



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:45 PM UTC

PDB ID : 6F7H / pdb_00006f7h
Title : Crystal structure of human AQP10
Authors : Gotfryd, K.; Wang, K.; Missel, J.W.; Pedersen, P.A.; Gourdon, P.
Deposited on : 2017-12-08
Resolution : 2.30 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

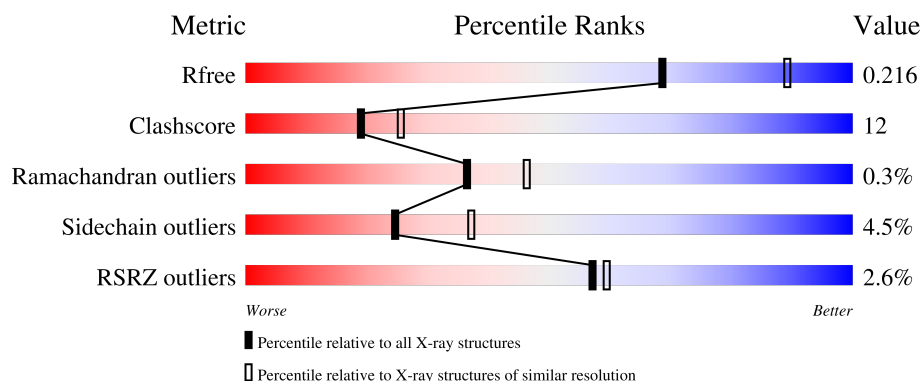
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	301	0.2% 65% 17% 17%
1	B	301	4% 66% 14% 16%
1	C	301	3% 68% 14% 16%
1	D	301	2% 69% 14% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BNG	A	401	X	-	-	-
2	BNG	A	402	X	-	-	-
2	BNG	A	403	X	-	-	-
2	BNG	B	401	X	-	-	-
2	BNG	B	402	X	-	-	-
2	BNG	B	403	X	-	-	-
2	BNG	B	404	X	-	-	-
2	BNG	B	405	X	-	-	-
2	BNG	B	406	X	-	-	-
2	BNG	C	401	X	-	-	-
2	BNG	C	402	X	-	-	-
2	BNG	C	403	X	-	X	-
2	BNG	C	404	X	-	-	-
2	BNG	D	401	X	-	-	-
2	BNG	D	402	X	-	-	-
2	BNG	D	403	X	-	X	-

2 Entry composition [i](#)

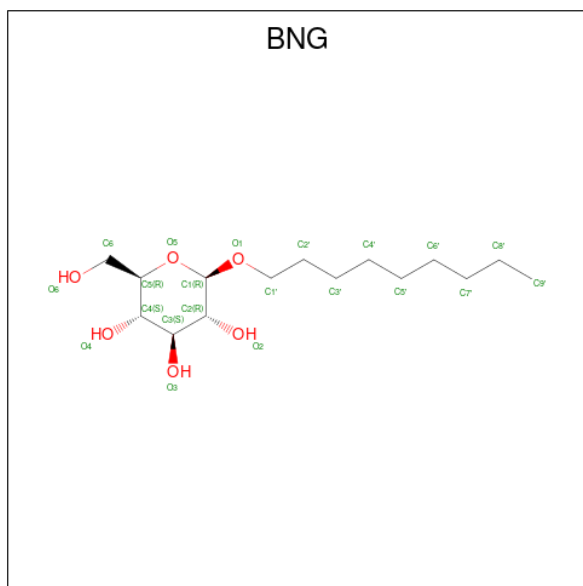
There are 4 unique types of molecules in this entry. The entry contains 8150 atoms, of which 2 are hydrogens and 0 are deuteriums.

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 Aquaporin-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	1	0
			1862	1223	305	324	10			
1	B	252	Total	C	N	O	S	0	0	0
			1863	1224	305	324	10			
1	C	253	Total	C	N	O	S	0	0	0
			1875	1231	309	325	10			
1	D	256	Total	C	N	O	S	0	0	0
			1904	1249	317	328	10			

- Molecule 2 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: C₁₅H₃₀O₆).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 21 15 6	0	0
2	B	1	Total C H O 22 15 1 6	0	0
2	B	1	Total C O 21 15 6	0	0
2	B	1	Total C O 21 15 6	0	0
2	B	1	Total C O 21 15 6	0	0
2	B	1	Total C O 21 15 6	0	0
2	B	1	Total C O 21 15 6	0	0
2	C	1	Total C O 21 15 6	0	0
2	C	1	Total C O 21 15 6	0	0
2	C	1	Total C O 21 15 6	0	0
2	C	1	Total C O 21 15 6	0	0
2	D	1	Total C H O 22 15 1 6	0	0
2	D	1	Total C O 21 15 6	0	0
2	D	1	Total C O 21 15 6	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

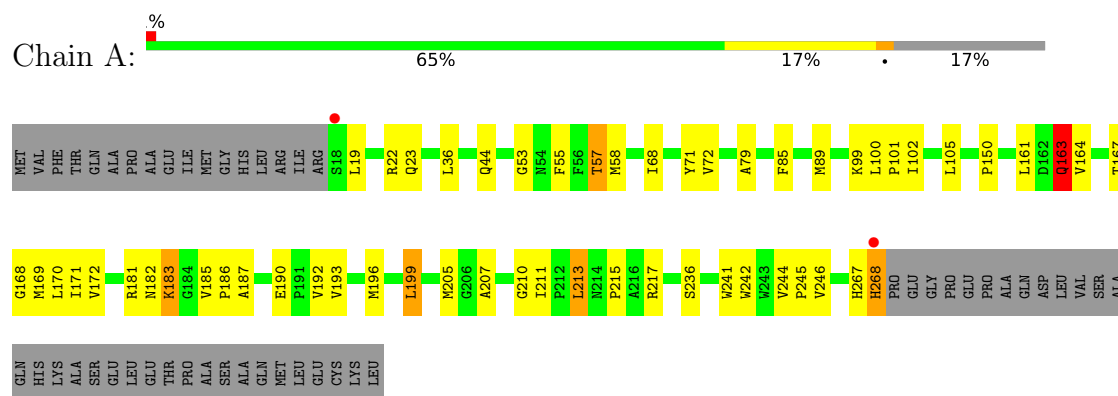
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	69	Total	O	0	0
			69	69		
4	C	55	Total	O	0	0
			55	55		
4	D	69	Total	O	0	0
			69	69		

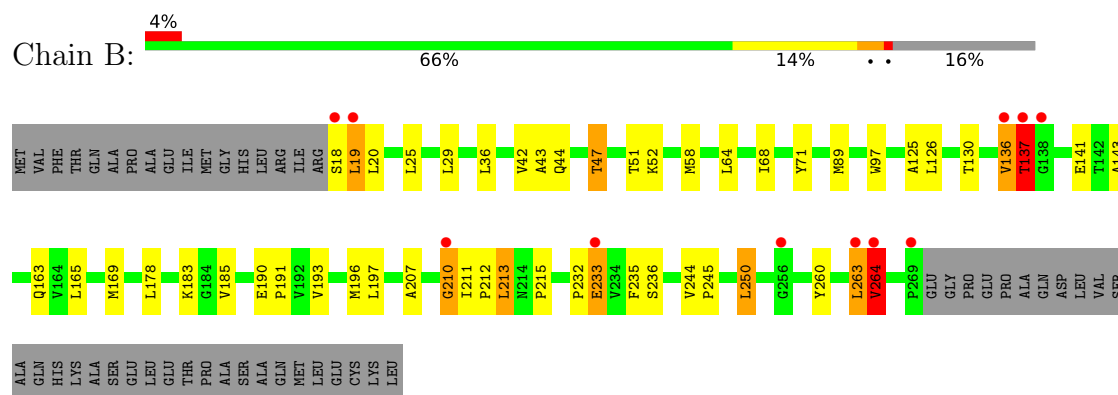
3 Residue-property plots

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.

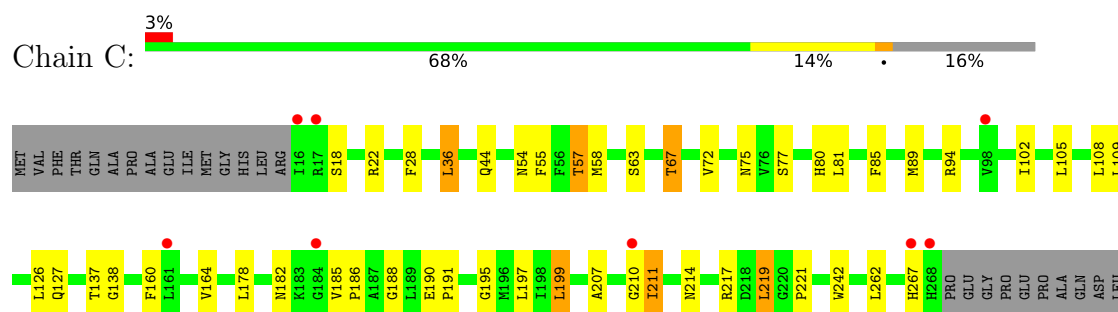
• Molecule 1: Aquaporin-10



• Molecule 1: Aquaporin-10



• Molecule 1: Aquaporin-10



VAL	SER	ALA	GLN	HIS	LYS	ALA	SER	GLU	GLU	GLY	THR	PRO	ALA	SER	ALA	GLN	MET	LEU	GLU	CYS	LYS	LEU
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● Molecule 1: Aquaporin-10



MET	VAL	PHE	THR	GLN	ALA	PRO	ALA	GLU	ILE	MET	GLY	H13	L14	R15	I16	R17	L36	V42	A43	Q44	A45	V46	E50	N54	T57	M58	L64	N82	P83	R94	I104	L105	L121	T135	E141	S144	A147	P150	Q163	V164	L165	R180
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K183	G194	E190	P191	Y192	V193	L197	L201	A207	T211	P212	L213	N214	R217	Y226	V241	V242	P245	T259	L262	L263	V264	A265	L266	H267	H268	PRO	GLU	GLY	PRO	GLU	PRO	ALA	GLN	ASP	LEU	VAL	SER	ALA	GLN	HIS	LYS	ALA	SER	GLU	LEU	GLU	THR
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO	ALA	SER	ALA	GLN	MET	LEU	GLU	CYS	LYS	LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.07Å 116.84Å 138.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.53 – 2.30 48.53 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.53-2.30) 99.6 (48.53-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.12rc2_2821: ???)	Depositor
R, R_{free}	0.189 , 0.212 0.193 , 0.216	Depositor DCC
R_{free} test set	3497 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8150	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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, GOL

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	0.92	6/1912 (0.3%)	1.28	9/2619 (0.3%)
1	B	0.66	0/1911	0.75	5/2619 (0.2%)
1	C	0.46	0/1922	0.57	0/2632
1	D	0.53	0/1952	0.66	3/2672 (0.1%)
All	All	0.66	6/7697 (0.1%)	0.86	17/10542 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163[A]	GLN	CA-C	15.44	1.75	1.52
1	A	163[B]	GLN	CA-C	15.44	1.75	1.52
1	A	163[A]	GLN	N-CA	-9.01	1.34	1.46
1	A	163[B]	GLN	N-CA	-9.01	1.34	1.46
1	A	163[A]	GLN	C-N	8.22	1.43	1.33
1	A	163[B]	GLN	C-N	8.22	1.43	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163[A]	GLN	CA-C-O	-32.36	81.49	119.35
1	A	163[B]	GLN	CA-C-O	-32.36	81.49	119.35
1	A	163[A]	GLN	O-C-N	-18.91	98.70	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163[B]	GLN	O-C-N	-18.91	98.70	122.34
1	A	163[A]	GLN	CB-CA-C	-11.56	90.78	110.09
1	A	163[B]	GLN	CB-CA-C	-11.56	90.78	110.09
1	D	265	ALA	N-CA-C	-11.10	91.31	108.96
1	B	263	LEU	N-CA-C	-10.34	93.33	109.76
1	B	210	GLY	N-CA-C	-8.03	97.60	112.62
1	A	163[A]	GLN	N-CA-C	7.85	122.58	112.92
1	A	163[B]	GLN	N-CA-C	7.85	122.58	112.92
1	B	137	THR	N-CA-C	7.44	126.65	110.80
1	A	183	LYS	N-CA-C	-6.75	98.23	108.96
1	D	211	ILE	N-CA-C	5.59	120.96	108.88
1	B	136	VAL	N-CA-C	-5.54	100.50	108.48
1	D	264	VAL	N-CA-C	-5.24	105.27	110.62
1	B	264	VAL	N-CA-C	-5.20	98.53	109.34

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163[A]	GLN	Mainchain
1	A	163[B]	GLN	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1862	0	1910	47	0
1	B	1863	0	1909	42	0
1	C	1875	0	1926	52	0
1	D	1904	0	1957	51	0
2	A	63	0	90	6	0
2	B	126	1	180	13	0
2	C	84	0	120	19	0
2	D	63	1	90	16	0
3	A	12	0	16	2	0
3	B	12	0	16	0	0
3	C	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	8	1	0
4	A	79	0	0	5	0
4	B	69	0	0	3	0
4	C	55	0	0	11	0
4	D	69	0	0	9	0
All	All	8148	2	8230	190	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 12.

All (190) 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)
2:C:401:BNG:H4'2	2:D:403:BNG:H8'2	1.22	1.19
1:B:260:TYR:O	1:B:263:LEU:O	1.66	1.12
1:C:75:ASN:HD22	2:C:403:BNG:H62	1.10	1.08
1:C:210:GLY:O	4:C:501:HOH:O	1.82	0.97
1:C:55:PHE:HA	1:C:58:MET:HE3	1.48	0.94
1:D:265:ALA:HA	4:D:501:HOH:O	1.68	0.93
1:C:94:ARG:NE	4:C:503:HOH:O	2.00	0.93
1:C:75:ASN:ND2	2:C:403:BNG:H62	1.85	0.91
1:D:265:ALA:CA	4:D:501:HOH:O	2.19	0.91
1:D:266:LEU:N	4:D:501:HOH:O	1.83	0.87
1:D:242:TRP:CZ2	2:D:402:BNG:H3'1	2.09	0.87
1:A:22:ARG:NH2	2:A:401:BNG:O3	2.09	0.86
1:C:182:ASN:OD1	2:C:404:BNG:H2	1.76	0.85
1:B:43:ALA:O	1:B:47:THR:HB	1.77	0.83
1:A:55:PHE:HA	1:A:58:MET:HE3	1.61	0.82
1:A:99:LYS:NZ	4:A:502:HOH:O	2.11	0.81
1:D:94:ARG:NE	4:D:505:HOH:O	2.13	0.81
1:B:136:VAL:O	1:B:137:THR:OG1	2.00	0.80
1:B:137:THR:H	1:B:141:GLU:HG3	1.49	0.78
1:A:163[A]:GLN:CA	1:A:164:VAL:N	2.47	0.78
2:C:403:BNG:H8'1	1:D:193:VAL:CG1	2.13	0.78
1:C:67:THR:HB	1:C:191:PRO:O	1.83	0.77
2:C:403:BNG:H8'1	1:D:193:VAL:HG13	1.68	0.76
1:C:138:GLY:N	4:C:502:HOH:O	1.84	0.76
1:D:141:GLU:OE1	4:D:502:HOH:O	2.03	0.76
1:B:235:PHE:HB3	2:B:402:BNG:H1'2	1.68	0.76
1:D:45:ALA:CB	1:D:58:MET:HE2	2.16	0.75
1:A:170:LEU:HD21	3:A:404:GOL:H11	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ARG:CD	4:C:503:HOH:O	2.32	0.74
1:C:72:VAL:HG13	2:D:403:BNG:H9'1	1.69	0.73
1:D:263:LEU:HD13	2:D:403:BNG:H6'1	1.71	0.73
2:C:401:BNG:H6'2	2:D:403:BNG:H9'2	1.70	0.71
1:C:94:ARG:HD2	4:C:503:HOH:O	1.91	0.71
1:B:193:VAL:HA	1:B:196:MET:HE2	1.73	0.71
1:C:44:GLN:HG3	1:D:207:ALA:HB2	1.72	0.71
1:A:79:ALA:O	4:A:501:HOH:O	2.07	0.71
2:C:401:BNG:C4'	2:D:403:BNG:H8'2	2.13	0.70
1:A:207:ALA:HB2	1:D:44:GLN:HG3	1.73	0.70
1:B:19:LEU:HA	4:B:501:HOH:O	1.94	0.68
1:C:55:PHE:HA	1:C:58:MET:CE	2.23	0.67
2:D:403:BNG:O2	4:D:503:HOH:O	2.04	0.67
1:A:99:LYS:HD2	4:A:502:HOH:O	1.94	0.67
1:D:226:TYR:O	4:D:504:HOH:O	2.12	0.66
1:B:47:THR:CG2	1:B:125:ALA:HB1	2.25	0.66
1:C:214:ASN:HD22	3:C:405:GOL:H32	1.61	0.66
1:D:50:GLU:OE2	4:D:506:HOH:O	2.13	0.65
2:C:403:BNG:H5	1:D:183:LYS:HB2	1.78	0.64
1:B:42:VAL:HG22	1:B:58:MET:HE3	1.79	0.63
2:C:404:BNG:O1	2:C:404:BNG:O6	2.13	0.62
1:B:137:THR:N	1:B:141:GLU:HG3	2.13	0.62
1:C:85:PHE:CE1	1:C:89:MET:HE3	2.34	0.62
1:A:19:LEU:O	1:A:23:GLN:HG3	1.99	0.62
1:A:199:LEU:HD13	1:D:64:LEU:HD11	1.83	0.61
1:A:182:ASN:HD21	2:A:403:BNG:H2'1	1.66	0.61
1:A:211:ILE:HB	1:A:213:LEU:HD22	1.82	0.61
1:B:193:VAL:HG12	2:B:403:BNG:H7'1	1.83	0.61
1:D:211:ILE:O	1:D:211:ILE:HG23	1.99	0.61
1:D:15:ARG:NH2	1:D:17:ARG:HG2	2.15	0.60
1:B:163:GLN:NE2	1:B:213:LEU:H	1.99	0.60
1:A:167:THR:O	1:A:171:ILE:HG12	2.01	0.60
1:B:193:VAL:CG1	2:B:403:BNG:H7'1	2.31	0.60
1:C:75:ASN:HB2	2:C:403:BNG:H4	1.84	0.59
1:D:264:VAL:HA	2:D:403:BNG:H1'2	1.84	0.59
1:C:54:ASN:C	1:C:58:MET:HE2	2.27	0.59
2:C:401:BNG:H6'2	2:D:403:BNG:C9'	2.32	0.59
1:B:18:SER:O	4:B:501:HOH:O	2.16	0.59
1:D:45:ALA:HB3	1:D:58:MET:HE2	1.83	0.59
1:A:163[B]:GLN:OE1	1:A:244:VAL:HG12	2.03	0.58
1:A:72:VAL:HG22	2:A:401:BNG:H6'2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:HD11	1:C:199:LEU:HD13	1.85	0.58
1:B:163:GLN:HE22	1:B:213:LEU:H	1.52	0.58
1:C:72:VAL:HG22	2:D:403:BNG:H9'1	1.86	0.58
1:C:18:SER:N	4:C:504:HOH:O	2.16	0.58
1:B:210:GLY:O	4:B:502:HOH:O	2.17	0.58
1:A:267:HIS:O	1:A:268:HIS:HB2	2.03	0.57
1:D:201:LEU:HB3	1:D:211:ILE:HD11	1.86	0.57
1:B:25:LEU:HD23	1:C:267:HIS:CE1	2.40	0.56
1:C:75:ASN:HD22	2:C:403:BNG:C6	2.00	0.56
1:C:137:THR:HA	4:C:502:HOH:O	2.04	0.56
1:A:242:TRP:CZ2	2:A:402:BNG:H3'2	2.41	0.56
1:B:47:THR:HG23	1:B:125:ALA:HB1	1.88	0.56
1:B:89:MET:HE2	1:B:89:MET:HA	1.87	0.56
1:A:196:MET:HG2	3:A:405:GOL:H2	1.88	0.56
1:C:102:ILE:N	1:C:102:ILE:HD12	2.20	0.56
1:D:259:THR:HA	1:D:262:LEU:CD2	2.36	0.56
1:C:85:PHE:CZ	1:C:89:MET:HE3	2.40	0.56
1:A:44:GLN:HG3	1:B:207:ALA:HB2	1.89	0.55
1:B:47:THR:HG21	1:B:125:ALA:HB1	1.87	0.55
1:B:244:VAL:HB	1:B:245:PRO:HD3	1.89	0.55
1:C:182:ASN:HA	2:C:404:BNG:O3	2.07	0.54
1:C:242:TRP:CH2	2:C:402:BNG:H5'2	2.42	0.54
1:D:242:TRP:CH2	2:D:402:BNG:H3'1	2.43	0.54
1:C:18:SER:CB	4:C:504:HOH:O	2.55	0.54
1:D:105:LEU:C	1:D:105:LEU:HD13	2.32	0.54
1:D:150:PRO:HD3	1:D:241:TRP:CG	2.43	0.53
1:D:15:ARG:HH22	1:D:17:ARG:HG2	1.74	0.53
1:C:137:THR:CA	4:C:502:HOH:O	2.57	0.53
1:C:217:ARG:O	1:C:221:PRO:HG2	2.09	0.52
1:D:54:ASN:H	1:D:57:THR:HB	1.72	0.52
1:C:72:VAL:HG13	2:D:403:BNG:C9'	2.38	0.52
1:C:72:VAL:CG1	2:D:403:BNG:H9'1	2.38	0.52
1:B:97:TRP:CZ3	2:B:405:BNG:H3'2	2.45	0.51
1:D:211:ILE:HG12	1:D:213:LEU:HD11	1.93	0.51
1:C:67:THR:HG22	1:C:195:GLY:HA3	1.93	0.51
1:C:108:LEU:HD11	1:C:219:LEU:HB3	1.93	0.50
1:B:178:LEU:HG	2:B:404:BNG:H3'1	1.93	0.50
1:B:44:GLN:HG3	1:C:207:ALA:HB2	1.93	0.50
1:A:85:PHE:CZ	1:A:89:MET:HE3	2.47	0.50
1:D:263:LEU:CD1	2:D:403:BNG:H6'1	2.41	0.50
1:C:160:PHE:O	1:C:164:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PRO:HD3	1:A:241:TRP:CG	2.48	0.49
1:A:217:ARG:HD3	1:A:217:ARG:C	2.37	0.49
1:A:53:GLY:HA2	1:A:57:THR:HG21	1.95	0.48
1:C:102:ILE:HD12	1:C:102:ILE:H	1.79	0.48
1:A:102:ILE:HD12	1:A:102:ILE:H	1.78	0.48
1:C:211:ILE:HD11	4:C:527:HOH:O	2.12	0.48
1:A:99:LYS:CE	4:A:502:HOH:O	2.59	0.48
1:C:75:ASN:HB2	2:C:403:BNG:C4	2.44	0.48
1:B:163:GLN:NE2	1:B:212:PRO:HG2	2.29	0.47
1:C:77:SER:HA	1:C:178:LEU:HD21	1.96	0.47
1:A:244:VAL:HB	1:A:245:PRO:HD3	1.97	0.47
1:B:178:LEU:HG	2:B:404:BNG:C3'	2.45	0.47
1:C:54:ASN:H	1:C:57:THR:HB	1.79	0.47
1:D:259:THR:O	1:D:262:LEU:HD23	2.15	0.47
1:A:236:SER:HA	2:A:402:BNG:H3	1.98	0.47
1:D:265:ALA:O	1:D:266:LEU:HB2	2.14	0.47
1:B:64:LEU:O	1:B:68:ILE:HG12	2.16	0.46
1:A:68:ILE:HG12	2:B:403:BNG:H8'1	1.98	0.46
1:C:109:LEU:C	1:C:109:LEU:HD23	2.41	0.46
1:A:185:VAL:HG23	1:A:190:GLU:HG3	1.97	0.46
1:D:42:VAL:O	1:D:46:VAL:HG23	2.15	0.46
1:D:217:ARG:C	1:D:217:ARG:HD3	2.41	0.46
1:D:259:THR:HA	1:D:262:LEU:HD21	1.97	0.46
1:C:80:HIS:O	1:C:81:LEU:HB2	2.15	0.45
1:D:201:LEU:HB3	1:D:211:ILE:CD1	2.45	0.45
1:B:136:VAL:HG21	1:B:233:GLU:HB3	1.99	0.45
1:B:190:GLU:HB2	1:B:191:PRO:HD3	1.99	0.45
1:D:82:ASN:HD22	3:D:404:GOL:H11	1.82	0.44
1:A:205:MET:HE2	1:D:36:LEU:HG	1.99	0.44
1:A:215:PRO:HB3	1:A:246:VAL:HA	1.99	0.44
1:B:165:LEU:O	1:B:169:MET:HG3	2.18	0.44
1:D:150:PRO:HD3	1:D:241:TRP:CD1	2.53	0.44
1:A:169:MET:SD	1:A:205:MET:HE1	2.58	0.44
1:C:182:ASN:CA	2:C:404:BNG:O3	2.64	0.43
1:D:214:ASN:HB3	1:D:217:ARG:HB3	1.99	0.43
1:A:71:TYR:HB3	2:B:403:BNG:H4'2	2.00	0.43
1:C:185:VAL:CG1	1:C:186:PRO:HD2	2.49	0.43
1:D:45:ALA:HB1	1:D:58:MET:HE2	1.98	0.43
1:D:83:PRO:HB3	1:D:104:ILE:HG12	2.01	0.43
1:D:242:TRP:O	1:D:245:PRO:HD2	2.19	0.43
1:B:232:PRO:HB3	2:B:406:BNG:H2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:N	1:A:101:PRO:HD2	2.34	0.42
1:B:141:GLU:OE2	1:B:143:ALA:N	2.53	0.42
1:C:22:ARG:O	4:C:505:HOH:O	2.22	0.42
1:C:36:LEU:HD11	1:D:165:LEU:HD21	2.01	0.42
1:A:99:LYS:CD	4:A:502:HOH:O	2.59	0.42
1:B:51:THR:O	1:B:52:LYS:HD2	2.20	0.42
1:A:101:PRO:HG2	1:A:102:ILE:HD12	2.00	0.42
1:A:186:PRO:O	1:A:187:ALA:C	2.62	0.42
1:A:192:VAL:HG22	1:B:196:MET:HE1	2.02	0.42
1:C:190:GLU:HB2	1:C:191:PRO:HD3	2.02	0.42
1:A:53:GLY:CA	1:A:57:THR:HG21	2.49	0.42
1:B:126:LEU:O	1:B:130:THR:HG23	2.20	0.41
1:B:263:LEU:O	1:B:264:VAL:CB	2.68	0.41
1:D:262:LEU:HA	1:D:265:ALA:HB3	2.01	0.41
1:D:144:SER:HA	1:D:147:ALA:O	2.20	0.41
1:D:190:GLU:HB2	1:D:191:PRO:HD3	2.01	0.41
1:C:63:SER:HB2	1:C:195:GLY:O	2.21	0.41
1:A:205:MET:HG2	1:D:121:LEU:HD21	2.02	0.41
1:A:210:GLY:O	1:A:211:ILE:C	2.63	0.41
1:B:215:PRO:HG2	1:B:250:LEU:HD13	2.03	0.41
2:B:401:BNG:H2	2:C:404:BNG:H1	2.02	0.41
1:D:135:THR:OG1	1:D:141:GLU:HA	2.20	0.41
1:B:183:LYS:HD3	1:B:183:LYS:HA	1.87	0.41
2:B:402:BNG:O2	2:B:406:BNG:H61	2.21	0.41
1:B:236:SER:CB	2:B:402:BNG:H3	2.50	0.41
1:D:265:ALA:O	1:D:266:LEU:CB	2.68	0.41
1:D:94:ARG:CZ	4:D:505:HOH:O	2.62	0.40
1:A:185:VAL:HG11	1:A:193:VAL:HG21	2.03	0.40
2:A:403:BNG:H1'1	2:D:401:BNG:H2	2.03	0.40
1:B:71:TYR:HB3	2:B:401:BNG:H6'2	2.02	0.40
1:C:72:VAL:CG2	2:D:403:BNG:H9'1	2.49	0.40
1:C:28:PHE:HE2	1:C:109:LEU:CD2	2.34	0.40
1:D:163:GLN:CD	1:D:212:PRO:HD2	2.46	0.40
1:C:188:GLY:HA2	2:C:403:BNG:H61	2.01	0.40
1:A:168:GLY:O	1:A:172:VAL:HG23	2.22	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	250/301 (83%)	242 (97%)	8 (3%)	0	100	100
1	B	250/301 (83%)	242 (97%)	6 (2%)	2 (1%)	16	20
1	C	251/301 (83%)	243 (97%)	8 (3%)	0	100	100
1	D	254/301 (84%)	245 (96%)	8 (3%)	1 (0%)	30	38
All	All	1005/1204 (84%)	972 (97%)	30 (3%)	3 (0%)	36	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	264	VAL
1	D	266	LEU
1	B	137	THR

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	193/233 (83%)	184 (95%)	9 (5%)	23	35
1	B	193/233 (83%)	182 (94%)	11 (6%)	18	27
1	C	194/233 (83%)	183 (94%)	11 (6%)	18	27
1	D	197/233 (84%)	193 (98%)	4 (2%)	48	67
All	All	777/932 (83%)	742 (96%)	35 (4%)	24	37

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	57	THR
1	A	105	LEU
1	A	161	LEU
1	A	181	ARG
1	A	183	LYS
1	A	199	LEU
1	A	213	LEU
1	A	268	HIS
1	B	19	LEU
1	B	20	LEU
1	B	29	LEU
1	B	36	LEU
1	B	47	THR
1	B	185	VAL
1	B	197	LEU
1	B	211	ILE
1	B	213	LEU
1	B	233	GLU
1	B	250	LEU
1	C	36	LEU
1	C	57	THR
1	C	67	THR
1	C	105	LEU
1	C	126	LEU
1	C	127	GLN
1	C	197	LEU
1	C	199	LEU
1	C	211	ILE
1	C	219	LEU
1	C	262	LEU
1	D	57	THR
1	D	180	ARG
1	D	197	LEU
1	D	266	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	B	163	GLN
1	C	127	GLN
1	C	268	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 ⓘ

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BNG	D	403	-	21,21,21	0.58	0	26,26,26	1.05	1 (3%)
2	BNG	C	403	-	21,21,21	0.89	1 (4%)	26,26,26	2.22	7 (26%)
3	GOL	A	404	-	5,5,5	1.00	0	5,5,5	1.39	1 (20%)
2	BNG	D	401	-	21,21,21	0.99	1 (4%)	26,26,26	1.85	6 (23%)
2	BNG	C	401	-	21,21,21	0.70	0	26,26,26	1.52	6 (23%)
3	GOL	C	405	-	5,5,5	0.40	0	5,5,5	0.68	0
2	BNG	A	403	-	21,21,21	0.61	0	26,26,26	0.97	1 (3%)
2	BNG	A	402	-	21,21,21	0.99	1 (4%)	26,26,26	1.13	1 (3%)
3	GOL	B	407	-	5,5,5	1.11	0	5,5,5	0.86	0
2	BNG	B	405	-	21,21,21	0.86	0	26,26,26	1.33	3 (11%)
2	BNG	A	401	-	21,21,21	0.75	0	26,26,26	1.33	5 (19%)
2	BNG	B	403	-	21,21,21	0.88	1 (4%)	26,26,26	1.71	5 (19%)
2	BNG	B	402	-	21,21,21	0.58	0	26,26,26	1.26	2 (7%)
2	BNG	C	404	-	21,21,21	0.78	1 (4%)	26,26,26	1.54	3 (11%)
2	BNG	B	401	-	21,21,21	0.75	0	26,26,26	1.35	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BNG	B	406	-	21,21,21	0.74	0	26,26,26	1.23	2 (7%)
2	BNG	D	402	-	21,21,21	0.65	0	26,26,26	0.96	1 (3%)
3	GOL	B	408	-	5,5,5	0.51	0	5,5,5	1.15	1 (20%)
3	GOL	D	404	-	5,5,5	0.45	0	5,5,5	0.64	0
2	BNG	B	404	-	21,21,21	0.63	0	26,26,26	0.96	0
2	BNG	C	402	-	21,21,21	0.68	0	26,26,26	1.24	4 (15%)
3	GOL	A	405	-	5,5,5	0.44	0	5,5,5	1.03	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BNG	D	403	-	1/1/5/5	6/12/32/32	0/1/1/1
2	BNG	C	403	-	1/1/5/5	9/12/32/32	0/1/1/1
3	GOL	A	404	-	-	4/4/4/4	-
2	BNG	D	401	-	1/1/5/5	7/12/32/32	0/1/1/1
2	BNG	C	401	-	1/1/5/5	5/12/32/32	0/1/1/1
3	GOL	C	405	-	-	1/4/4/4	-
2	BNG	A	403	-	1/1/5/5	6/12/32/32	0/1/1/1
2	BNG	A	402	-	1/1/5/5	6/12/32/32	0/1/1/1
3	GOL	B	407	-	-	2/4/4/4	-
2	BNG	B	405	-	1/1/5/5	5/12/32/32	0/1/1/1
2	BNG	A	401	-	1/1/5/5	5/12/32/32	0/1/1/1
2	BNG	B	403	-	1/1/5/5	3/12/32/32	0/1/1/1
2	BNG	B	402	-	1/1/5/5	9/12/32/32	0/1/1/1
2	BNG	C	404	-	1/1/5/5	10/12/32/32	0/1/1/1
2	BNG	B	401	-	1/1/5/5	3/12/32/32	0/1/1/1
2	BNG	B	406	-	1/1/5/5	10/12/32/32	0/1/1/1
2	BNG	D	402	-	1/1/5/5	8/12/32/32	0/1/1/1
3	GOL	B	408	-	-	2/4/4/4	-
3	GOL	D	404	-	-	2/4/4/4	-
2	BNG	B	404	-	1/1/5/5	5/12/32/32	0/1/1/1
2	BNG	C	402	-	1/1/5/5	7/12/32/32	0/1/1/1
3	GOL	A	405	-	-	3/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	BNG	O5-C5	-2.64	1.37	1.44
2	B	403	BNG	O5-C5	-2.45	1.38	1.44
2	D	401	BNG	O1-C1	2.29	1.44	1.40
2	C	404	BNG	O5-C5	-2.12	1.39	1.44
2	C	403	BNG	O3-C3	-2.04	1.37	1.43

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	403	BNG	C1-O5-C5	-6.11	101.79	113.72
2	D	401	BNG	O1-C1-C2	5.66	116.86	108.27
2	C	404	BNG	O1-C1-C2	5.38	116.45	108.27
2	C	403	BNG	C4-C3-C2	4.82	119.30	110.83
2	B	403	BNG	C1-O5-C5	-4.75	104.44	113.72
2	C	403	BNG	O5-C5-C6	4.44	117.44	106.44
2	B	402	BNG	C1-O5-C5	-4.29	105.34	113.72
2	D	401	BNG	C1-O5-C5	-4.06	105.79	113.72
2	C	401	BNG	C1-O5-C5	-3.66	106.58	113.72
2	C	401	BNG	C6-C5-C4	-3.51	104.41	113.02
2	C	402	BNG	C1-O5-C5	-3.45	106.98	113.72
2	B	403	BNG	C6-C5-C4	-3.28	104.96	113.02
2	C	401	BNG	C4-C3-C2	3.26	116.55	110.83
2	D	401	BNG	C4-C3-C2	3.20	116.45	110.83
2	A	401	BNG	C4-C3-C2	3.19	116.42	110.83
2	B	406	BNG	C3-C4-C5	-3.17	104.48	110.23
2	B	405	BNG	C4-C3-C2	3.14	116.34	110.83
2	C	403	BNG	O5-C1-O1	3.08	117.33	110.04
2	A	401	BNG	C3-C4-C5	3.04	115.74	110.23
2	B	401	BNG	C4-C3-C2	3.03	116.14	110.83
2	A	401	BNG	C6-C5-C4	-2.97	105.72	113.02
2	B	405	BNG	C1-O5-C5	-2.97	107.92	113.72
2	B	406	BNG	O5-C5-C6	2.78	113.33	106.44
2	C	403	BNG	O3-C3-C4	-2.77	103.86	110.38
2	A	402	BNG	C4-C3-C2	2.72	115.61	110.83
2	C	403	BNG	C6-C5-C4	-2.68	106.45	113.02
2	B	403	BNG	C6'-C5'-C4'	-2.68	100.85	114.37
2	B	401	BNG	C1-O5-C5	-2.61	108.63	113.72
2	C	404	BNG	O2-C2-C1	-2.58	103.93	110.08
2	B	401	BNG	C1-C2-C3	2.58	115.44	110.01
2	B	401	BNG	C3-C4-C5	2.50	114.77	110.23
2	C	401	BNG	C3-C4-C5	2.46	114.70	110.23
2	D	401	BNG	O5-C1-C2	-2.45	105.33	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	BNG	C1'-O1-C1	2.37	117.73	113.68
2	C	404	BNG	O6-C6-C5	-2.37	103.26	111.33
2	C	402	BNG	C4-C3-C2	2.37	114.99	110.83
2	B	402	BNG	O5-C5-C6	2.36	112.29	106.44
2	D	402	BNG	C3'-C2'-C1'	-2.36	103.23	113.47
2	B	403	BNG	C4-C3-C2	2.35	114.96	110.83
3	A	404	GOL	C3-C2-C1	-2.33	103.25	111.80
2	B	403	BNG	O1-C1-C2	2.28	111.73	108.27
2	B	401	BNG	C6-C5-C4	-2.21	107.60	113.02
2	C	402	BNG	C3-C4-C5	2.18	114.18	110.23
2	D	403	BNG	C1-O5-C5	-2.17	109.48	113.72
2	A	403	BNG	C6-C5-C4	-2.14	107.77	113.02
2	D	401	BNG	C6-C5-C4	-2.13	107.78	113.02
2	A	401	BNG	C1-C2-C3	2.12	114.47	110.01
2	A	401	BNG	C1-O5-C5	-2.11	109.60	113.72
2	C	403	BNG	C1'-O1-C1	2.11	117.28	113.68
2	D	401	BNG	O3-C3-C2	2.10	115.33	110.38
2	B	405	BNG	O3-C3-C2	-2.09	105.44	110.38
2	C	402	BNG	O1-C1-C2	2.06	111.41	108.27
2	C	401	BNG	C1-C2-C3	2.01	114.24	110.01
3	B	408	GOL	C3-C2-C1	-2.01	104.42	111.80

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	BNG	C3
2	A	402	BNG	C3
2	A	403	BNG	C3
2	B	401	BNG	C3
2	B	402	BNG	C3
2	B	403	BNG	C3
2	B	404	BNG	C3
2	B	405	BNG	C3
2	B	406	BNG	C3
2	C	401	BNG	C3
2	C	402	BNG	C3
2	C	403	BNG	C3
2	C	404	BNG	C3
2	D	401	BNG	C3
2	D	402	BNG	C3
2	D	403	BNG	C3

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	402	BNG	O5-C1-O1-C1'
2	B	402	BNG	C2'-C1'-O1-C1
2	C	402	BNG	C2'-C1'-O1-C1
2	C	403	BNG	O5-C1-O1-C1'
2	C	403	BNG	C2'-C1'-O1-C1
2	C	404	BNG	O5-C1-O1-C1'
3	A	404	GOL	O1-C1-C2-C3
3	A	404	GOL	C1-C2-C3-O3
3	A	404	GOL	O2-C2-C3-O3
3	A	405	GOL	O1-C1-C2-C3
3	B	408	GOL	O1-C1-C2-C3
3	D	404	GOL	C1-C2-C3-O3
2	B	405	BNG	O5-C5-C6-O6
2	C	403	BNG	O5-C5-C6-O6
2	C	402	BNG	C4-C5-C6-O6
2	D	403	BNG	O5-C5-C6-O6
2	B	402	BNG	O5-C5-C6-O6
2	C	403	BNG	C4-C5-C6-O6
2	A	401	BNG	O5-C1-O1-C1'
2	B	406	BNG	O5-C1-O1-C1'
2	C	401	BNG	O5-C1-O1-C1'
2	C	402	BNG	O5-C1-O1-C1'
2	B	406	BNG	O5-C5-C6-O6
2	D	402	BNG	C4'-C5'-C6'-C7'
2	C	404	BNG	O5-C5-C6-O6
2	B	405	BNG	C4-C5-C6-O6
2	D	403	BNG	C4-C5-C6-O6
2	B	402	BNG	C2-C1-O1-C1'
2	B	406	BNG	C2-C1-O1-C1'
2	C	402	BNG	C2-C1-O1-C1'
2	C	403	BNG	C2-C1-O1-C1'
2	D	401	BNG	C2-C1-O1-C1'
2	C	402	BNG	O5-C5-C6-O6
2	B	402	BNG	C4-C5-C6-O6
2	B	406	BNG	C4-C5-C6-O6
3	B	407	GOL	O2-C2-C3-O3
2	B	404	BNG	O1-C1'-C2'-C3'
2	B	405	BNG	C5'-C6'-C7'-C8'
2	A	401	BNG	C4-C5-C6-O6
2	A	403	BNG	O5-C1-O1-C1'
2	B	401	BNG	C3'-C4'-C5'-C6'
2	C	401	BNG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	402	BNG	O1-C1'-C2'-C3'
2	D	401	BNG	C4'-C5'-C6'-C7'
2	A	401	BNG	O5-C5-C6-O6
2	C	404	BNG	C4-C5-C6-O6
2	C	401	BNG	O5-C5-C6-O6
2	B	401	BNG	C4-C5-C6-O6
2	D	402	BNG	C2'-C3'-C4'-C5'
3	B	407	GOL	C1-C2-C3-O3
2	D	402	BNG	C4-C5-C6-O6
2	B	406	BNG	O1-C1'-C2'-C3'
2	B	403	BNG	C5'-C6'-C7'-C8'
2	B	404	BNG	C1'-C2'-C3'-C4'
2	B	405	BNG	C4'-C5'-C6'-C7'
2	A	401	BNG	C6'-C7'-C8'-C9'
3	A	404	GOL	O1-C1-C2-O2
3	B	408	GOL	O1-C1-C2-O2
2	B	406	BNG	C2'-C3'-C4'-C5'
2	B	402	BNG	C2'-C3'-C4'-C5'
2	C	404	BNG	C2'-C3'-C4'-C5'
2	B	402	BNG	O1-C1'-C2'-C3'
2	C	403	BNG	C1'-C2'-C3'-C4'
2	D	403	BNG	C5'-C6'-C7'-C8'
2	B	406	BNG	C3'-C4'-C5'-C6'
2	C	404	BNG	C1'-C2'-C3'-C4'
2	B	406	BNG	C5'-C6'-C7'-C8'
2	C	403	BNG	C5'-C6'-C7'-C8'
2	B	404	BNG	C3'-C4'-C5'-C6'
2	C	404	BNG	C5'-C6'-C7'-C8'
2	B	401	BNG	O5-C5-C6-O6
2	C	402	BNG	C3'-C4'-C5'-C6'
2	C	403	BNG	C4'-C5'-C6'-C7'
2	A	402	BNG	C2'-C3'-C4'-C5'
2	C	403	BNG	C3'-C4'-C5'-C6'
2	C	401	BNG	O1-C1'-C2'-C3'
2	A	402	BNG	O1-C1'-C2'-C3'
2	D	401	BNG	O1-C1'-C2'-C3'
2	A	401	BNG	O1-C1'-C2'-C3'
2	D	401	BNG	C3'-C4'-C5'-C6'
2	D	402	BNG	O5-C5-C6-O6
2	A	403	BNG	C6'-C7'-C8'-C9'
2	A	402	BNG	C6'-C7'-C8'-C9'
2	B	403	BNG	C2'-C1'-O1-C1

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Mol	Chain	Res	Type	Atoms
2	B	404	BNG	C2'-C1'-O1-C1
2	C	404	BNG	C2'-C1'-O1-C1
2	B	402	BNG	C1'-C2'-C3'-C4'
2	C	404	BNG	C2-C1-O1-C1'
2	D	401	BNG	C4-C5-C6-O6
2	D	403	BNG	C6'-C7'-C8'-C9'
2	A	402	BNG	C3'-C4'-C5'-C6'
2	D	401	BNG	C1'-C2'-C3'-C4'
2	A	402	BNG	C4'-C5'-C6'-C7'
2	B	404	BNG	C4'-C5'-C6'-C7'
2	B	402	BNG	C5'-C6'-C7'-C8'
2	C	404	BNG	C6'-C7'-C8'-C9'
3	A	405	GOL	O1-C1-C2-O2
3	A	405	GOL	O2-C2-C3-O3
3	C	405	GOL	O1-C1-C2-O2
2	B	405	BNG	C6'-C7'-C8'-C9'
2	D	402	BNG	C3'-C4'-C5'-C6'
2	A	403	BNG	C1'-C2'-C3'-C4'
2	B	406	BNG	C4'-C5'-C6'-C7'
2	D	402	BNG	C6'-C7'-C8'-C9'
2	A	403	BNG	C2'-C3'-C4'-C5'
2	D	402	BNG	C5'-C6'-C7'-C8'
2	A	402	BNG	C5'-C6'-C7'-C8'
2	D	401	BNG	O5-C5-C6-O6
2	A	403	BNG	C4'-C5'-C6'-C7'
2	D	403	BNG	C2'-C1'-O1-C1
2	A	403	BNG	C5'-C6'-C7'-C8'
2	B	406	BNG	C1'-C2'-C3'-C4'
2	B	403	BNG	C3'-C4'-C5'-C6'
2	C	404	BNG	C3'-C4'-C5'-C6'
2	D	403	BNG	O1-C1'-C2'-C3'
2	C	401	BNG	C1'-C2'-C3'-C4'
2	D	402	BNG	O5-C1-O1-C1'
3	D	404	GOL	O2-C2-C3-O3

There are no ring outliers.

20 monomers are involved in 52 short contacts:

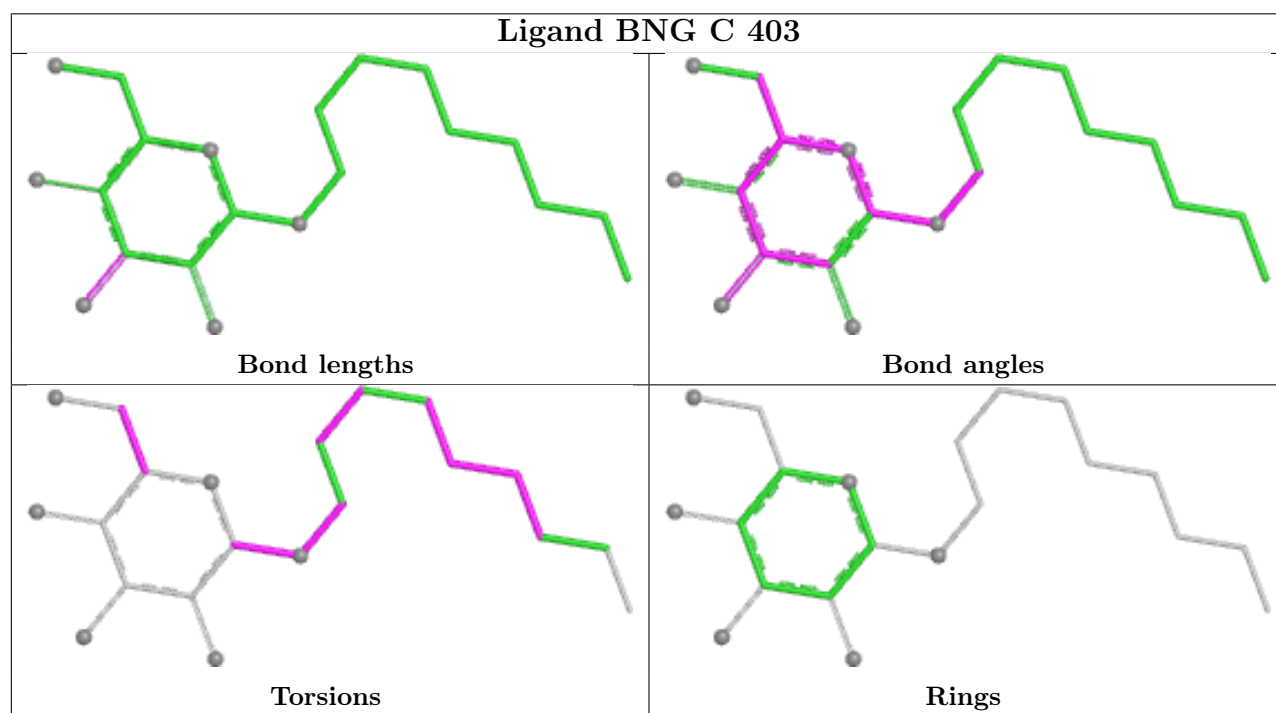
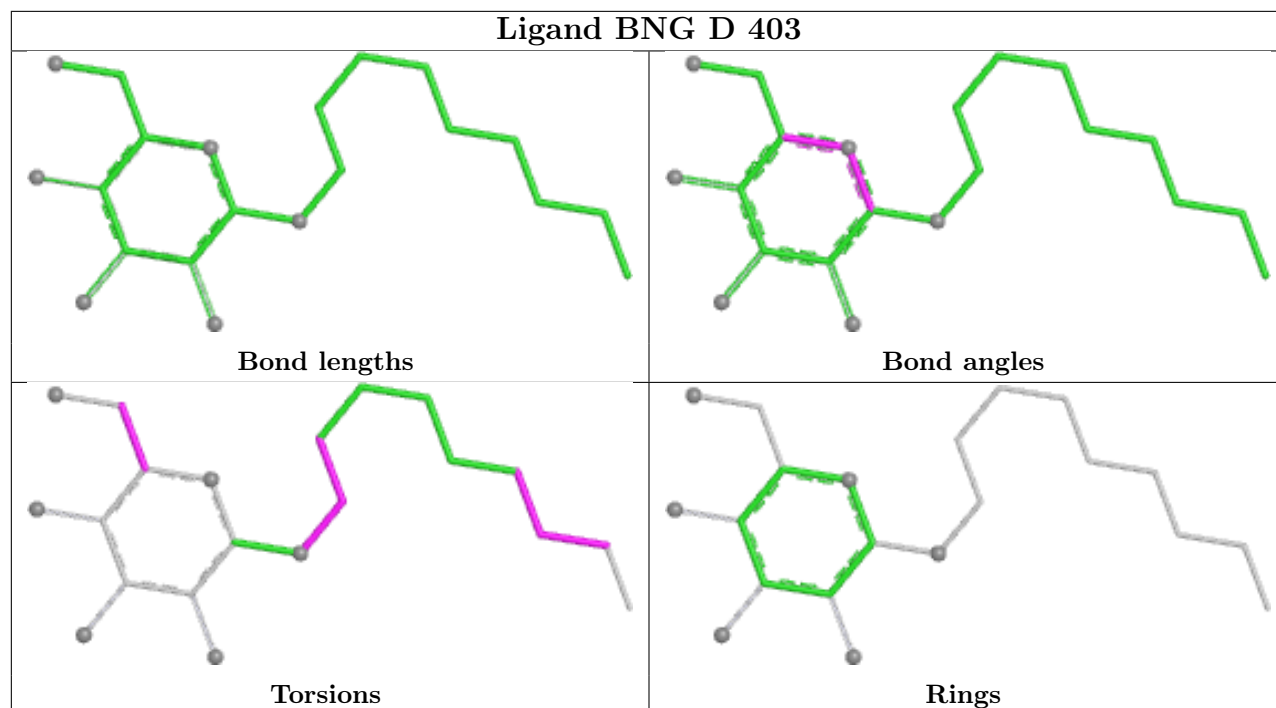
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	403	BNG	13	0
2	C	403	BNG	9	0
3	A	404	GOL	1	0

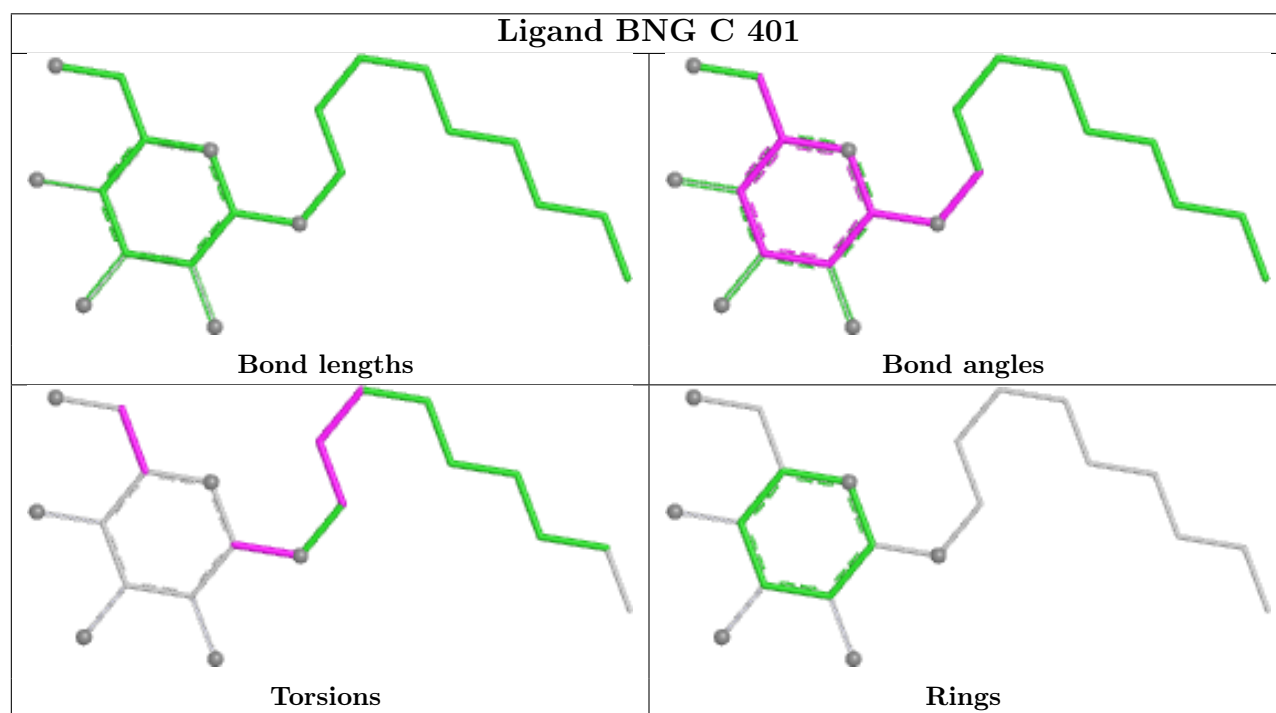
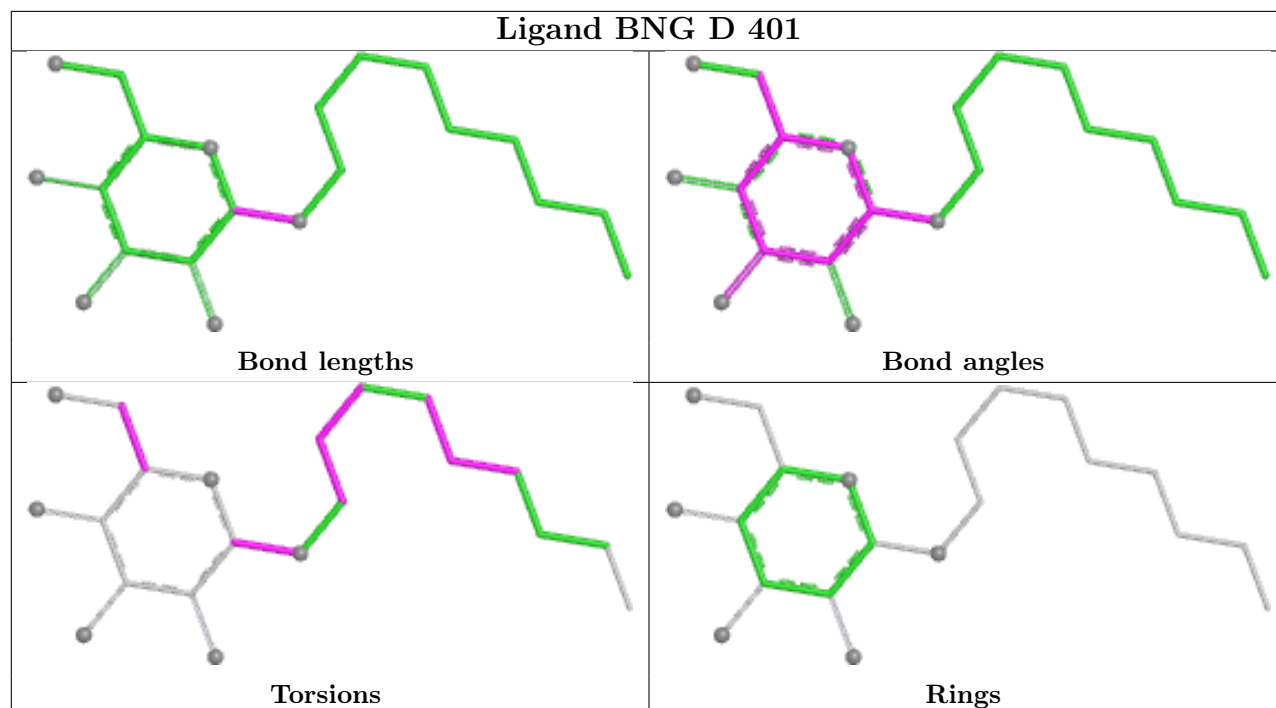
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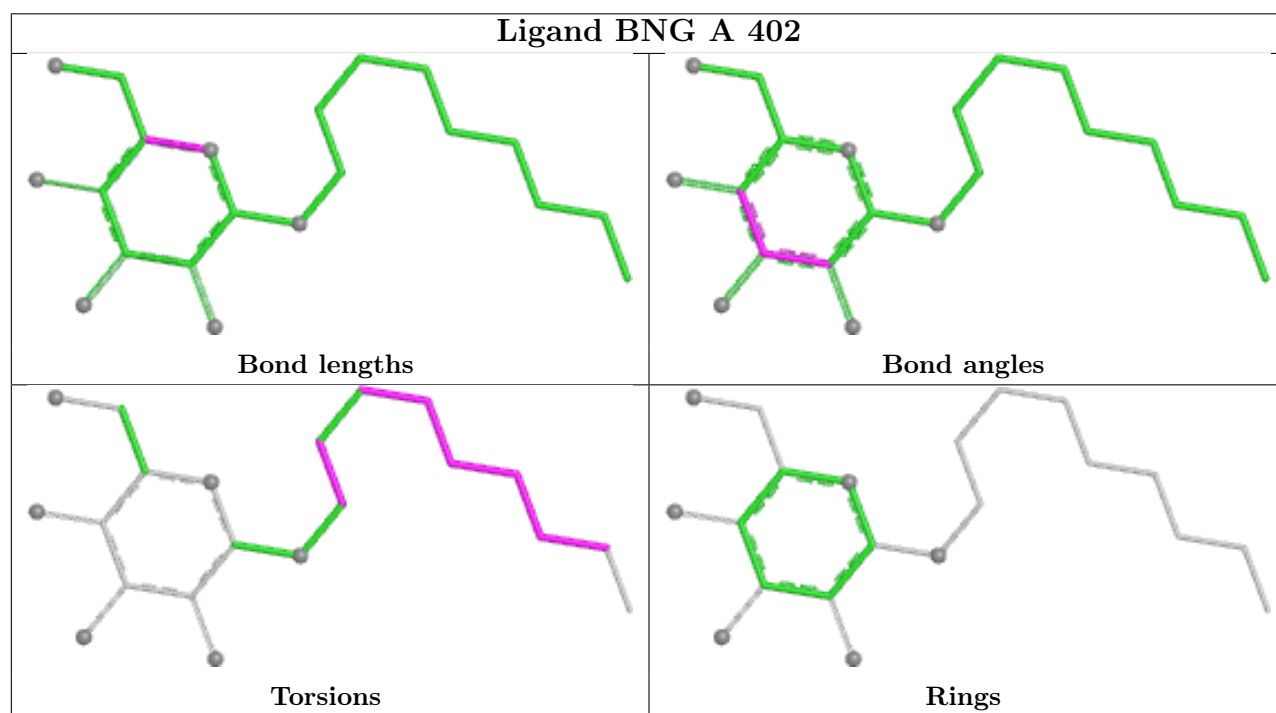
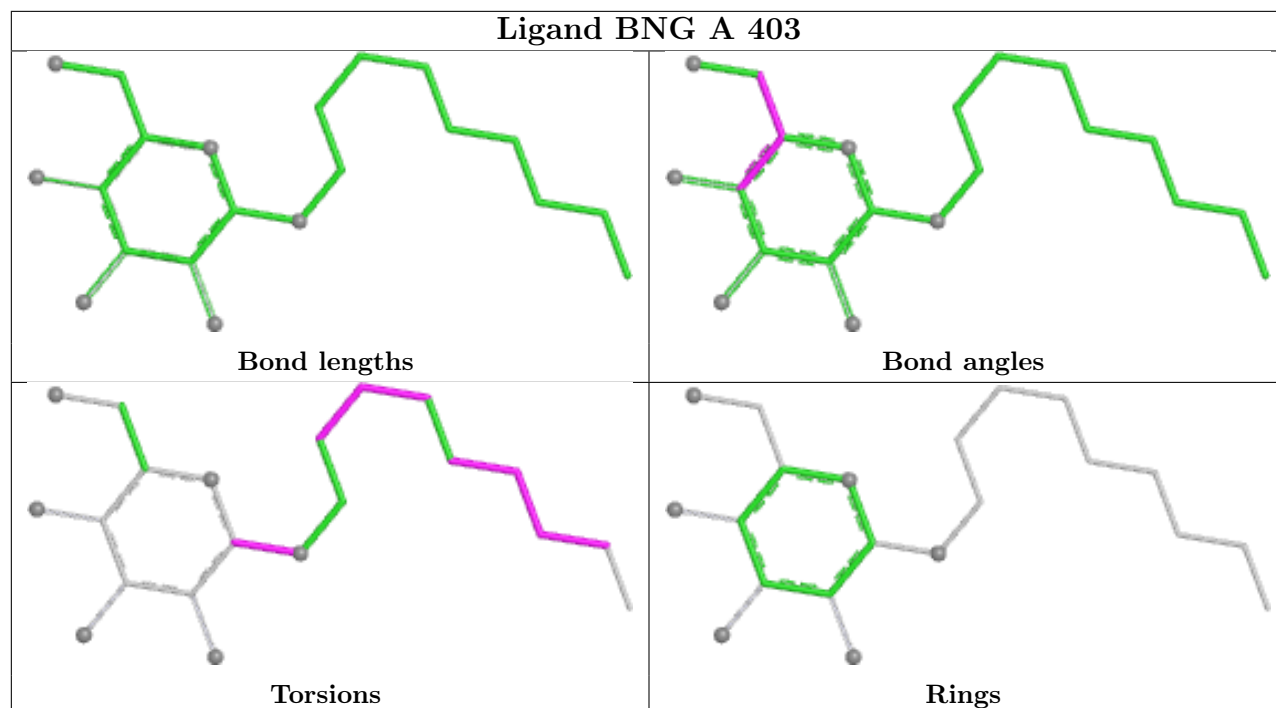
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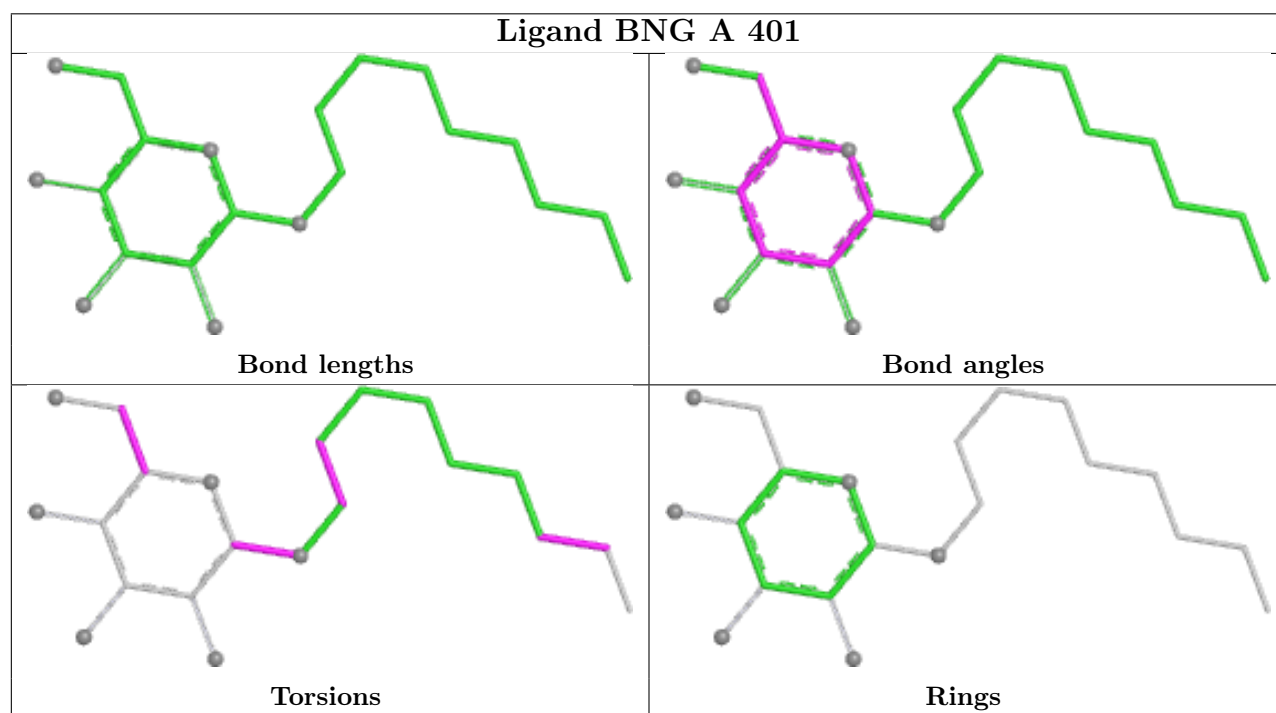
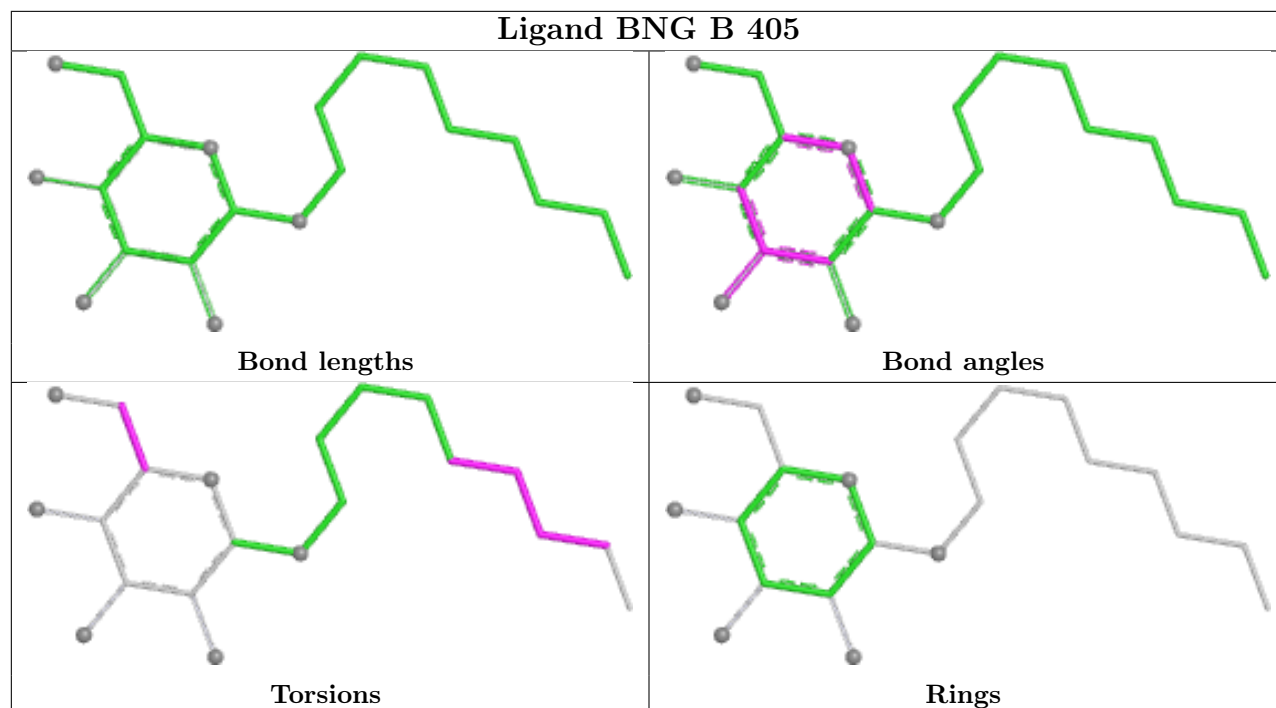
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	BNG	1	0
2	C	401	BNG	4	0
3	C	405	GOL	1	0
2	A	403	BNG	2	0
2	A	402	BNG	2	0
2	B	405	BNG	1	0
2	A	401	BNG	2	0
2	B	403	BNG	4	0
2	B	402	BNG	3	0
2	C	404	BNG	5	0
2	B	401	BNG	2	0
2	B	406	BNG	2	0
2	D	402	BNG	2	0
3	D	404	GOL	1	0
2	B	404	BNG	2	0
2	C	402	BNG	1	0
3	A	405	GOL	1	0

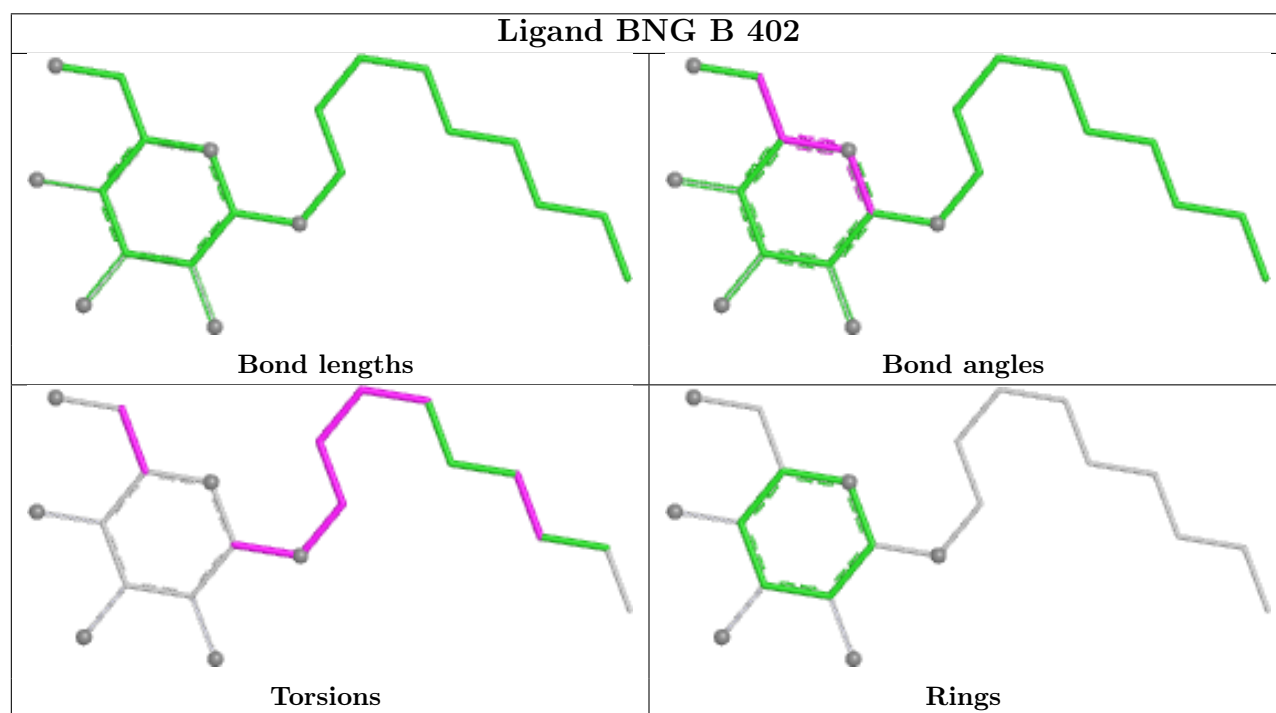
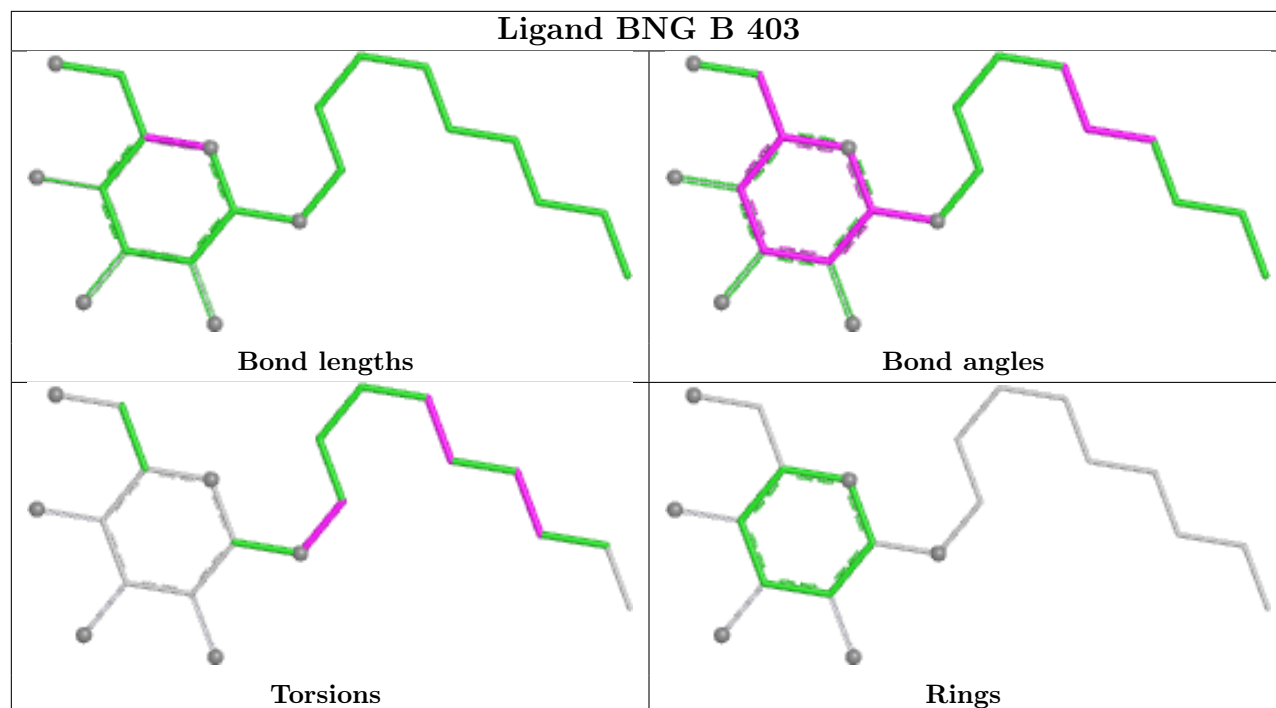
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

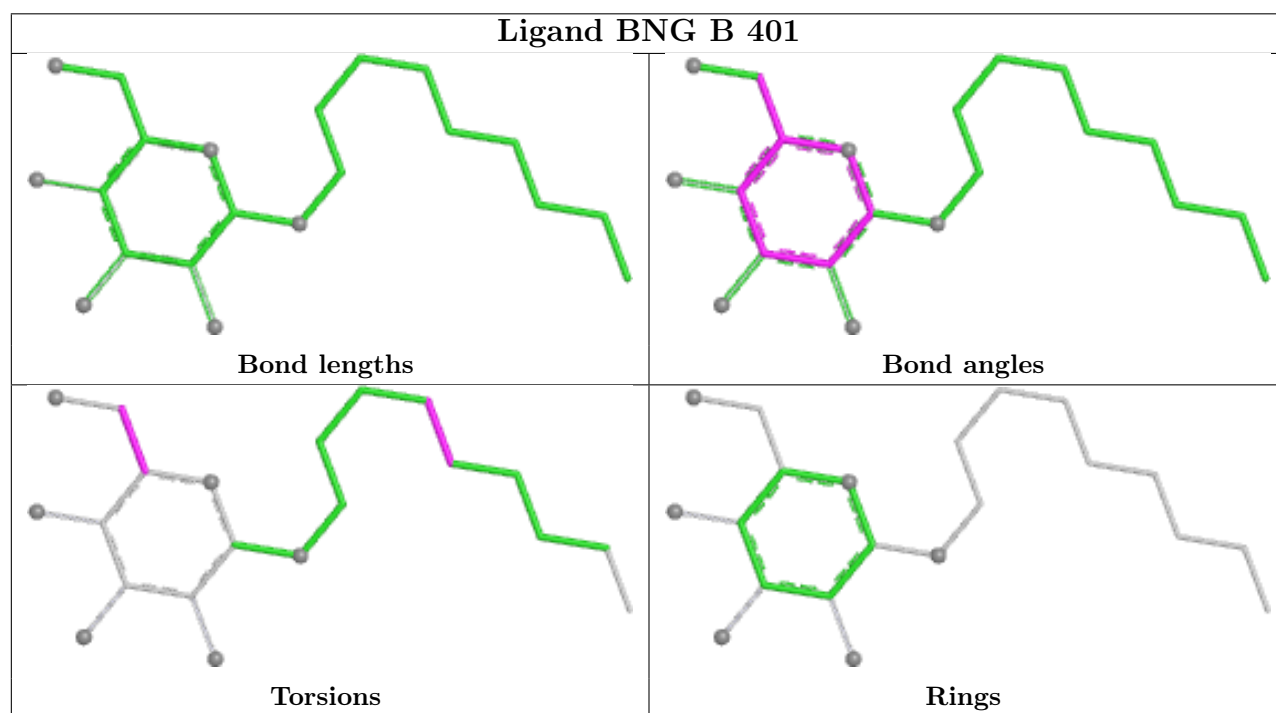
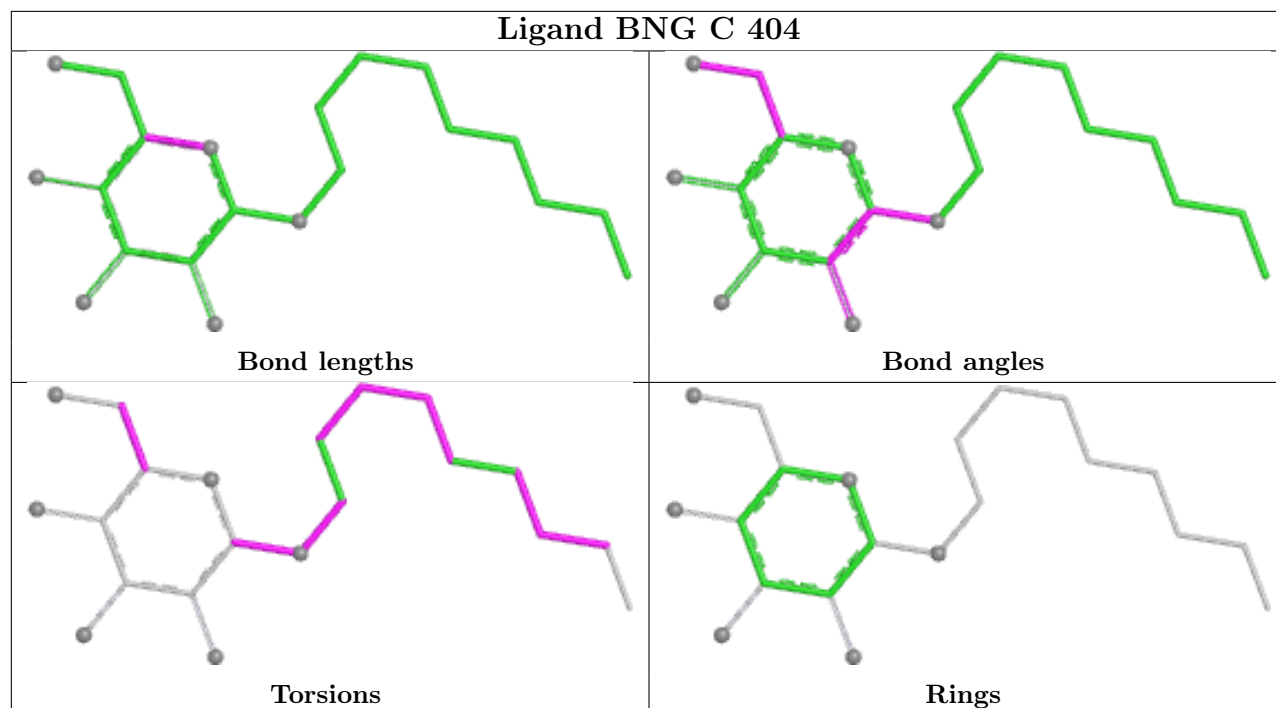


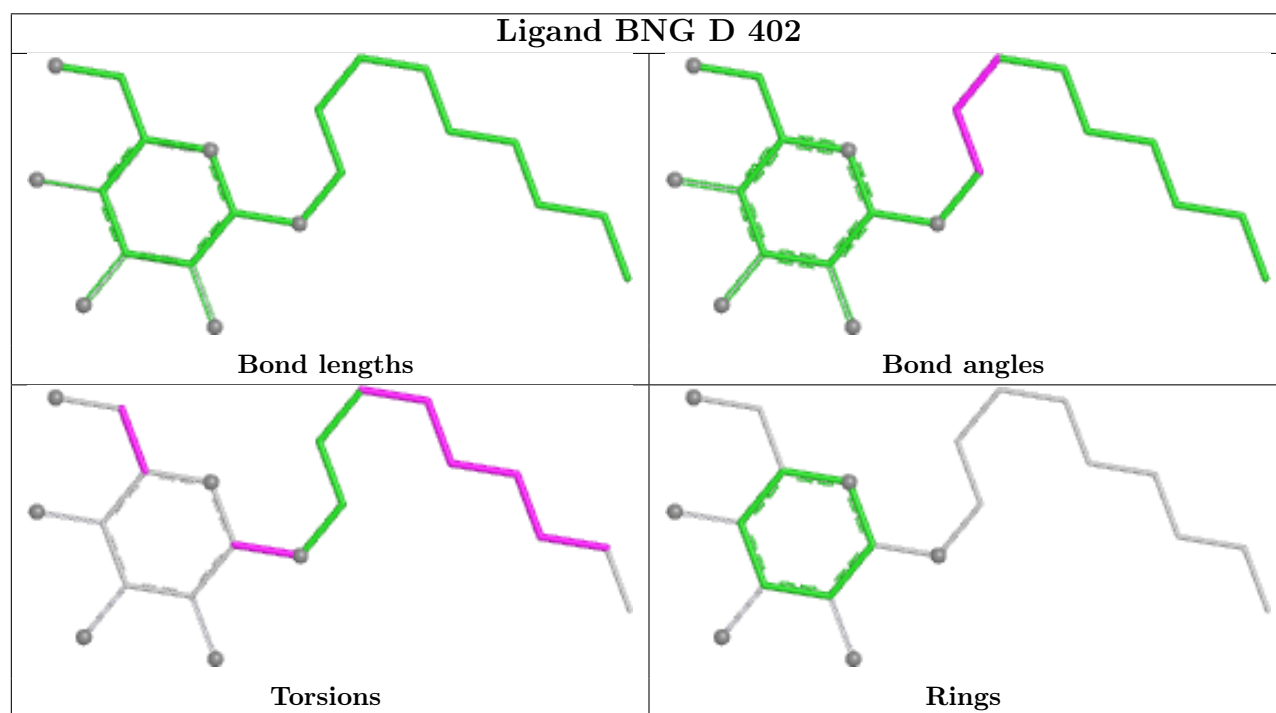
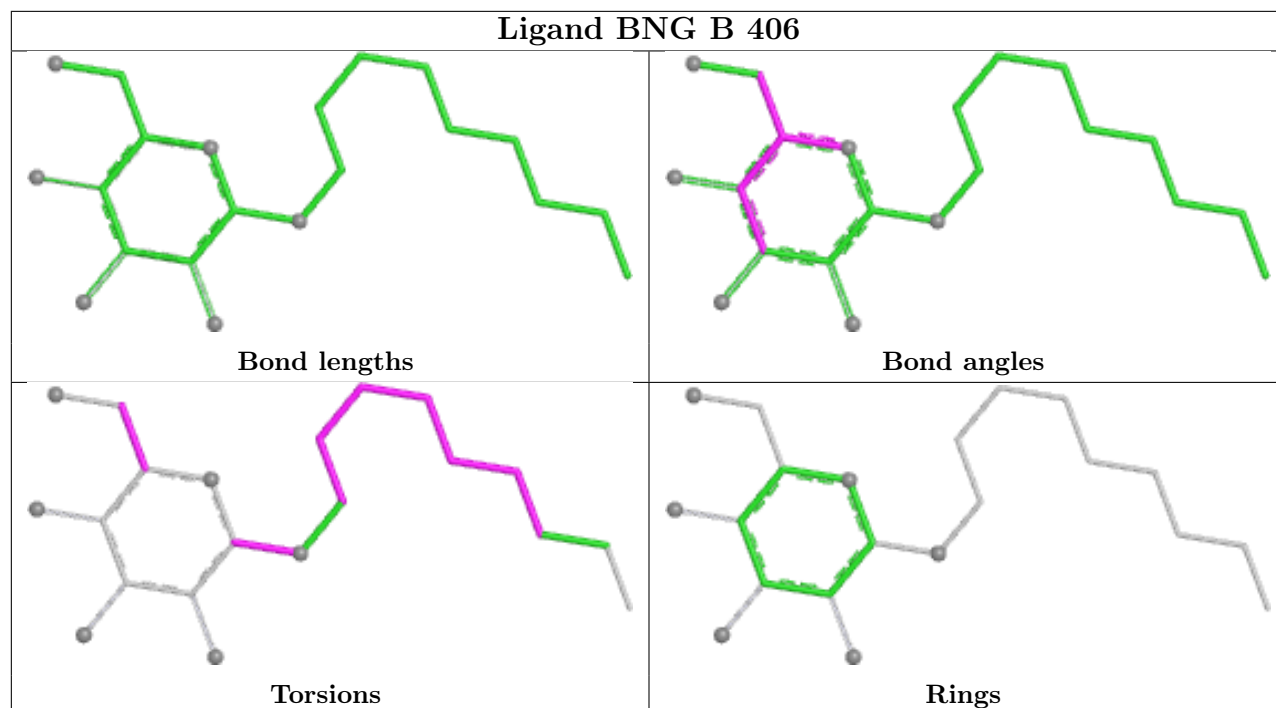


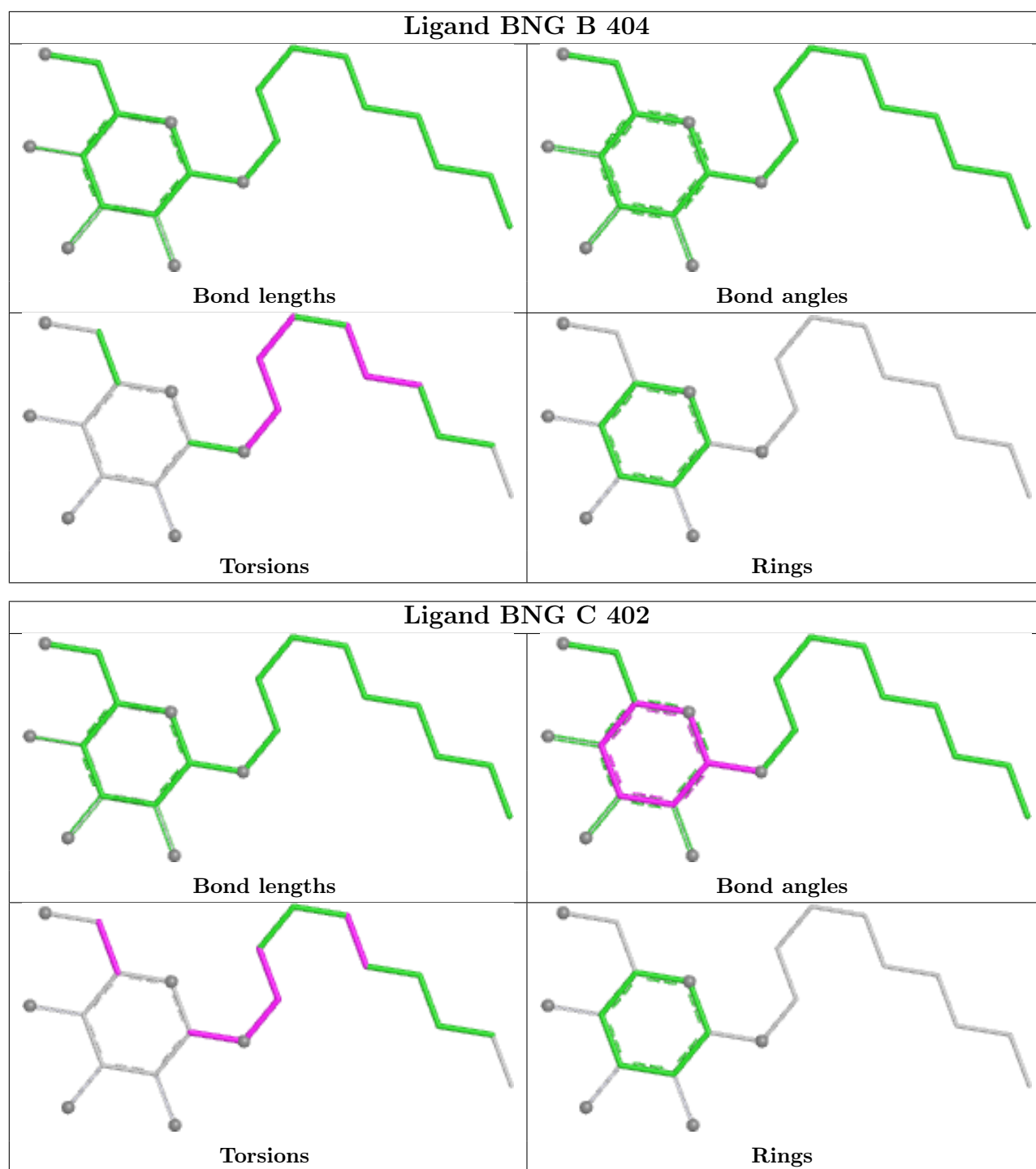












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	251/301 (83%)	-0.09	2 (0%) 82 83	27, 46, 61, 90	1 (0%)
1	B	252/301 (83%)	0.02	11 (4%) 39 41	34, 44, 63, 80	0
1	C	253/301 (84%)	0.09	8 (3%) 50 52	35, 50, 68, 91	0
1	D	256/301 (85%)	0.02	5 (1%) 65 66	35, 50, 68, 97	0
All	All	1012/1204 (84%)	0.01	26 (2%) 57 59	27, 48, 66, 97	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	268	HIS	4.5
1	A	268	HIS	4.2
1	B	269	PRO	4.2
1	C	98	VAL	3.6
1	B	210	GLY	3.6
1	B	137	THR	3.5
1	D	265	ALA	3.5
1	D	268	HIS	3.4
1	D	184	GLY	3.2
1	B	18	SER	3.0
1	C	210	GLY	3.0
1	B	256	GLY	2.9
1	C	17	ARG	2.8
1	B	264	VAL	2.6
1	C	267	HIS	2.5
1	D	262	LEU	2.5
1	D	17	ARG	2.4
1	C	184	GLY	2.3
1	C	161	LEU	2.2
1	B	263	LEU	2.2
1	B	138	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	19	LEU	2.1
1	C	16	ILE	2.1
1	B	136	VAL	2.1
1	A	18	SER	2.0
1	B	233	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BNG	B	406	21/21	0.71	0.21	74,88,99,102	0
2	BNG	B	405	21/21	0.75	0.21	78,88,94,94	0
2	BNG	C	404	21/21	0.79	0.20	66,79,89,91	0
2	BNG	C	403	21/21	0.83	0.17	47,69,75,81	0
2	BNG	D	403	21/21	0.84	0.21	80,92,101,102	0
2	BNG	B	402	21/21	0.85	0.17	53,75,88,89	0
2	BNG	B	404	21/21	0.85	0.18	61,74,79,80	0
2	BNG	C	402	21/21	0.85	0.17	70,80,86,87	0
2	BNG	D	402	21/21	0.86	0.16	59,72,78,86	0
2	BNG	A	402	21/21	0.86	0.15	64,72,81,86	0
3	GOL	D	404	6/6	0.86	0.21	54,59,63,65	0
3	GOL	A	404	6/6	0.87	0.18	50,58,62,68	0
2	BNG	A	403	21/21	0.87	0.16	66,80,94,97	0
2	BNG	B	403	21/21	0.88	0.14	48,58,65,66	0
3	GOL	B	408	6/6	0.91	0.17	70,71,72,73	0
3	GOL	C	405	6/6	0.92	0.15	55,56,58,62	0
3	GOL	B	407	6/6	0.93	0.14	54,55,59,60	0
3	GOL	A	405	6/6	0.93	0.13	53,60,64,67	0

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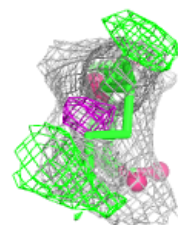
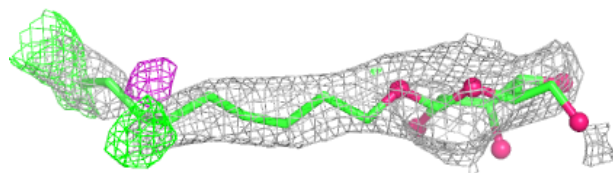
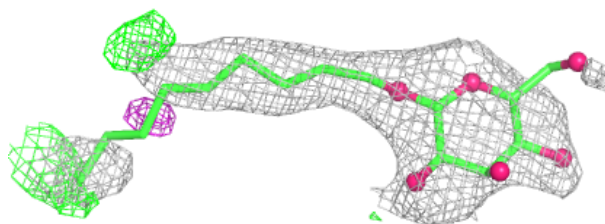
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BNG	D	401	21/21	0.94	0.11	49,57,61,66	0
2	BNG	C	401	21/21	0.94	0.11	49,58,62,64	0
2	BNG	A	401	21/21	0.94	0.11	52,56,60,61	0
2	BNG	B	401	21/21	0.95	0.11	57,61,68,74	0

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.

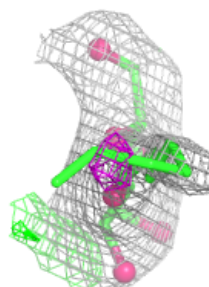
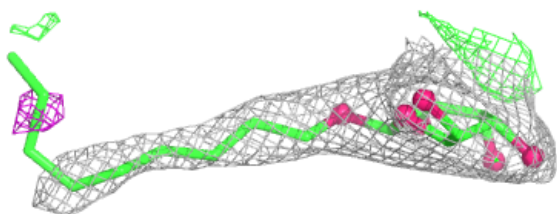
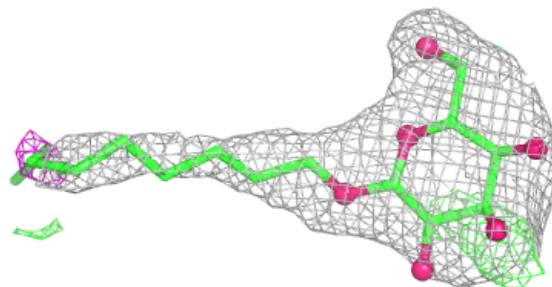
Electron density around BNG B 406:

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

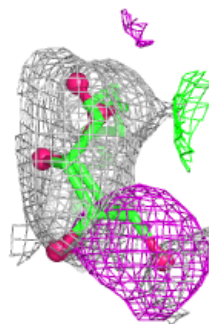
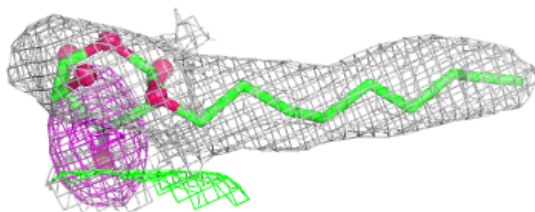
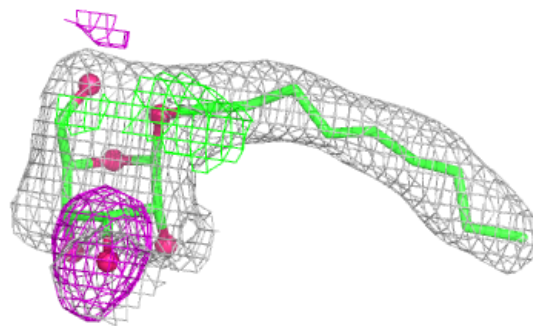


Electron density around BNG B 405:

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

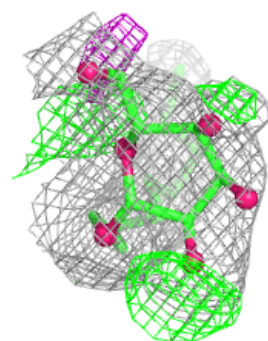
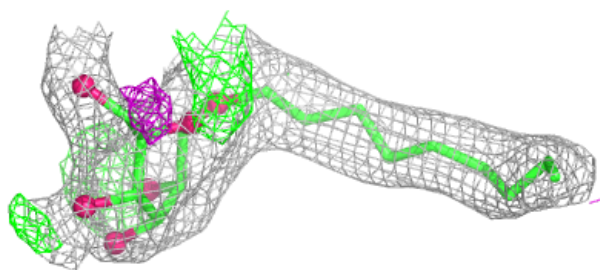
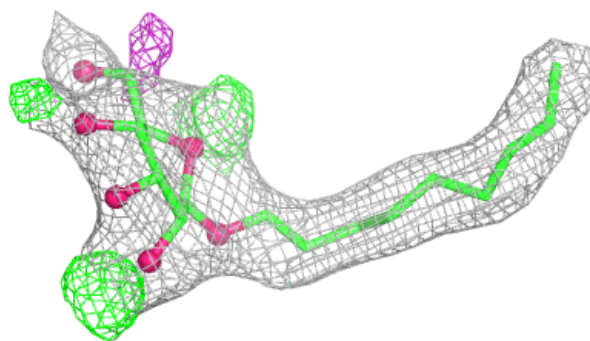
**Electron density around BNG C 404:**

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

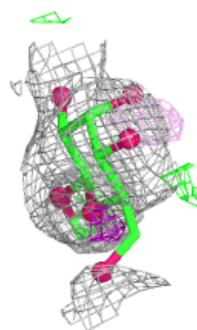
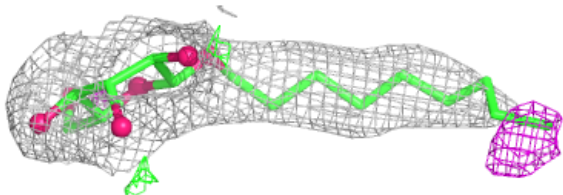
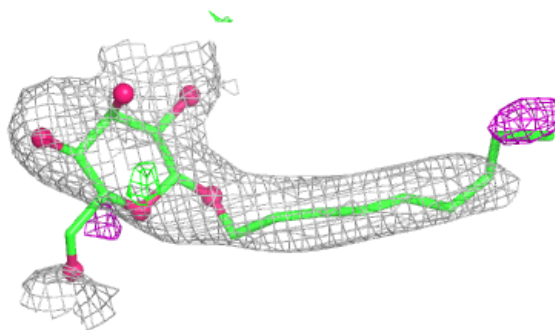


Electron density around BNG C 403:

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

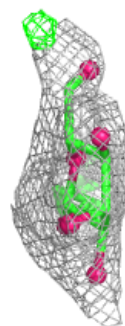
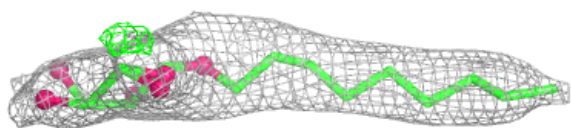
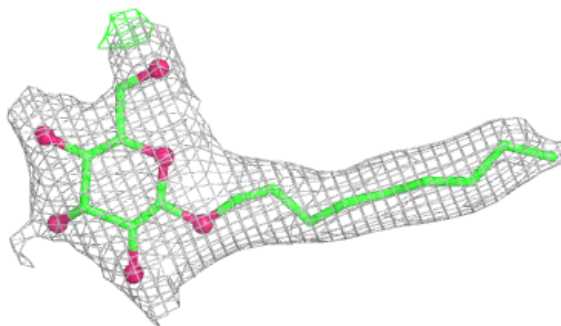
**Electron density around BNG D 403:**

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

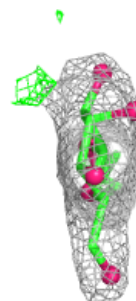
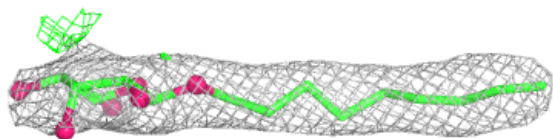
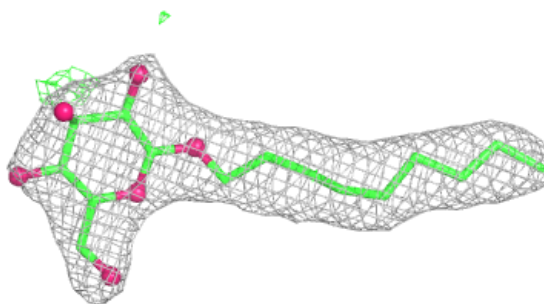


Electron density around BNG B 402:

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

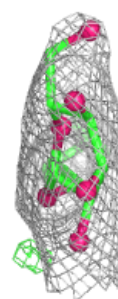
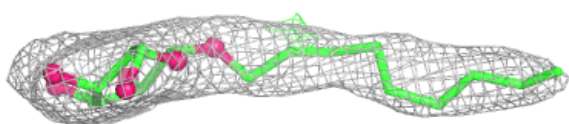
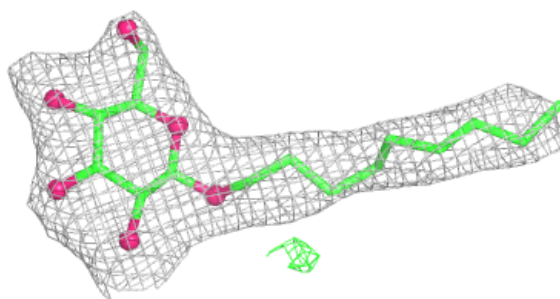
**Electron density around BNG B 404:**

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

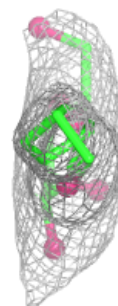
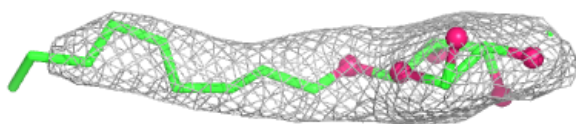
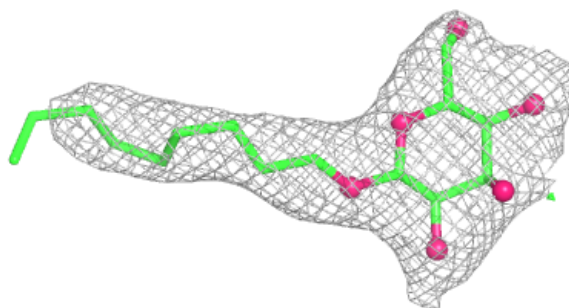


Electron density around BNG C 402:

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

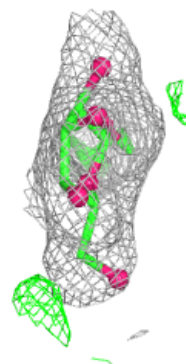
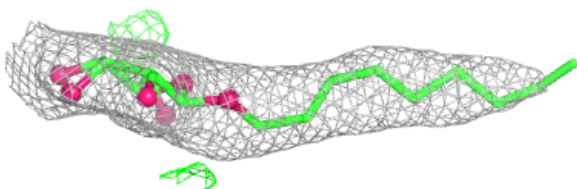
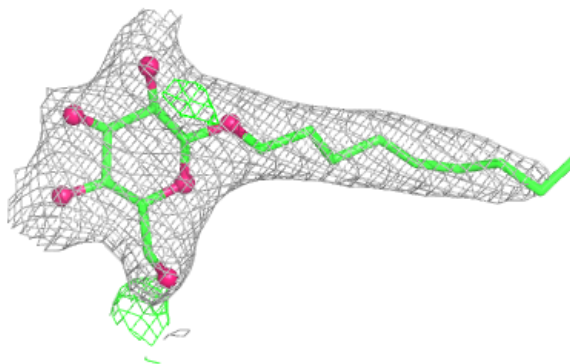
**Electron density around BNG D 402:**

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

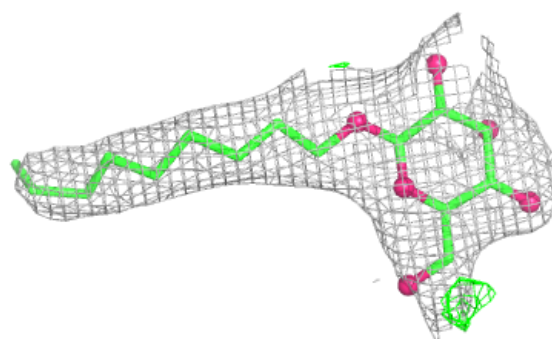


Electron density around BNG A 402:

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

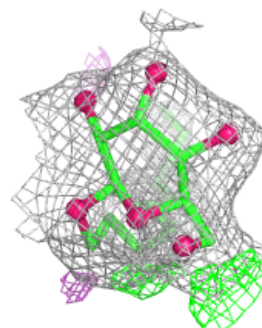
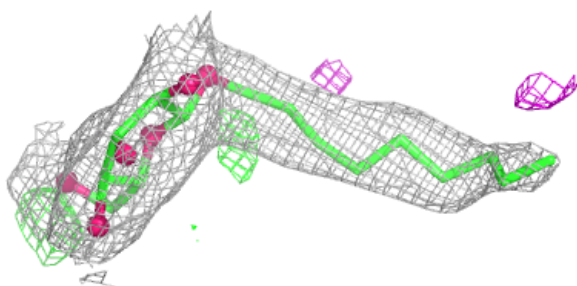
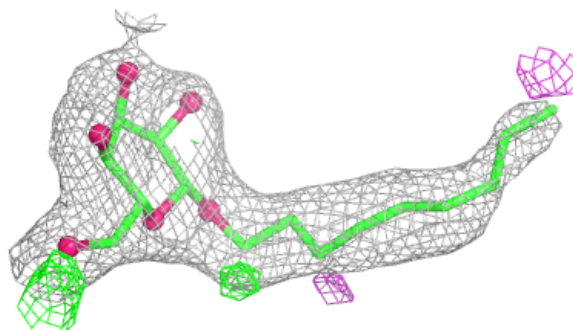
**Electron density around BNG A 403:**

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

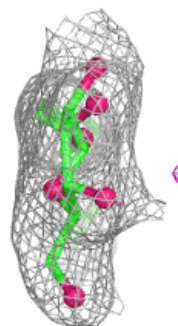
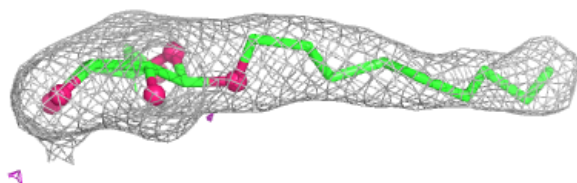
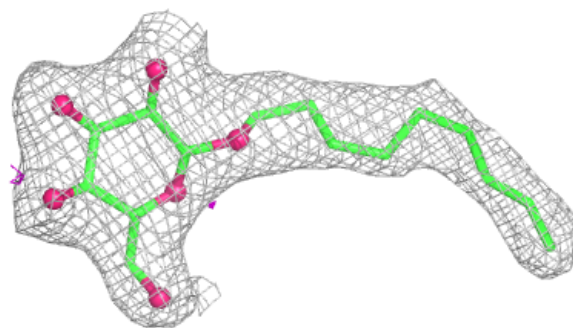


Electron density around BNG B 403:

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

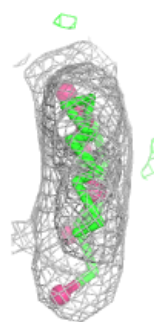
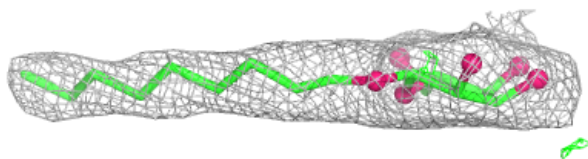
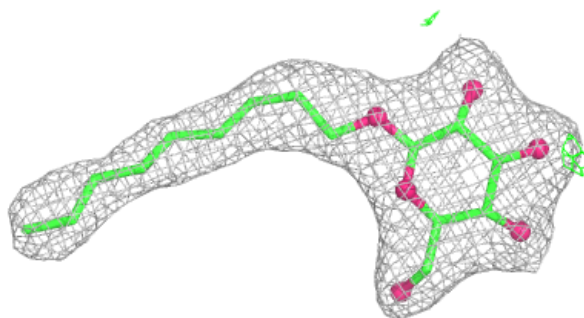
**Electron density around BNG D 401:**

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

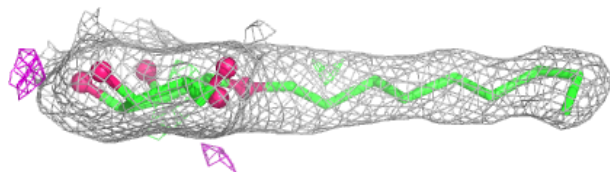
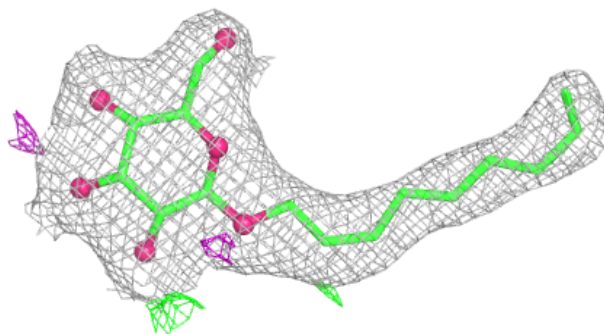


Electron density around BNG C 401:

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

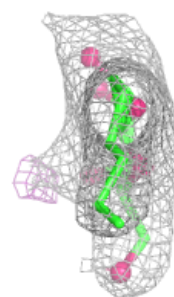
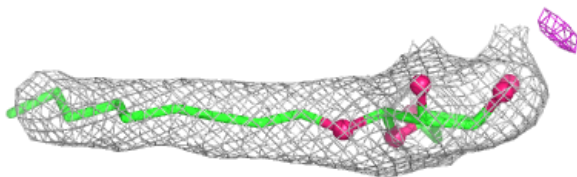
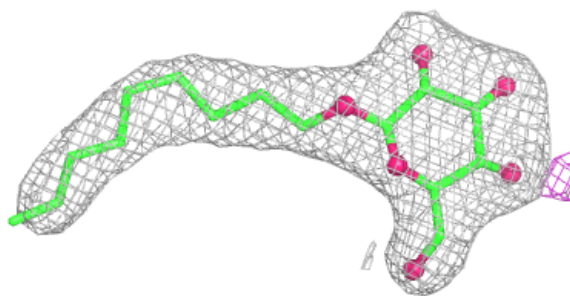
**Electron density around BNG A 401:**

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



Electron density around BNG B 401:

$2mF_o-DF_c$ (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.