



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:14 PM UTC

PDB ID : 6YU5 / pdb_00006yu5
Title : Crystal structure of MhsT in complex with L-valine
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Deposited on : 2020-04-25
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

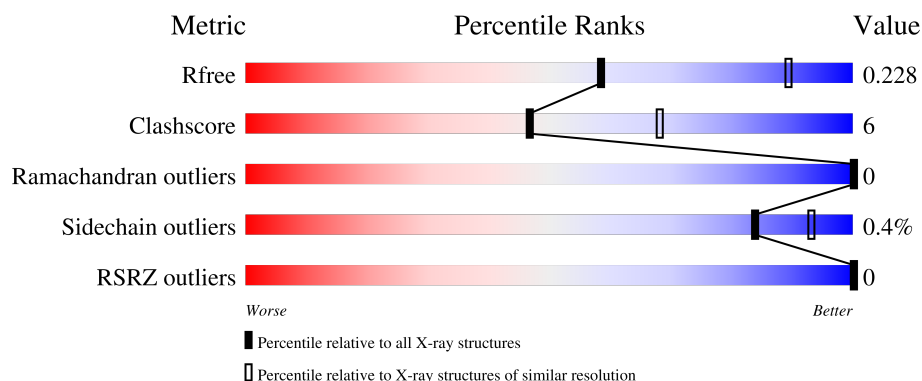
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	455	 85% 12% •
1	B	455	 85% 12% •

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7124 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.

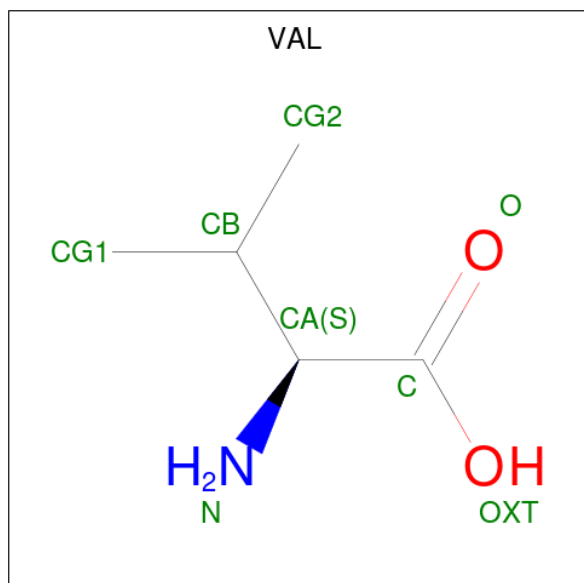
- Molecule 1 is a protein called Sodium-dependent transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3315	2235	512	560	8			
1	B	445	Total	C	N	O	S	0	0	0
			3359	2266	518	567	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A0A4Y7X244
A	0	MET	-	expression tag	UNP A0A4Y7X244
A	1	ALA	-	expression tag	UNP A0A4Y7X244
B	-1	SER	-	expression tag	UNP A0A4Y7X244
B	0	MET	-	expression tag	UNP A0A4Y7X244
B	1	ALA	-	expression tag	UNP A0A4Y7X244

- Molecule 2 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$) (labeled as "Ligand of Interest" by depositor).

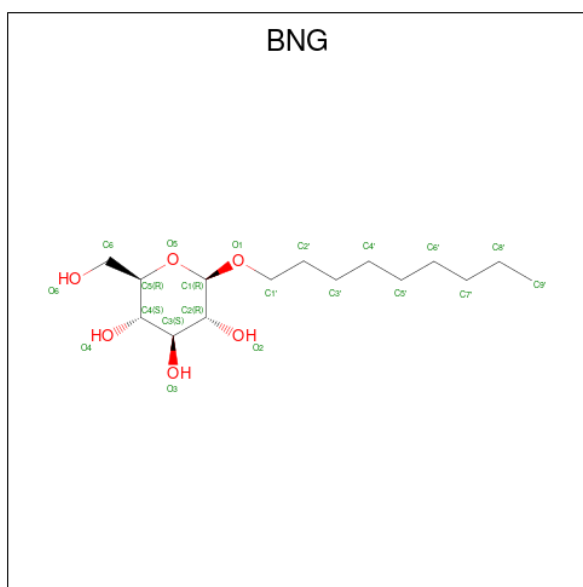


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	5	1	2		
2	B	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	B	2	Total	Na	0	0
			2	2		

- Molecule 4 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: C₁₅H₃₀O₆).



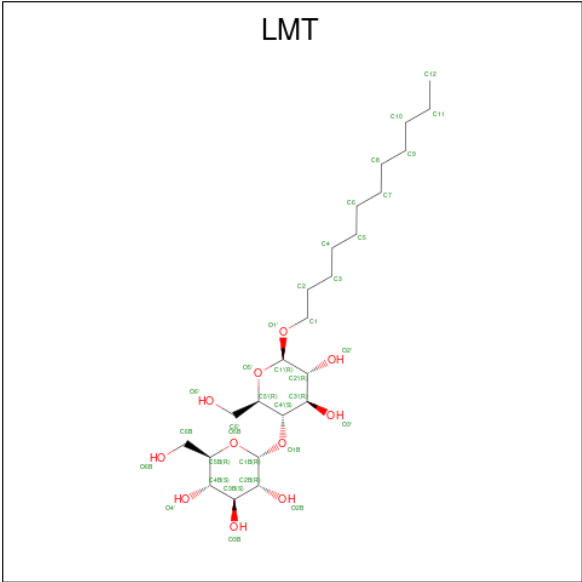
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	15	6		
4	A	1	Total	C	O	0	0
			21	15	6		
4	A	1	Total	C	O	0	0
			21	15	6		
4	A	1	Total	C	O	0	0
			21	15	6		
4	A	1	Total	C	O	0	0
			21	15	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 9 1	0	0
4	A	1	Total C O 21 15 6	0	0
4	A	1	Total C O 10 9 1	0	0
4	A	1	Total C O 10 9 1	0	0
4	A	1	Total C O 10 9 1	0	0
4	A	1	Total C 9 9	0	0
4	A	1	Total C O 21 15 6	0	0
4	A	1	Total C O 21 15 6	0	0
4	B	1	Total C O 21 15 6	0	0
4	B	1	Total C O 10 9 1	0	0
4	B	1	Total C O 10 9 1	0	0
4	B	1	Total C O 21 15 6	0	0
4	B	1	Total C O 10 9 1	0	0
4	B	1	Total C O 21 15 6	0	0
4	B	1	Total C O 21 15 6	0	0

- Molecule 5 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	12	1		
5	A	1	Total	C	O	0	0
			13	12	1		

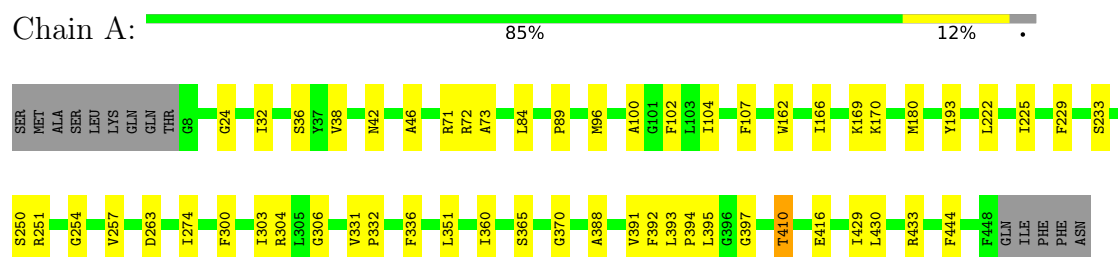
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	38	Total	O	0	0
			38	38		
6	B	35	Total	O	0	0
			35	35		

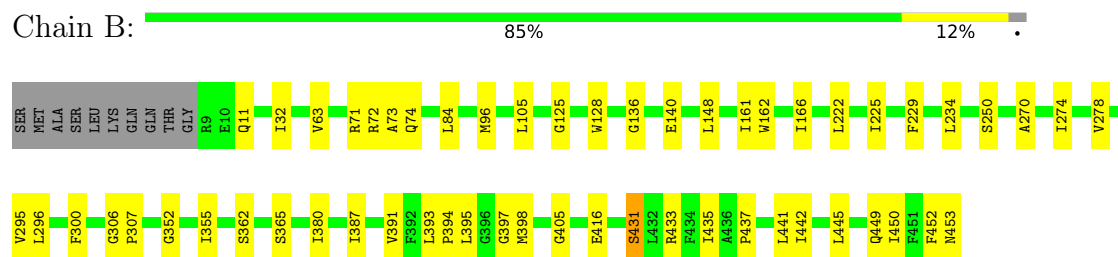
3 Residue-property plots [i](#)

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: Sodium-dependent transporter



- Molecule 1: Sodium-dependent transporter



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.16Å 216.03Å 50.36Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	49.05 – 2.60 49.05 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.05-2.60) 99.3 (49.05-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.207 , 0.237 (Not available) , 0.228	Depositor DCC
R_{free} test set	1404 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.205 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7124	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, NA, 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	0.13	0/3407	0.32	0/4642
1	B	0.13	0/3453	0.32	0/4703
All	All	0.13	0/6860	0.32	0/9345

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

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	3315	0	3430	45	0
1	B	3359	0	3470	40	0
2	A	8	0	8	1	0
2	B	8	0	8	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	217	0	333	11	0
4	B	114	0	177	2	0
5	A	26	0	50	2	0
6	A	38	0	0	3	0
6	B	35	0	0	0	0
All	All	7124	0	7476	83	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 6.

All (83) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:PRO:HB2	1:A:351:LEU:HD23	1.74	0.69
1:B:72:ARG:HD2	1:B:416:GLU:HG3	1.74	0.68
4:A:504:BNG:H3'2	4:A:510:BNG:H2'1	1.77	0.65
1:A:433:ARG:NH1	1:B:450:ILE:O	2.30	0.65
1:A:38:VAL:O	1:A:42:ASN:ND2	2.32	0.63
1:B:449:GLN:O	1:B:453:ASN:HB2	2.00	0.61
1:A:71:ARG:NH1	1:A:250:SER:O	2.34	0.60
1:B:96:MET:HE1	1:B:395:LEU:HB3	1.84	0.60
1:A:72:ARG:HB2	1:A:416:GLU:HG2	1.84	0.60
1:A:89:PRO:HG2	4:A:513:BNG:H5'1	1.85	0.58
1:A:303:ILE:HG23	4:A:510:BNG:H1'2	1.85	0.58
4:A:507:BNG:H7'2	4:A:511:BNG:H9'2	1.86	0.58
1:A:433:ARG:HH12	1:B:453:ASN:HB3	1.69	0.58
1:A:433:ARG:HH22	1:B:453:ASN:HB3	1.69	0.57
1:A:24:GLY:HA2	1:A:180:MET:HE1	1.87	0.57
1:B:63:VAL:HG22	1:B:234:LEU:HD11	1.87	0.57
1:A:331:VAL:HB	1:A:332:PRO:HD3	1.86	0.56
1:A:410:THR:OG1	1:A:433:ARG:NH2	2.39	0.56
1:A:162:TRP:O	1:A:166:ILE:HG12	2.06	0.55
1:B:105:LEU:HD23	1:B:355:ILE:HD13	1.88	0.55
1:B:431:SER:HA	1:B:435:ILE:HB	1.89	0.55
1:A:336:PHE:CD1	1:A:351:LEU:HD21	2.42	0.54
1:B:162:TRP:O	1:B:166:ILE:HG12	2.07	0.54
1:A:233:SER:HG	2:A:501:VAL:N	2.08	0.52
1:A:300:PHE:O	1:A:306:GLY:HA3	2.09	0.52
1:A:360:ILE:HD11	4:A:511:BNG:H2'2	1.93	0.51
1:B:274:ILE:HD13	1:B:296:LEU:HD21	1.93	0.51
1:B:393:LEU:HB2	1:B:394:PRO:HD3	1.93	0.51
1:A:193:TYR:HD1	4:A:504:BNG:H2'1	1.77	0.50
4:A:505:BNG:H9'1	4:A:514:BNG:H6'1	1.92	0.50
1:B:365:SER:HB3	1:B:380:ILE:HB	1.93	0.50
1:A:32:ILE:O	1:A:36:SER:OG	2.24	0.50
1:A:393:LEU:HB2	1:A:394:PRO:HD3	1.93	0.50
1:B:442:ILE:HG22	4:B:506:BNG:H7'2	1.94	0.49
1:A:388:ALA:O	1:A:393:LEU:HG	2.14	0.48
1:B:71:ARG:NH2	1:B:416:GLU:O	2.46	0.48
4:A:504:BNG:H5'2	4:A:510:BNG:H4'2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLN:NE2	1:B:74:GLN:OE1	2.44	0.47
1:B:405:GLY:O	1:B:433:ARG:NE	2.43	0.47
1:B:234:LEU:O	1:B:393:LEU:HD22	2.15	0.47
4:A:512:BNG:H1'2	4:A:513:BNG:H2'1	1.97	0.47
1:B:73:ALA:HB2	1:B:84:LEU:HD11	1.97	0.46
1:B:222:LEU:HA	1:B:225:ILE:HG22	1.98	0.46
1:A:391:VAL:O	1:A:395:LEU:HB2	2.16	0.46
5:A:517:LMT:H42	5:A:517:LMT:H11	1.72	0.46
1:A:251:ARG:NH1	5:A:518:LMT:O1'	2.49	0.45
1:A:433:ARG:NH1	1:B:453:ASN:HB3	2.31	0.45
1:A:433:ARG:NH2	1:B:453:ASN:HB3	2.32	0.45
1:B:229:PHE:HE2	1:B:397:GLY:HA3	1.82	0.45
1:B:300:PHE:O	1:B:306:GLY:HA3	2.15	0.45
1:A:169:LYS:NZ	6:A:609:HOH:O	2.50	0.45
1:A:429:ILE:HG21	1:B:453:ASN:OXT	2.17	0.45
1:A:166:ILE:HG22	1:A:170:LYS:HB2	2.00	0.44
1:A:251:ARG:NH2	1:A:254:GLY:HA3	2.33	0.44
1:B:128:TRP:CE2	1:B:307:PRO:HB3	2.53	0.44
1:B:136:GLY:O	1:B:140:GLU:HG2	2.18	0.44
1:B:398:MET:HG3	1:B:437:PRO:HA	1.99	0.44
1:A:430:LEU:HD22	1:B:452:PHE:HE1	1.83	0.43
1:B:32:ILE:HD13	1:B:270:ALA:HB2	2.00	0.43
1:A:46:ALA:HB3	6:A:615:HOH:O	2.19	0.43
1:B:148:LEU:HD13	4:B:505:BNG:H4'1	2.01	0.43
1:B:125:GLY:HA2	1:B:128:TRP:CD1	2.54	0.43
1:A:96:MET:O	1:A:100:ALA:N	2.41	0.42
1:B:362:SER:O	1:B:365:SER:OG	2.31	0.42
1:B:387:ILE:O	1:B:391:VAL:HB	2.18	0.42
1:A:257:VAL:HG12	4:A:509:BNG:H5'2	2.01	0.42
1:A:263:ASP:OD2	6:A:601:HOH:O	2.21	0.42
1:A:73:ALA:HB2	1:A:84:LEU:HG	2.02	0.42
1:A:104:ILE:HA	1:A:107:PHE:CE2	2.55	0.42
1:B:441:LEU:O	1:B:445:LEU:HG	2.20	0.41
1:A:222:LEU:HA	1:A:225:ILE:HG22	2.02	0.41
1:A:229:PHE:HE2	1:A:397:GLY:HA3	1.83	0.41
1:A:102:PHE:CE2	1:A:332:PRO:HB3	2.55	0.41
1:B:391:VAL:O	1:B:395:LEU:HB2	2.21	0.41
1:A:395:LEU:HG	1:A:444:PHE:CE2	2.55	0.41
1:A:96:MET:HE2	1:A:392:PHE:HA	2.02	0.41
1:A:304:ARG:HB2	4:A:510:BNG:O3	2.21	0.41
1:A:410:THR:HG1	1:A:433:ARG:HH22	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ARG:HH12	1:B:453:ASN:CB	2.34	0.41
1:B:71:ARG:NH1	1:B:250:SER:O	2.54	0.41
1:B:161:ILE:HG12	1:B:352:GLY:HA3	2.03	0.40
1:A:365:SER:O	1:A:370:GLY:HA2	2.22	0.40
1:B:278:VAL:HG22	1:B:295:VAL:HG21	2.04	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	439/455 (96%)	424 (97%)	15 (3%)	0	100	100
1	B	443/455 (97%)	426 (96%)	17 (4%)	0	100	100
All	All	882/910 (97%)	850 (96%)	32 (4%)	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	335/348 (96%)	333 (99%)	2 (1%)	78	91
1	B	340/348 (98%)	339 (100%)	1 (0%)	86	94
All	All	675/696 (97%)	672 (100%)	3 (0%)	84	93

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

Mol	Chain	Res	Type
1	A	274	ILE
1	A	410	THR
1	B	431	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BNG	B	510	-	21,21,21	1.28	2 (9%)	26,26,26	0.93	0
5	LMT	A	518	-	12,12,36	0.67	0	11,11,47	0.85	0
4	BNG	A	509	-	9,9,21	0.89	0	8,8,26	0.78	0
4	BNG	A	514	-	8,8,21	0.87	0	7,7,26	0.75	0
4	BNG	B	504	-	21,21,21	1.27	3 (14%)	26,26,26	1.02	3 (11%)
4	BNG	A	506	-	21,21,21	1.27	2 (9%)	26,26,26	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BNG	B	506	-	9,9,21	0.86	0	8,8,26	0.84	0
4	BNG	A	507	-	21,21,21	1.27	2 (9%)	26,26,26	0.88	0
4	BNG	A	508	-	21,21,21	1.31	3 (14%)	26,26,26	0.91	0
4	BNG	A	504	-	21,21,21	1.31	2 (9%)	26,26,26	0.84	0
4	BNG	A	516	-	21,21,21	1.25	2 (9%)	26,26,26	1.09	1 (3%)
4	BNG	B	508	-	9,9,21	0.87	0	8,8,26	0.79	0
4	BNG	A	505	-	21,21,21	1.28	1 (4%)	26,26,26	0.95	1 (3%)
4	BNG	A	513	-	9,9,21	0.86	0	8,8,26	0.81	0
4	BNG	A	512	-	9,9,21	0.86	0	8,8,26	0.85	0
4	BNG	A	510	-	21,21,21	1.35	3 (14%)	26,26,26	1.13	2 (7%)
5	LMT	A	517	-	12,12,36	0.68	0	11,11,47	0.85	0
4	BNG	B	505	-	9,9,21	0.87	0	8,8,26	0.81	0
2	VAL	A	501	3	6,7,7	0.87	0	8,9,9	0.92	0
4	BNG	B	509	-	21,21,21	1.30	2 (9%)	26,26,26	0.85	1 (3%)
2	VAL	B	501	3	6,7,7	0.85	0	8,9,9	0.97	1 (12%)
4	BNG	A	515	-	21,21,21	1.33	3 (14%)	26,26,26	0.91	1 (3%)
4	BNG	B	507	-	21,21,21	1.23	2 (9%)	26,26,26	1.17	3 (11%)
4	BNG	A	511	-	9,9,21	0.85	0	8,8,26	0.85	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
4	BNG	B	510	-	-	2/12/32/32	0/1/1/1
5	LMT	A	518	-	-	5/10/10/61	-
4	BNG	A	509	-	-	2/7/7/32	-
4	BNG	A	514	-	-	4/6/6/32	-
4	BNG	B	504	-	-	5/12/32/32	0/1/1/1
4	BNG	A	506	-	-	3/12/32/32	0/1/1/1
4	BNG	B	506	-	-	1/7/7/32	-
4	BNG	A	507	-	-	2/12/32/32	0/1/1/1
4	BNG	A	508	-	-	8/12/32/32	0/1/1/1
4	BNG	A	504	-	-	2/12/32/32	0/1/1/1
4	BNG	A	516	-	-	5/12/32/32	0/1/1/1
4	BNG	B	508	-	-	5/7/7/32	-
4	BNG	A	505	-	-	6/12/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BNG	A	513	-	-	4/7/7/32	-
4	BNG	A	512	-	-	3/7/7/32	-
4	BNG	A	510	-	-	5/12/32/32	0/1/1/1
5	LMT	A	517	-	-	9/10/10/61	-
4	BNG	B	505	-	-	2/7/7/32	-
2	VAL	A	501	3	-	3/8/8/8	-
4	BNG	B	509	-	-	8/12/32/32	0/1/1/1
2	VAL	B	501	3	-	0/8/8/8	-
4	BNG	A	515	-	-	4/12/32/32	0/1/1/1
4	BNG	B	507	-	-	4/12/32/32	0/1/1/1
4	BNG	A	511	-	-	6/7/7/32	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	510	BNG	O5-C1	3.66	1.51	1.41
4	A	515	BNG	O5-C1	3.64	1.51	1.41
4	B	509	BNG	O5-C1	3.63	1.51	1.41
4	A	505	BNG	O5-C1	3.55	1.51	1.41
4	A	508	BNG	O5-C1	3.54	1.50	1.41
4	B	510	BNG	O5-C1	3.52	1.50	1.41
4	A	504	BNG	O5-C1	3.46	1.50	1.41
4	A	507	BNG	O5-C1	3.45	1.50	1.41
4	B	507	BNG	O5-C1	3.33	1.50	1.41
4	A	506	BNG	O5-C1	3.33	1.50	1.41
4	A	516	BNG	O5-C1	3.31	1.50	1.41
4	B	504	BNG	O5-C1	3.30	1.50	1.41
4	A	504	BNG	O1-C1	-2.62	1.35	1.40
4	A	506	BNG	O1-C1	-2.49	1.36	1.40
4	A	516	BNG	O1-C1	-2.46	1.36	1.40
4	A	507	BNG	O1-C1	-2.46	1.36	1.40
4	A	510	BNG	O1-C1	-2.41	1.36	1.40
4	A	508	BNG	O1-C1	-2.33	1.36	1.40
4	A	515	BNG	O1-C1	-2.32	1.36	1.40
4	B	507	BNG	O1-C1	-2.32	1.36	1.40
4	B	504	BNG	O1-C1	-2.28	1.36	1.40
4	B	509	BNG	O1-C1	-2.24	1.36	1.40
4	A	510	BNG	O5-C5	2.18	1.49	1.44
4	A	515	BNG	O5-C5	2.06	1.49	1.44
4	B	510	BNG	O1-C1	-2.02	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	BNG	O5-C5	2.01	1.49	1.44
4	A	508	BNG	O5-C5	2.00	1.49	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	507	BNG	C1-C2-C3	2.95	116.22	110.01
4	A	510	BNG	C1-C2-C3	-2.63	104.48	110.01
4	B	504	BNG	O5-C5-C4	2.53	114.26	109.70
4	A	510	BNG	O5-C5-C4	2.33	113.89	109.70
4	A	505	BNG	O1-C1-C2	2.32	111.80	108.27
4	B	507	BNG	O5-C1-C2	2.24	114.97	110.37
4	A	516	BNG	O1-C1-C2	2.17	111.58	108.27
4	B	504	BNG	O1-C1-C2	2.11	111.47	108.27
4	B	507	BNG	C4-C3-C2	2.09	114.50	110.83
4	B	504	BNG	C3-C4-C5	2.07	113.99	110.23
4	A	515	BNG	C1'-O1-C1	2.05	117.19	113.68
4	B	509	BNG	O5-C1-C2	2.00	114.49	110.37
2	B	501	VAL	OXT-C-O	-2.00	119.54	124.08

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	515	BNG	O5-C1-O1-C1'
4	A	516	BNG	O5-C5-C6-O6
4	A	508	BNG	C4-C5-C6-O6
4	A	516	BNG	C4-C5-C6-O6
4	A	508	BNG	O5-C5-C6-O6
4	A	508	BNG	O5-C1-O1-C1'
4	A	510	BNG	O5-C5-C6-O6
4	A	508	BNG	C2-C1-O1-C1'
4	A	504	BNG	O5-C5-C6-O6
4	A	510	BNG	C4-C5-C6-O6
4	A	505	BNG	O5-C5-C6-O6
5	A	517	LMT	C1-C2-C3-C4
4	B	509	BNG	O5-C1-O1-C1'
4	A	515	BNG	O5-C5-C6-O6
4	B	506	BNG	C3'-C4'-C5'-C6'
4	B	509	BNG	C1'-C2'-C3'-C4'
4	A	510	BNG	C2'-C3'-C4'-C5'
4	B	504	BNG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
4	B	504	BNG	C5'-C6'-C7'-C8'
4	A	506	BNG	O5-C5-C6-O6
4	A	507	BNG	C2'-C1'-O1-C1
4	A	509	BNG	C2'-C3'-C4'-C5'
4	A	511	BNG	C5'-C6'-C7'-C8'
4	B	509	BNG	C5'-C6'-C7'-C8'
4	A	511	BNG	C4'-C5'-C6'-C7'
4	B	507	BNG	O1-C1'-C2'-C3'
4	A	505	BNG	C2'-C3'-C4'-C5'
4	B	508	BNG	C4'-C5'-C6'-C7'
4	A	510	BNG	C2-C1-O1-C1'
4	B	508	BNG	C5'-C6'-C7'-C8'
5	A	517	LMT	C5-C6-C7-C8
4	B	507	BNG	O5-C5-C6-O6
5	A	517	LMT	C7-C8-C9-C10
4	A	504	BNG	C4-C5-C6-O6
4	A	509	BNG	O1-C1'-C2'-C3'
4	A	513	BNG	C5'-C6'-C7'-C8'
4	A	514	BNG	C3'-C4'-C5'-C6'
4	B	509	BNG	C2'-C3'-C4'-C5'
4	B	508	BNG	O1-C1'-C2'-C3'
4	B	510	BNG	O5-C5-C6-O6
5	A	517	LMT	C3-C4-C5-C6
4	A	516	BNG	C5'-C6'-C7'-C8'
4	A	511	BNG	C3'-C4'-C5'-C6'
4	B	509	BNG	C4'-C5'-C6'-C7'
4	A	515	BNG	C6'-C7'-C8'-C9'
4	B	508	BNG	C6'-C7'-C8'-C9'
5	A	517	LMT	C9-C10-C11-C12
5	A	517	LMT	O1'-C1-C2-C3
4	A	513	BNG	C6'-C7'-C8'-C9'
4	A	505	BNG	C2-C1-O1-C1'
4	B	508	BNG	C3'-C4'-C5'-C6'
4	A	508	BNG	C4'-C5'-C6'-C7'
4	A	514	BNG	C4'-C5'-C6'-C7'
2	A	501	VAL	O-C-CA-CB
2	A	501	VAL	OXT-C-CA-CB
4	A	505	BNG	O1-C1'-C2'-C3'
4	A	510	BNG	C3'-C4'-C5'-C6'
4	A	515	BNG	C5'-C6'-C7'-C8'
4	A	512	BNG	C1'-C2'-C3'-C4'
4	B	505	BNG	C5'-C6'-C7'-C8'

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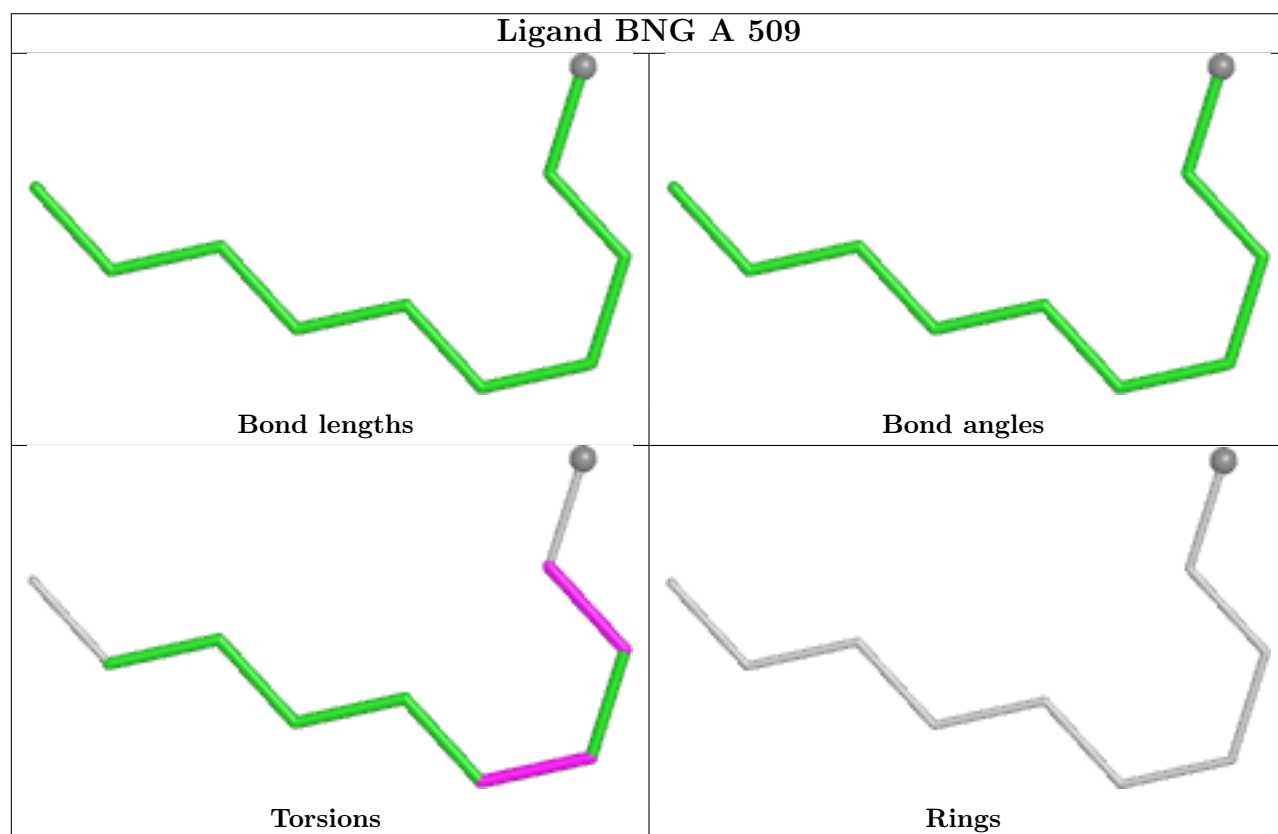
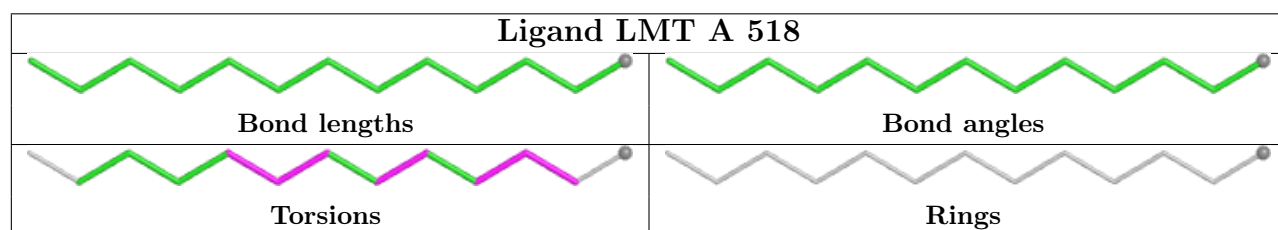
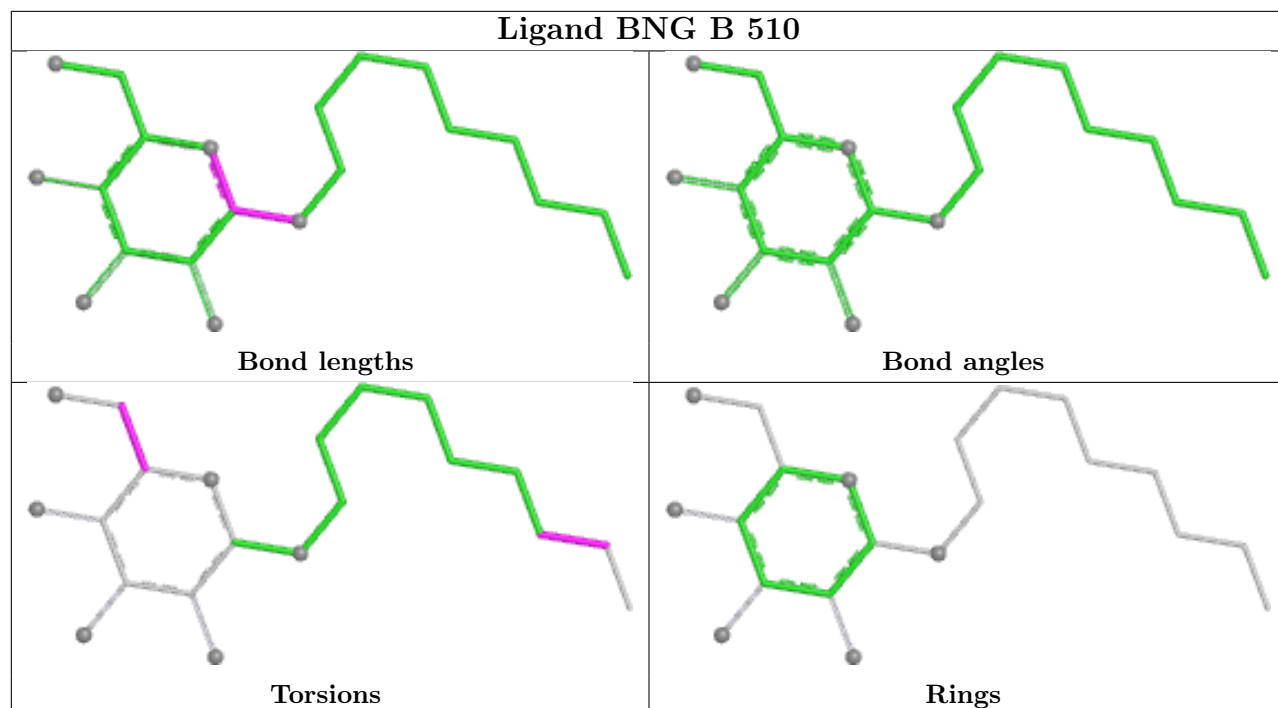
Mol	Chain	Res	Type	Atoms
5	A	518	LMT	C1-C2-C3-C4
4	A	512	BNG	C2'-C3'-C4'-C5'
4	A	514	BNG	C6'-C7'-C8'-C9'
4	A	513	BNG	C1'-C2'-C3'-C4'
4	A	508	BNG	C3'-C4'-C5'-C6'
4	A	505	BNG	C4-C5-C6-O6
4	A	505	BNG	C3'-C4'-C5'-C6'
4	A	508	BNG	O1-C1'-C2'-C3'
4	A	514	BNG	C1'-C2'-C3'-C4'
4	B	509	BNG	C4-C5-C6-O6
4	B	509	BNG	C6'-C7'-C8'-C9'
4	B	507	BNG	C2'-C3'-C4'-C5'
4	A	506	BNG	C4'-C5'-C6'-C7'
4	A	507	BNG	C1'-C2'-C3'-C4'
4	B	504	BNG	C3'-C4'-C5'-C6'
4	A	513	BNG	C4'-C5'-C6'-C7'
5	A	518	LMT	O1'-C1-C2-C3
5	A	517	LMT	C11-C10-C9-C8
5	A	517	LMT	C4-C5-C6-C7
5	A	517	LMT	C6-C7-C8-C9
4	A	511	BNG	C2'-C3'-C4'-C5'
4	A	511	BNG	C6'-C7'-C8'-C9'
4	B	505	BNG	C4'-C5'-C6'-C7'
4	A	516	BNG	C6'-C7'-C8'-C9'
5	A	518	LMT	C3-C4-C5-C6
4	A	511	BNG	O1-C1'-C2'-C3'
4	B	509	BNG	C3'-C4'-C5'-C6'
5	A	518	LMT	C5-C6-C7-C8
4	B	510	BNG	C6'-C7'-C8'-C9'
4	A	516	BNG	C2'-C1'-O1-C1
4	B	504	BNG	O1-C1'-C2'-C3'
2	A	501	VAL	C-CA-CB-CG2
4	B	507	BNG	C5'-C6'-C7'-C8'
4	A	512	BNG	C6'-C7'-C8'-C9'
4	B	504	BNG	C4-C5-C6-O6
4	A	508	BNG	C5'-C6'-C7'-C8'
4	A	506	BNG	C4-C5-C6-O6
5	A	518	LMT	C6-C7-C8-C9

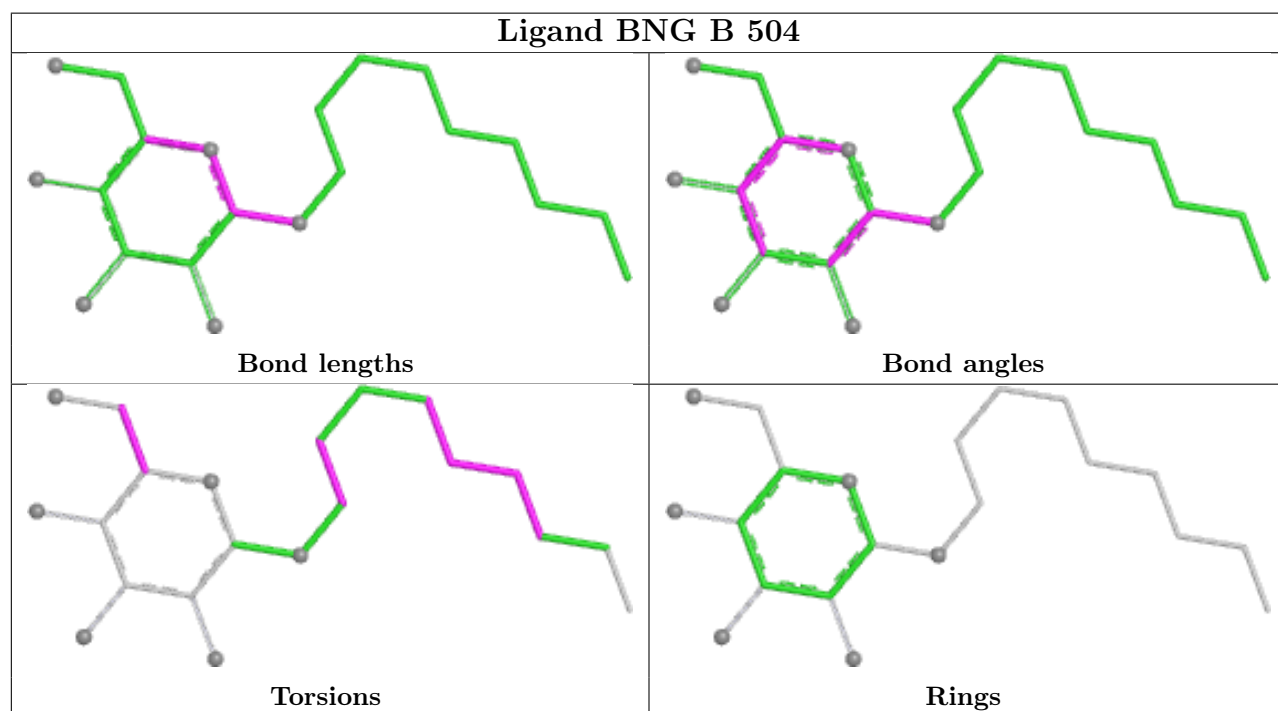
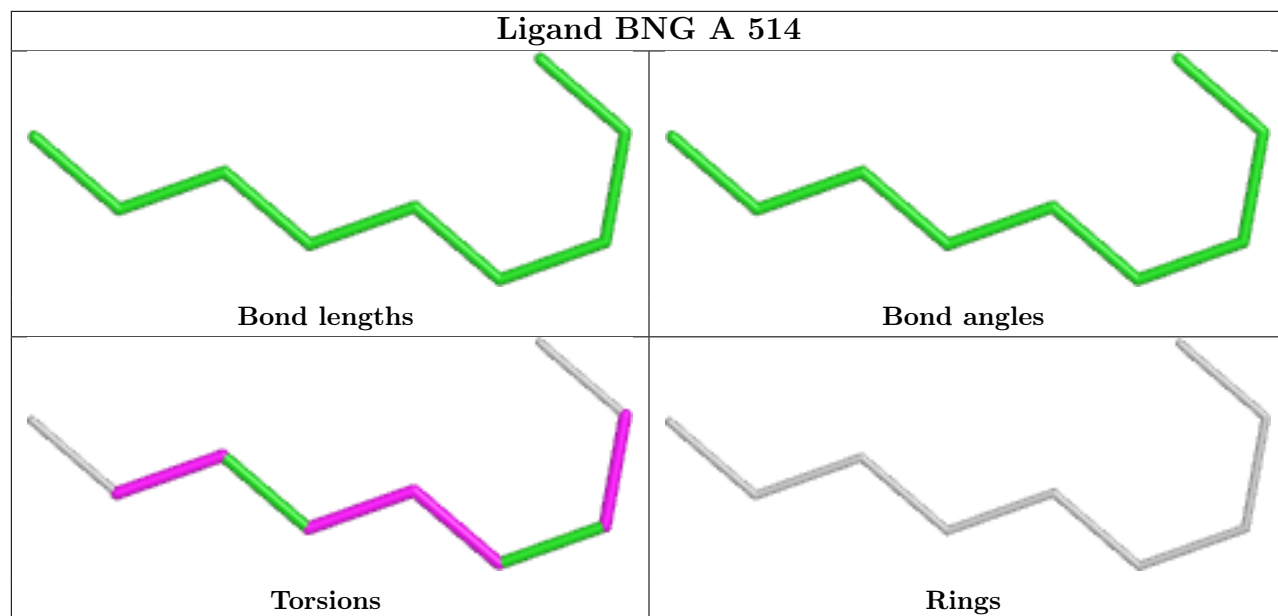
There are no ring outliers.

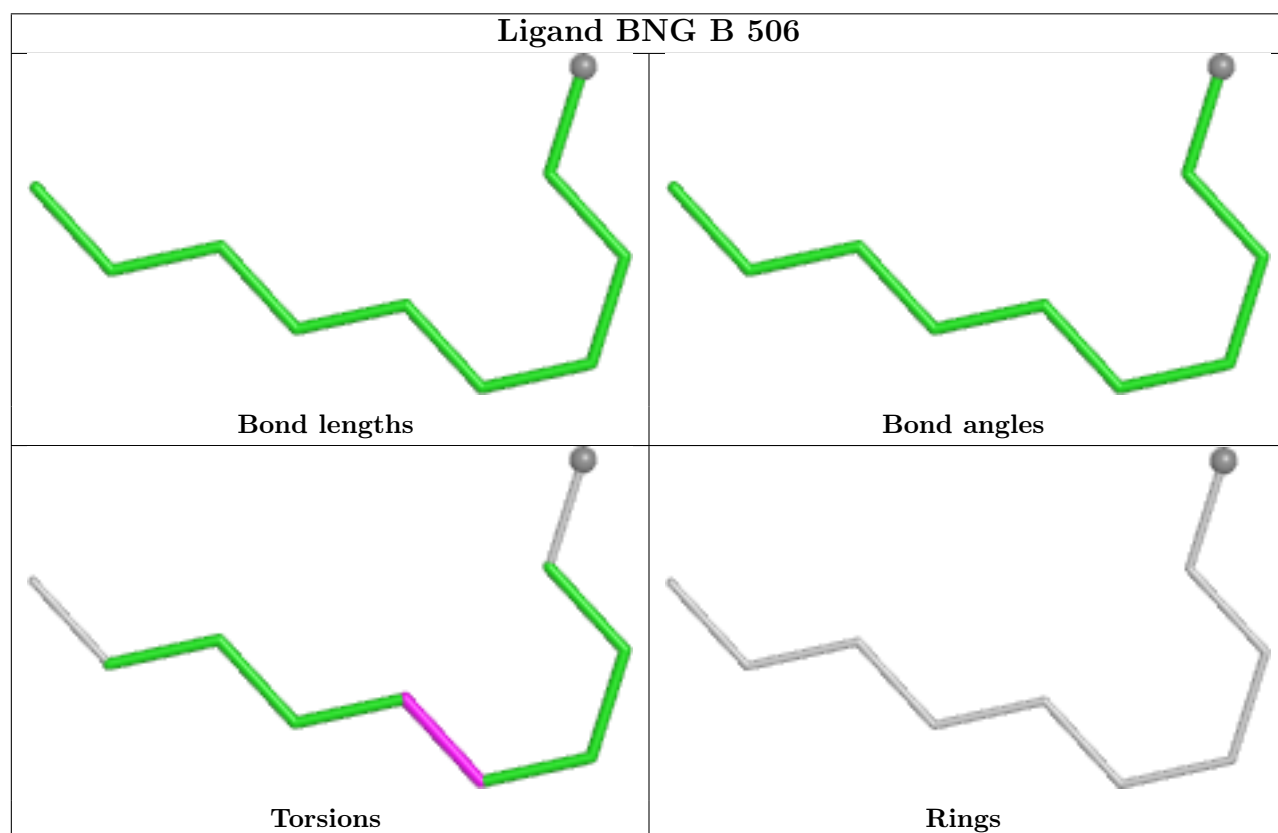
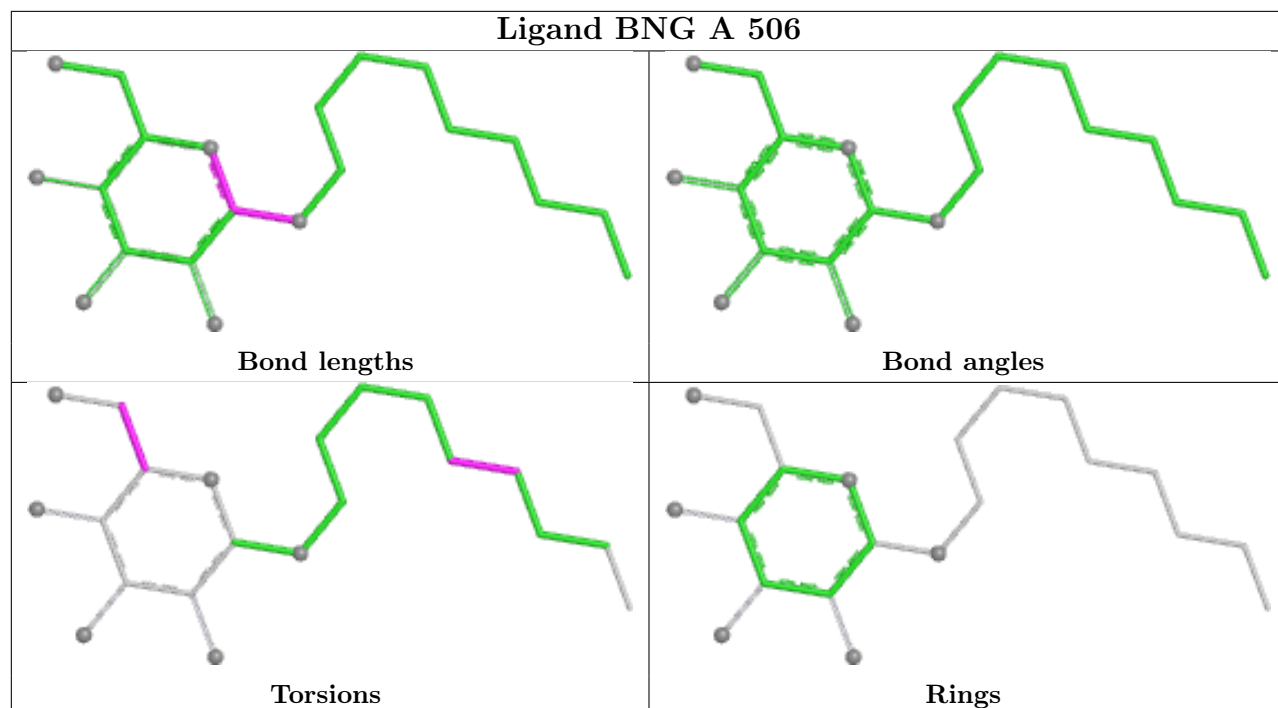
14 monomers are involved in 16 short contacts:

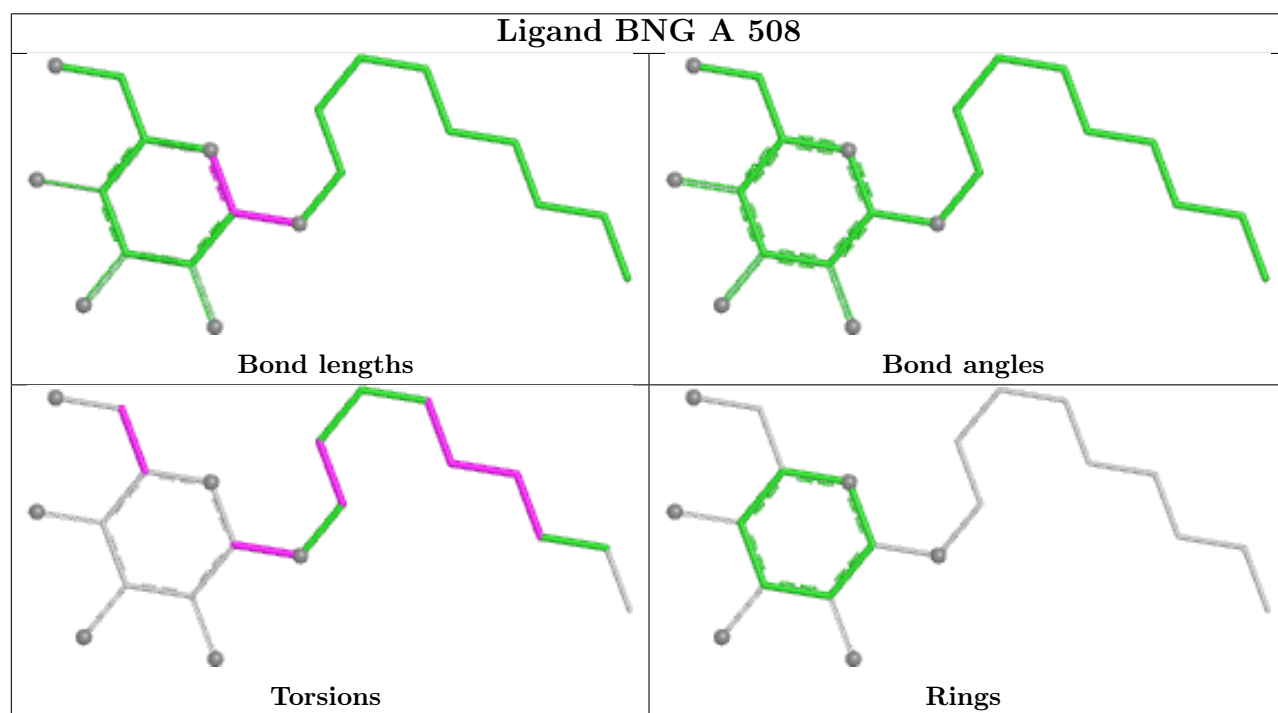
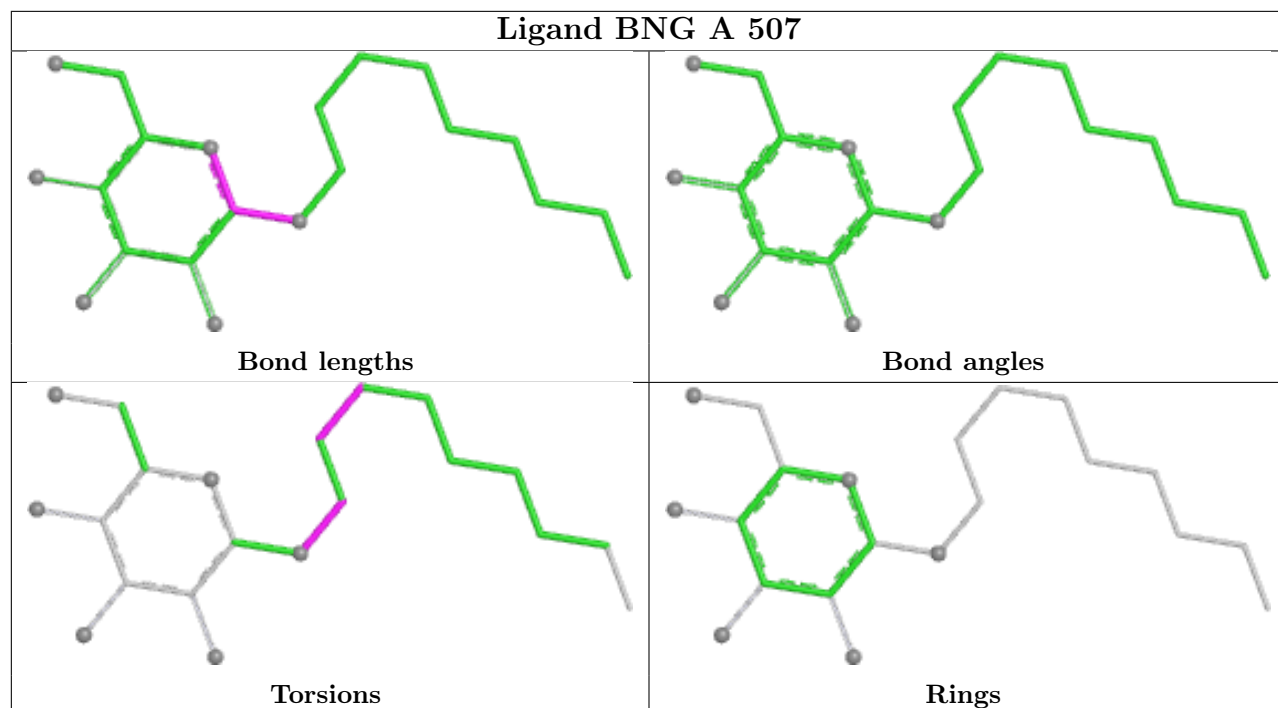
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	518	LMT	1	0
4	A	509	BNG	1	0
4	A	514	BNG	1	0
4	B	506	BNG	1	0
4	A	507	BNG	1	0
4	A	504	BNG	3	0
4	A	505	BNG	1	0
4	A	513	BNG	2	0
4	A	512	BNG	1	0
4	A	510	BNG	4	0
5	A	517	LMT	1	0
4	B	505	BNG	1	0
2	A	501	VAL	1	0
4	A	511	BNG	2	0

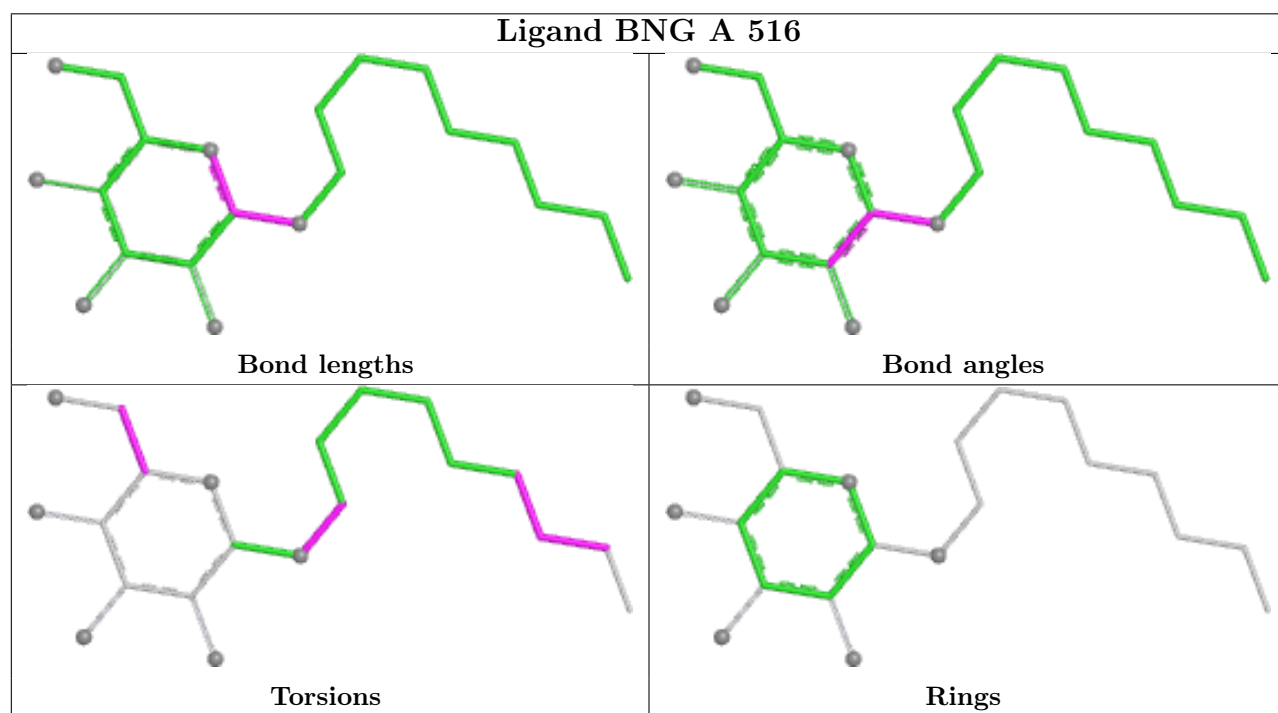
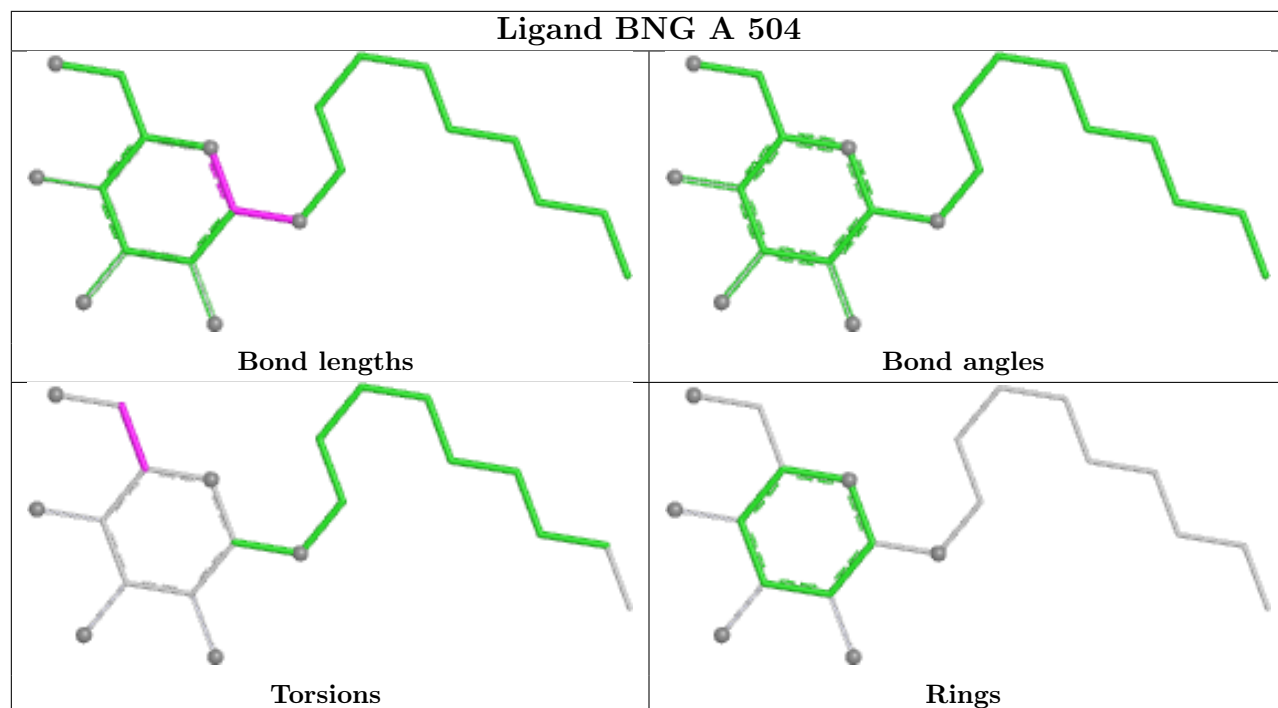
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

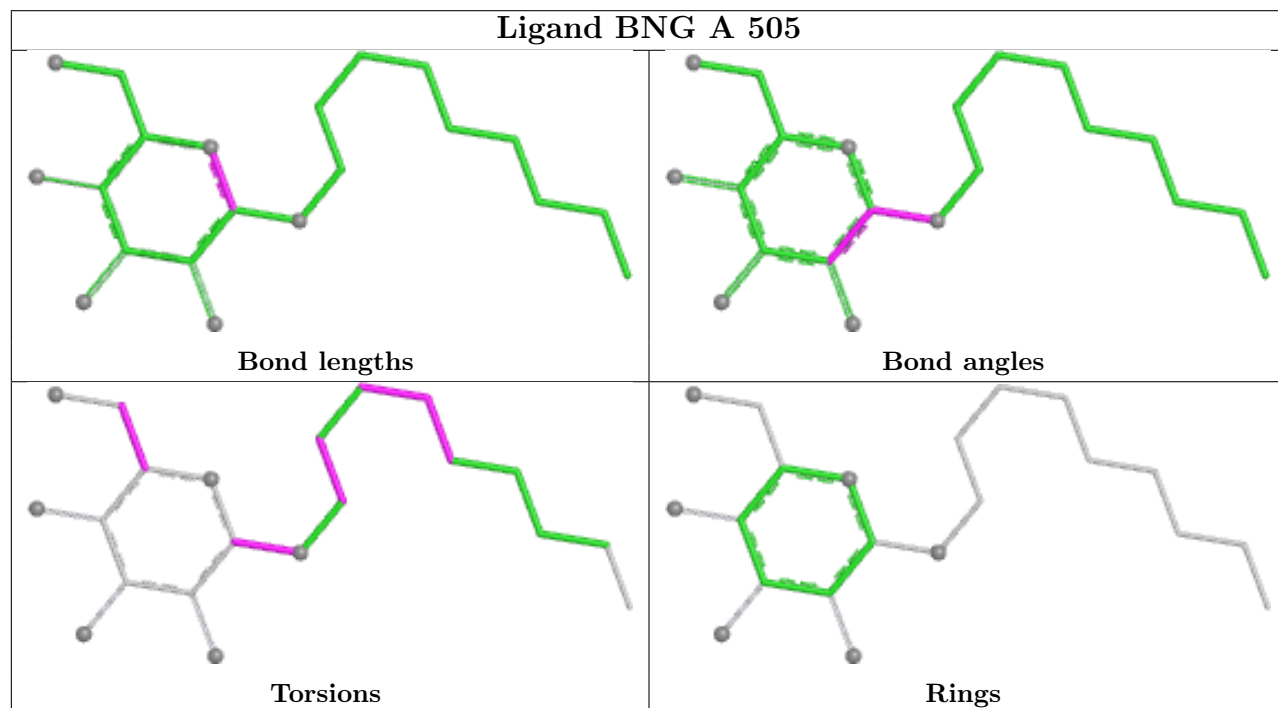
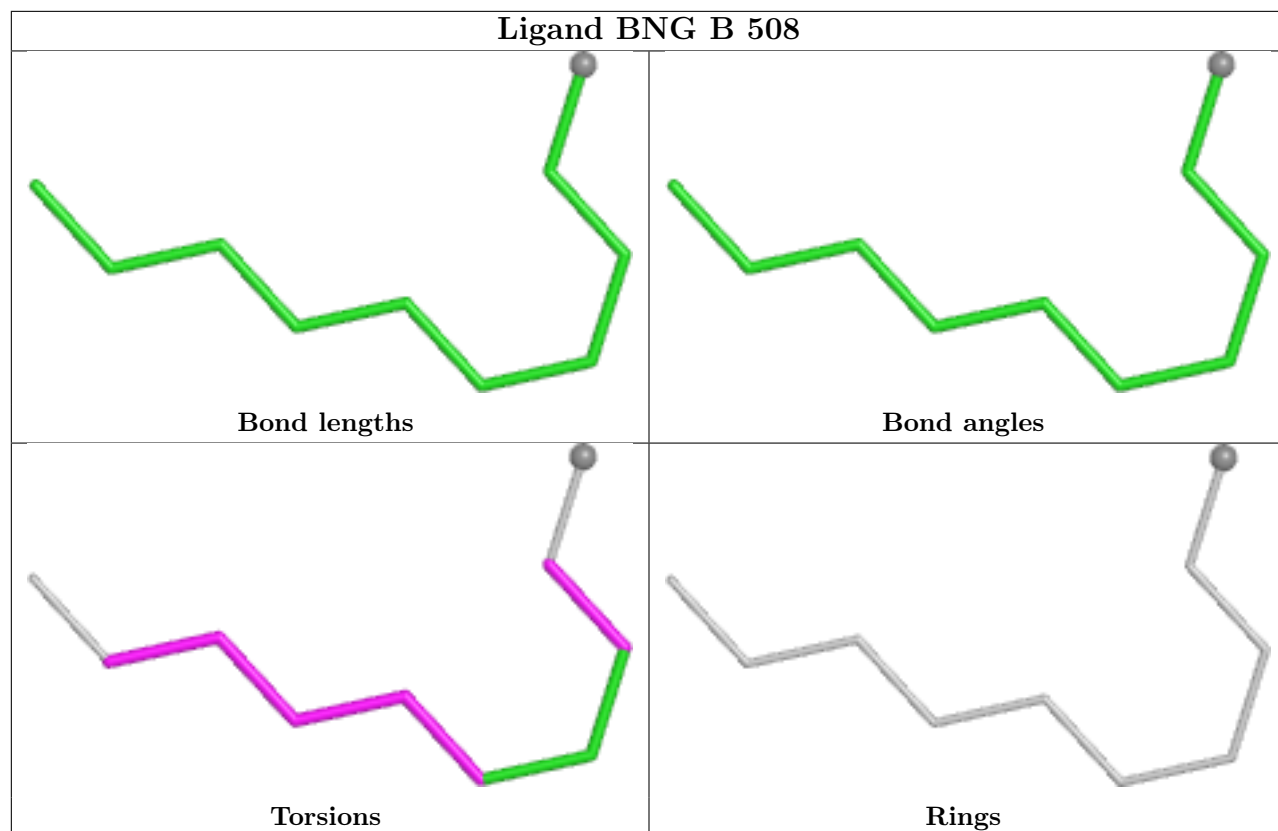


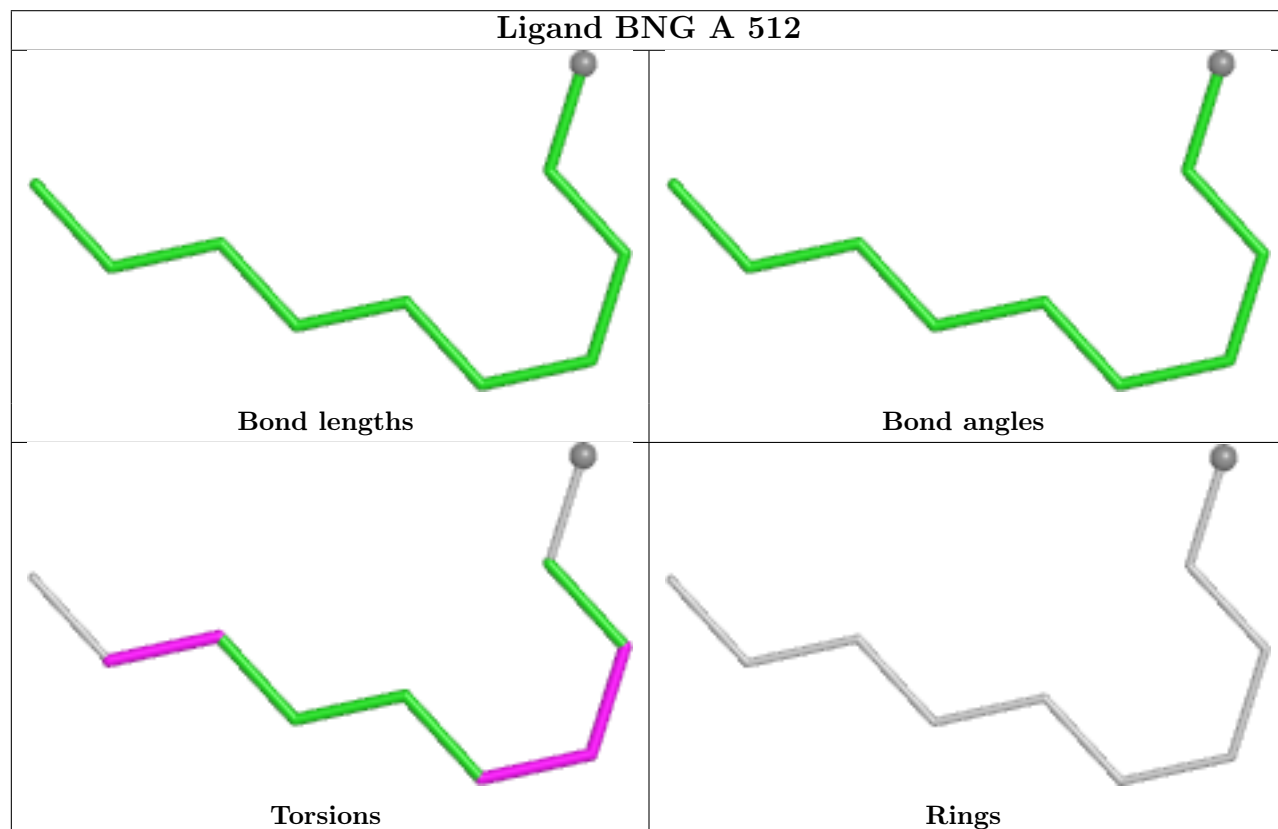
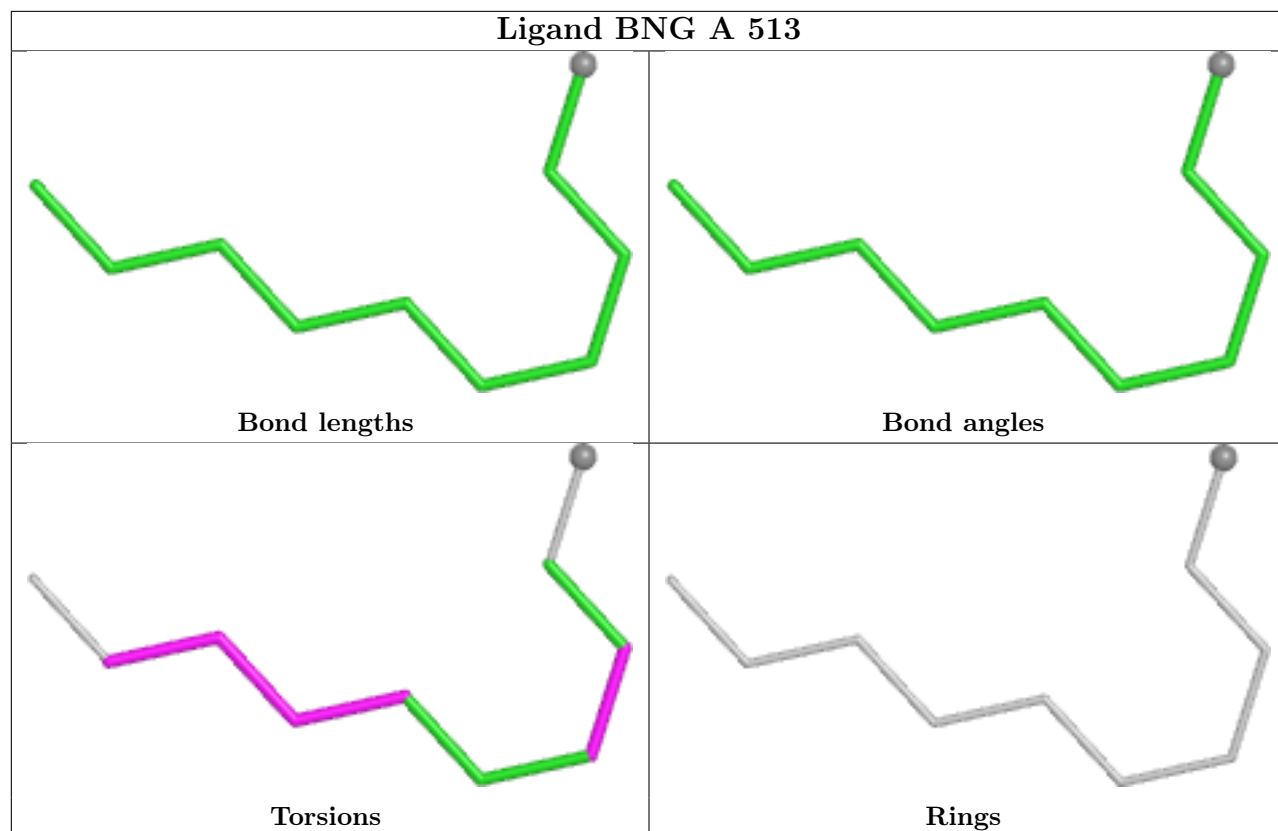


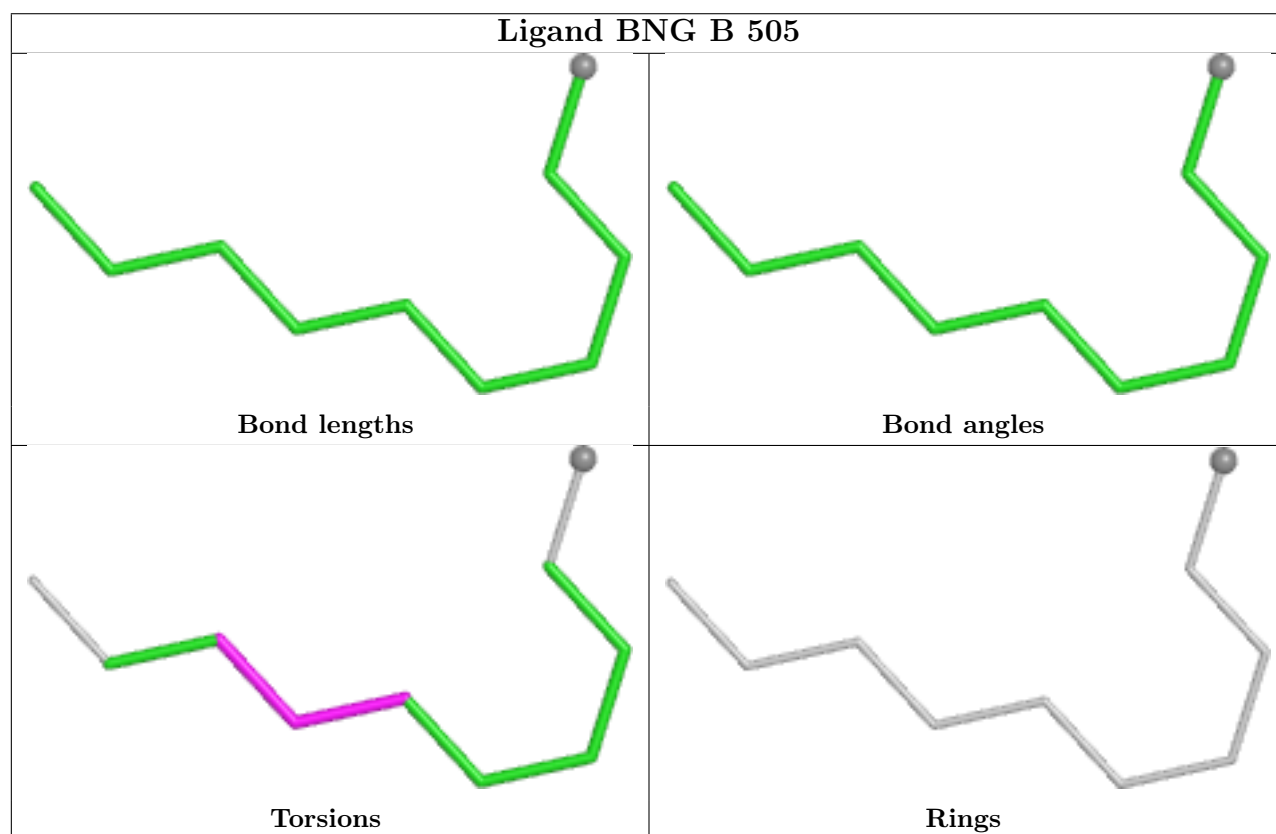
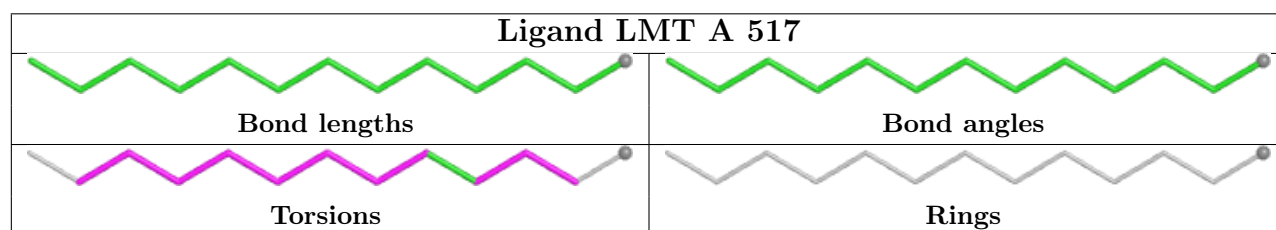
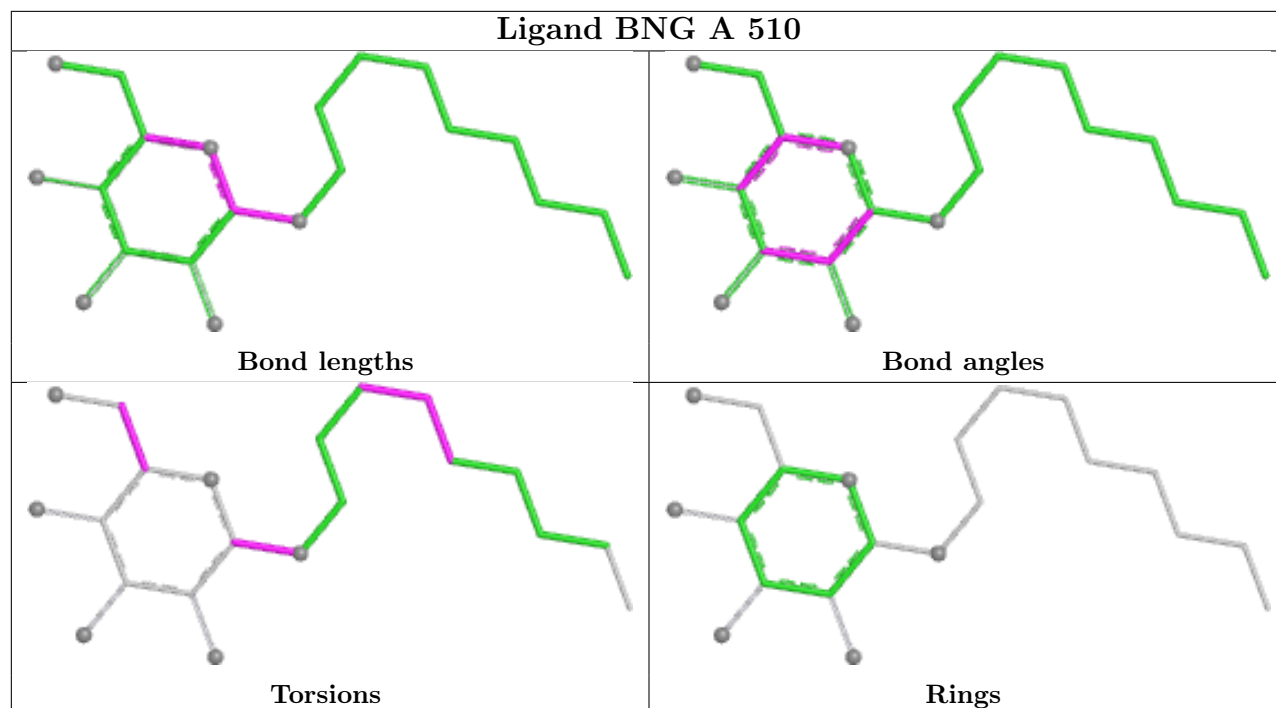




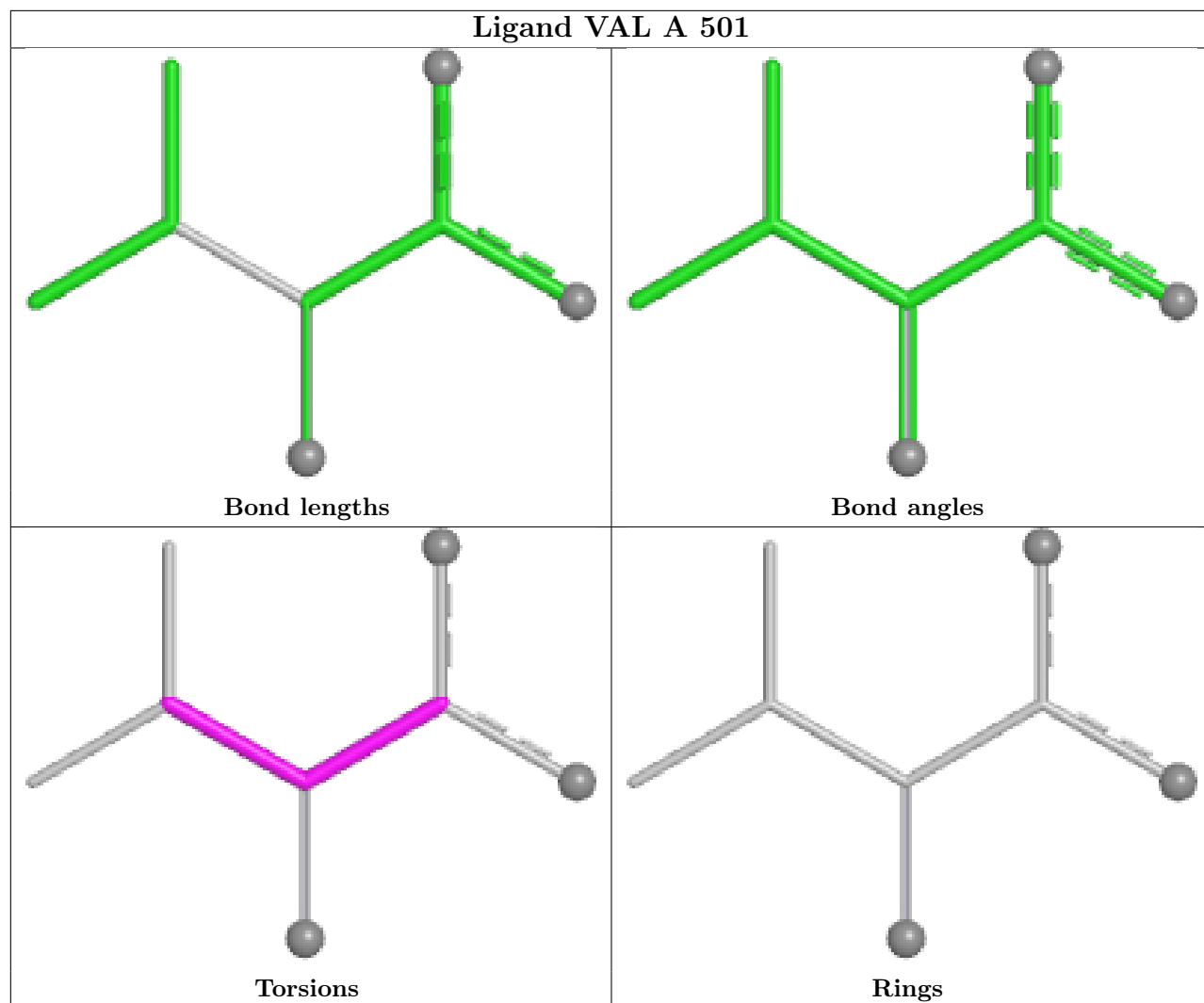




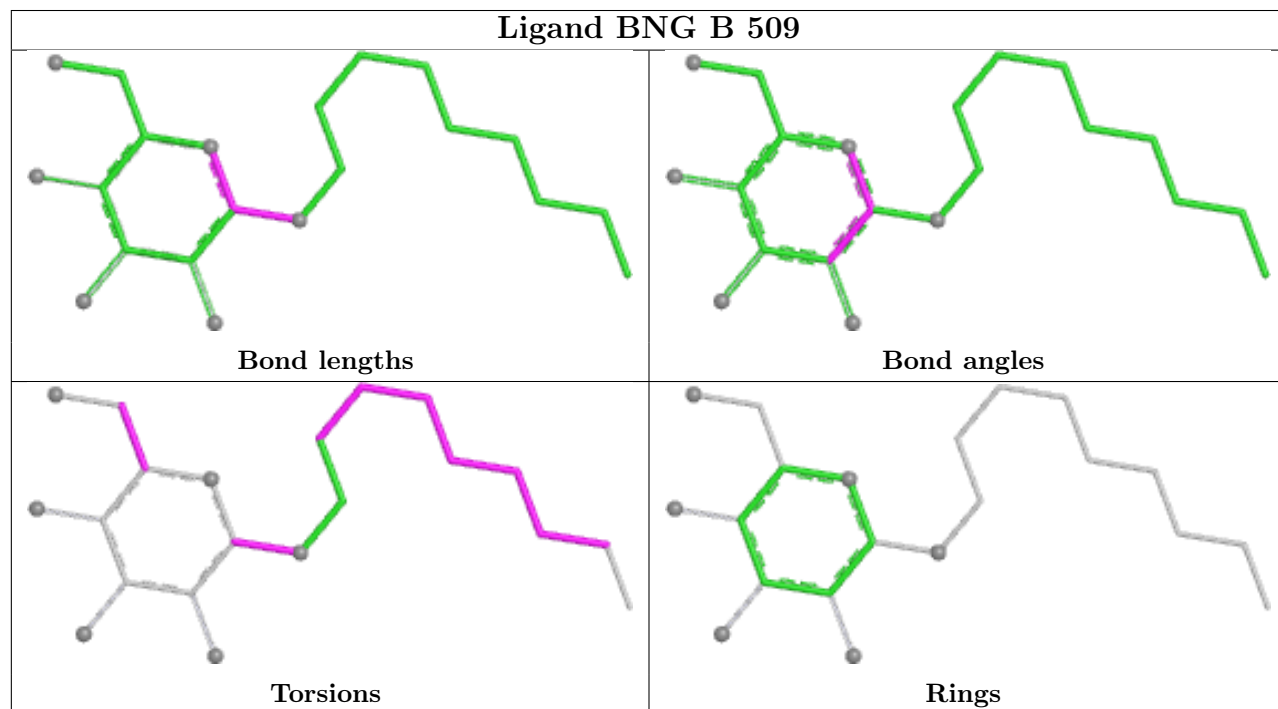




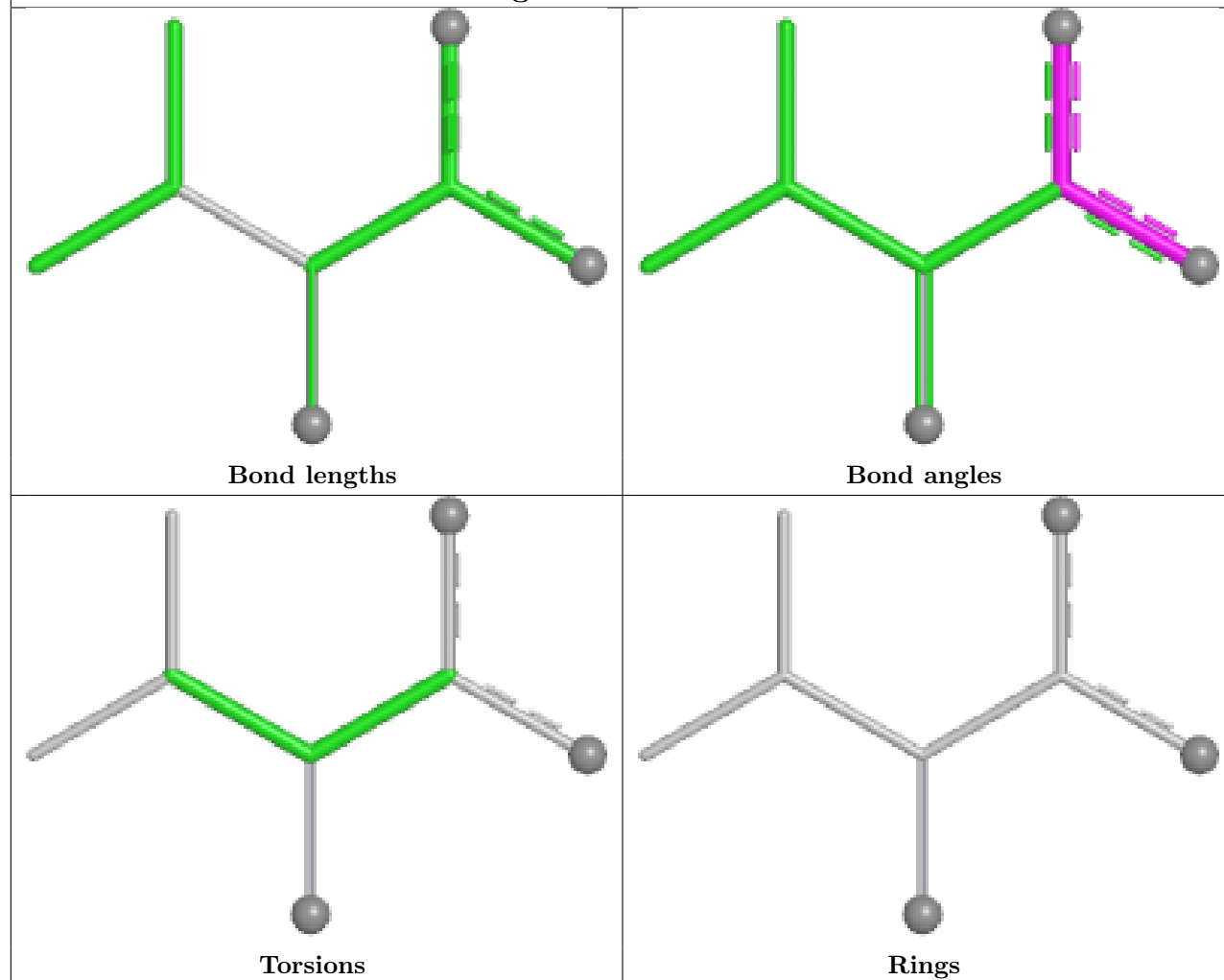
Ligand VAL A 501



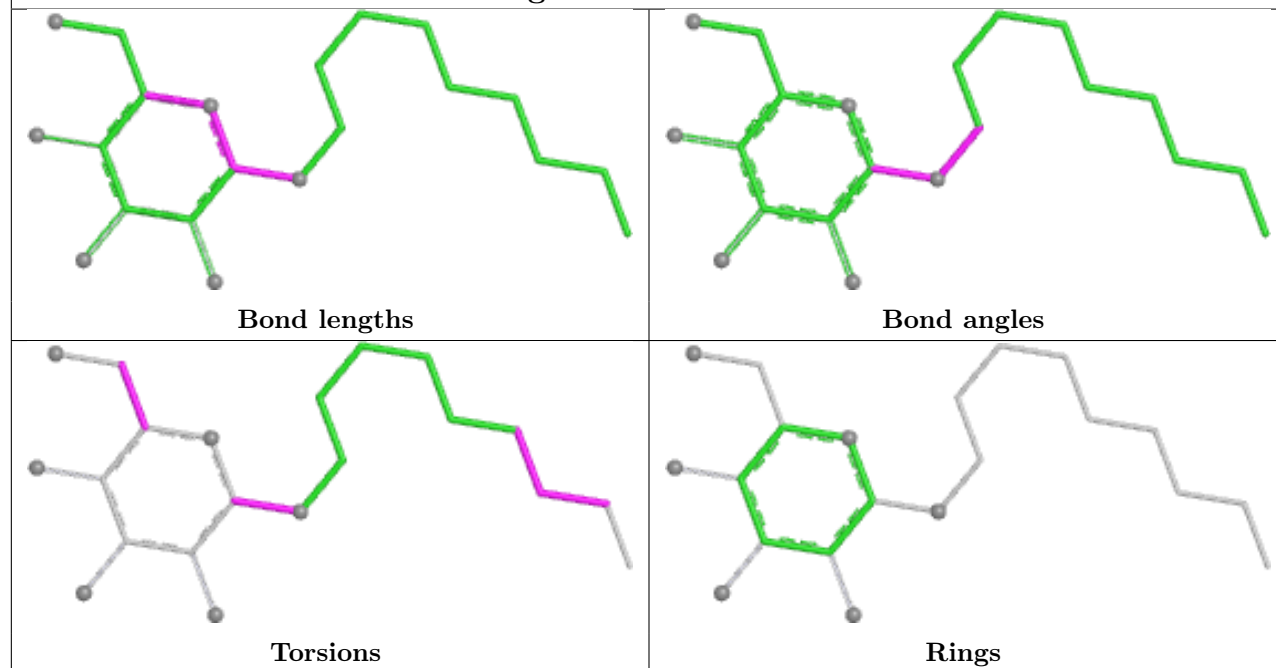
Ligand BNG B 509

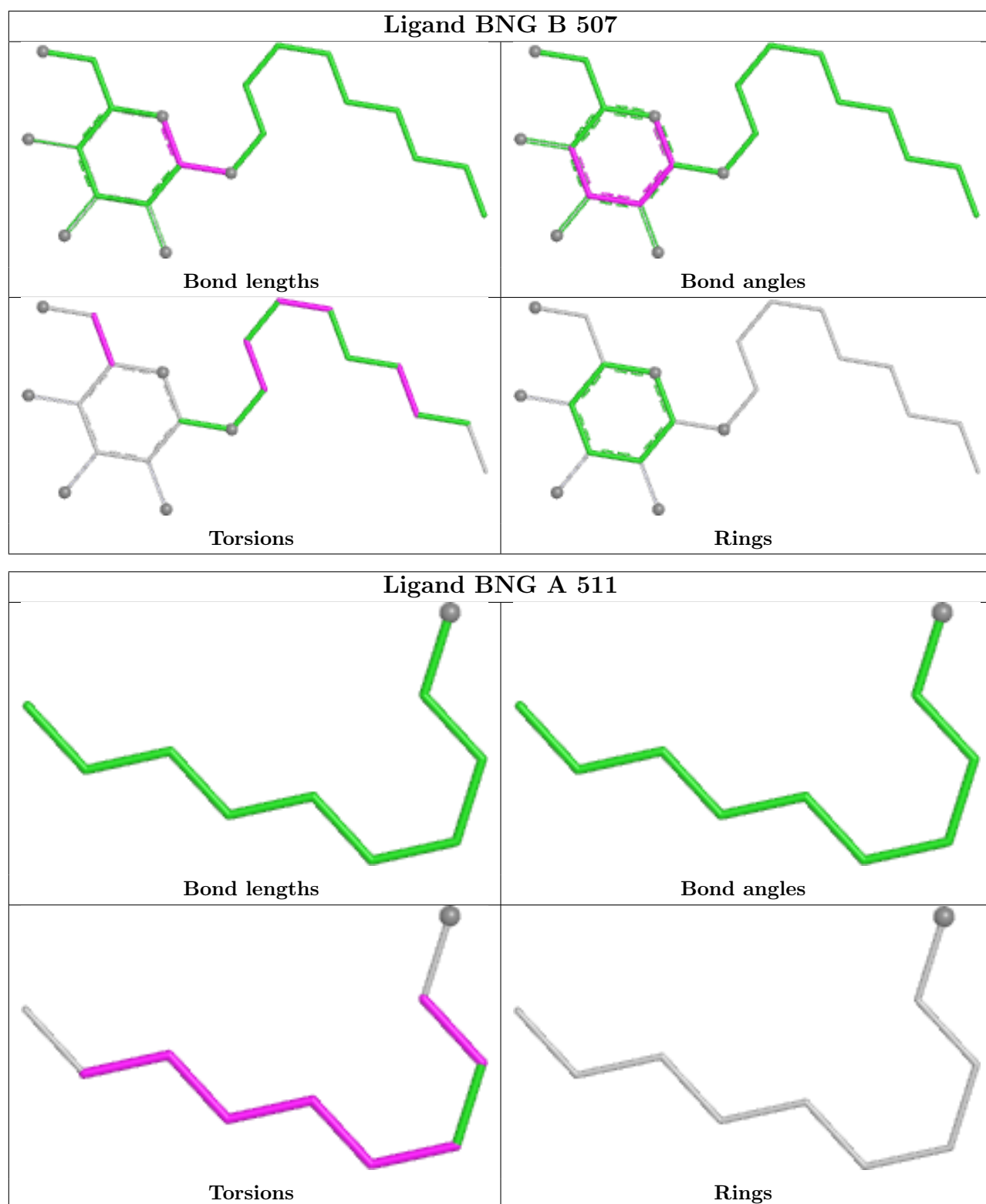


Ligand VAL B 501



Ligand BNG A 515





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	441/455 (96%)	-1.45	0 100 100	43, 54, 69, 80	0
1	B	445/455 (97%)	-1.40	0 100 100	42, 56, 73, 91	0
All	All	886/910 (97%)	-1.43	0 100 100	42, 55, 72, 91	0

There are no RSRZ outliers to report.

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
4	BNG	B	507	21/21	0.96	0.06	60,71,77,86	0
4	BNG	A	508	21/21	0.97	0.06	50,68,79,83	0
4	BNG	A	507	21/21	0.97	0.05	53,81,89,90	0
4	BNG	B	508	10/21	0.97	0.07	51,61,73,76	0
4	BNG	B	509	21/21	0.97	0.04	63,85,93,96	0
4	BNG	A	509	10/21	0.98	0.06	57,63,69,71	0
4	BNG	A	510	21/21	0.98	0.06	58,70,75,81	0

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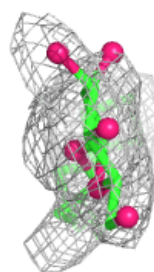
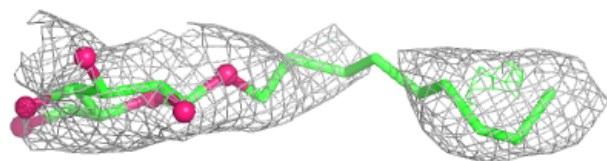
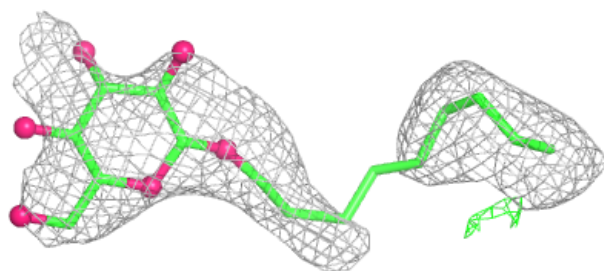
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BNG	A	511	10/21	0.98	0.05	56,58,65,68	0
4	BNG	A	512	10/21	0.98	0.06	59,64,72,72	0
4	BNG	A	514	9/21	0.98	0.06	51,53,57,59	0
4	BNG	A	515	21/21	0.98	0.05	51,82,96,96	0
4	BNG	A	516	21/21	0.98	0.04	54,70,79,82	0
4	BNG	B	505	10/21	0.98	0.05	57,64,72,74	0
4	BNG	B	506	10/21	0.98	0.05	56,64,70,73	0
4	BNG	A	506	21/21	0.98	0.05	54,67,73,75	0
4	BNG	A	504	21/21	0.98	0.04	57,67,77,81	0
4	BNG	A	505	21/21	0.98	0.05	50,59,69,76	0
4	BNG	B	510	21/21	0.98	0.04	47,64,75,80	0
5	LMT	A	517	13/35	0.98	0.05	58,62,77,77	0
5	LMT	A	518	13/35	0.98	0.06	58,60,65,70	0
3	NA	A	503	1/1	0.99	0.05	51,51,51,51	0
4	BNG	B	504	21/21	0.99	0.04	52,68,78,78	0
4	BNG	A	513	10/21	0.99	0.05	58,68,74,76	0
2	VAL	A	501	8/8	0.99	0.04	42,47,48,49	0
2	VAL	B	501	8/8	0.99	0.03	45,50,51,53	0
3	NA	B	502	1/1	1.00	0.02	52,52,52,52	0
3	NA	B	503	1/1	1.00	0.02	48,48,48,48	0
3	NA	A	502	1/1	1.00	0.02	45,45,45,45	0

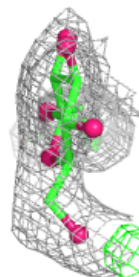
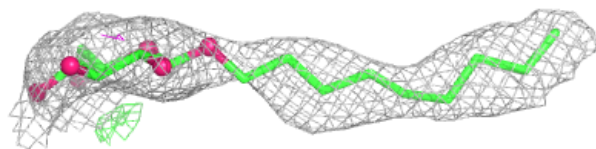
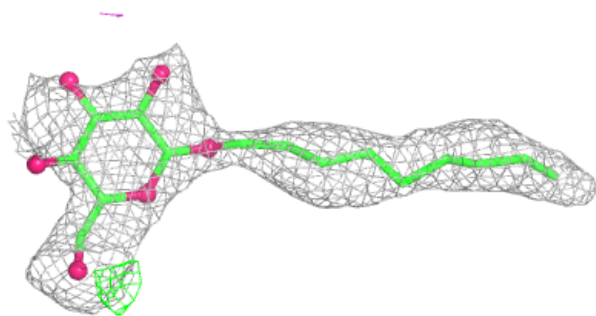
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BNG B 507:

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

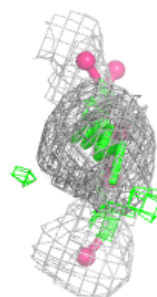
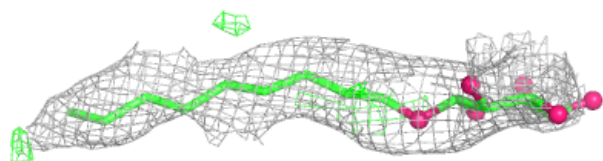
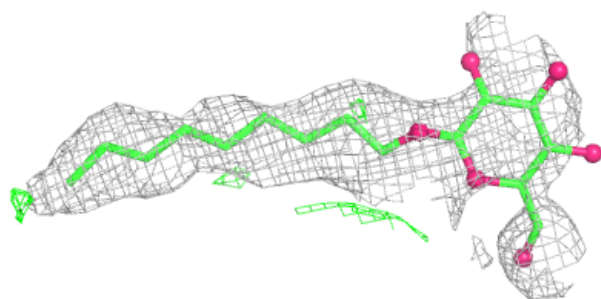
**Electron density around BNG A 508:**

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

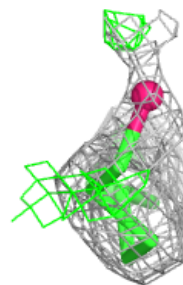
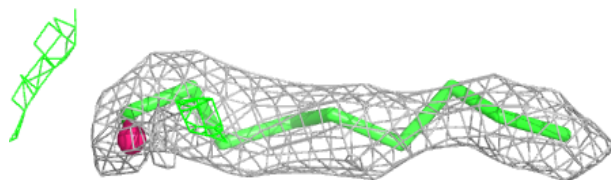
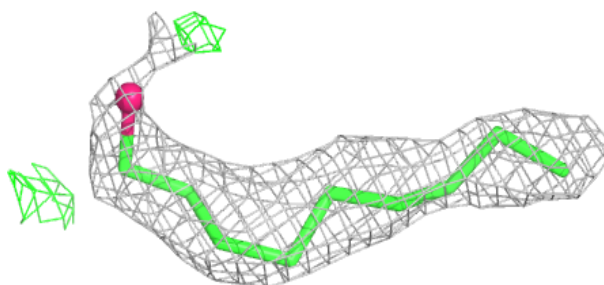


Electron density around BNG A 507:

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

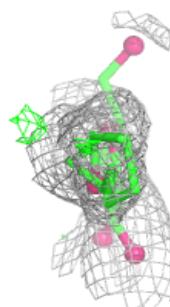
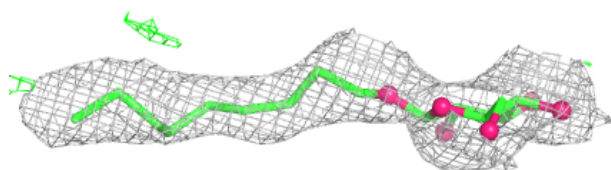
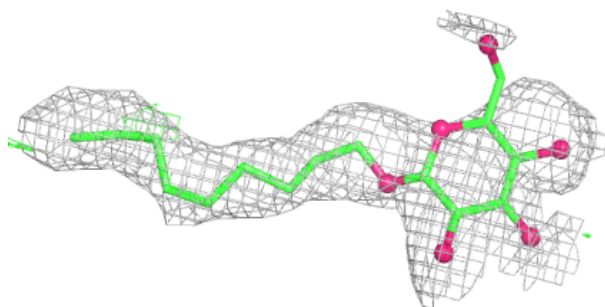
**Electron density around BNG B 508:**

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

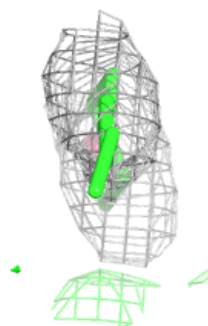
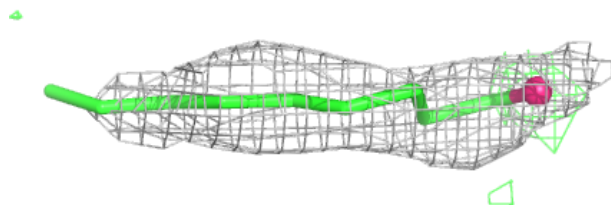
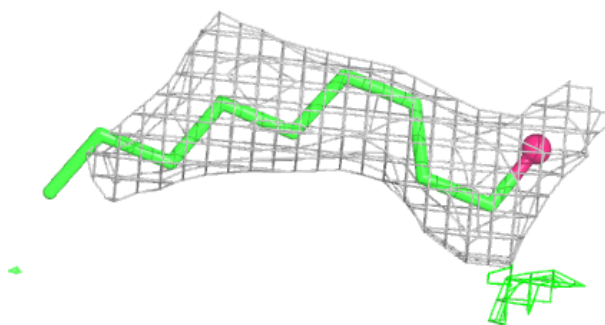


Electron density around BNG B 509:

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

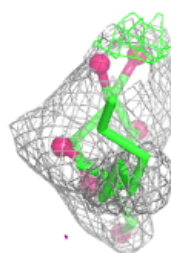
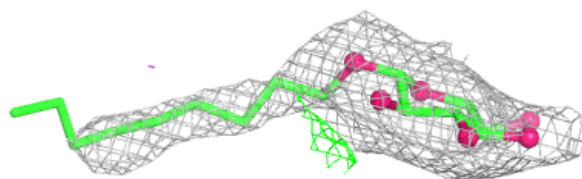
**Electron density around BNG A 509:**

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

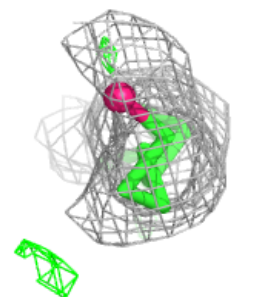
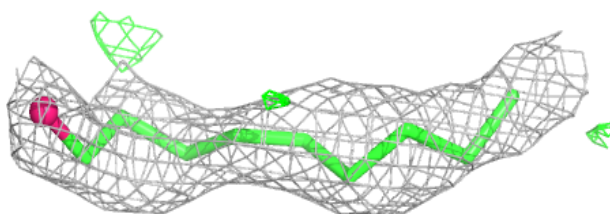
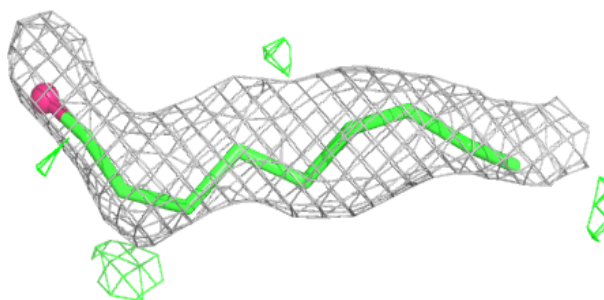


Electron density around BNG A 510:

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

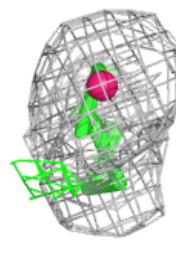
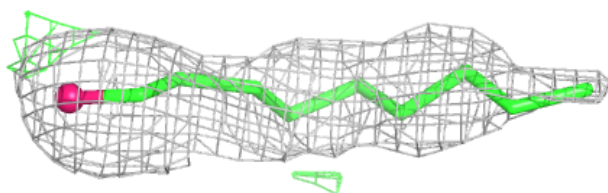
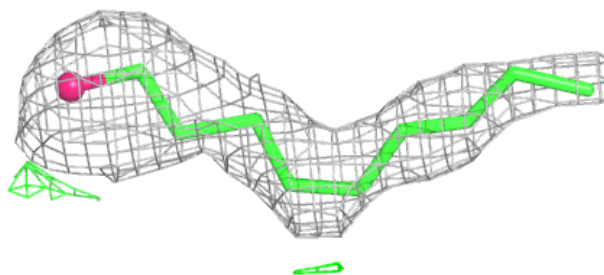
**Electron density around BNG A 511:**

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

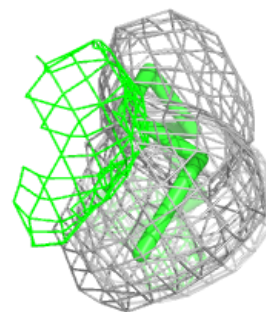
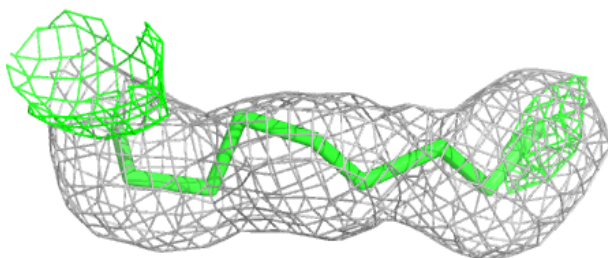
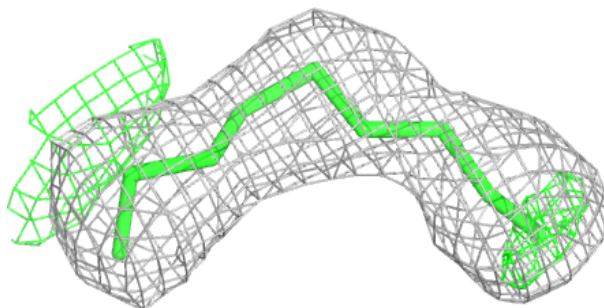


Electron density around BNG A 512:

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

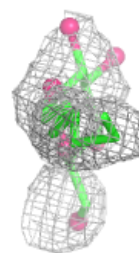
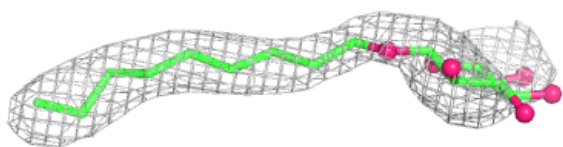
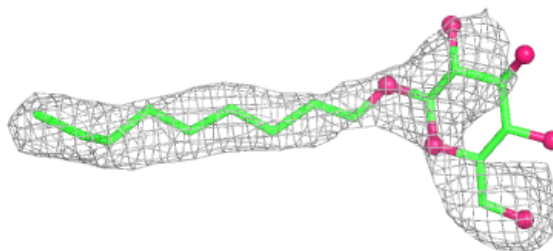
**Electron density around BNG A 514:**

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

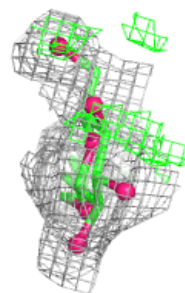
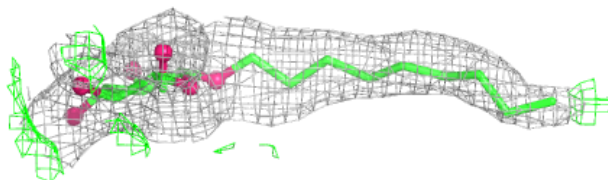


Electron density around BNG A 515:

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

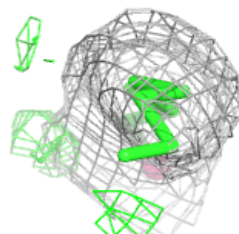
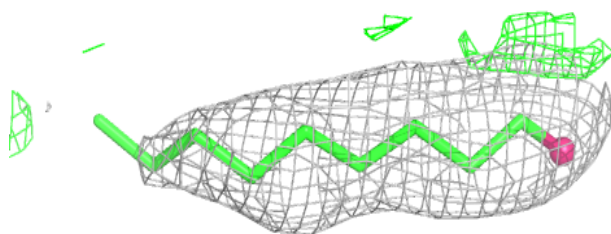
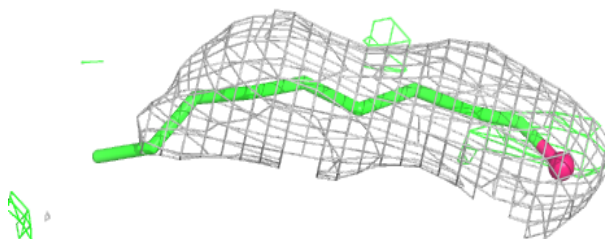
**Electron density around BNG A 516:**

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

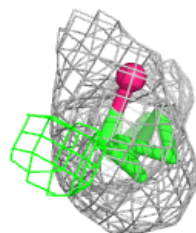
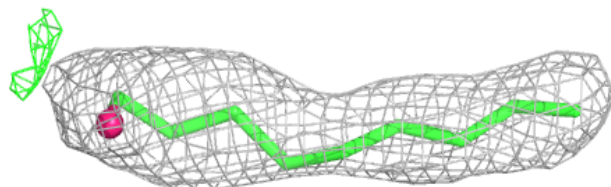
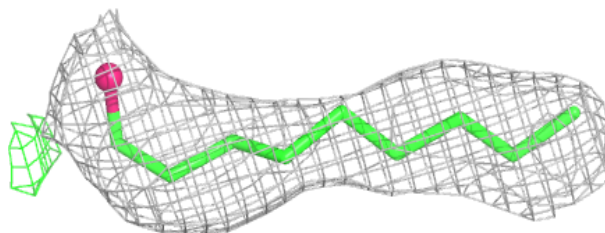


Electron density around BNG B 505:

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

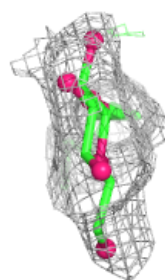
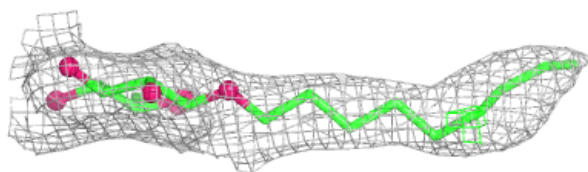
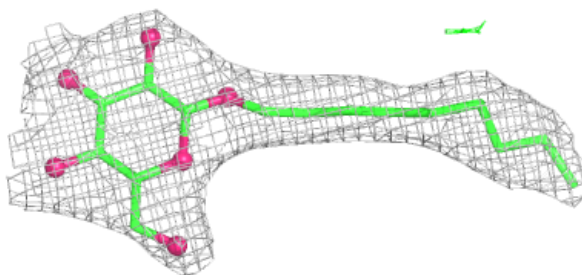
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

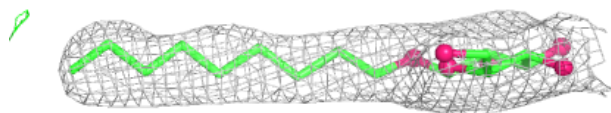
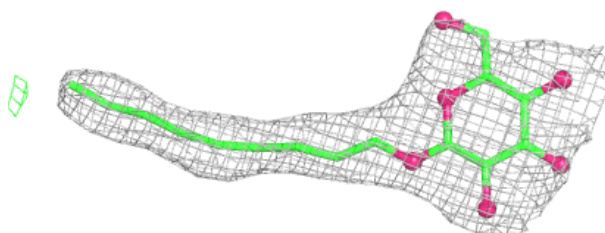


Electron density around BNG A 506:

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and green (positive)

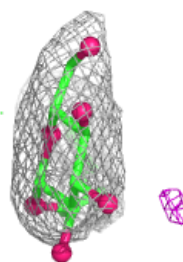
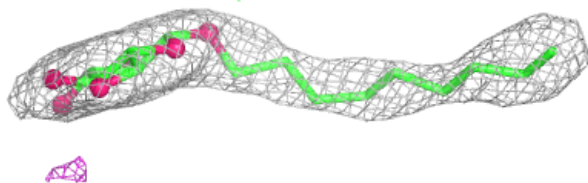
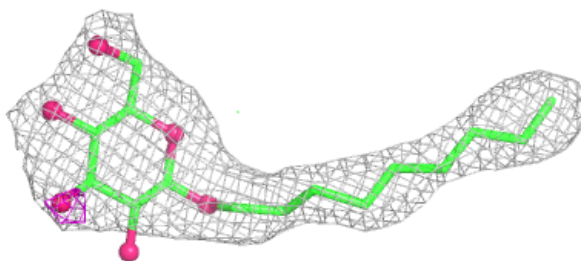
**Electron density around BNG A 504:**

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and green (positive)

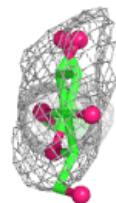
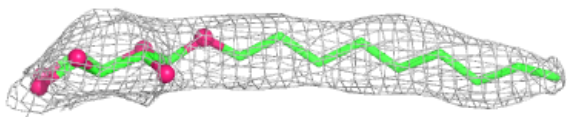
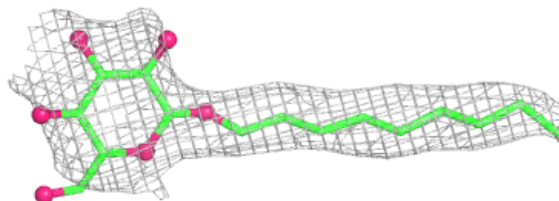


Electron density around BNG A 505:

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

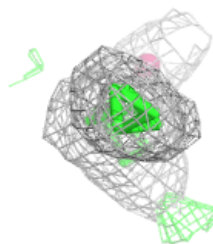
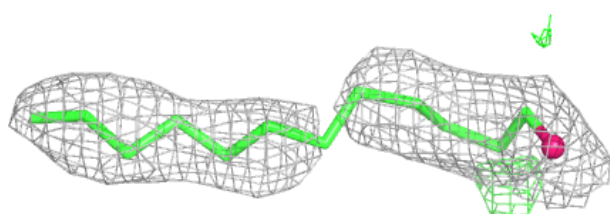
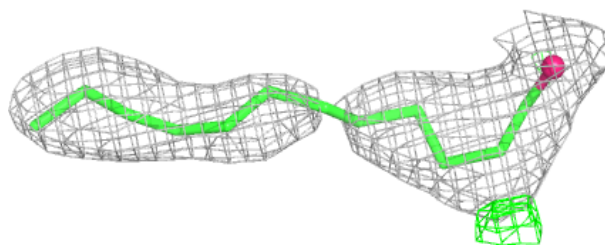
**Electron density around BNG B 510:**

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

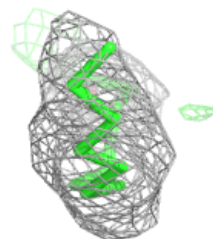
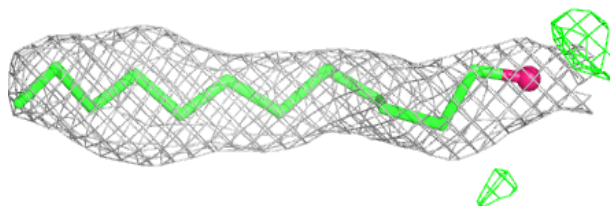
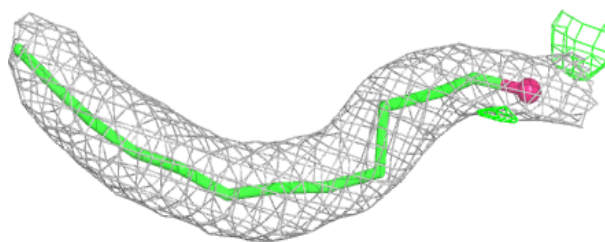


Electron density around LMT A 517:

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

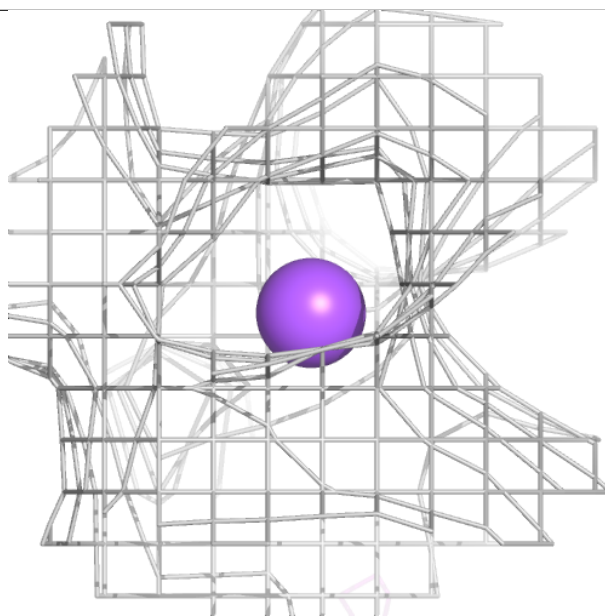
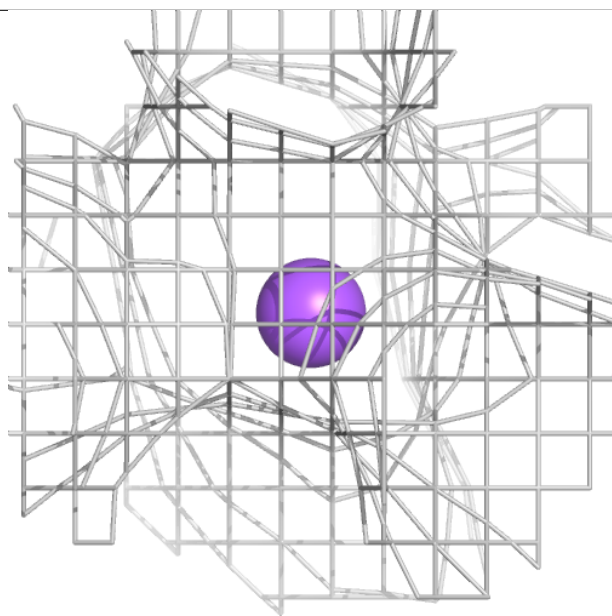
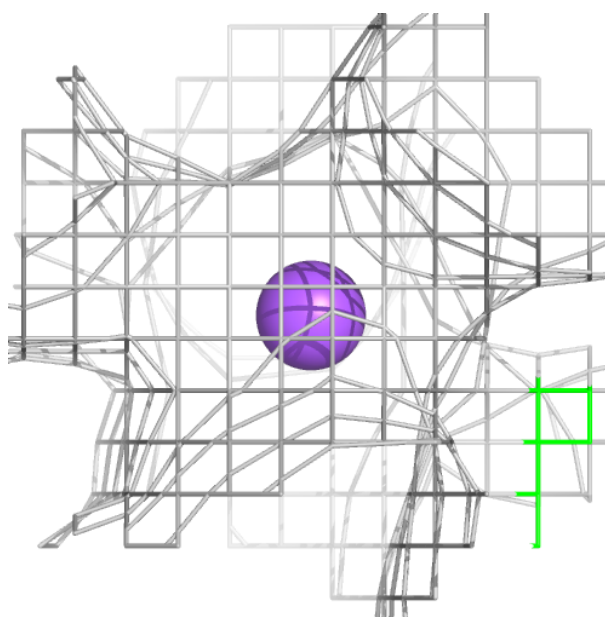
**Electron density around LMT A 518:**

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



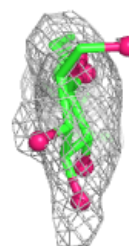
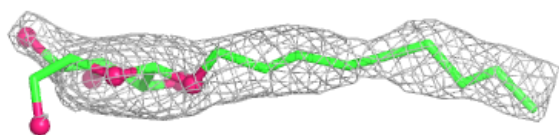
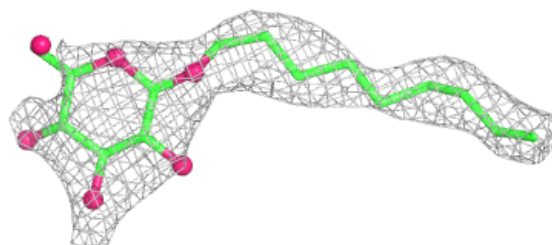
Electron density around NA A 503:

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and green (positive)

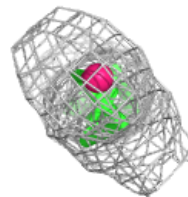
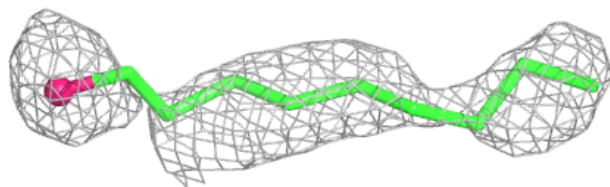
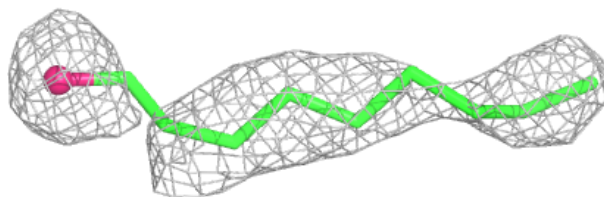


Electron density around BNG B 504:

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

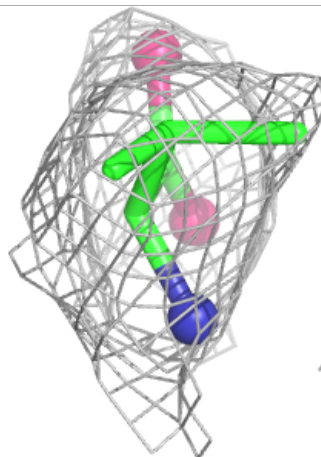
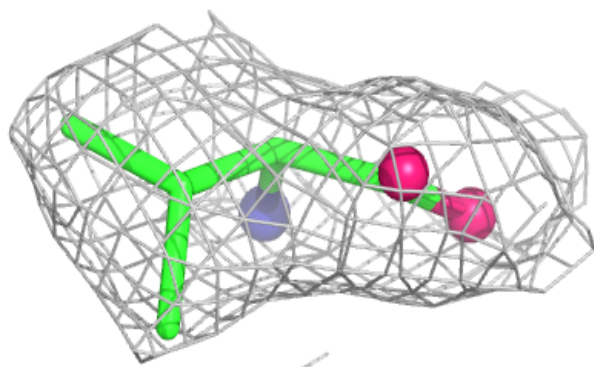
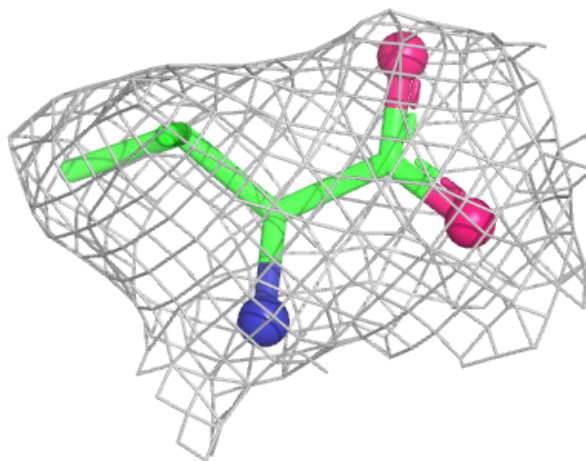
**Electron density around BNG A 513:**

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



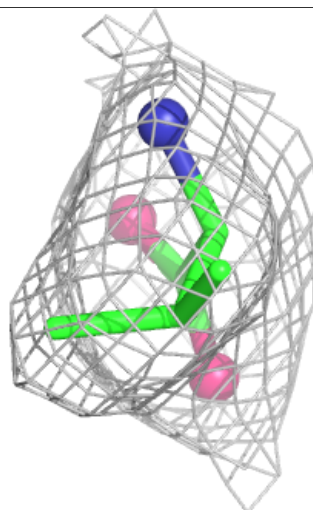
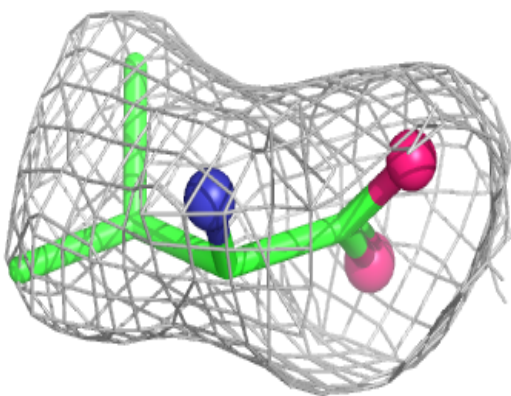
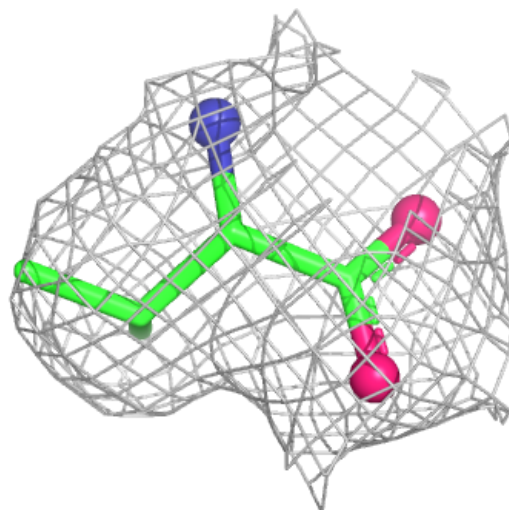
Electron density around VAL A 501:

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



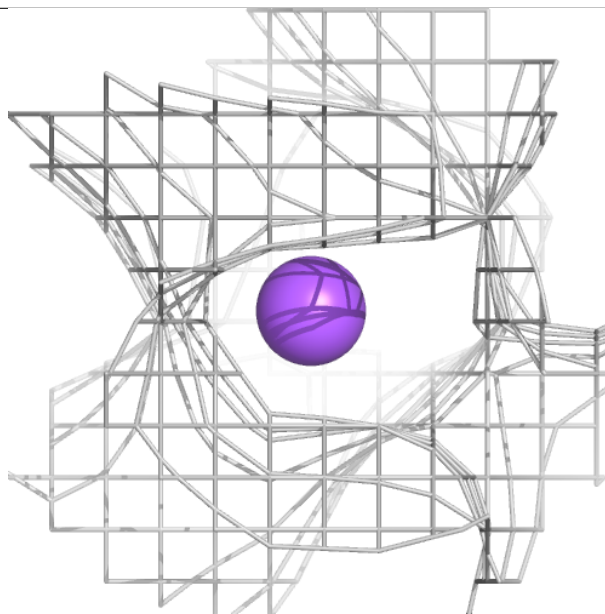
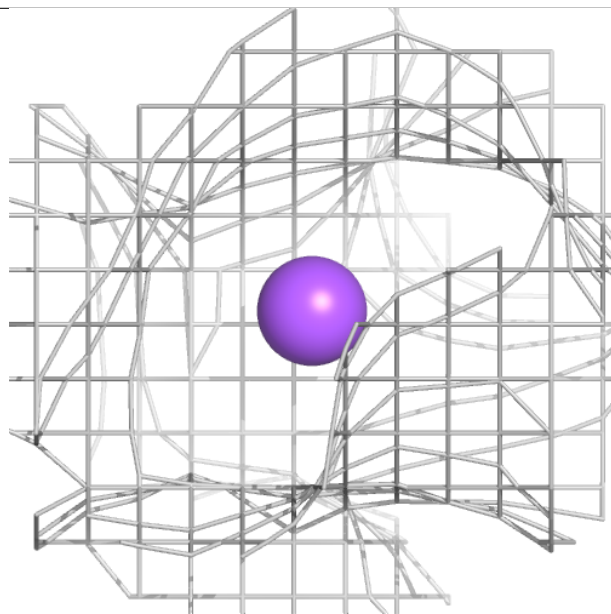
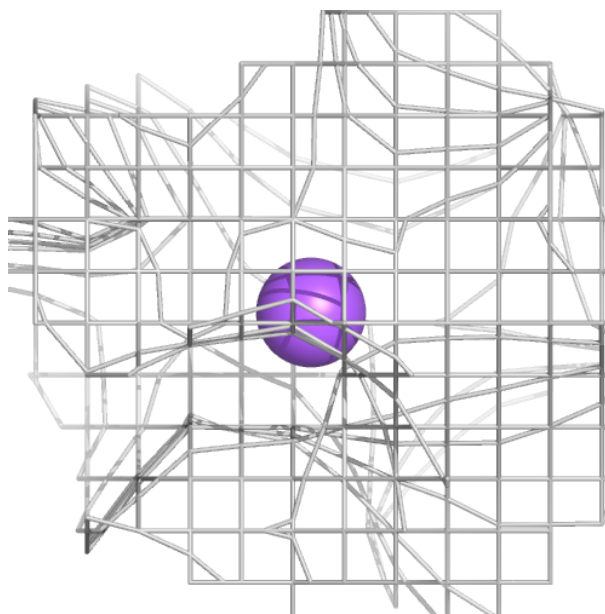
Electron density around VAL B 501:

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



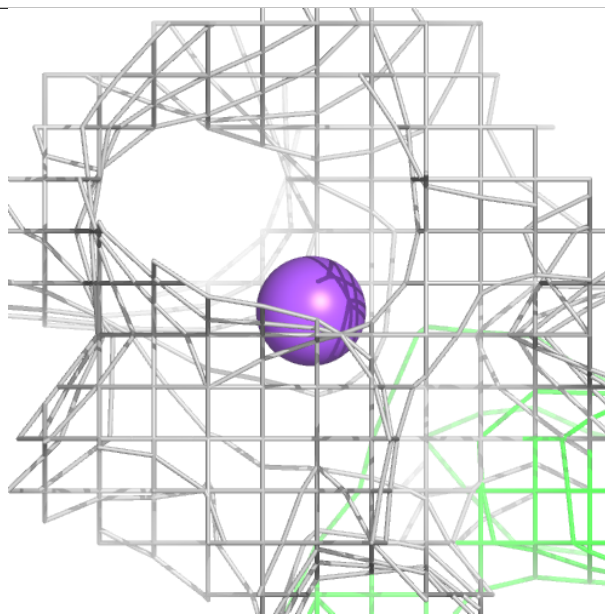
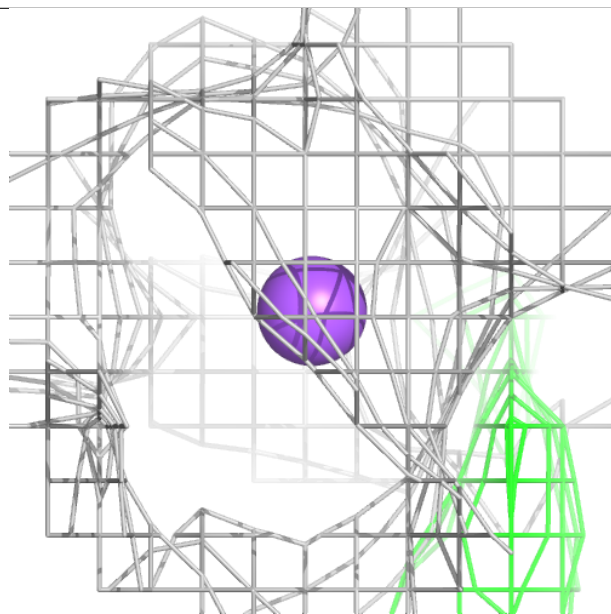
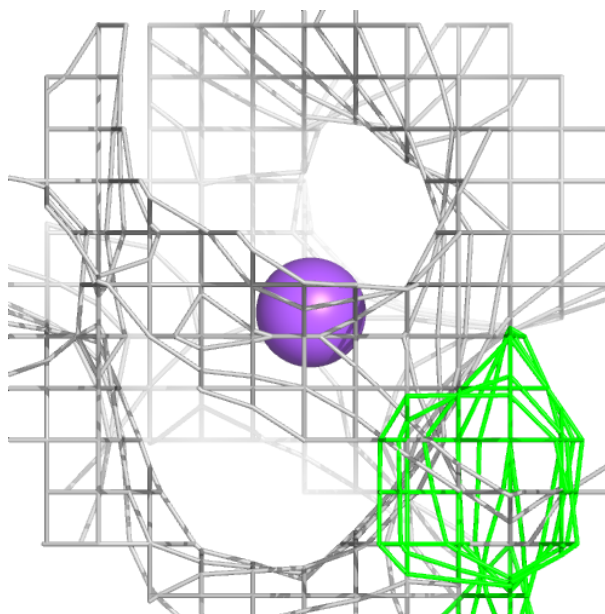
Electron density around NA B 502:

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



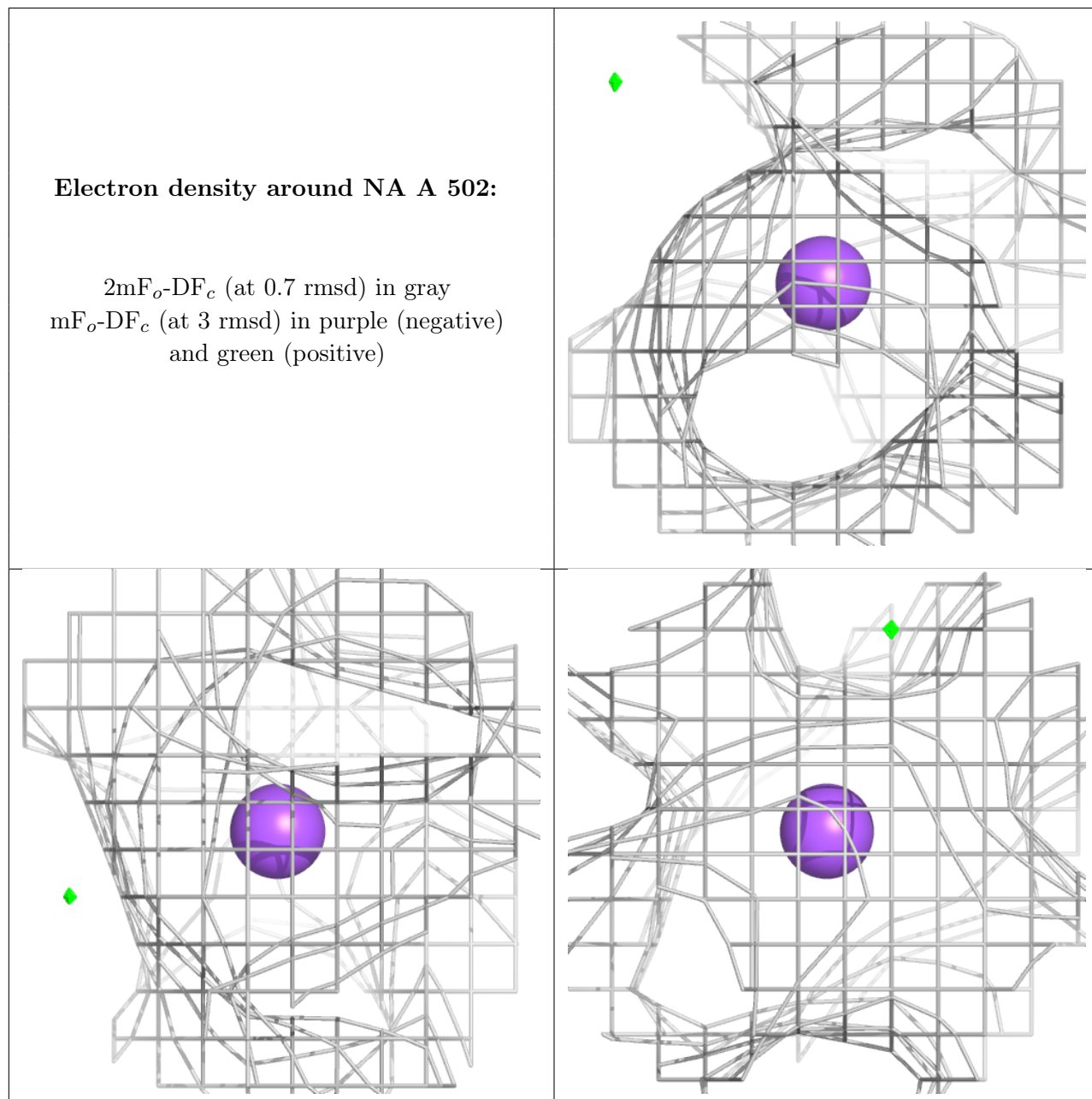
Electron density around NA B 503:

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



Electron density around NA A 502:

$2mF_o-DF_c$ (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.