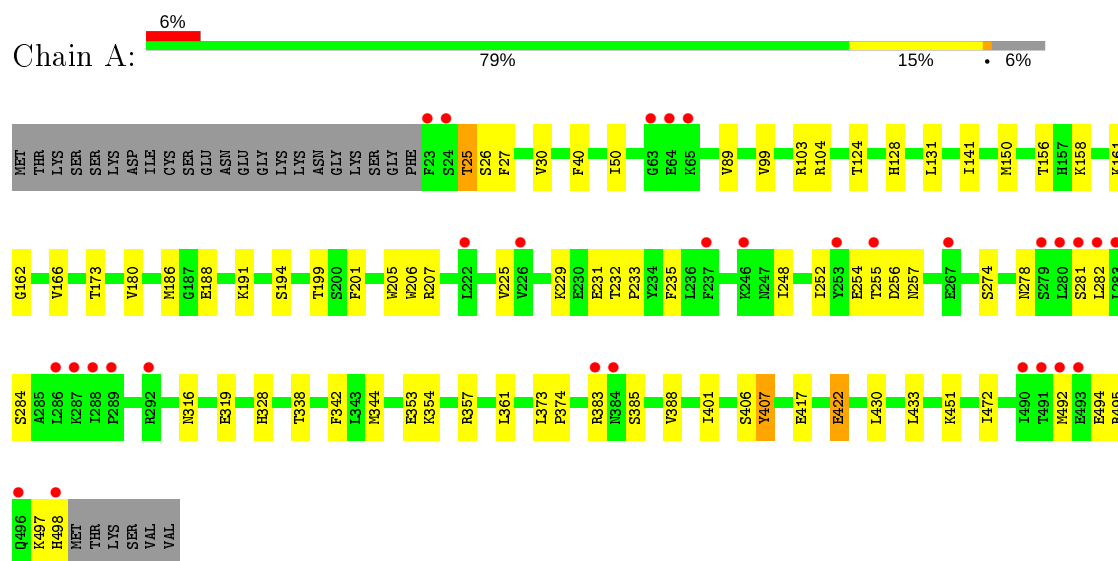
- Molecule 4 is water.

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		

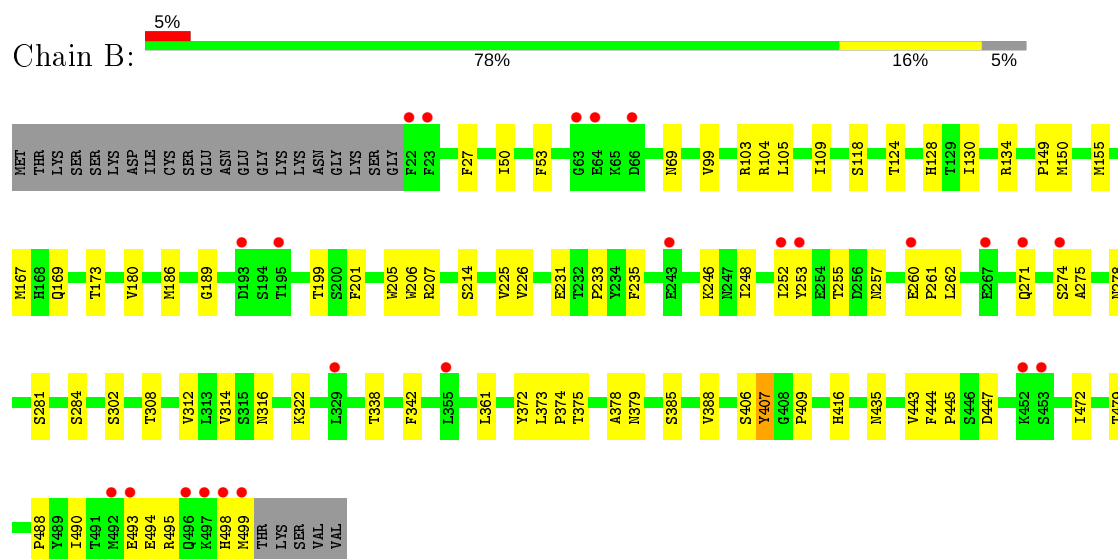
3 Residue-property plots [i](#)

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.

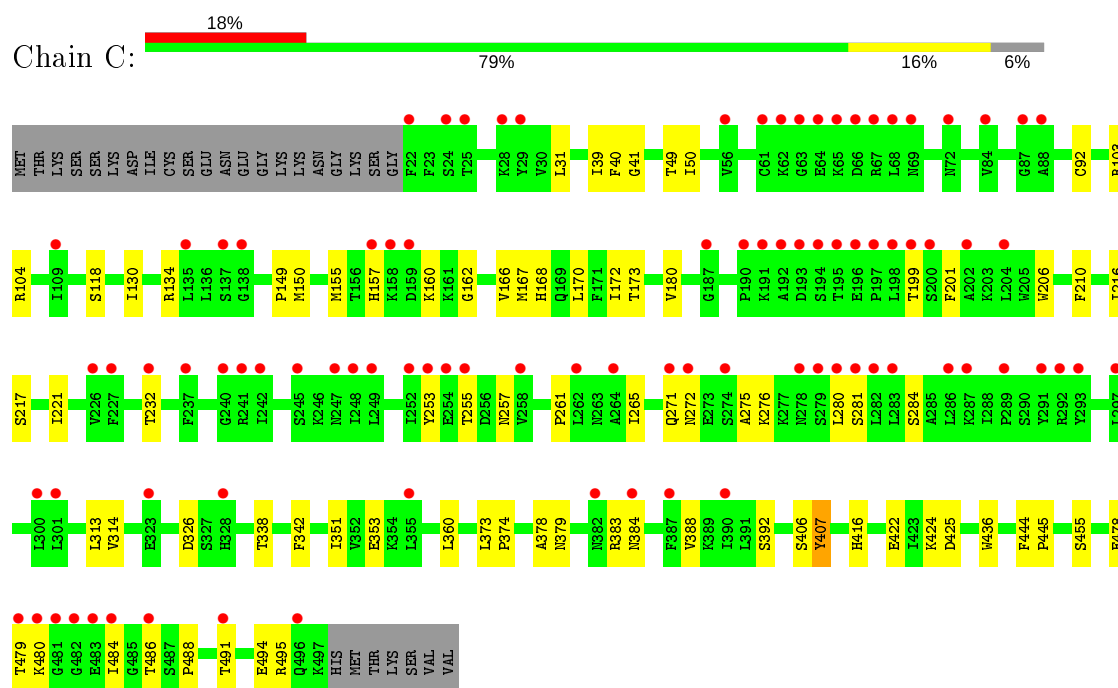
• Molecule 1: Hexose transporter 1



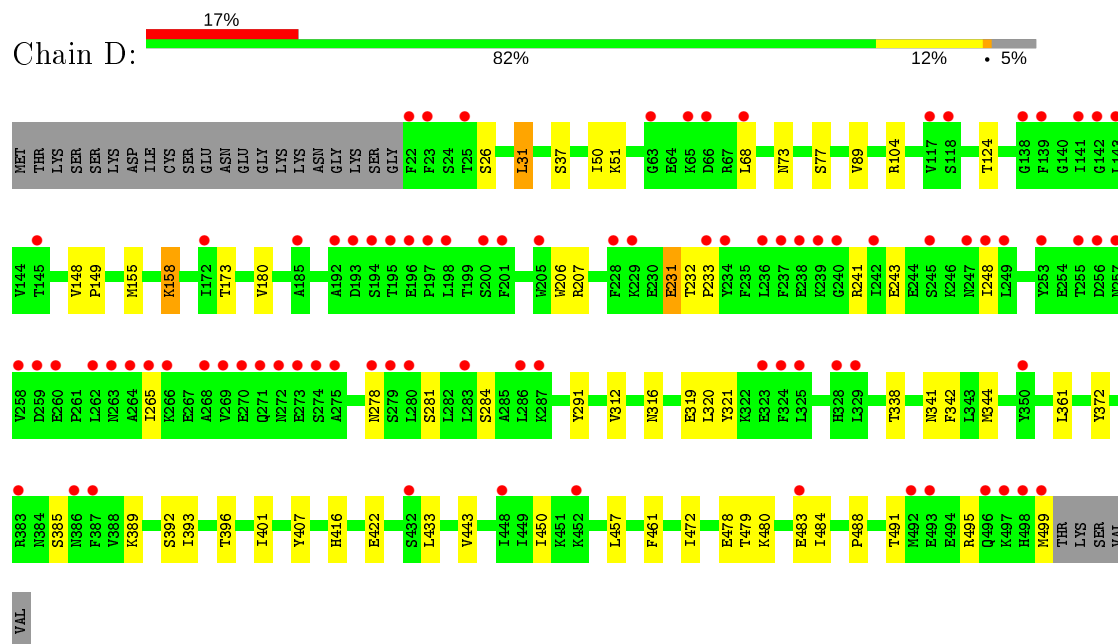
• Molecule 1: Hexose transporter 1



• 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 46.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.60) 98.6 (46.43-2.60)	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 0.254 , 0.272	Depositor DCC
R_{free} test set	4222 reflections (5.00%)	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)	0.33 , 72.9	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	0.92	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: BGC, BNG

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	0.28	0/3841	0.37	0/5213
1	B	0.23	0/3852	0.37	0/5227
1	C	0.25	0/3788	0.38	0/5152
1	D	0.26	0/3826	0.37	0/5195
All	All	0.26	0/15307	0.37	0/20787

There are no bond length outliers.

There are no bond angle outliers.

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	63	0
1	B	3759	0	3851	66	0
1	C	3696	0	3740	58	0
1	D	3733	0	3811	49	0
2	A	12	0	12	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	235	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 (235) 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	1.16	1.08
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: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:B:27:PHE:CE1	1:B:167:MET:HE1	2.08	0.88
1:D:491:THR:O	1:D:495:ARG:HG3	1.74	0.87
1:A:383:ARG:HH11	1:A:383:ARG:HG3	1.41	0.85
1:B:27:PHE:CE1	1:B:167:MET:CE	2.60	0.84
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HG2	1:A:497:LYS:O	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: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:B:27:PHE:CE1	1:B:167:MET:HE3	2.34	0.62
1:A:188:GLU:HG2	1:A:188:GLU:O	1.99	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:HG2	1:B:322:LYS:O	2.02	0.59
1:C:424:LYS:HE3	1:C:425:ASP:OD1	2.03	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:SER:HB3	1:B:388:VAL:HG23	1.87	0.57
1:D:31:LEU:O	1:D:31:LEU:HD12	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:A:357:ARG:HH11	1:A:417:GLU:CD	2.09	0.56
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:186:MET:HE2	1:B:205:TRP:HB3	1.89	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:491:THR:C	1:D:495:ARG:HG3	2.26	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:180:VAL:HG21	1:A:338:THR:HG21	1.90	0.54
1:B:275:ALA:HB2	1:B:499:MET:HE1	1.89	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: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
1:A:406:SER:OG	1:A:407:TYR:N	2.41	0.52
1:B:271:GLN:O	1:B:499:MET:HE1	2.09	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:D:158:LYS:HZ2	1:D:484:ILE:HB	1.75	0.52
1:A:131:LEU:HD23	3:A:605:BNG:H8'1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:422:GLU:H	1:A:422:GLU:CD	2.09	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:26:SER:OG	1:D:155:MET:O	2.25	0.50
1:D:173:THR:HG22	1:D:342:PHE:CB	2.41	0.49
1:D:158:LYS:HE3	1:D:483:GLU:HA	1.93	0.49
1:D:180:VAL:HG13	3:D:603:BNG:H61	1.93	0.49
1:A:27:PHE:CD1	1:A:27:PHE:C	2.85	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:B:27:PHE:CD1	1:B:167:MET:HE3	2.47	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:N	1:A:422:GLU:OE1	2.25	0.49
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: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:231:GLU:HG2	1:B:235:PHE:CD2	2.50	0.47
1:B:69:ASN:OD1	1:B:322:LYS:NZ	2.43	0.47
1:A:255:THR:HG22	1:A:257:ASN:H	1.79	0.47
1:A:492:MET:HA	1:A:495:ARG:HD3	1.97	0.47
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:MET:HE2	1:A:205:TRP:HB3	1.97	0.46
1:A:104:ARG:N	1:A:231:GLU:OE2	2.45	0.46
1:A:89:VAL:HG13	1:A:433:LEU:HG	1.98	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: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:233:PRO:HG3	1:A:248:ILE:HG23	1.97	0.45
1:A:27:PHE:CD1	1:A:27:PHE:O	2.70	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:D:319:GLU:HG3	1:D:319:GLU:O	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: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:373:LEU:HB3	1:B:374:PRO:HD3	2.00	0.44
1:B:312:VAL:HG22	1:B:443:VAL:HA	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:393:ILE:O	1:D:396:THR:OG1	2.33	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:A:25:THR:C	1:A:27:PHE:N	2.72	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:PHE:HB2	1:C:445:PRO:HD3	2.01	0.42
1:B:155:MET:HE3	1:B:252:ILE:HG21	2.01	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
3:A:604:BNG:H5'2	1:B:128:HIS:CD2	2.55	0.41
1:A:254:GLU:HG2	1:C:384:ASN:ND2	2.35	0.41
1:D:243:GLU:OE2	1:D:243:GLU:HA	2.19	0.41
1:D:281:SER:H	1:D:284:SER:HG	1.59	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:344:MET:HG3	1:D:401:ILE:HG12	2.01	0.41
1:D:50:ILE:H	1:D:50:ILE:HG13	1.80	0.41
1:A:354:LYS:HD2	1:A:354:LYS:HA	1.92	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:351:ILE:HG21	1:C:360:LEU:HD13	2.03	0.41
1:A:353:GLU:OE2	1:A:353:GLU:HA	2.21	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:C:92:CYS:HG	1:C:436:TRP:HD1	1.69	0.41
1:A:225:VAL:O	1:A:229:LYS:NZ	2.54	0.41
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:186:MET:HE1	1:B:206:TRP:HB3	2.04	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:444:PHE:HB2	1:B:445:PRO:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	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 [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	416/447 (93%)	413 (99%)	3 (1%)	84	94
1	B	416/447 (93%)	414 (100%)	2 (0%)	88	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	402/447 (90%)	399 (99%)	3 (1%)	84	94
1	D	409/447 (92%)	404 (99%)	5 (1%)	71	87
All	All	1643/1788 (92%)	1630 (99%)	13 (1%)	81	92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	THR
1	A	407	TYR
1	A	422	GLU
1	B	407	TYR
1	B	493	GLU
1	C	31	LEU
1	C	40	PHE
1	C	407	TYR
1	D	31	LEU
1	D	158	LYS
1	D	231	GLU
1	D	241	ARG
1	D	407	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	416	HIS
1	B	128	HIS
1	B	168	HIS
1	B	271	GLN
1	D	278	ASN
1	D	306	GLN
1	D	311	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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	D	603	-	21,21,21	0.48	0	26,26,26	0.85	1 (3%)
3	BNG	D	604	-	21,21,21	0.49	0	26,26,26	0.83	1 (3%)
3	BNG	C	602	-	21,21,21	0.47	0	26,26,26	0.92	1 (3%)
2	BGC	B	601[B]	-	12,12,12	1.09	0	17,17,17	1.68	4 (23%)
3	BNG	C	604	-	21,21,21	0.47	0	26,26,26	0.83	1 (3%)
3	BNG	C	603	-	21,21,21	0.47	0	26,26,26	0.87	1 (3%)
3	BNG	B	603	-	21,21,21	0.51	0	26,26,26	0.89	1 (3%)
3	BNG	A	603	-	21,21,21	0.48	0	26,26,26	0.86	1 (3%)
3	BNG	A	604	-	21,21,21	0.47	0	26,26,26	0.88	1 (3%)
3	BNG	D	602	-	21,21,21	0.50	0	26,26,26	0.91	1 (3%)
3	BNG	B	602	-	21,21,21	0.48	0	26,26,26	0.91	1 (3%)
2	BGC	A	601[B]	-	12,12,12	1.10	0	17,17,17	1.67	4 (23%)
3	BNG	A	605	-	21,21,21	0.52	0	26,26,26	1.09	1 (3%)
3	BNG	C	605	-	21,21,21	0.48	0	26,26,26	0.80	1 (3%)
2	BGC	D	601[B]	-	12,12,12	1.08	0	17,17,17	1.67	4 (23%)
2	BGC	C	601[B]	-	12,12,12	1.07	0	17,17,17	1.66	5 (29%)
3	BNG	A	602	-	21,21,21	0.47	0	26,26,26	0.87	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	D	603	-	-	4/12/32/32	0/1/1/1
3	BNG	D	604	-	-	3/12/32/32	0/1/1/1
3	BNG	C	602	-	-	9/12/32/32	0/1/1/1
2	BGC	B	601[B]	-	-	0/2/22/22	0/1/1/1
3	BNG	C	604	-	-	5/12/32/32	0/1/1/1
3	BNG	C	603	-	-	3/12/32/32	0/1/1/1
3	BNG	B	603	-	-	4/12/32/32	0/1/1/1
3	BNG	A	603	-	-	5/12/32/32	0/1/1/1
3	BNG	A	604	-	-	7/12/32/32	0/1/1/1
3	BNG	D	602	-	-	8/12/32/32	0/1/1/1
3	BNG	B	602	-	-	4/12/32/32	0/1/1/1
2	BGC	A	601[B]	-	-	0/2/22/22	0/1/1/1
3	BNG	A	605	-	-	2/12/32/32	0/1/1/1
3	BNG	C	605	-	-	1/12/32/32	0/1/1/1
2	BGC	D	601[B]	-	-	0/2/22/22	0/1/1/1
2	BGC	C	601[B]	-	-	0/2/22/22	0/1/1/1
3	BNG	A	602	-	-	6/12/32/32	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	-3.51	106.79	113.69
2	C	601[B]	BGC	C6-C5-C4	-3.32	105.23	113.00
2	D	601[B]	BGC	C6-C5-C4	-3.21	105.50	113.00
2	B	601[B]	BGC	C6-C5-C4	-3.18	105.55	113.00
2	A	601[B]	BGC	C6-C5-C4	-3.17	105.57	113.00
3	D	602	BNG	C1-O5-C5	-3.11	107.58	113.69
2	A	601[B]	BGC	C1-C2-C3	-3.03	104.03	110.31
3	A	602	BNG	C1-O5-C5	-2.99	107.82	113.69
2	B	601[B]	BGC	C1-C2-C3	-2.93	104.23	110.31
2	D	601[B]	BGC	C1-C2-C3	-2.91	104.28	110.31
3	C	603	BNG	C1-O5-C5	-2.85	108.09	113.69
3	C	602	BNG	C1-O5-C5	-2.82	108.15	113.69
3	A	603	BNG	C1-O5-C5	-2.81	108.17	113.69
3	D	603	BNG	C1-O5-C5	-2.78	108.23	113.69
3	B	602	BNG	C1-O5-C5	-2.78	108.23	113.69
2	C	601[B]	BGC	C1-C2-C3	-2.68	104.76	110.31
3	D	604	BNG	C1-O5-C5	-2.56	108.66	113.69
2	C	601[B]	BGC	O1-C1-C2	-2.55	101.86	109.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	604	BNG	C1-O5-C5	-2.53	108.72	113.69
2	A	601[B]	BGC	O1-C1-C2	-2.46	102.10	109.03
2	D	601[B]	BGC	O1-C1-C2	-2.46	102.11	109.03
2	B	601[B]	BGC	O1-C1-C2	-2.44	102.17	109.03
2	A	601[B]	BGC	C4-C3-C2	-2.43	106.58	110.82
3	A	604	BNG	C1-O5-C5	-2.39	109.00	113.69
3	C	605	BNG	C1-O5-C5	-2.34	109.10	113.69
2	D	601[B]	BGC	C4-C3-C2	-2.30	106.81	110.82
2	B	601[B]	BGC	C4-C3-C2	-2.30	106.81	110.82
2	C	601[B]	BGC	C4-C3-C2	-2.13	107.11	110.82
3	B	603	BNG	C1-O5-C5	-2.05	109.67	113.69
2	C	601[B]	BGC	O3-C3-C4	-2.03	105.65	110.35

There are no chirality outliers.

All (61) torsion outliers are listed below:

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

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

There are no ring outliers.

9 monomers are involved in 18 short contacts:

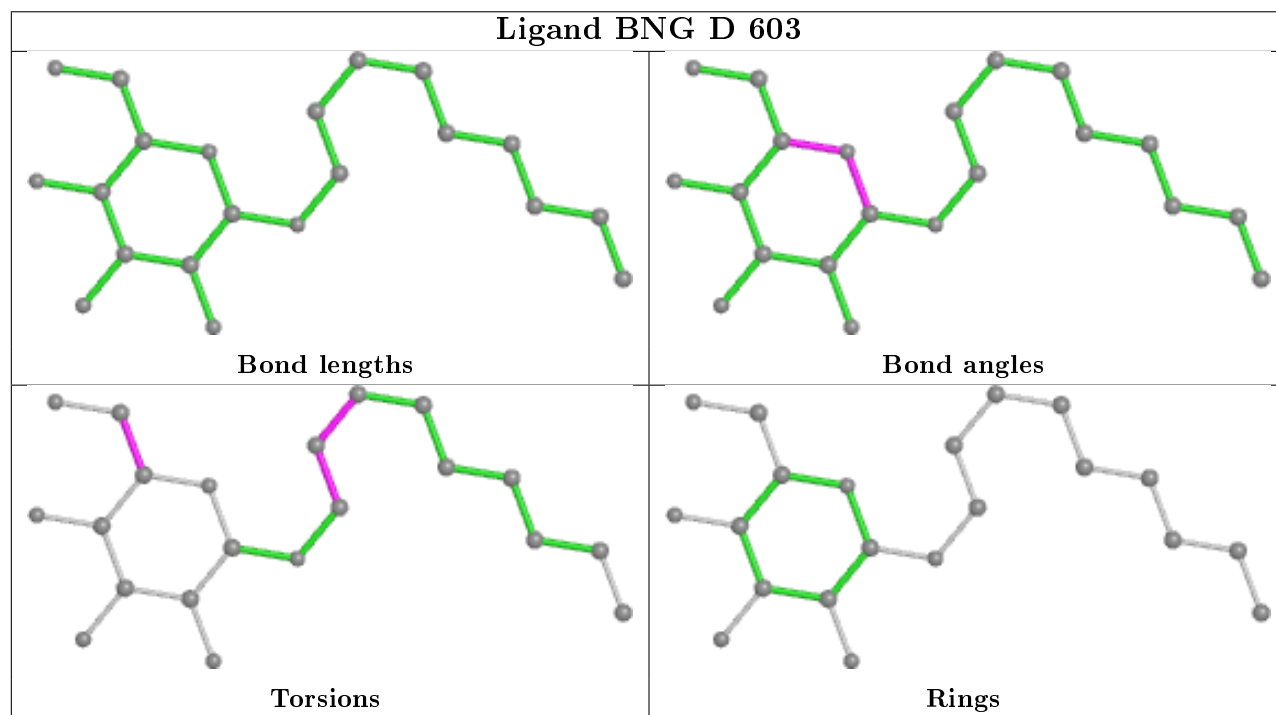
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	603	BNG	1	0

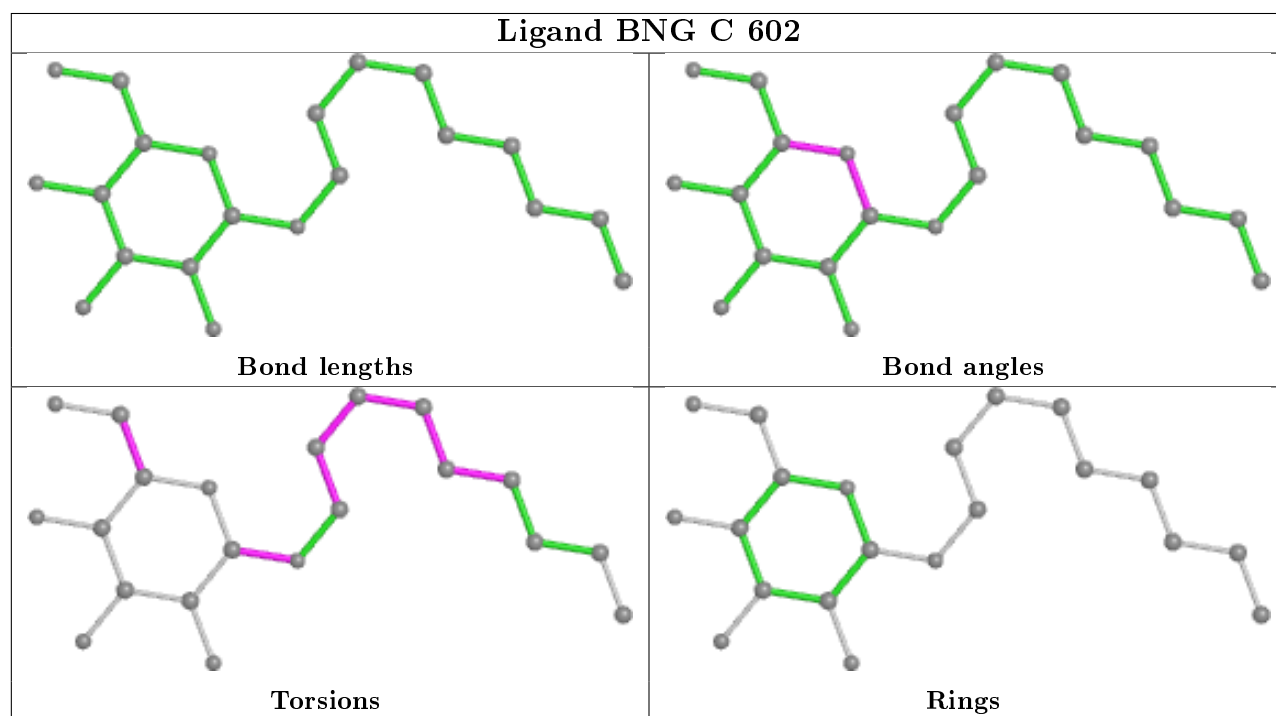
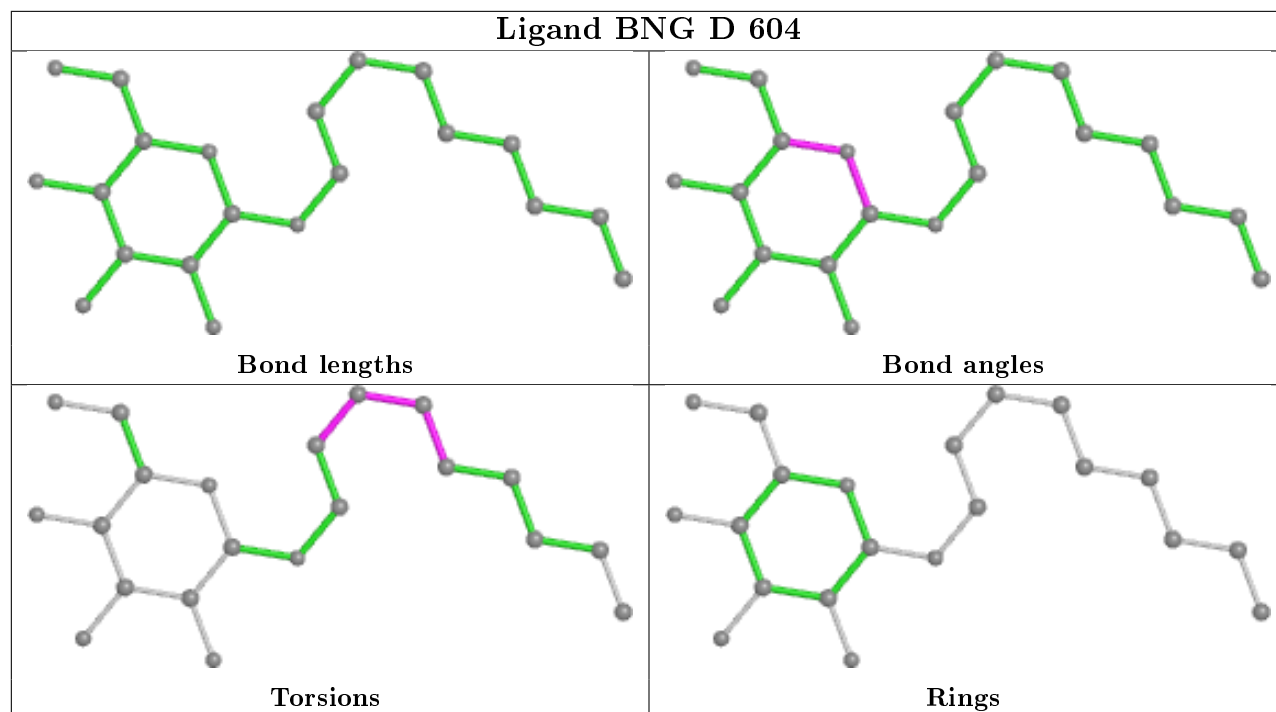
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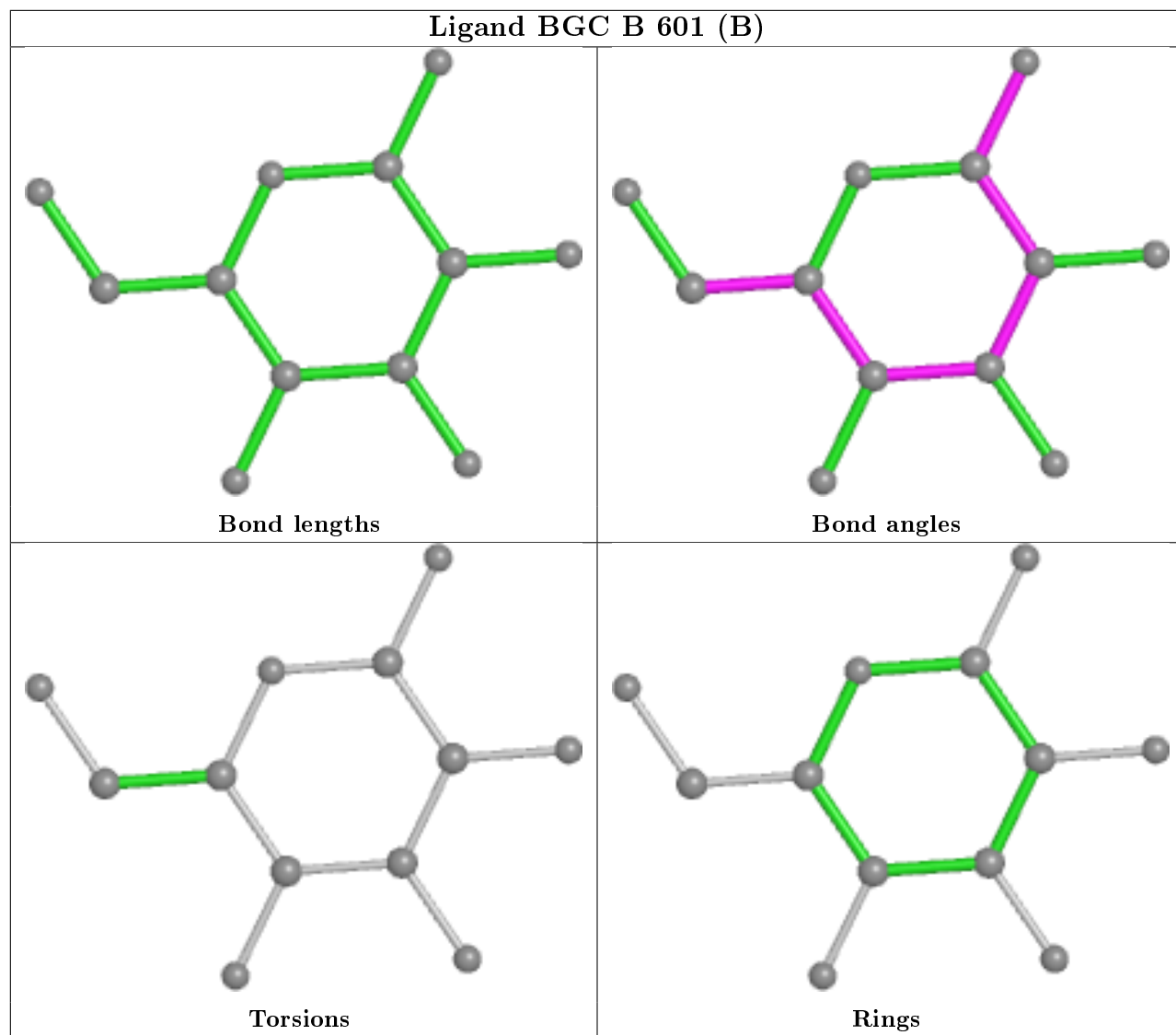
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	BNG	1	0
3	C	604	BNG	1	0
3	C	603	BNG	5	0
3	B	603	BNG	1	0
3	A	603	BNG	1	0
3	A	604	BNG	3	0
3	D	602	BNG	3	0
3	A	605	BNG	2	0

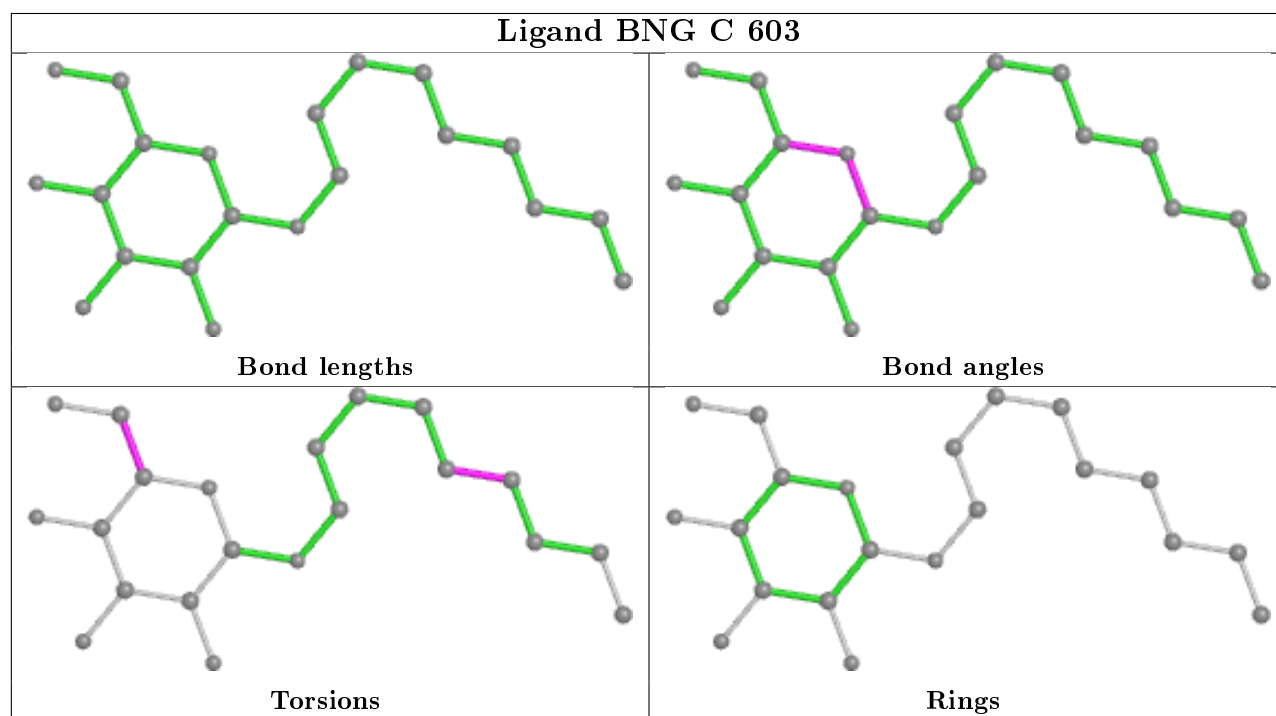
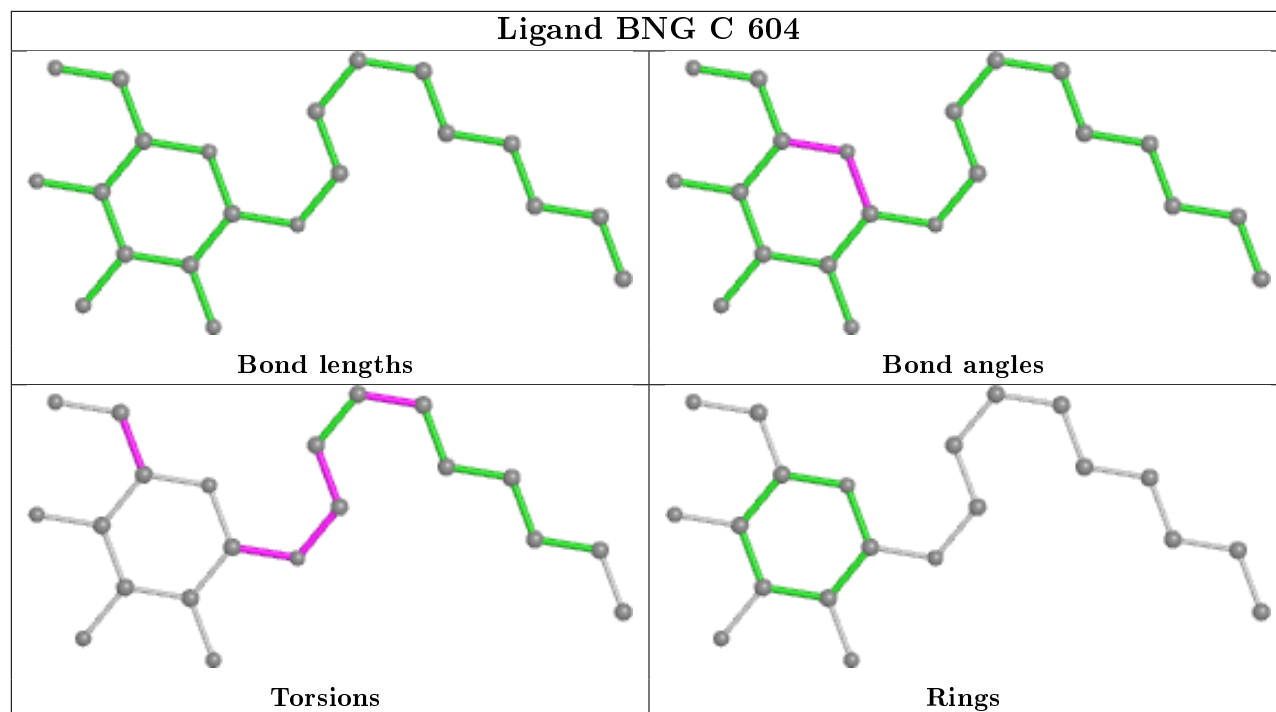
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

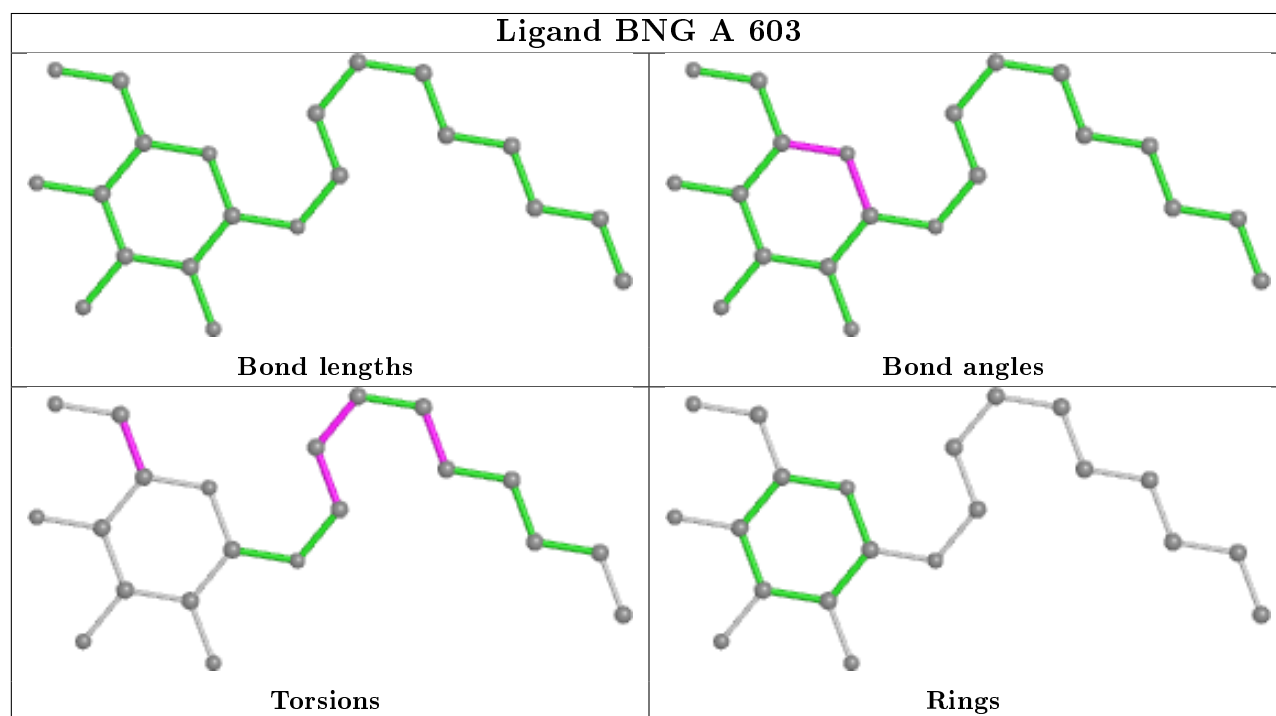
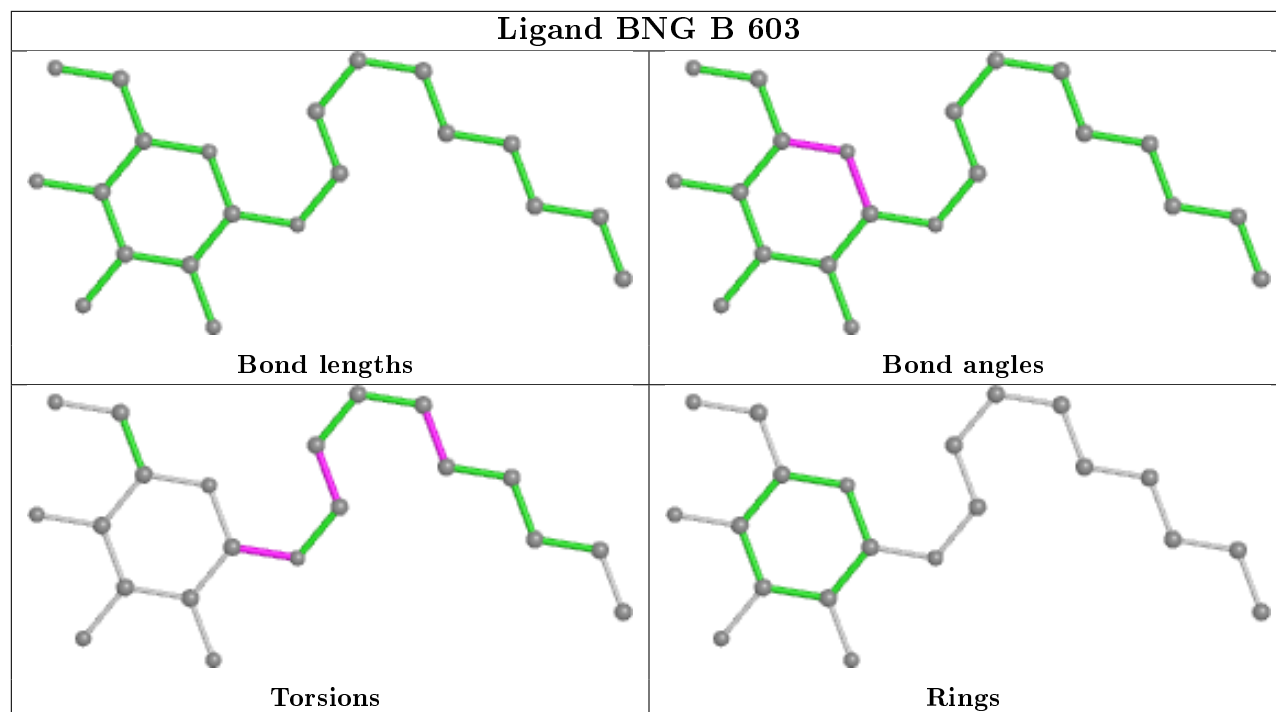


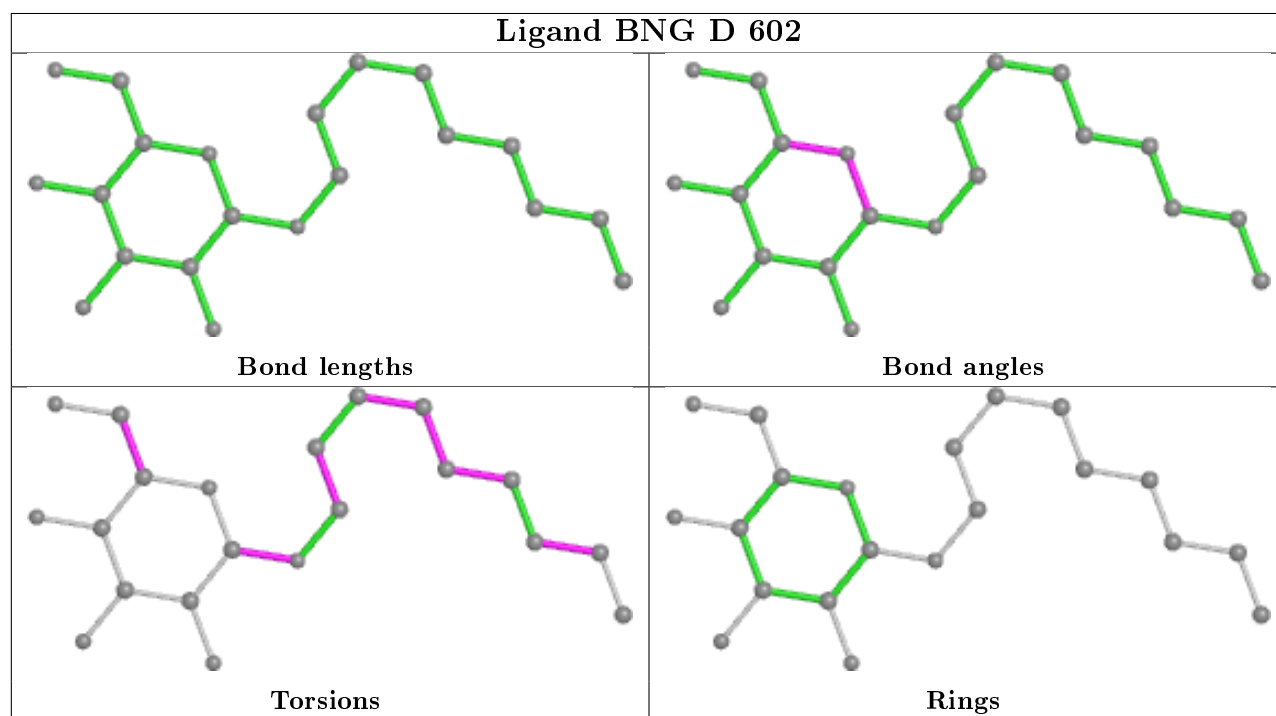
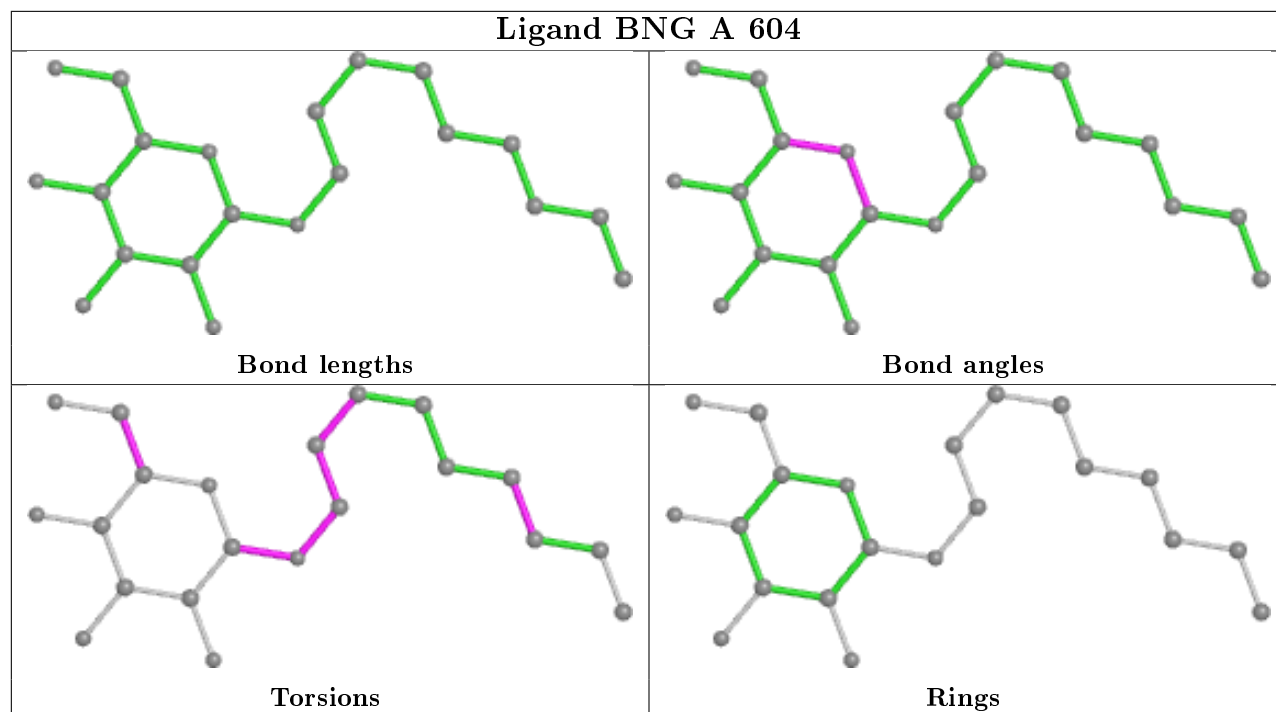


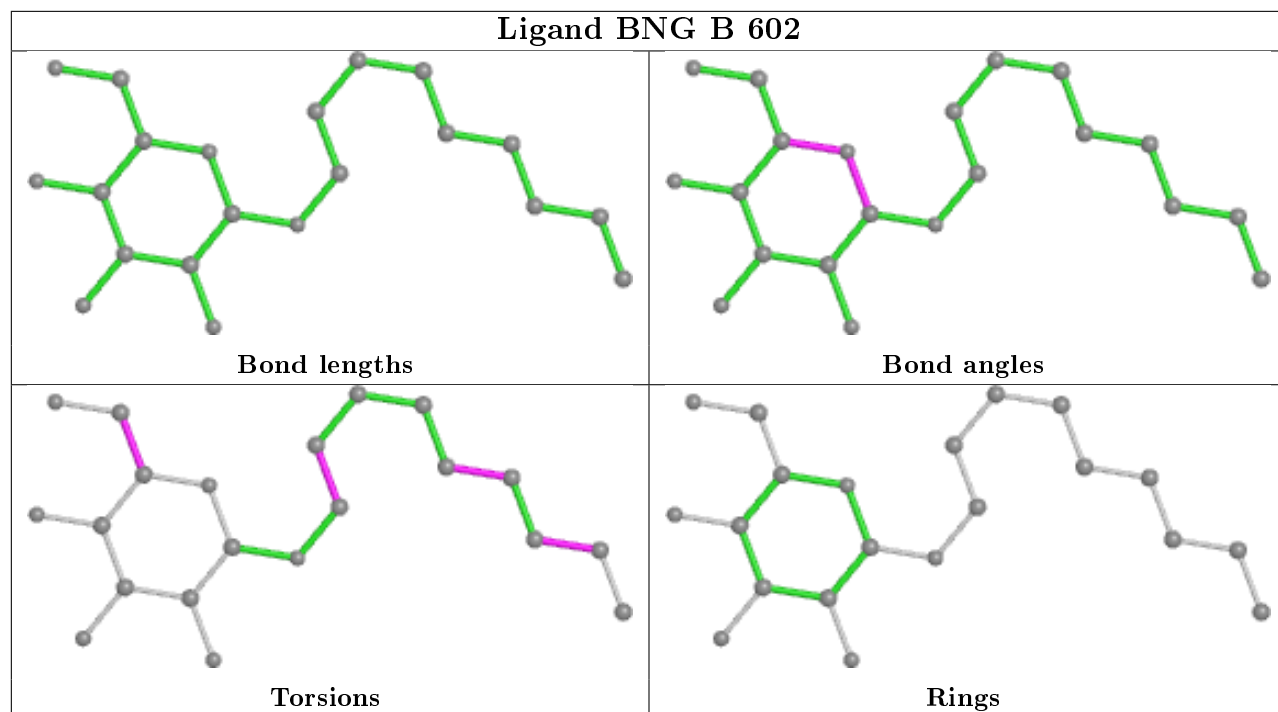
Ligand BGC B 601 (B)



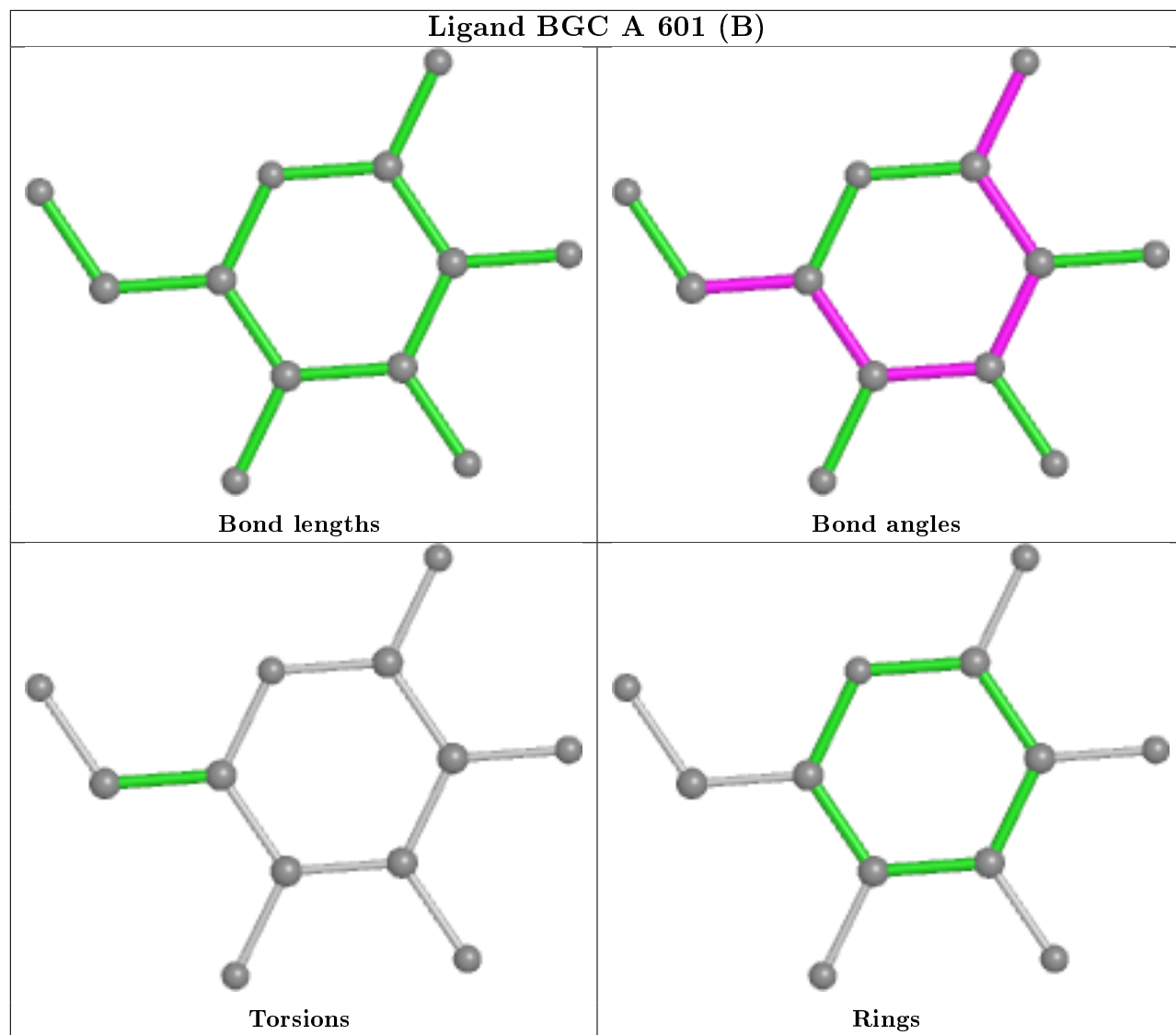


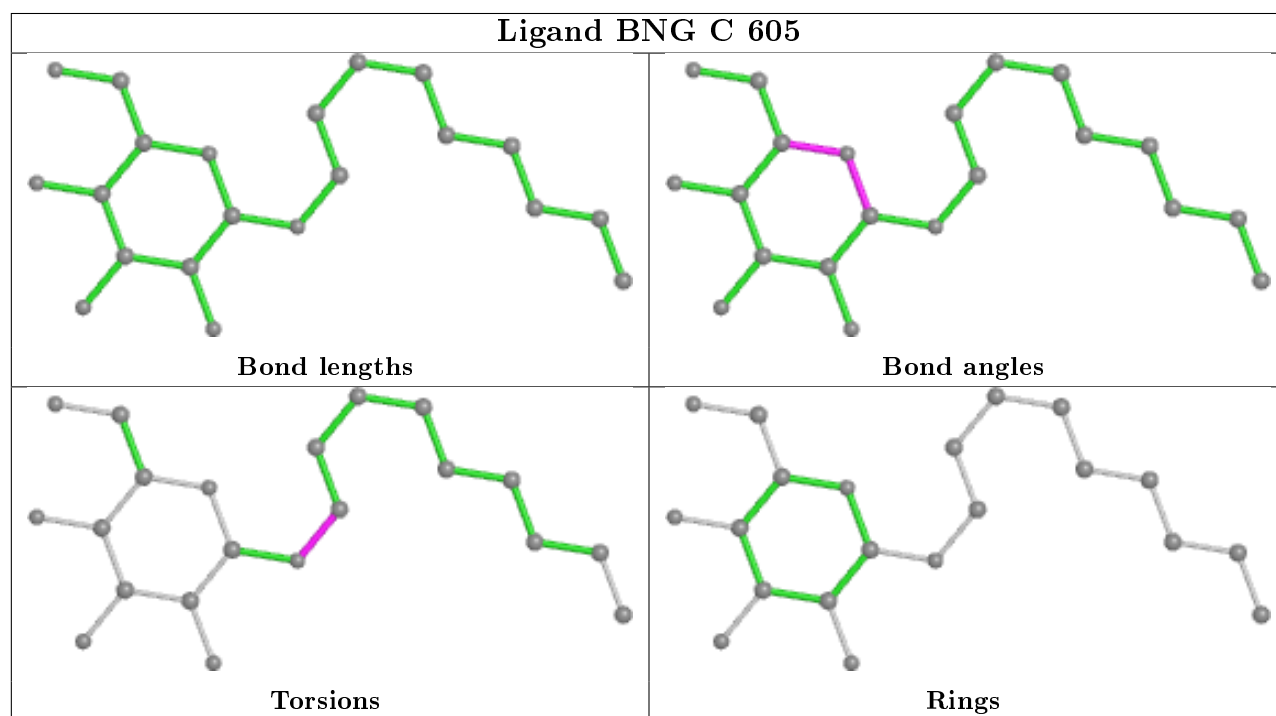
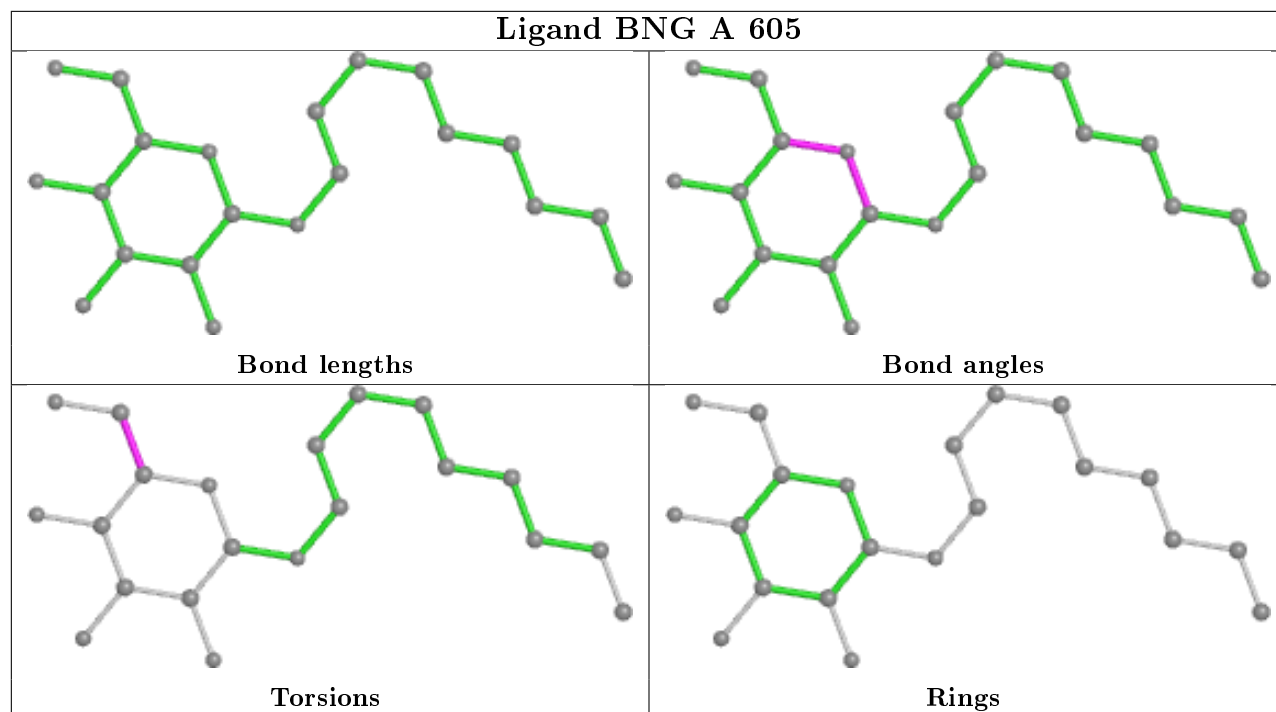




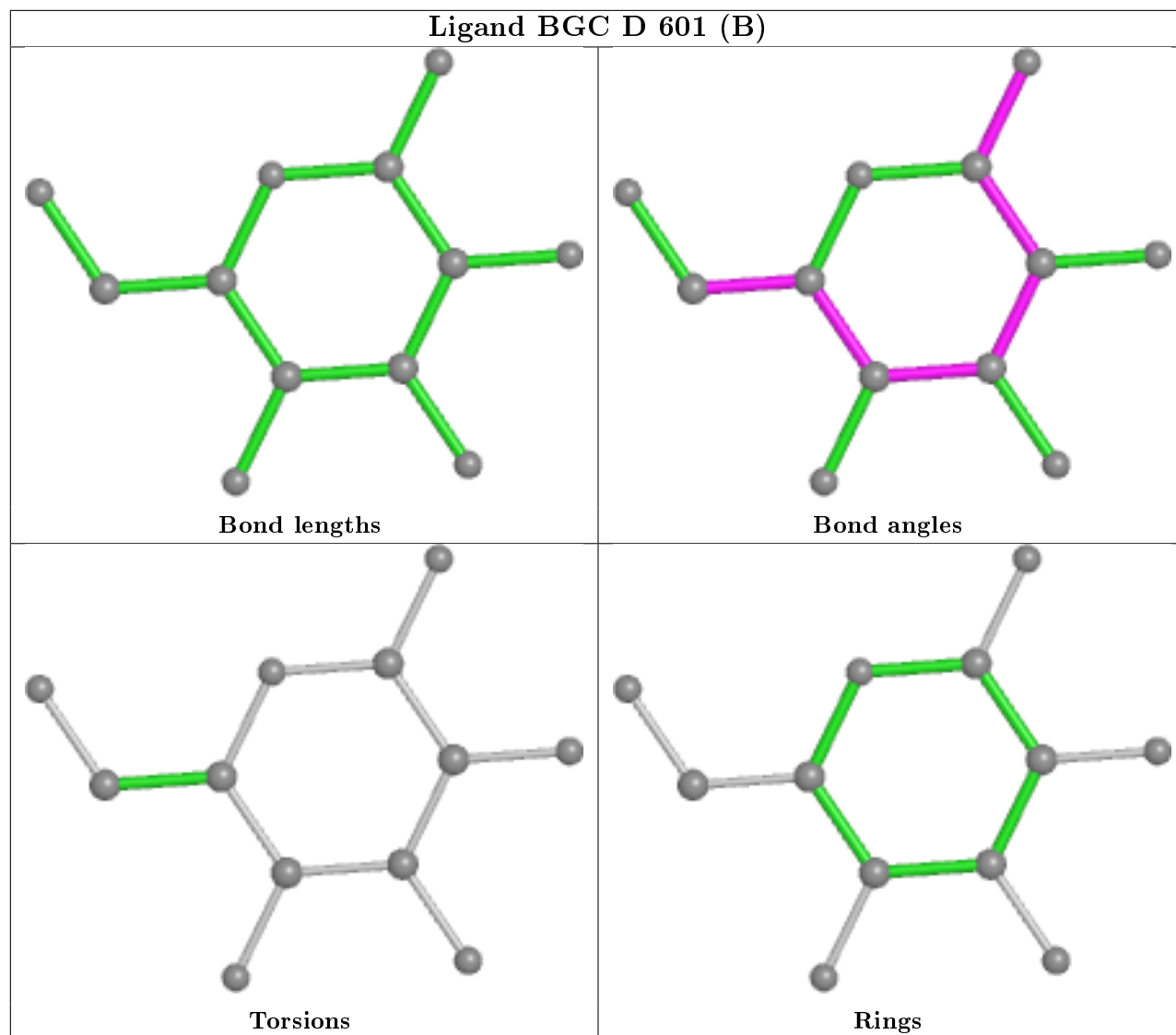


Ligand BGC A 601 (B)

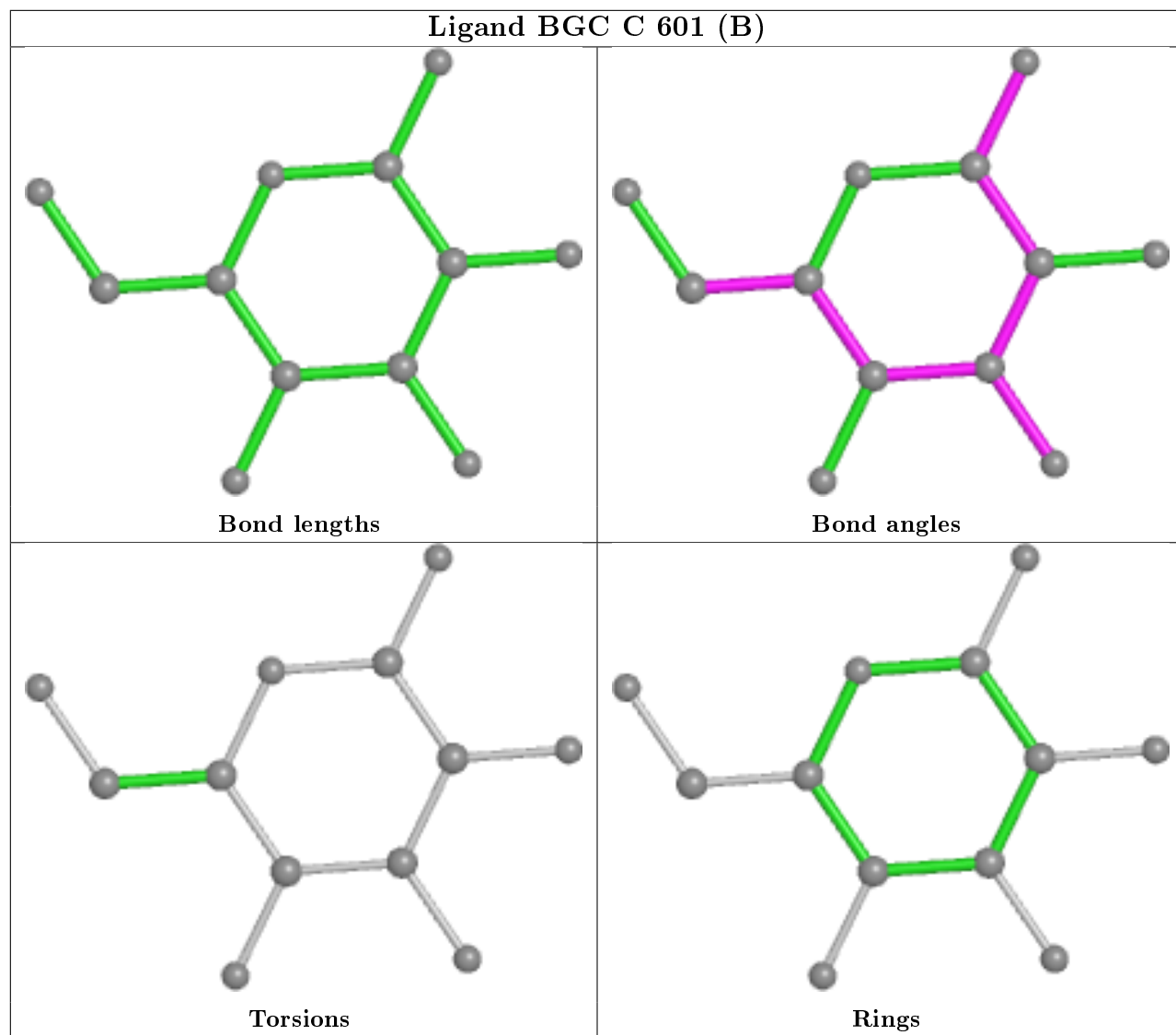


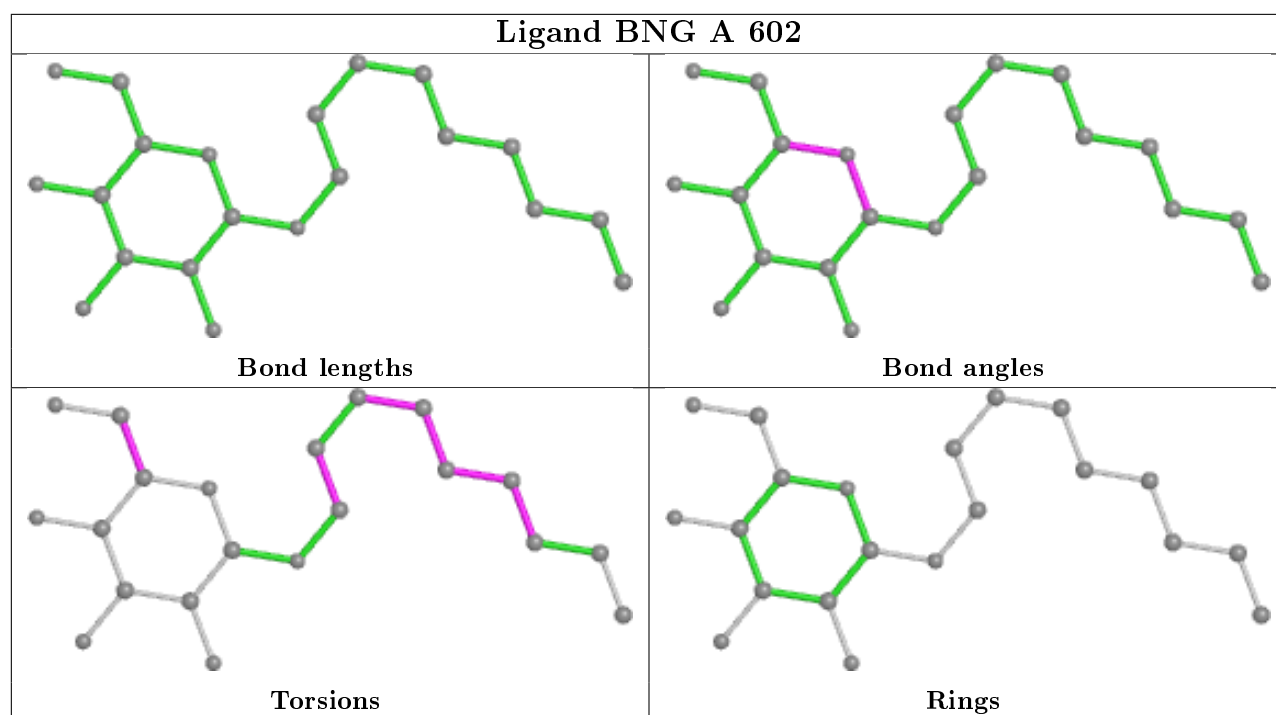


Ligand BGC D 601 (B)



Ligand BGC C 601 (B)





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	476/504 (94%)	0.36	30 (6%) 20 15	52, 71, 100, 127	0
1	B	478/504 (94%)	0.33	24 (5%) 28 23	49, 68, 100, 119	0
1	C	476/504 (94%)	1.03	92 (19%) 1 0	63, 94, 139, 161	0
1	D	478/504 (94%)	0.97	86 (17%) 1 0	62, 85, 132, 164	0
All	All	1908/2016 (94%)	0.67	232 (12%) 4 2	49, 79, 127, 164	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	193	ASP	12.1
1	D	237	PHE	9.0
1	C	252	ILE	8.5
1	C	193	ASP	8.2
1	C	194	SER	7.5
1	D	263	ASN	7.5
1	C	197	PRO	7.0
1	A	23	PHE	6.9
1	B	496	GLN	6.9
1	A	498	HIS	6.8
1	A	286	LEU	6.8
1	A	280	LEU	6.7
1	C	253	TYR	6.5
1	D	259	ASP	6.4
1	D	23	PHE	6.4
1	D	22	PHE	6.3
1	D	269	VAL	6.3
1	A	383	ARG	6.3
1	D	194	SER	6.2
1	C	64	GLU	6.2
1	D	249	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	286	LEU	6.0
1	D	242	ILE	5.9
1	C	63	GLY	5.9
1	C	157	HIS	5.9
1	D	492	MET	5.8
1	C	62	LYS	5.8
1	B	63	GLY	5.8
1	D	280	LEU	5.7
1	D	192	ALA	5.7
1	C	248	ILE	5.7
1	C	281	SER	5.6
1	C	282	LEU	5.5
1	A	282	LEU	5.4
1	C	272	ASN	5.4
1	C	483	GLU	5.4
1	D	238	GLU	5.4
1	C	479	THR	5.3
1	C	249	LEU	5.0
1	D	258	VAL	4.9
1	C	25	THR	4.9
1	A	63	GLY	4.9
1	B	23	PHE	4.8
1	D	265	ILE	4.8
1	C	283	LEU	4.8
1	D	262	LEU	4.7
1	C	482	GLY	4.7
1	D	197	PRO	4.7
1	A	64	GLU	4.6
1	C	195	THR	4.6
1	D	245	SER	4.6
1	C	297	LEU	4.6
1	D	499	MET	4.6
1	A	492	MET	4.5
1	A	283	LEU	4.5
1	C	481	GLY	4.5
1	B	253	TYR	4.4
1	C	255	THR	4.3
1	D	236	LEU	4.3
1	D	266	LYS	4.2
1	A	288	ILE	4.2
1	D	257	ASN	4.2
1	D	493	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	499	MET	4.2
1	A	491	THR	4.2
1	C	291	TYR	4.1
1	C	289	PRO	4.1
1	B	492	MET	4.1
1	D	498	HIS	4.1
1	C	280	LEU	3.9
1	D	275	ALA	3.9
1	D	329	LEU	3.9
1	B	498	HIS	3.9
1	D	272	ASN	3.9
1	D	240	GLY	3.9
1	B	22	PHE	3.9
1	D	452	LYS	3.8
1	C	29	TYR	3.8
1	C	486	THR	3.8
1	D	260	GLU	3.7
1	C	61	CYS	3.7
1	C	384	ASN	3.7
1	A	287	LYS	3.7
1	D	195	THR	3.7
1	C	254	GLU	3.6
1	B	329	LEU	3.6
1	D	68	LEU	3.6
1	C	196	GLU	3.6
1	A	253	TYR	3.6
1	C	191	LYS	3.6
1	D	270	GLU	3.6
1	D	248	ILE	3.6
1	C	245	SER	3.6
1	C	293	TYR	3.6
1	C	65	LYS	3.6
1	B	193	ASP	3.5
1	C	159	ASP	3.5
1	C	198	LEU	3.5
1	A	279	SER	3.5
1	D	286	LEU	3.4
1	C	480	LYS	3.4
1	A	226	VAL	3.4
1	C	158	LYS	3.3
1	C	200	SER	3.3
1	C	355	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	255	THR	3.3
1	D	256	ASP	3.3
1	C	278	ASN	3.3
1	D	386	ASN	3.3
1	C	227	PHE	3.3
1	C	22	PHE	3.3
1	C	258	VAL	3.2
1	C	287	LYS	3.2
1	C	66	ASP	3.2
1	C	382	ASN	3.1
1	C	271	GLN	3.1
1	D	278	ASN	3.1
1	B	274	SER	3.1
1	D	287	LYS	3.1
1	C	242	ILE	3.1
1	D	65	LYS	3.1
1	D	234	TYR	3.1
1	D	496	GLN	3.1
1	D	279	SER	3.0
1	D	448	ILE	3.0
1	D	233	PRO	3.0
1	A	289	PRO	3.0
1	D	25	THR	3.0
1	C	264	ALA	3.0
1	C	72	ASN	3.0
1	A	267	GLU	3.0
1	B	493	GLU	3.0
1	C	323	GLU	3.0
1	D	271	GLN	2.9
1	D	273	GLU	2.9
1	C	240	GLY	2.9
1	C	247	ASN	2.9
1	C	491	THR	2.9
1	C	496	GLN	2.9
1	C	202	ALA	2.9
1	C	28	LYS	2.9
1	D	497	LYS	2.9
1	A	281	SER	2.9
1	B	267	GLU	2.9
1	C	84	VAL	2.9
1	D	142	GLY	2.9
1	B	252	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	205	TRP	2.8
1	D	274	SER	2.8
1	D	247	ASN	2.7
1	D	196	GLU	2.7
1	D	268	ALA	2.7
1	A	246	LYS	2.7
1	C	87	GLY	2.7
1	C	300	LEU	2.7
1	C	301	LEU	2.7
1	C	204	LEU	2.6
1	D	324	PHE	2.6
1	D	350	TYR	2.6
1	D	201	PHE	2.6
1	B	260	GLU	2.6
1	C	192	ALA	2.6
1	D	283	LEU	2.5
1	D	387	PHE	2.5
1	C	328	HIS	2.5
1	C	69	ASN	2.5
1	C	187	GLY	2.5
1	A	237	PHE	2.5
1	D	383	ARG	2.5
1	C	390	ILE	2.5
1	D	198	LEU	2.5
1	D	66	ASP	2.5
1	C	109	ILE	2.5
1	B	355	LEU	2.5
1	D	141	ILE	2.5
1	D	117	VAL	2.5
1	D	328	HIS	2.4
1	C	68	LEU	2.4
1	A	222	LEU	2.4
1	C	262	LEU	2.4
1	C	274	SER	2.4
1	C	484	ILE	2.4
1	C	292	ARG	2.4
1	C	199	THR	2.3
1	D	185	ALA	2.3
1	D	253	TYR	2.3
1	C	135	LEU	2.3
1	C	24	SER	2.3
1	A	496	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	497	LYS	2.3
1	C	137	SER	2.3
1	C	241	ARG	2.3
1	D	143	LEU	2.3
1	D	145	THR	2.3
1	B	64	GLU	2.2
1	B	195	THR	2.2
1	C	226	VAL	2.2
1	C	279	SER	2.2
1	D	325	LEU	2.2
1	A	24	SER	2.2
1	C	190	PRO	2.2
1	D	139	PHE	2.2
1	A	493	GLU	2.2
1	A	490	ILE	2.2
1	D	172	ILE	2.2
1	C	232	THR	2.2
1	C	237	PHE	2.2
1	D	229	LYS	2.2
1	A	384	ASN	2.1
1	D	118	SER	2.1
1	D	323	GLU	2.1
1	B	66	ASP	2.1
1	A	65	LYS	2.1
1	D	264	ALA	2.1
1	D	432	SER	2.1
1	D	63	GLY	2.1
1	B	452	LYS	2.1
1	D	483	GLU	2.1
1	A	292	ARG	2.1
1	B	453	SER	2.1
1	C	67	ARG	2.1
1	C	88	ALA	2.1
1	D	239	LYS	2.1
1	C	138	GLY	2.0
1	C	387	PHE	2.0
1	D	228	PHE	2.0
1	C	56	VAL	2.0
1	B	271	GLN	2.0
1	B	243	GLU	2.0
1	D	138	GLY	2.0
1	D	200	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	255	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

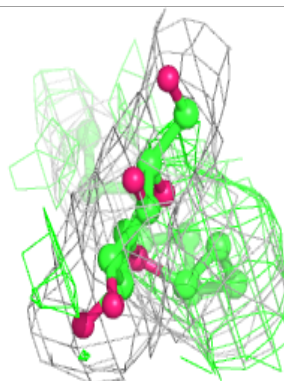
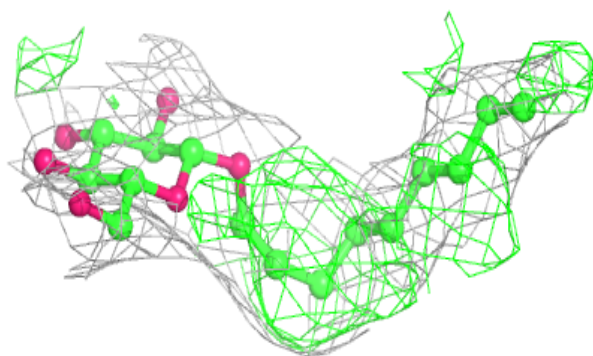
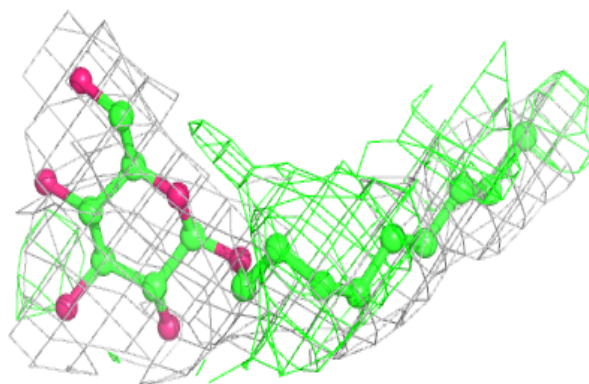
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BNG	C	604	21/21	0.70	0.29	83,94,108,114	0
3	BNG	A	604	21/21	0.83	0.21	62,77,86,92	0
3	BNG	C	603	21/21	0.85	0.36	86,97,106,109	0
3	BNG	C	605	21/21	0.86	0.20	73,84,91,98	0
3	BNG	A	605	21/21	0.87	0.28	75,85,110,127	0
3	BNG	D	604	21/21	0.88	0.15	77,91,102,106	0
3	BNG	C	602	21/21	0.89	0.34	96,103,111,118	0
3	BNG	A	602	21/21	0.89	0.20	65,76,94,101	0
3	BNG	A	603	21/21	0.90	0.19	61,78,93,102	0
3	BNG	B	603	21/21	0.90	0.17	67,79,83,86	0
3	BNG	D	602	21/21	0.90	0.25	78,99,102,104	0
3	BNG	B	602	21/21	0.92	0.17	69,82,90,103	0
3	BNG	D	603	21/21	0.92	0.15	77,94,106,107	0
2	BGC	C	601[B]	12/12	0.93	0.23	69,75,80,80	0
2	BGC	D	601[B]	12/12	0.94	0.24	60,64,73,76	0
2	BGC	B	601[B]	12/12	0.95	0.22	57,62,71,74	0
2	BGC	A	601[B]	12/12	0.95	0.22	58,65,72,77	0

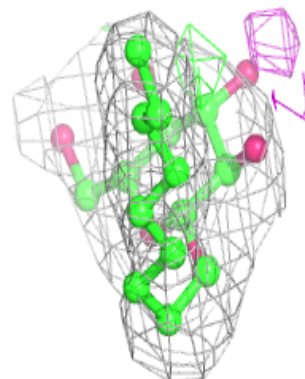
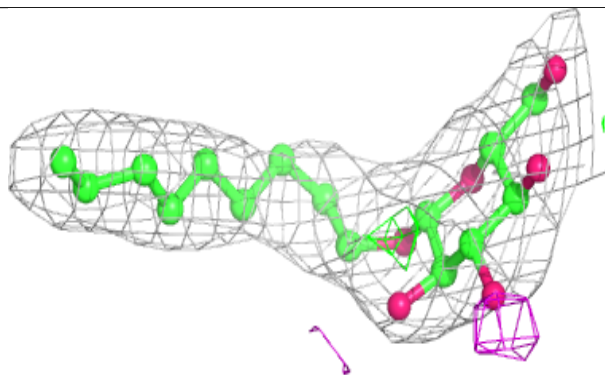
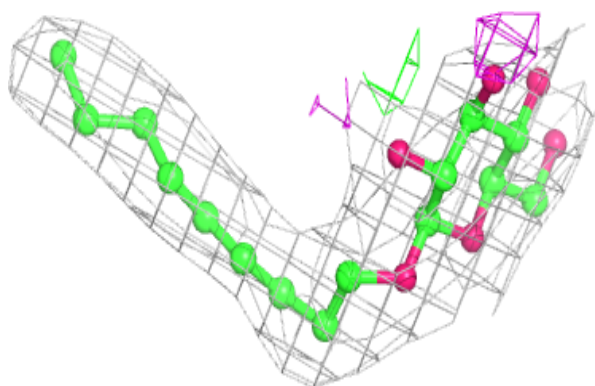
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

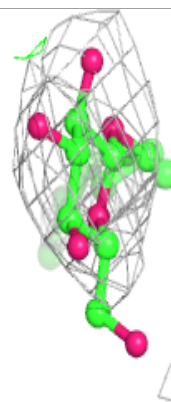
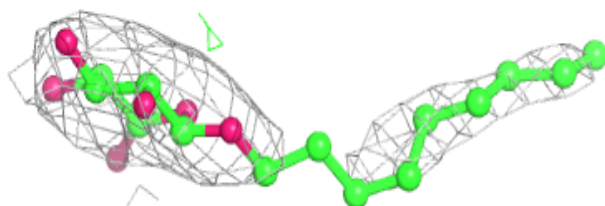
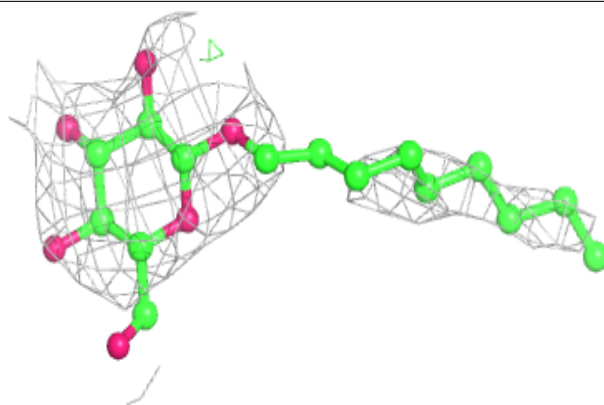
**Electron density around BNG A 604:**

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

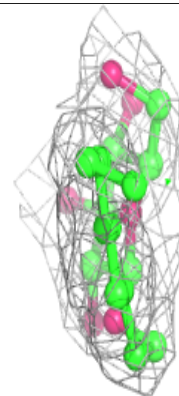
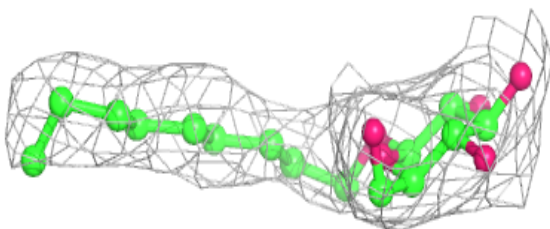
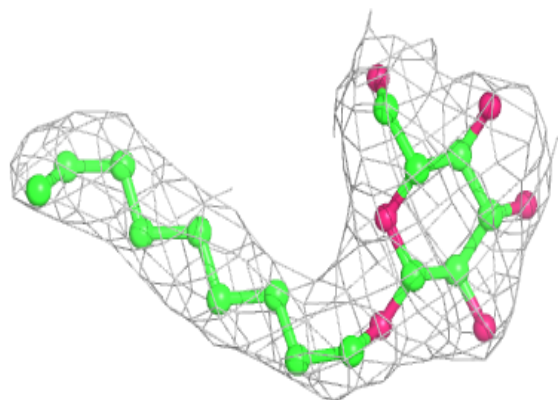


Electron density around BNG C 603:

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

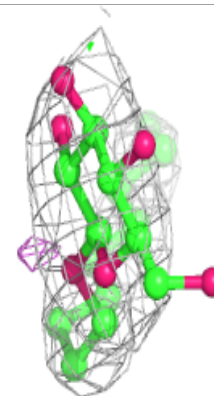
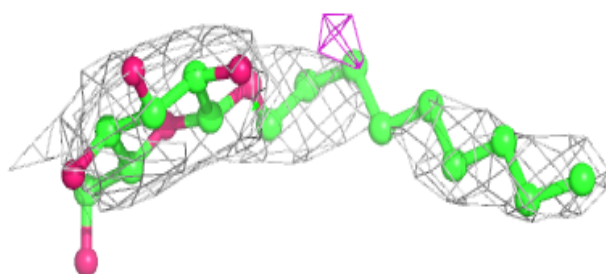
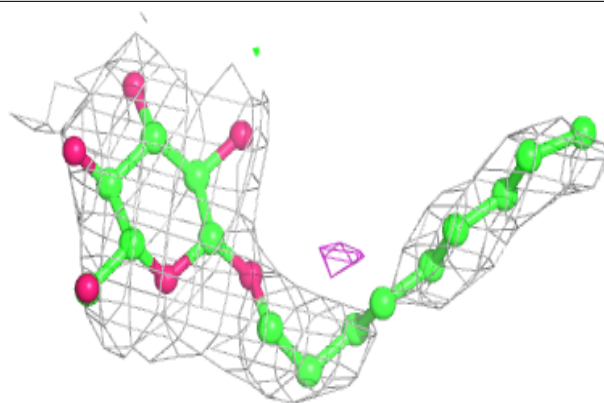
**Electron density around BNG C 605:**

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

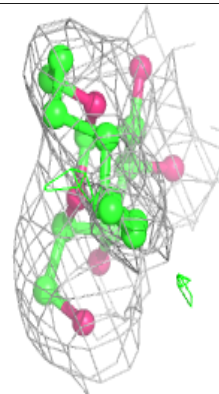
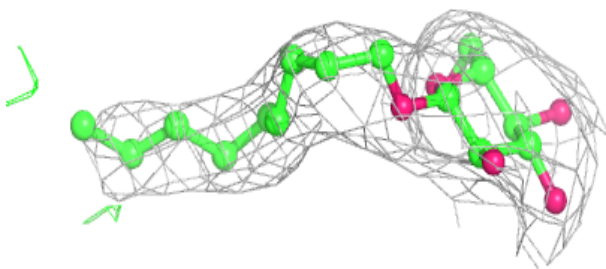
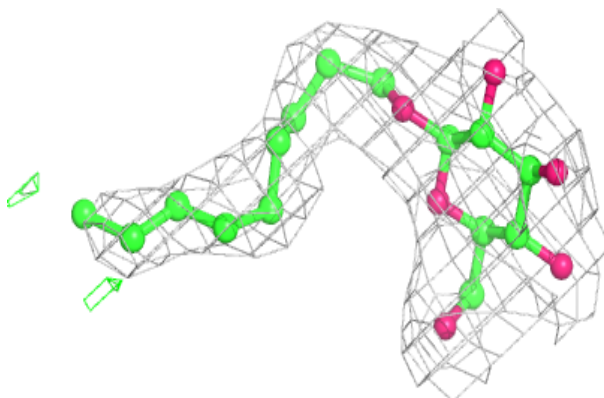


Electron density around BNG A 605:

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

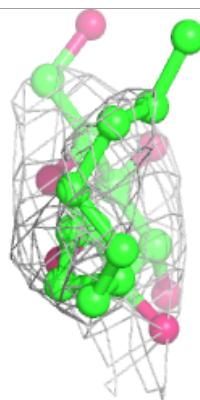
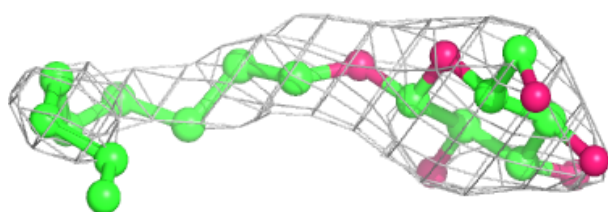
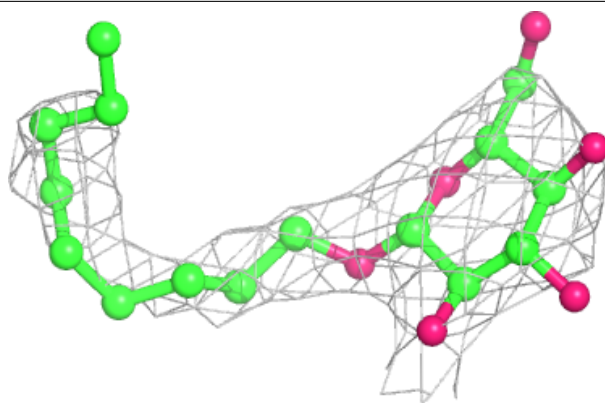
**Electron density around BNG D 604:**

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

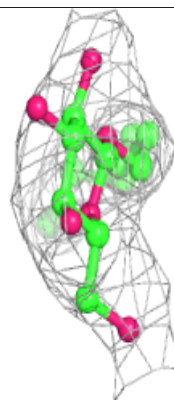
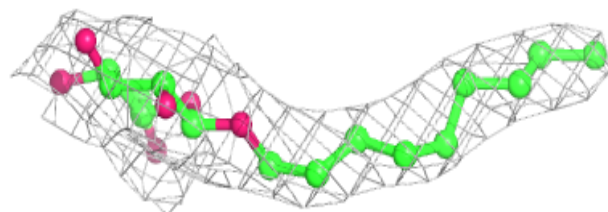
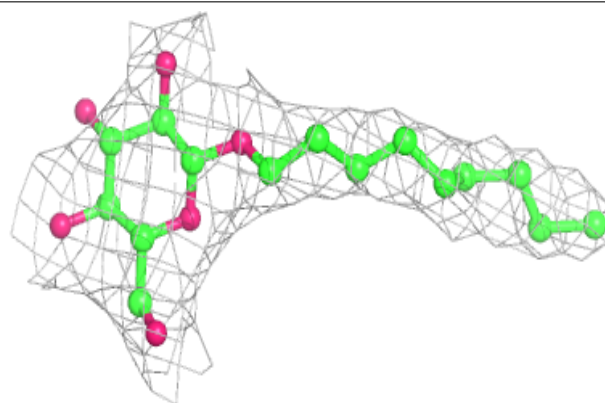


Electron density around BNG C 602:

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

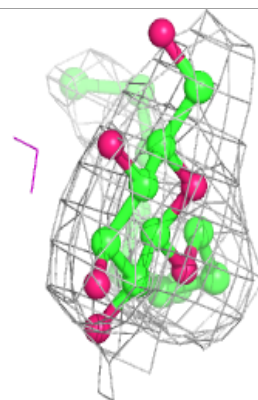
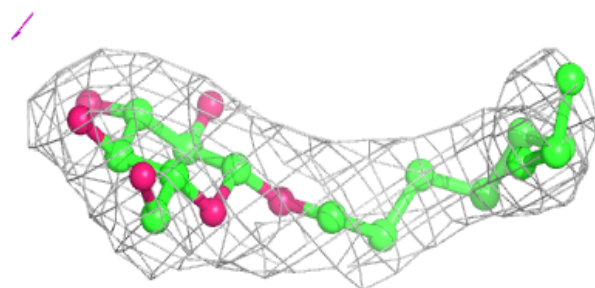
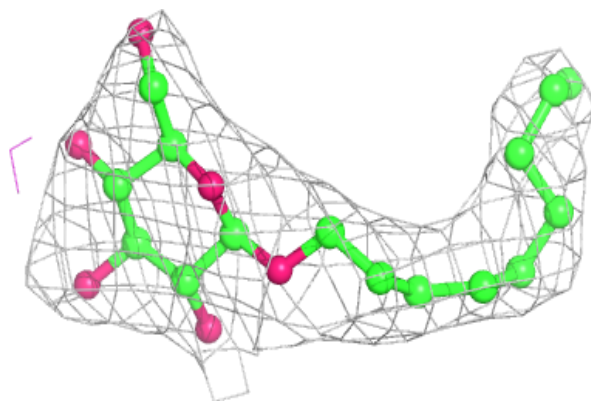
**Electron density around BNG A 602:**

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

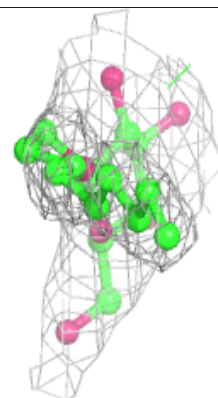
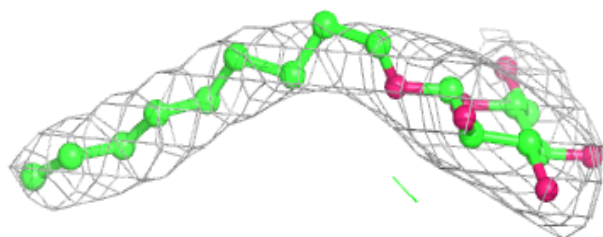
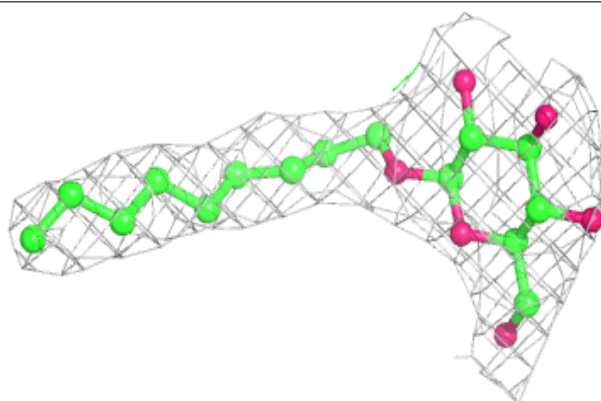


Electron density around BNG A 603:

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

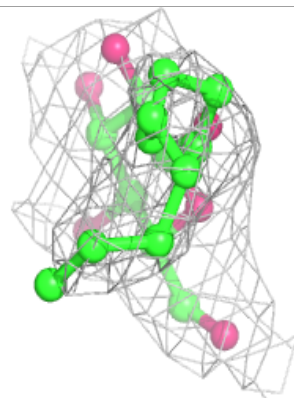
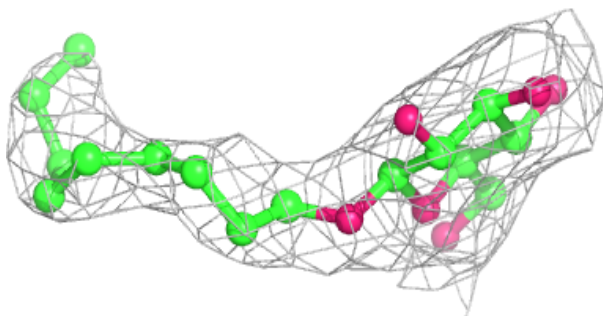
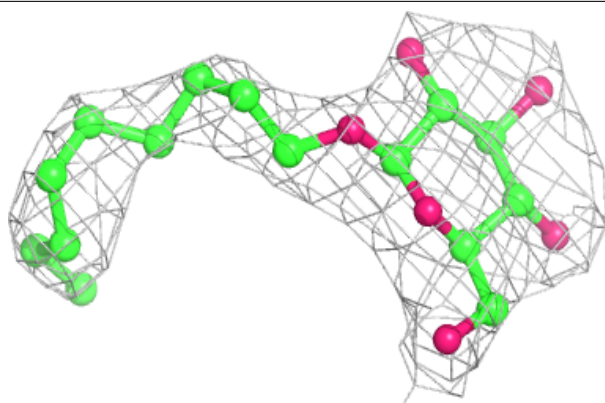
**Electron density around BNG B 603:**

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

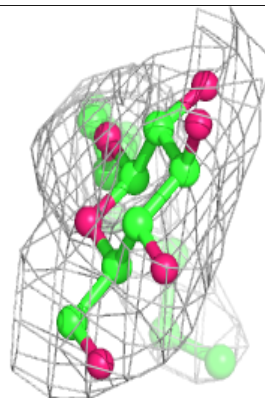
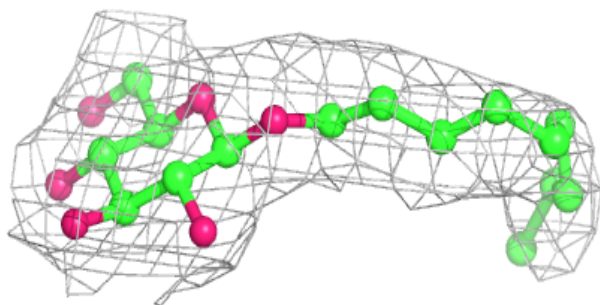
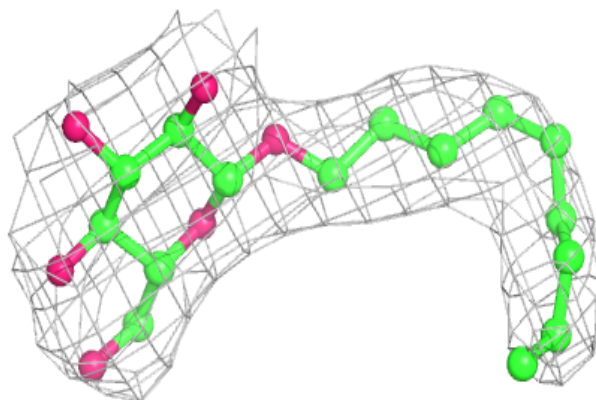


Electron density around BNG D 602:

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

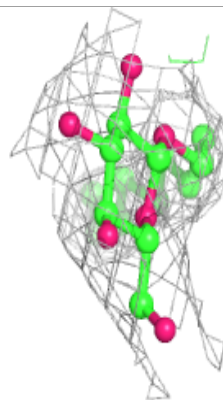
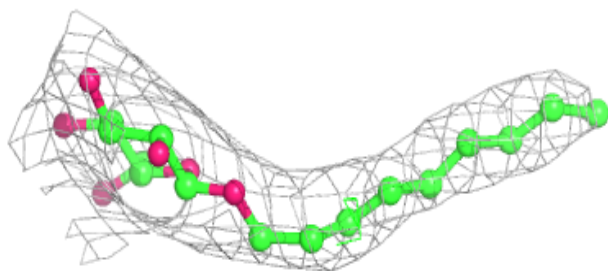
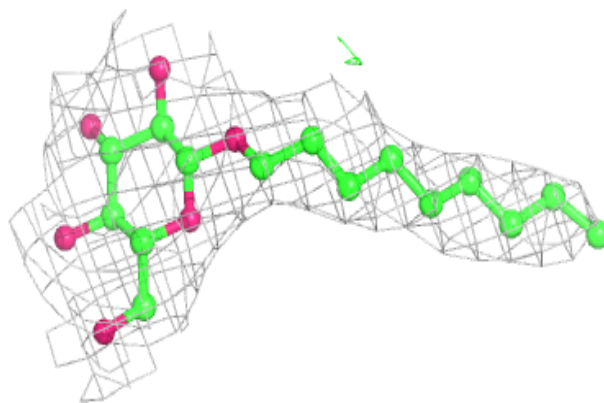
**Electron density around BNG B 602:**

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



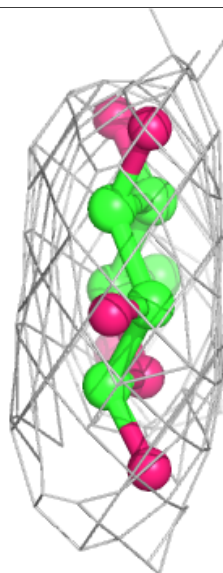
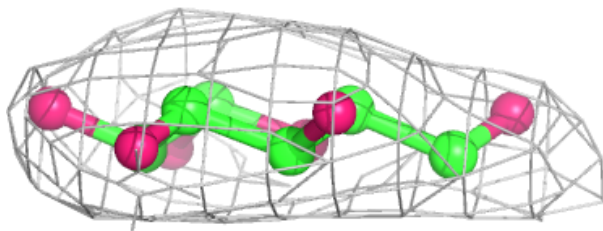
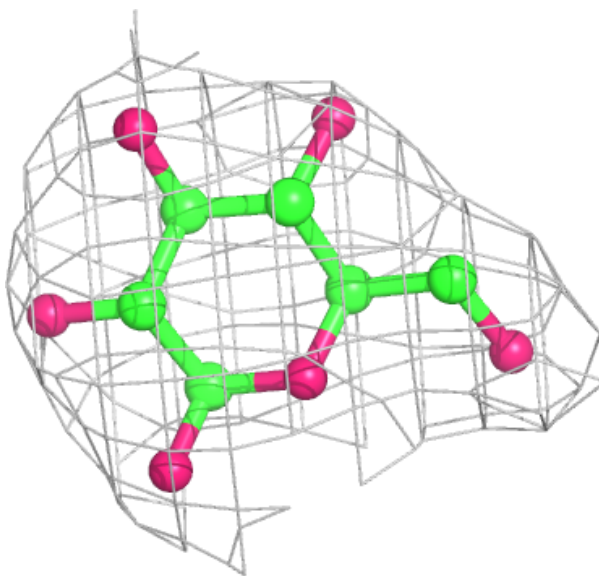
Electron density around BNG D 603:

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



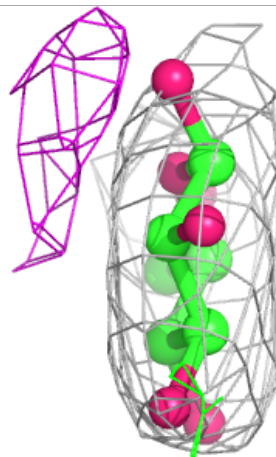
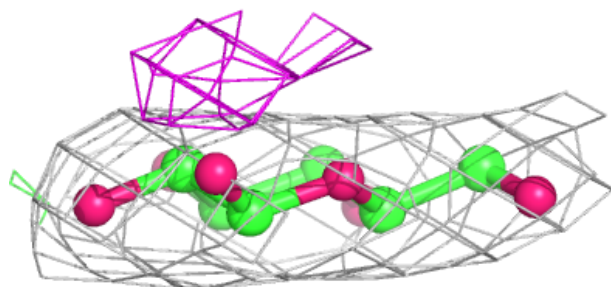
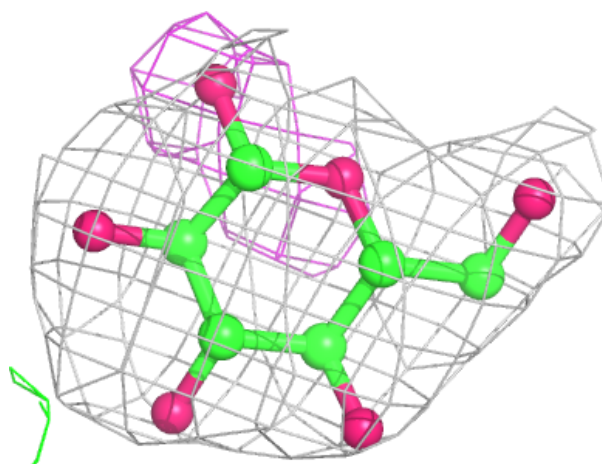
Electron density around BGC C 601 (B):

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



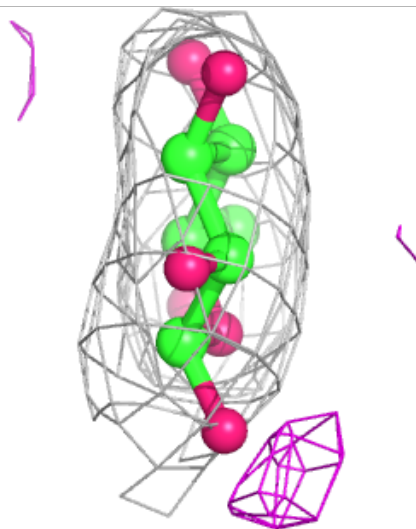
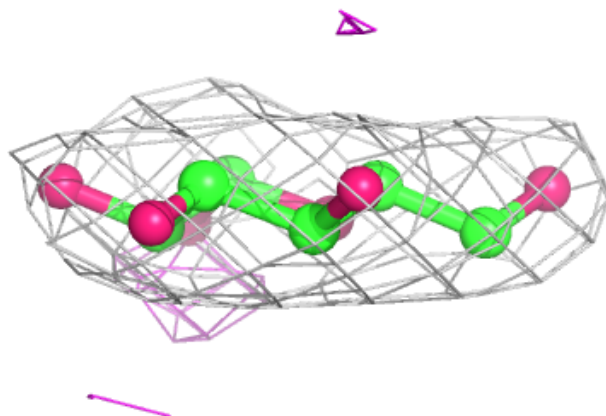
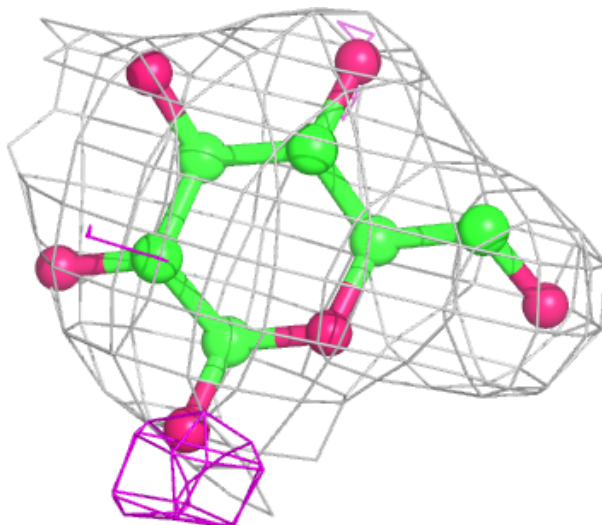
Electron density around BGC D 601 (B):

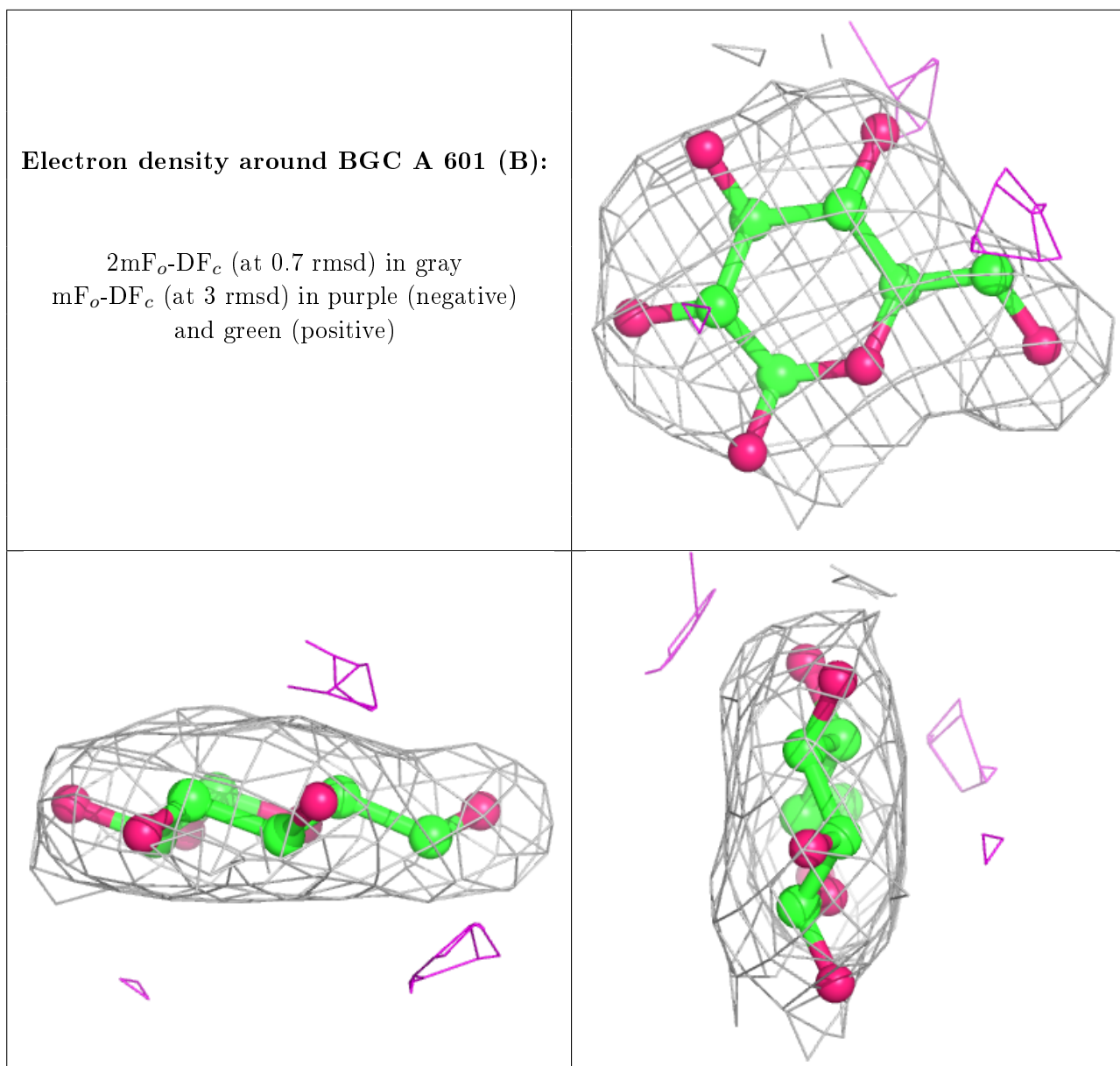
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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 ⓘ

There are no such residues in this entry.