



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 05:12 PM JST

PDB ID : 7F8N
EMDB ID : EMD-31490
Title : Human pannexin-1 showing a conformational change in the N-terminal domain and blocked pore
Authors : Kuzuya, M.; Hirano, H.; Hayashida, K.; Watanabe, M.; Kobayashi, K.; Tani, K.; Fujiyoshi, Y.; Oshima, A.
Deposited on : 2021-07-02
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

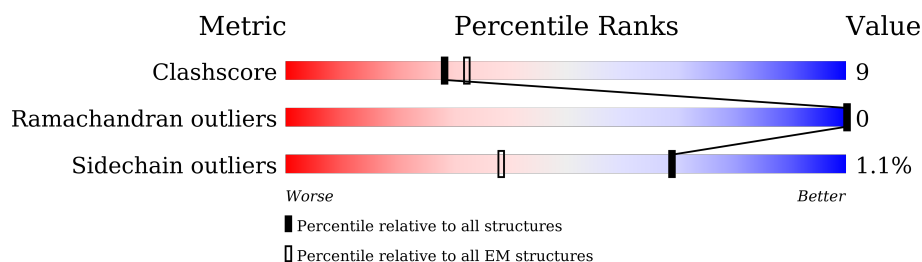
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	426	<div> <div>8%</div> <div>54%</div> <div>18%</div> <div>27%</div> </div>
1	B	426	<div> <div>9%</div> <div>54%</div> <div>18%</div> <div>27%</div> </div>
1	C	426	<div> <div>9%</div> <div>54%</div> <div>18%</div> <div>27%</div> </div>
1	D	426	<div> <div>10%</div> <div>54%</div> <div>18%</div> <div>27%</div> </div>
1	E	426	<div> <div>9%</div> <div>55%</div> <div>17%</div> <div>27%</div> </div>
1	F	426	<div> <div>8%</div> <div>54%</div> <div>18%</div> <div>27%</div> </div>
1	G	426	<div> <div>9%</div> <div>54%</div> <div>18%</div> <div>27%</div> </div>

2 Entry composition [i](#)

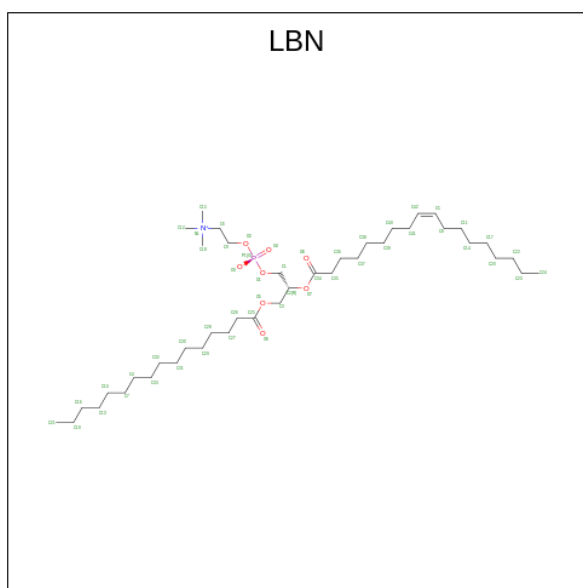
There are 2 unique types of molecules in this entry. The entry contains 18522 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Pannexin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	309	Total	C	N	O	S	0	0
			2467	1644	384	428	11		
1	B	309	Total	C	N	O	S	0	0
			2467	1644	384	428	11		
1	C	309	Total	C	N	O	S	0	0
			2467	1644	384	428	11		
1	D	309	Total	C	N	O	S	0	0
			2467	1644	384	428	11		
1	E	309	Total	C	N	O	S	0	0
			2467	1644	384	428	11		
1	F	309	Total	C	N	O	S	0	0
			2467	1644	384	428	11		
1	G	309	Total	C	N	O	S	0	0
			2467	1644	384	428	11		

- Molecule 2 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (three-letter code: LBN) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	A	1	Total	C	N	O	P	0
			28	19	1	7	1	
2	A	1	Total	C				0
			12	12				
2	A	1	Total	C				0
			11	11				
2	A	1	Total	C	O			0
			16	14	2			
2	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
2	B	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
2	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	B	1	Total	C	N	O	P	0
			28	19	1	7	1	
2	B	1	Total	C				0
			12	12				
2	B	1	Total	C				0
			11	11				
2	B	1	Total	C	O			0
			16	14	2			
2	C	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
2	C	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	C	1	Total	C	N	O	P	0
			28	19	1	7	1	
2	C	1	Total	C				0
			12	12				
2	C	1	Total	C	O			0
			16	14	2			
2	D	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	D	1	Total	C	N	O	P	0
			35	25	1	8	1	
2	D	1	Total	C				0
			11	11				

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	D	1	Total	C				0
			12	12				
2	D	1	Total	C	O			0
			16	14	2			
2	E	1	Total	C	N	O	P	0
			28	19	1	7	1	
2	E	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	E	1	Total	C	N	O	P	0
			35	25	1	8	1	
2	E	1	Total	C				0
			11	11				
2	E	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	E	1	Total	C	N	O	P	0
			28	19	1	7	1	
2	E	1	Total	C				0
			12	12				
2	E	1	Total	C				0
			11	11				
2	E	1	Total	C	O			0
			16	14	2			
2	F	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	F	1	Total	C	N	O	P	0
			35	25	1	8	1	
2	F	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	F	1	Total	C	N	O	P	0
			28	19	1	7	1	
2	F	1	Total	C				0
			12	12				
2	F	1	Total	C				0
			11	11				
2	F	1	Total	C	O			0
			16	14	2			
2	G	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	G	1	Total	C	N	O	P	0
			35	25	1	8	1	

Continued on next page...

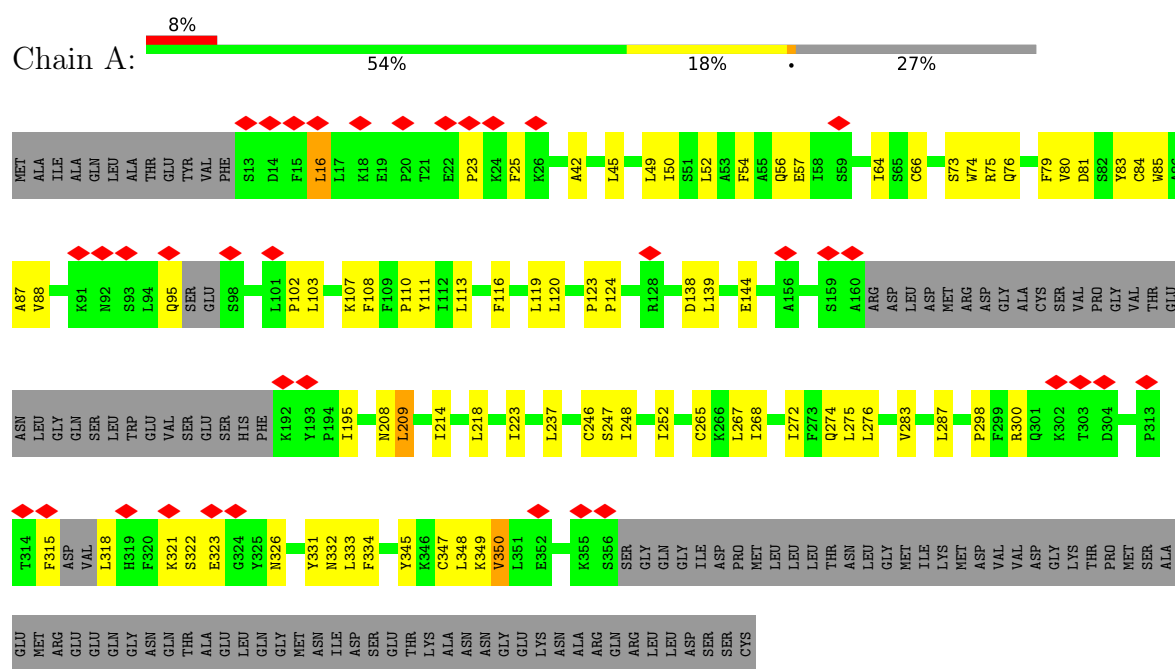
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	G	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	G	1	Total	C	N	O	P	0
			28	19	1	7	1	
2	G	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	G	1	Total	C				0
			12	12				
2	G	1	Total	C				0
			11	11				
2	G	1	Total	C	O			0
			16	14	2			

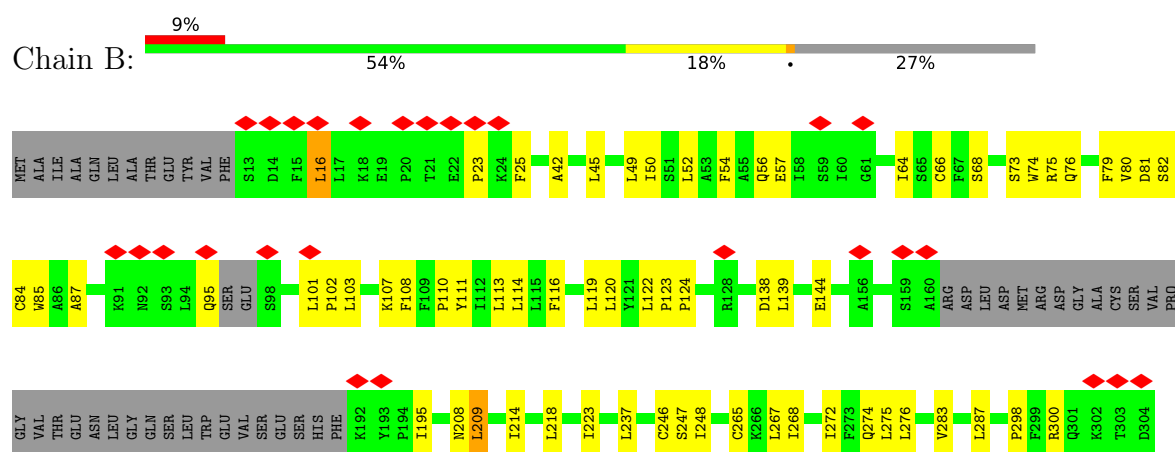
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

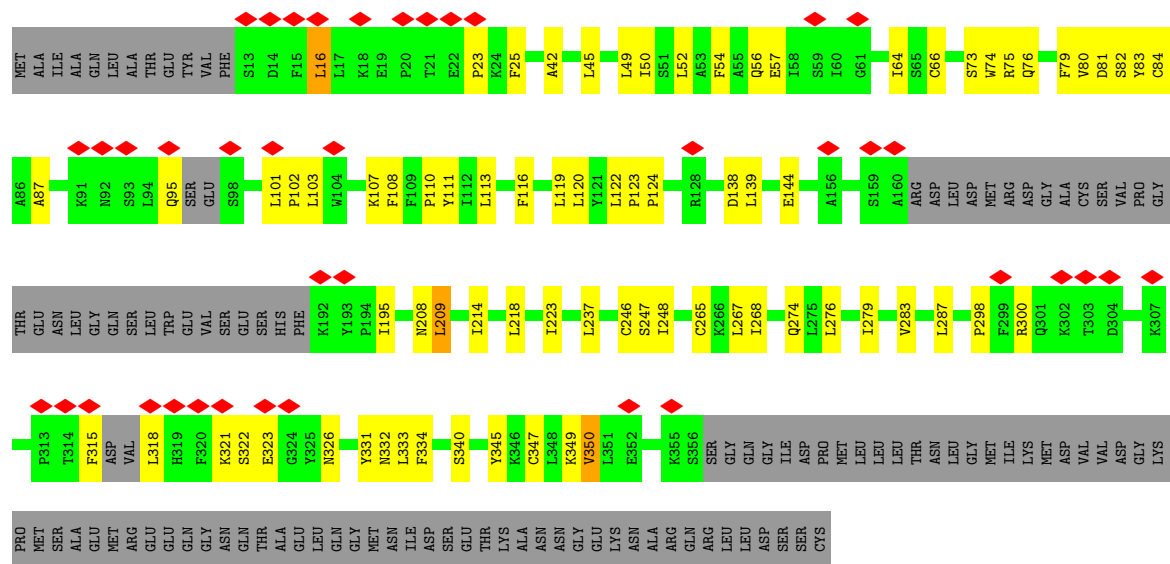
• Molecule 1: Pannexin-1



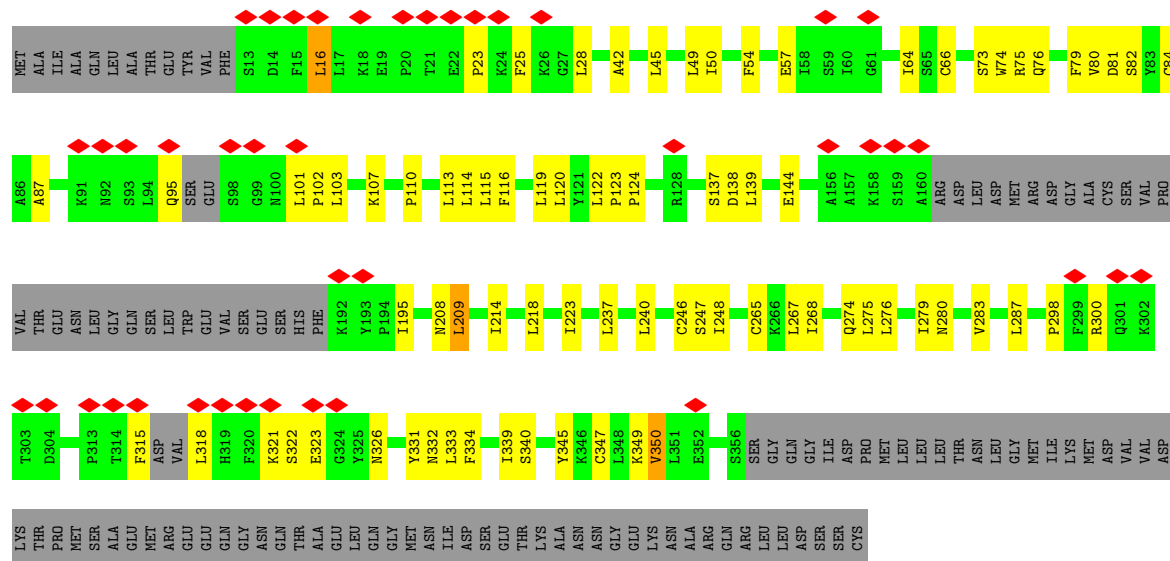
• Molecule 1: Pannexin-1



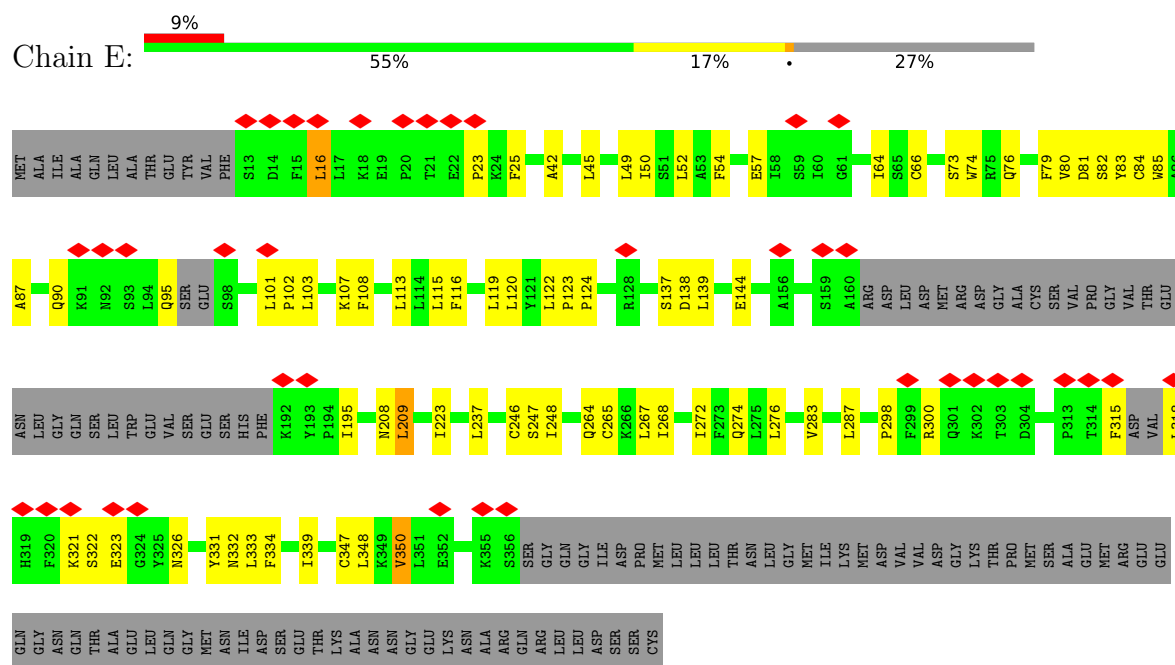
- Molecule 1: Pannexin-1



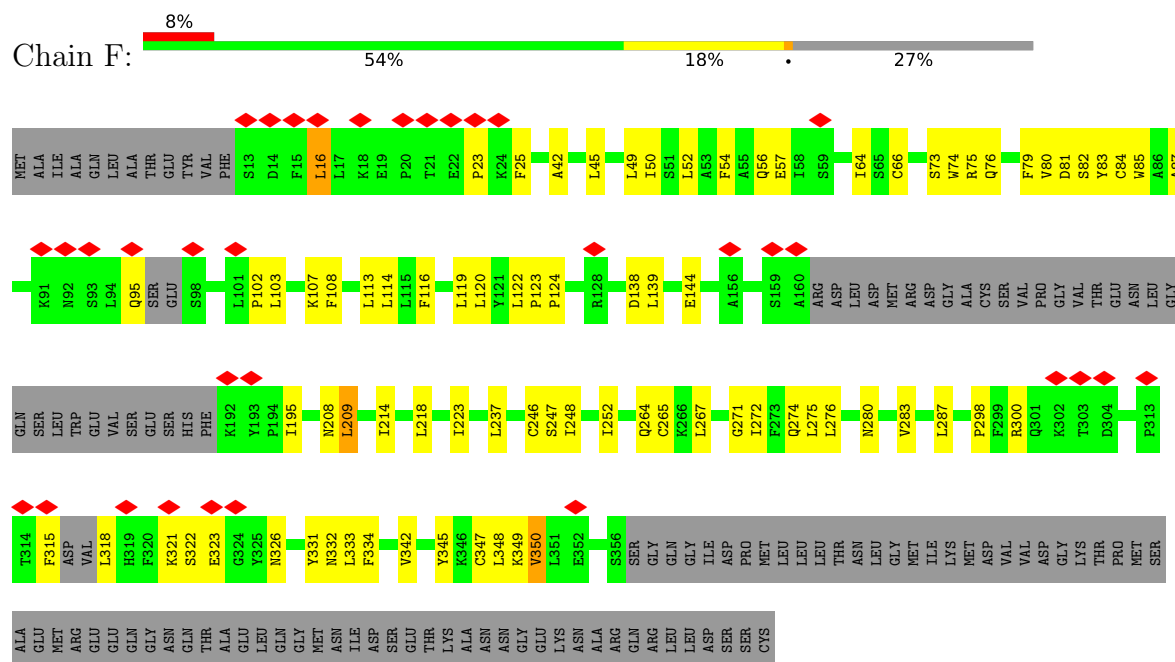
- Molecule 1: Pannexin-1



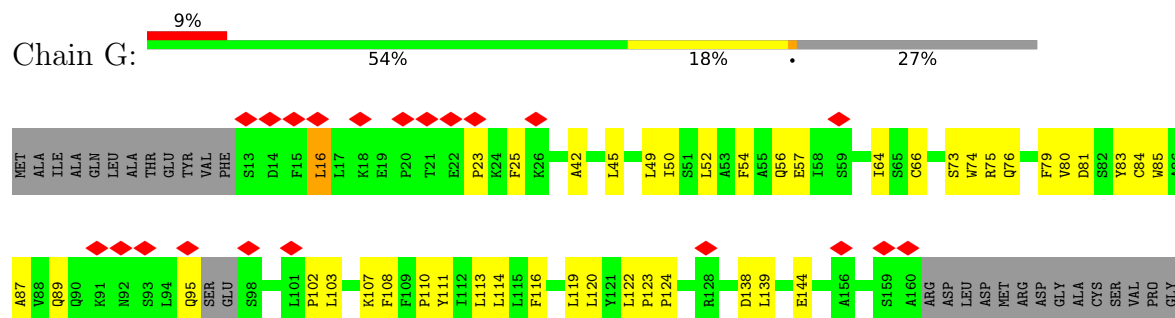
- Molecule 1: Pannexin-1

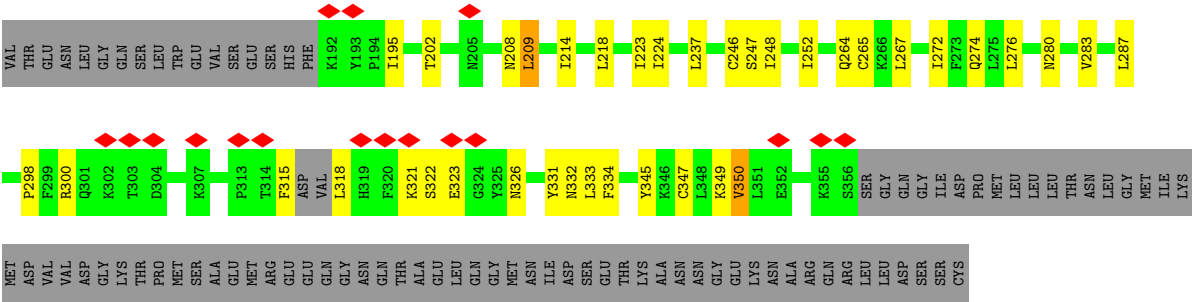


• Molecule 1: Pannexin-1



• Molecule 1: Pannexin-1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	19897	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.131	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (\AA)	226.8, 226.8, 226.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LBN

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	0.26	0/2523	0.42	1/3422 (0.0%)
1	B	0.26	0/2523	0.42	1/3422 (0.0%)
1	C	0.26	0/2523	0.42	1/3422 (0.0%)
1	D	0.26	0/2523	0.42	1/3422 (0.0%)
1	E	0.26	0/2523	0.42	1/3422 (0.0%)
1	F	0.26	0/2523	0.42	1/3422 (0.0%)
1	G	0.26	0/2523	0.42	1/3422 (0.0%)
All	All	0.26	0/17661	0.42	7/23954 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	PRO	N-CA-CB	6.18	110.72	103.30
1	F	23	PRO	N-CA-CB	6.18	110.72	103.30
1	D	23	PRO	N-CA-CB	6.17	110.71	103.30
1	E	23	PRO	N-CA-CB	6.17	110.71	103.30
1	B	23	PRO	N-CA-CB	6.16	110.69	103.30
1	G	23	PRO	N-CA-CB	6.16	110.69	103.30
1	A	23	PRO	N-CA-CB	6.15	110.68	103.30

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	2467	0	2546	60	0
1	B	2467	0	2546	56	0
1	C	2467	0	2546	56	0
1	D	2467	0	2546	59	0
1	E	2467	0	2546	53	0
1	F	2467	0	2546	56	0
1	G	2467	0	2546	63	0
2	A	139	0	0	0	0
2	B	179	0	0	0	0
2	C	168	0	0	0	0
2	D	151	0	0	0	0
2	E	218	0	0	1	0
2	F	179	0	0	0	0
2	G	219	0	0	0	0
All	All	18522	0	17822	337	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 9.

All (337) 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:F:74:TRP:HZ3	1:G:75:ARG:HH11	1.20	0.85
1:D:268:ILE:HG21	1:E:82:SER:HB3	1.67	0.77
1:A:116:PHE:HA	1:A:119:LEU:HB2	1.66	0.77
1:D:116:PHE:HA	1:D:119:LEU:HB2	1.66	0.77
1:G:116:PHE:HA	1:G:119:LEU:HB2	1.66	0.77
1:F:116:PHE:HA	1:F:119:LEU:HB2	1.66	0.76
1:C:116:PHE:HA	1:C:119:LEU:HB2	1.66	0.76
1:E:116:PHE:HA	1:E:119:LEU:HB2	1.66	0.76
1:C:268:ILE:HG21	1:D:82:SER:HB3	1.67	0.75
1:B:116:PHE:HA	1:B:119:LEU:HB2	1.66	0.75
1:B:268:ILE:HG21	1:C:82:SER:HB3	1.71	0.71
1:F:272:ILE:HG22	1:G:108:PHE:HE1	1.55	0.71
1:B:139:LEU:HD11	1:B:334:PHE:HB3	1.74	0.69
1:A:139:LEU:HD11	1:A:334:PHE:HB3	1.74	0.69
1:A:272:ILE:HG22	1:B:108:PHE:HE1	1.58	0.69
1:C:139:LEU:HD11	1:C:334:PHE:HB3	1.74	0.69
1:E:139:LEU:HD11	1:E:334:PHE:HB3	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:LEU:HD11	1:D:334:PHE:HB3	1.74	0.68
1:G:139:LEU:HD11	1:G:334:PHE:HB3	1.74	0.68
1:F:139:LEU:HD11	1:F:334:PHE:HB3	1.74	0.68
1:E:315:PHE:HB2	1:E:318:LEU:HD11	1.76	0.67
1:A:315:PHE:HB2	1:A:318:LEU:HD11	1.77	0.67
1:F:315:PHE:HB2	1:F:318:LEU:HD11	1.77	0.67
1:B:315:PHE:HB2	1:B:318:LEU:HD11	1.76	0.67
1:G:315:PHE:HB2	1:G:318:LEU:HD11	1.77	0.67
1:D:315:PHE:HB2	1:D:318:LEU:HD11	1.76	0.67
1:C:315:PHE:HB2	1:C:318:LEU:HD11	1.77	0.67
1:B:102:PRO:HB3	1:B:237:LEU:HD22	1.78	0.66
1:G:102:PRO:HB3	1:G:237:LEU:HD22	1.78	0.66
1:A:102:PRO:HB3	1:A:237:LEU:HD22	1.78	0.66
1:G:42:ALA:HB1	1:G:120:LEU:HD13	1.78	0.66
1:A:42:ALA:HB1	1:A:120:LEU:HD13	1.78	0.66
1:F:102:PRO:HB3	1:F:237:LEU:HD22	1.78	0.66
1:C:102:PRO:HB3	1:C:237:LEU:HD22	1.78	0.66
1:F:42:ALA:HB1	1:F:120:LEU:HD13	1.78	0.66
1:E:102:PRO:HB3	1:E:237:LEU:HD22	1.78	0.66
1:A:75:ARG:HD3	1:G:74:TRP:HZ3	1.60	0.65
1:D:102:PRO:HB3	1:D:237:LEU:HD22	1.78	0.65
1:A:108:PHE:HE1	1:G:272:ILE:HG22	1.60	0.65
1:D:42:ALA:HB1	1:D:120:LEU:HD13	1.78	0.65
1:B:42:ALA:HB1	1:B:120:LEU:HD13	1.78	0.65
1:C:81:ASP:OD2	1:D:75:ARG:NH2	2.30	0.65
1:E:42:ALA:HB1	1:E:120:LEU:HD13	1.78	0.65
1:C:42:ALA:HB1	1:C:120:LEU:HD13	1.78	0.64
1:B:119:LEU:HB3	1:B:223:ILE:HD13	1.79	0.64
1:A:119:LEU:HB3	1:A:223:ILE:HD13	1.79	0.64
1:C:279:ILE:HD13	1:D:115:LEU:HD11	1.80	0.64
1:C:119:LEU:HB3	1:C:223:ILE:HD13	1.79	0.64
1:G:119:LEU:HB3	1:G:223:ILE:HD13	1.79	0.64
1:D:49:LEU:HD22	1:D:276:LEU:HD22	1.80	0.64
1:C:49:LEU:HD22	1:C:276:LEU:HD22	1.80	0.63
1:A:49:LEU:HD22	1:A:276:LEU:HD22	1.80	0.63
1:G:49:LEU:HD22	1:G:276:LEU:HD22	1.80	0.63
1:E:49:LEU:HD22	1:E:276:LEU:HD22	1.80	0.63
1:E:119:LEU:HB3	1:E:223:ILE:HD13	1.79	0.63
1:F:119:LEU:HB3	1:F:223:ILE:HD13	1.79	0.63
1:C:80:VAL:HA	1:C:248:ILE:HD11	1.81	0.63
1:D:80:VAL:HA	1:D:248:ILE:HD11	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:VAL:HA	1:B:248:ILE:HD11	1.81	0.62
1:F:49:LEU:HD22	1:F:276:LEU:HD22	1.80	0.62
1:B:49:LEU:HD22	1:B:276:LEU:HD22	1.80	0.62
1:D:119:LEU:HB3	1:D:223:ILE:HD13	1.79	0.62
1:A:80:VAL:HA	1:A:248:ILE:HD11	1.81	0.62
1:E:80:VAL:HA	1:E:248:ILE:HD11	1.81	0.61
1:A:74:TRP:HZ3	1:B:75:ARG:HH11	1.49	0.61
1:G:80:VAL:HA	1:G:248:ILE:HD11	1.81	0.61
1:F:80:VAL:HA	1:F:248:ILE:HD11	1.81	0.61
1:B:16:LEU:HD13	1:C:195:ILE:HB	1.83	0.60
1:C:340:SER:HB2	1:D:137:SER:HB3	1.85	0.59
1:E:321:LYS:O	1:E:332:ASN:ND2	2.37	0.58
1:F:321:LYS:O	1:F:332:ASN:ND2	2.37	0.58
1:D:321:LYS:O	1:D:332:ASN:ND2	2.37	0.58
1:C:321:LYS:O	1:C:332:ASN:ND2	2.37	0.57
1:A:64:ILE:HG21	1:A:85:TRP:HB2	1.86	0.57
1:G:321:LYS:O	1:G:332:ASN:ND2	2.37	0.57
1:B:321:LYS:O	1:B:332:ASN:ND2	2.37	0.57
1:D:64:ILE:HG21	1:D:85:TRP:HB2	1.86	0.57
1:A:321:LYS:O	1:A:332:ASN:ND2	2.37	0.57
1:G:64:ILE:HG21	1:G:85:TRP:HB2	1.86	0.57
1:A:75:ARG:HD3	1:G:74:TRP:CZ3	2.38	0.57
1:B:68:SER:O	1:C:76:GLN:NE2	2.34	0.57
1:B:64:ILE:HG21	1:B:85:TRP:HB2	1.85	0.56
1:C:64:ILE:HG21	1:C:85:TRP:HB2	1.86	0.56
1:D:16:LEU:HD13	1:E:195:ILE:HB	1.87	0.56
1:E:16:LEU:HD13	1:F:195:ILE:HB	1.86	0.56
1:E:64:ILE:HG21	1:E:85:TRP:HB2	1.86	0.56
1:F:52:LEU:HD21	1:G:114:LEU:HD22	1.86	0.56
1:F:64:ILE:HG21	1:F:85:TRP:HB2	1.86	0.56
1:D:95:GLN:HE22	1:D:103:LEU:HD11	1.71	0.56
1:E:66:CYS:N	1:E:81:ASP:OD1	2.39	0.56
1:D:138:ASP:OD2	1:D:331:TYR:OH	2.22	0.55
1:F:95:GLN:HE22	1:F:103:LEU:HD11	1.71	0.55
1:G:95:GLN:HE22	1:G:103:LEU:HD11	1.71	0.55
1:C:95:GLN:HE22	1:C:103:LEU:HD11	1.72	0.55
1:C:138:ASP:OD2	1:C:331:TYR:OH	2.22	0.55
1:A:52:LEU:HD21	1:B:114:LEU:HD22	1.89	0.55
1:A:74:TRP:HZ3	1:B:75:ARG:HD3	1.72	0.55
1:D:350:VAL:HG11	1:E:195:ILE:HD11	1.90	0.54
1:D:66:CYS:N	1:D:81:ASP:OD1	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:CYS:N	1:A:81:ASP:OD1	2.38	0.54
1:B:95:GLN:HE22	1:B:103:LEU:HD11	1.71	0.54
1:C:340:SER:HB2	1:D:137:SER:CB	2.38	0.54
1:A:95:GLN:HE22	1:A:103:LEU:HD11	1.71	0.54
1:B:237:LEU:O	1:B:274:GLN:NE2	2.41	0.54
1:E:95:GLN:HE22	1:E:103:LEU:HD11	1.71	0.54
1:D:279:ILE:HD13	1:E:115:LEU:HD11	1.88	0.54
1:A:237:LEU:O	1:A:274:GLN:NE2	2.41	0.54
1:C:237:LEU:O	1:C:274:GLN:NE2	2.41	0.53
1:A:56:GLN:HE22	1:B:110:PRO:HG2	1.74	0.53
1:E:237:LEU:O	1:E:274:GLN:NE2	2.41	0.53
1:G:237:LEU:O	1:G:274:GLN:NE2	2.41	0.53
1:G:66:CYS:N	1:G:81:ASP:OD1	2.39	0.53
1:C:66:CYS:N	1:C:81:ASP:OD1	2.39	0.53
1:F:237:LEU:O	1:F:274:GLN:NE2	2.41	0.53
1:B:138:ASP:OD2	1:B:331:TYR:OH	2.22	0.52
1:C:52:LEU:HD21	1:D:114:LEU:HD22	1.91	0.52
1:D:237:LEU:O	1:D:274:GLN:NE2	2.41	0.52
1:E:74:TRP:HZ3	1:F:75:ARG:HH11	1.56	0.52
1:D:50:ILE:HG13	1:D:113:LEU:HD23	1.92	0.51
1:E:50:ILE:HG13	1:E:113:LEU:HD23	1.92	0.51
1:A:110:PRO:HG2	1:G:56:GLN:HE22	1.75	0.51
1:A:252:ILE:HG12	1:G:264:GLN:HB2	1.93	0.51
1:B:66:CYS:N	1:B:81:ASP:OD1	2.39	0.51
1:F:50:ILE:HG13	1:F:113:LEU:HD23	1.92	0.51
1:A:74:TRP:CZ3	1:B:75:ARG:HD3	2.46	0.51
1:C:50:ILE:HG13	1:C:113:LEU:HD23	1.92	0.51
1:B:52:LEU:HB3	1:C:111:TYR:CE1	2.46	0.50
1:B:50:ILE:HG13	1:B:113:LEU:HD23	1.92	0.50
1:A:50:ILE:HG13	1:A:113:LEU:HD23	1.92	0.50
1:F:138:ASP:OD2	1:F:331:TYR:OH	2.22	0.50
1:F:323:GLU:O	1:F:326:ASN:ND2	2.45	0.50
1:G:50:ILE:HG13	1:G:113:LEU:HD23	1.92	0.50
1:B:323:GLU:O	1:B:326:ASN:ND2	2.45	0.49
1:A:138:ASP:OD2	1:A:331:TYR:OH	2.22	0.49
1:D:240:LEU:HA	1:E:90:GLN:NE2	2.27	0.49
1:A:323:GLU:O	1:A:326:ASN:ND2	2.45	0.49
1:D:323:GLU:O	1:D:326:ASN:ND2	2.45	0.49
1:F:74:TRP:CZ3	1:G:75:ARG:HD3	2.47	0.49
1:G:323:GLU:O	1:G:326:ASN:ND2	2.45	0.49
1:C:323:GLU:O	1:C:326:ASN:ND2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:GLU:O	1:E:326:ASN:ND2	2.45	0.49
1:F:66:CYS:N	1:F:81:ASP:OD1	2.39	0.49
1:D:350:VAL:HG11	1:E:195:ILE:CD1	2.42	0.49
1:A:111:TYR:CE1	1:G:52:LEU:HB3	2.47	0.49
1:E:268:ILE:HG21	1:F:82:SER:HB3	1.95	0.48
1:G:138:ASP:OD2	1:G:331:TYR:OH	2.22	0.48
1:B:45:LEU:HD23	1:B:283:VAL:HG21	1.96	0.48
1:F:74:TRP:HZ3	1:G:75:ARG:HD3	1.79	0.47
1:A:45:LEU:HD23	1:A:283:VAL:HG21	1.96	0.47
1:C:45:LEU:HD23	1:C:283:VAL:HG21	1.96	0.47
1:B:246:CYS:SG	1:B:247:SER:N	2.88	0.47
1:C:246:CYS:SG	1:C:247:SER:N	2.88	0.47
1:B:298:PRO:HB3	1:B:322:SER:HB3	1.97	0.47
1:E:45:LEU:HD23	1:E:283:VAL:HG21	1.96	0.47
1:E:138:ASP:OD2	1:E:331:TYR:OH	2.22	0.47
1:A:298:PRO:HB3	1:A:322:SER:HB3	1.97	0.47
1:C:298:PRO:HB3	1:C:322:SER:HB3	1.97	0.47
1:B:56:GLN:HE22	1:C:110:PRO:HG2	1.80	0.46
1:D:45:LEU:HD23	1:D:283:VAL:HG21	1.96	0.46
1:D:246:CYS:SG	1:D:247:SER:N	2.88	0.46
1:G:246:CYS:SG	1:G:247:SER:N	2.88	0.46
1:A:75:ARG:HH11	1:G:74:TRP:HZ3	1.61	0.46
1:G:298:PRO:HB3	1:G:322:SER:HB3	1.97	0.46
1:A:300:ARG:HG3	1:A:333:LEU:HD21	1.98	0.46
1:B:275:LEU:HD22	1:C:108:PHE:CG	2.51	0.46
1:B:300:ARG:HG3	1:B:333:LEU:HD21	1.98	0.46
1:A:214:ILE:O	1:A:218:LEU:N	2.41	0.46
1:F:45:LEU:HD23	1:F:283:VAL:HG21	1.96	0.46
1:A:246:CYS:SG	1:A:247:SER:N	2.88	0.46
1:F:246:CYS:SG	1:F:247:SER:N	2.88	0.46
1:G:45:LEU:HD23	1:G:283:VAL:HG21	1.96	0.46
1:E:246:CYS:SG	1:E:247:SER:N	2.88	0.46
1:G:300:ARG:HG3	1:G:333:LEU:HD21	1.98	0.46
1:D:85:TRP:CZ2	1:D:107:LYS:HG3	2.51	0.46
1:F:298:PRO:HB3	1:F:322:SER:HB3	1.97	0.46
1:E:66:CYS:HA	1:E:265:CYS:HA	1.98	0.45
1:C:85:TRP:CZ2	1:C:107:LYS:HG3	2.52	0.45
1:C:300:ARG:HG3	1:C:333:LEU:HD21	1.98	0.45
1:F:85:TRP:CZ2	1:F:107:LYS:HG3	2.52	0.45
1:A:111:TYR:HD1	1:G:52:LEU:HD22	1.81	0.45
1:B:85:TRP:CZ2	1:B:107:LYS:HG3	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:TRP:CZ2	1:E:107:LYS:HG3	2.51	0.45
1:F:66:CYS:HA	1:F:265:CYS:HA	1.98	0.45
1:F:56:GLN:HB2	1:G:111:TYR:OH	2.16	0.45
1:G:85:TRP:CZ2	1:G:107:LYS:HG3	2.52	0.45
1:D:298:PRO:HB3	1:D:322:SER:HB3	1.97	0.45
1:G:66:CYS:HA	1:G:265:CYS:HA	1.98	0.45
1:E:300:ARG:HG3	1:E:333:LEU:HD21	1.98	0.45
1:A:85:TRP:CZ2	1:A:107:LYS:HG3	2.52	0.45
1:D:66:CYS:HA	1:D:265:CYS:HA	1.98	0.45
1:A:208:ASN:OD1	1:A:209:LEU:N	2.50	0.45
1:D:208:ASN:OD1	1:D:209:LEU:N	2.50	0.45
1:A:75:ARG:HD2	1:A:75:ARG:HA	1.79	0.45
1:A:111:TYR:OH	1:G:56:GLN:HB2	2.17	0.45
1:C:208:ASN:OD1	1:C:209:LEU:N	2.50	0.45
1:G:208:ASN:OD1	1:G:209:LEU:N	2.50	0.44
1:E:208:ASN:OD1	1:E:209:LEU:N	2.50	0.44
1:D:214:ILE:O	1:D:218:LEU:N	2.41	0.44
1:E:85:TRP:HZ3	1:E:267:LEU:HD23	1.82	0.44
1:E:298:PRO:HB3	1:E:322:SER:HB3	1.97	0.44
1:B:208:ASN:OD1	1:B:209:LEU:N	2.50	0.44
1:F:54:PHE:HA	1:F:57:GLU:HG2	1.99	0.44
1:A:110:PRO:HG2	1:G:56:GLN:NE2	2.31	0.44
1:A:268:ILE:HG21	1:B:82:SER:HB3	1.99	0.44
1:D:85:TRP:HZ3	1:D:267:LEU:HD23	1.82	0.44
1:D:300:ARG:HG3	1:D:333:LEU:HD21	1.98	0.44
1:F:275:LEU:HD22	1:G:108:PHE:CG	2.52	0.44
1:G:54:PHE:HA	1:G:57:GLU:HG2	1.99	0.44
1:B:54:PHE:HA	1:B:57:GLU:HG2	1.99	0.44
1:C:66:CYS:HA	1:C:265:CYS:HA	1.98	0.44
1:C:85:TRP:HZ3	1:C:267:LEU:HD23	1.82	0.44
1:F:85:TRP:HZ3	1:F:267:LEU:HD23	1.82	0.44
1:F:208:ASN:OD1	1:F:209:LEU:N	2.50	0.44
1:A:66:CYS:HA	1:A:265:CYS:HA	1.98	0.44
1:A:195:ILE:HB	1:G:16:LEU:HD13	2.00	0.44
1:F:300:ARG:HG3	1:F:333:LEU:HD21	1.98	0.44
1:G:214:ILE:O	1:G:218:LEU:N	2.41	0.44
1:B:123:PRO:HB2	1:B:124:PRO:HD3	1.99	0.44
1:D:54:PHE:HA	1:D:57:GLU:HG2	1.99	0.44
1:G:85:TRP:HZ3	1:G:267:LEU:HD23	1.82	0.44
1:A:16:LEU:HD13	1:B:195:ILE:HB	2.00	0.43
1:C:54:PHE:HA	1:C:57:GLU:HG2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:348:LEU:HD13	1:F:348:LEU:HA	1.90	0.43
1:G:84:CYS:HA	1:G:87:ALA:HB3	2.00	0.43
1:C:123:PRO:HB2	1:C:124:PRO:HD3	2.00	0.43
1:E:54:PHE:HA	1:E:57:GLU:HG2	1.99	0.43
1:G:123:PRO:HB2	1:G:124:PRO:HD3	2.00	0.43
1:B:66:CYS:HA	1:B:265:CYS:HA	1.98	0.43
1:B:79:PHE:HE2	1:B:248:ILE:HG21	1.83	0.43
1:E:84:CYS:HA	1:E:87:ALA:HB3	2.00	0.43
1:F:84:CYS:HA	1:F:87:ALA:HB3	2.00	0.43
1:F:123:PRO:HB2	1:F:124:PRO:HD3	2.00	0.43
1:G:75:ARG:HA	1:G:75:ARG:HD2	1.79	0.43
1:A:54:PHE:HA	1:A:57:GLU:HG2	1.99	0.43
1:A:85:TRP:HZ3	1:A:267:LEU:HD23	1.82	0.43
1:A:348:LEU:HD13	1:A:348:LEU:HA	1.90	0.43
1:C:79:PHE:HE2	1:C:248:ILE:HG21	1.83	0.43
1:D:123:PRO:HB2	1:D:124:PRO:HD3	1.99	0.43
1:E:348:LEU:HD13	1:E:348:LEU:HA	1.90	0.43
1:D:275:LEU:HD22	1:E:108:PHE:CG	2.53	0.43
1:E:79:PHE:HE2	1:E:248:ILE:HG21	1.84	0.43
1:G:79:PHE:HE2	1:G:248:ILE:HG21	1.83	0.43
1:E:123:PRO:HB2	1:E:124:PRO:HD3	2.00	0.43
1:A:84:CYS:HA	1:A:87:ALA:HB3	2.00	0.43
1:C:283:VAL:O	1:C:287:LEU:N	2.51	0.43
1:B:85:TRP:HZ3	1:B:267:LEU:HD23	1.82	0.43
1:D:340:SER:HB2	1:E:137:SER:HB3	2.01	0.43
1:F:79:PHE:HE2	1:F:248:ILE:HG21	1.83	0.43
1:A:123:PRO:HB2	1:A:124:PRO:HD3	2.00	0.42
1:D:84:CYS:HA	1:D:87:ALA:HB3	2.00	0.42
1:E:272:ILE:HG22	1:F:108:PHE:HE1	1.83	0.42
1:B:84:CYS:HA	1:B:87:ALA:HB3	2.00	0.42
1:C:16:LEU:HD13	1:D:195:ILE:HB	2.01	0.42
1:D:79:PHE:HE2	1:D:248:ILE:HG21	1.83	0.42
1:C:350:VAL:HG11	1:D:195:ILE:CD1	2.49	0.42
1:F:16:LEU:HD13	1:G:195:ILE:HB	2.00	0.42
1:B:272:ILE:HG22	1:C:108:PHE:HE1	1.83	0.42
1:C:84:CYS:HA	1:C:87:ALA:HB3	2.00	0.42
1:D:75:ARG:HA	1:D:75:ARG:HD2	1.79	0.42
1:G:25:PHE:CE2	1:G:144:GLU:HG3	2.54	0.42
1:G:347:CYS:O	1:G:350:VAL:HG13	2.20	0.42
1:A:79:PHE:HE2	1:A:248:ILE:HG21	1.83	0.42
1:D:25:PHE:CE2	1:D:144:GLU:HG3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:CYS:O	1:A:350:VAL:HG13	2.20	0.42
1:E:115:LEU:HG	2:E:502:LBN:O4	2.20	0.42
1:E:347:CYS:O	1:E:350:VAL:HG13	2.20	0.42
1:F:214:ILE:O	1:F:218:LEU:N	2.41	0.42
1:F:347:CYS:O	1:F:350:VAL:HG13	2.20	0.42
1:B:214:ILE:O	1:B:218:LEU:N	2.41	0.42
1:B:347:CYS:O	1:B:350:VAL:HG13	2.20	0.42
1:C:74:TRP:CE3	1:D:74:TRP:NE1	2.88	0.42
1:C:25:PHE:CE2	1:C:144:GLU:HG3	2.55	0.42
1:E:73:SER:H	1:E:76:GLN:HB2	1.85	0.42
1:E:339:ILE:HD12	1:E:339:ILE:HA	1.96	0.42
1:A:52:LEU:HB3	1:B:111:TYR:CE1	2.55	0.42
1:F:25:PHE:CE2	1:F:144:GLU:HG3	2.55	0.42
1:E:25:PHE:CE2	1:E:144:GLU:HG3	2.54	0.41
1:E:52:LEU:HD21	1:F:114:LEU:HD22	2.01	0.41
1:A:25:PHE:CE2	1:A:144:GLU:HG3	2.55	0.41
1:D:73:SER:H	1:D:76:GLN:HB2	1.85	0.41
1:E:283:VAL:O	1:E:287:LEU:N	2.51	0.41
1:B:283:VAL:O	1:B:287:LEU:N	2.51	0.41
1:A:321:LYS:O	1:A:322:SER:OG	2.39	0.41
1:B:25:PHE:CE2	1:B:144:GLU:HG3	2.54	0.41
1:B:73:SER:H	1:B:76:GLN:HB2	1.85	0.41
1:C:73:SER:H	1:C:76:GLN:HB2	1.85	0.41
1:F:73:SER:H	1:F:76:GLN:HB2	1.85	0.41
1:F:264:GLN:HB2	1:G:252:ILE:HG12	2.03	0.41
1:F:349:LYS:HB3	1:G:202:THR:HG21	2.03	0.41
1:A:73:SER:H	1:A:76:GLN:HB2	1.85	0.41
1:E:264:GLN:HB2	1:F:252:ILE:HG12	2.03	0.41
1:G:283:VAL:O	1:G:287:LEU:N	2.51	0.41
1:C:347:CYS:O	1:C:350:VAL:HG13	2.20	0.41
1:D:347:CYS:O	1:D:350:VAL:HG13	2.20	0.41
1:B:321:LYS:O	1:B:322:SER:OG	2.39	0.41
1:C:122:LEU:HB2	1:C:123:PRO:HD3	2.02	0.41
1:C:214:ILE:O	1:C:218:LEU:N	2.41	0.41
1:E:321:LYS:O	1:E:322:SER:OG	2.39	0.41
1:F:83:TYR:CD1	1:F:248:ILE:HG12	2.56	0.41
1:F:122:LEU:HB2	1:F:123:PRO:HD3	2.02	0.41
1:B:122:LEU:HB2	1:B:123:PRO:HD3	2.02	0.41
1:D:28:LEU:HD23	1:D:28:LEU:HA	1.94	0.41
1:D:113:LEU:HD11	1:D:280:ASN:HD22	1.86	0.41
1:E:83:TYR:CD1	1:E:248:ILE:HG12	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:LEU:HD11	1:F:280:ASN:HD22	1.86	0.41
1:G:83:TYR:CD1	1:G:248:ILE:HG12	2.56	0.41
1:G:122:LEU:HB2	1:G:123:PRO:HD3	2.02	0.41
1:F:345:TYR:CZ	1:F:349:LYS:HD3	2.56	0.40
1:G:73:SER:H	1:G:76:GLN:HB2	1.85	0.40
1:A:83:TYR:CD1	1:A:248:ILE:HG12	2.56	0.40
1:A:345:TYR:CZ	1:A:349:LYS:HD3	2.56	0.40
1:B:345:TYR:CZ	1:B:349:LYS:HD3	2.56	0.40
1:C:56:GLN:HE22	1:D:110:PRO:HG2	1.87	0.40
1:C:101:LEU:N	1:C:102:PRO:HD2	2.37	0.40
1:D:339:ILE:HD12	1:D:339:ILE:HA	1.96	0.40
1:D:345:TYR:CZ	1:D:349:LYS:HD3	2.56	0.40
1:E:122:LEU:HB2	1:E:123:PRO:HD3	2.02	0.40
1:F:283:VAL:O	1:F:287:LEU:N	2.51	0.40
1:G:321:LYS:O	1:G:322:SER:OG	2.39	0.40
1:A:275:LEU:HD22	1:B:108:PHE:CG	2.56	0.40
1:B:83:TYR:CD1	1:B:248:ILE:HG12	2.56	0.40
1:D:122:LEU:HB2	1:D:123:PRO:HD3	2.02	0.40
1:F:56:GLN:HE22	1:G:110:PRO:HG2	1.87	0.40
1:F:271:GLY:HA3	1:G:89:GLN:HG3	2.03	0.40
1:A:283:VAL:O	1:A:287:LEU:N	2.51	0.40
1:C:81:ASP:OD2	1:D:75:ARG:CZ	2.69	0.40
1:C:83:TYR:CD1	1:C:248:ILE:HG12	2.56	0.40
1:D:101:LEU:N	1:D:102:PRO:HD2	2.37	0.40
1:A:88:VAL:HG13	1:A:103:LEU:HB3	2.03	0.40
1:B:74:TRP:HZ3	1:C:75:ARG:HD3	1.86	0.40
1:B:101:LEU:N	1:B:102:PRO:HD2	2.37	0.40
1:C:345:TYR:CZ	1:C:349:LYS:HD3	2.56	0.40
1:D:283:VAL:O	1:D:287:LEU:N	2.51	0.40
1:E:101:LEU:N	1:E:102:PRO:HD2	2.37	0.40
1:G:113:LEU:HD11	1:G:280:ASN:HD22	1.86	0.40
1:G:120:LEU:HD21	1:G:224:ILE:HG13	2.03	0.40
1:G:345:TYR:CZ	1:G:349:LYS:HD3	2.56	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 PDB entries followed by that with respect to all EM entries.

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	301/426 (71%)	287 (95%)	14 (5%)	0	100	100
1	B	301/426 (71%)	287 (95%)	14 (5%)	0	100	100
1	C	301/426 (71%)	287 (95%)	14 (5%)	0	100	100
1	D	301/426 (71%)	287 (95%)	14 (5%)	0	100	100
1	E	301/426 (71%)	287 (95%)	14 (5%)	0	100	100
1	F	301/426 (71%)	287 (95%)	14 (5%)	0	100	100
1	G	301/426 (71%)	287 (95%)	14 (5%)	0	100	100
All	All	2107/2982 (71%)	2009 (95%)	98 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	275/381 (72%)	272 (99%)	3 (1%)	70	81
1	B	275/381 (72%)	272 (99%)	3 (1%)	70	81
1	C	275/381 (72%)	272 (99%)	3 (1%)	70	81
1	D	275/381 (72%)	272 (99%)	3 (1%)	70	81
1	E	275/381 (72%)	272 (99%)	3 (1%)	70	81
1	F	275/381 (72%)	271 (98%)	4 (2%)	60	76
1	G	275/381 (72%)	272 (99%)	3 (1%)	70	81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1925/2667 (72%)	1903 (99%)	22 (1%)	69 81

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	209	LEU
1	A	350	VAL
1	B	16	LEU
1	B	209	LEU
1	B	350	VAL
1	C	16	LEU
1	C	209	LEU
1	C	350	VAL
1	D	16	LEU
1	D	209	LEU
1	D	350	VAL
1	E	16	LEU
1	E	209	LEU
1	E	350	VAL
1	F	16	LEU
1	F	209	LEU
1	F	342	VAL
1	F	350	VAL
1	G	16	LEU
1	G	209	LEU
1	G	350	VAL

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

Mol	Chain	Res	Type
1	A	56	GLN
1	A	92	ASN
1	A	95	GLN
1	A	100	ASN
1	A	280	ASN
1	A	353	ASN
1	B	56	GLN
1	B	92	ASN
1	B	95	GLN
1	B	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	280	ASN
1	B	353	ASN
1	C	56	GLN
1	C	92	ASN
1	C	100	ASN
1	C	280	ASN
1	C	353	ASN
1	D	92	ASN
1	D	95	GLN
1	D	100	ASN
1	D	280	ASN
1	D	353	ASN
1	E	92	ASN
1	E	95	GLN
1	E	100	ASN
1	E	280	ASN
1	E	353	ASN
1	F	56	GLN
1	F	92	ASN
1	F	95	GLN
1	F	100	ASN
1	F	280	ASN
1	F	353	ASN
1	G	56	GLN
1	G	90	GLN
1	G	92	ASN
1	G	95	GLN
1	G	100	ASN
1	G	280	ASN
1	G	353	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

49 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	LBN	E	507	-	11,11,51	1.49	1 (9%)	10,10,59	0.60	0
2	LBN	D	505	-	11,11,51	1.49	1 (9%)	10,10,59	0.60	0
2	LBN	E	509	-	15,15,51	1.01	1 (6%)	15,15,59	0.80	1 (6%)
2	LBN	E	504	-	10,10,51	0.69	0	9,9,59	0.19	0
2	LBN	C	505	-	11,11,51	1.49	1 (9%)	10,10,59	0.60	0
2	LBN	F	502	-	34,34,51	1.55	4 (11%)	40,42,59	1.23	6 (15%)
2	LBN	F	505	-	11,11,51	1.49	1 (9%)	10,10,59	0.60	0
2	LBN	E	508	-	10,10,51	0.69	0	9,9,59	0.18	0
2	LBN	E	501	-	27,27,51	1.68	4 (14%)	32,34,59	1.14	3 (9%)
2	LBN	E	502	-	39,39,51	1.47	4 (10%)	45,47,59	1.19	6 (13%)
2	LBN	A	503	-	11,11,51	1.49	1 (9%)	10,10,59	0.60	0
2	LBN	C	504	-	27,27,51	1.68	4 (14%)	32,34,59	1.14	3 (9%)
2	LBN	E	505	-	36,36,51	1.49	4 (11%)	42,44,59	1.20	6 (14%)
2	LBN	B	501	-	39,39,51	1.47	4 (10%)	45,47,59	1.18	6 (13%)
2	LBN	F	507	-	15,15,51	1.02	1 (6%)	15,15,59	0.79	1 (6%)
2	LBN	A	505	-	15,15,51	1.02	1 (6%)	15,15,59	0.79	1 (6%)
2	LBN	E	503	-	34,34,51	1.55	4 (11%)	40,42,59	1.23	6 (15%)
2	LBN	D	503	-	10,10,51	0.69	0	9,9,59	0.19	0
2	LBN	G	501	-	39,39,51	1.47	4 (10%)	45,47,59	1.19	6 (13%)
2	LBN	F	501	-	39,39,51	1.47	4 (10%)	45,47,59	1.19	6 (13%)
2	LBN	A	501	-	36,36,51	1.49	4 (11%)	42,44,59	1.20	6 (14%)
2	LBN	C	506	-	15,15,51	1.02	1 (6%)	15,15,59	0.79	1 (6%)
2	LBN	F	506	-	10,10,51	0.69	0	9,9,59	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LBN	B	504	-	27,27,51	1.68	4 (14%)	32,34,59	1.14	3 (9%)
2	LBN	G	504	-	27,27,51	1.68	4 (14%)	32,34,59	1.14	3 (9%)
2	LBN	G	508	-	15,15,51	1.02	1 (6%)	15,15,59	0.80	1 (6%)
2	LBN	G	505	-	39,39,51	1.47	4 (10%)	45,47,59	1.19	6 (13%)
2	LBN	D	504	-	36,36,51	1.49	4 (11%)	42,44,59	1.20	6 (14%)
2	LBN	C	501	-	39,39,51	1.47	4 (10%)	45,47,59	1.18	6 (13%)
2	LBN	B	506	-	10,10,51	0.69	0	9,9,59	0.19	0
2	LBN	B	507	-	15,15,51	1.02	1 (6%)	15,15,59	0.79	1 (6%)
2	LBN	C	502	-	34,34,51	1.55	4 (11%)	40,42,59	1.23	6 (15%)
2	LBN	F	503	-	36,36,51	1.49	4 (11%)	42,44,59	1.20	6 (14%)
2	LBN	D	506	-	15,15,51	1.01	1 (6%)	15,15,59	0.80	1 (6%)
2	LBN	G	506	-	11,11,51	1.49	1 (9%)	10,10,59	0.60	0
2	LBN	G	502	-	34,34,51	1.55	4 (11%)	40,42,59	1.23	6 (15%)
2	LBN	G	507	-	10,10,51	0.69	0	9,9,59	0.19	0
2	LBN	B	502	-	34,34,51	1.55	4 (11%)	40,42,59	1.23	6 (15%)
2	LBN	B	505	-	11,11,51	1.49	1 (9%)	10,10,59	0.60	0
2	LBN	C	503	-	36,36,51	1.49	4 (11%)	42,44,59	1.20	6 (14%)
2	LBN	F	504	-	27,27,51	1.68	4 (14%)	32,34,59	1.14	3 (9%)
2	LBN	D	502	-	34,34,51	1.55	4 (11%)	40,42,59	1.23	6 (15%)
2	LBN	A	506	-	34,34,51	1.55	4 (11%)	40,42,59	1.23	6 (15%)
2	LBN	B	503	-	36,36,51	1.49	4 (11%)	42,44,59	1.20	6 (14%)
2	LBN	G	503	-	36,36,51	1.48	4 (11%)	42,44,59	1.20	6 (14%)
2	LBN	A	504	-	10,10,51	0.69	0	9,9,59	0.18	0
2	LBN	D	501	-	39,39,51	1.47	4 (10%)	45,47,59	1.19	6 (13%)
2	LBN	A	502	-	27,27,51	1.68	4 (14%)	32,34,59	1.14	3 (9%)
2	LBN	E	506	-	27,27,51	1.68	4 (14%)	32,34,59	1.14	3 (9%)

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	LBN	E	507	-	-	2/9/9/55	-
2	LBN	D	505	-	-	2/9/9/55	-
2	LBN	E	509	-	-	5/13/13/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LBN	E	504	-	-	5/8/8/55	-
2	LBN	C	505	-	-	2/9/9/55	-
2	LBN	F	502	-	-	15/38/38/55	-
2	LBN	F	505	-	-	2/9/9/55	-
2	LBN	E	508	-	-	5/8/8/55	-
2	LBN	E	501	-	-	18/30/30/55	-
2	LBN	E	502	-	-	22/43/43/55	-
2	LBN	A	503	-	-	2/9/9/55	-
2	LBN	C	504	-	-	18/30/30/55	-
2	LBN	E	505	-	-	15/40/40/55	-
2	LBN	B	501	-	-	22/43/43/55	-
2	LBN	F	507	-	-	5/13/13/55	-
2	LBN	A	505	-	-	5/13/13/55	-
2	LBN	E	503	-	-	15/38/38/55	-
2	LBN	D	503	-	-	5/8/8/55	-
2	LBN	G	501	-	-	22/43/43/55	-
2	LBN	F	501	-	-	22/43/43/55	-
2	LBN	A	501	-	-	15/40/40/55	-
2	LBN	C	506	-	-	5/13/13/55	-
2	LBN	F	506	-	-	5/8/8/55	-
2	LBN	B	504	-	-	18/30/30/55	-
2	LBN	G	504	-	-	18/30/30/55	-
2	LBN	G	508	-	-	5/13/13/55	-
2	LBN	G	505	-	-	22/43/43/55	-
2	LBN	D	504	-	-	15/40/40/55	-
2	LBN	C	501	-	-	22/43/43/55	-
2	LBN	B	506	-	-	5/8/8/55	-
2	LBN	B	507	-	-	5/13/13/55	-
2	LBN	C	502	-	-	15/38/38/55	-
2	LBN	F	503	-	-	15/40/40/55	-
2	LBN	D	506	-	-	5/13/13/55	-
2	LBN	G	506	-	-	2/9/9/55	-
2	LBN	G	502	-	-	15/38/38/55	-
2	LBN	G	507	-	-	5/8/8/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LBN	B	502	-	-	15/38/38/55	-
2	LBN	B	505	-	-	2/9/9/55	-
2	LBN	C	503	-	-	15/40/40/55	-
2	LBN	F	504	-	-	18/30/30/55	-
2	LBN	D	502	-	-	15/38/38/55	-
2	LBN	A	506	-	-	15/38/38/55	-
2	LBN	B	503	-	-	15/40/40/55	-
2	LBN	G	503	-	-	15/40/40/55	-
2	LBN	A	504	-	-	5/8/8/55	-
2	LBN	D	501	-	-	22/43/43/55	-
2	LBN	A	502	-	-	18/30/30/55	-
2	LBN	E	506	-	-	18/30/30/55	-

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	503	LBN	P1-O2	4.85	1.78	1.59
2	G	502	LBN	P1-O2	4.85	1.78	1.59
2	E	501	LBN	P1-O2	4.84	1.78	1.59
2	C	502	LBN	P1-O2	4.83	1.78	1.59
2	D	502	LBN	P1-O2	4.83	1.78	1.59
2	C	504	LBN	P1-O2	4.83	1.78	1.59
2	B	502	LBN	P1-O2	4.83	1.78	1.59
2	F	502	LBN	P1-O2	4.83	1.78	1.59
2	A	502	LBN	P1-O2	4.82	1.78	1.59
2	A	506	LBN	P1-O2	4.82	1.78	1.59
2	E	506	LBN	P1-O2	4.82	1.78	1.59
2	G	504	LBN	P1-O2	4.82	1.78	1.59
2	B	504	LBN	P1-O2	4.82	1.78	1.59
2	F	504	LBN	P1-O2	4.81	1.78	1.59
2	D	504	LBN	P1-O2	4.78	1.78	1.59
2	F	503	LBN	P1-O2	4.77	1.78	1.59
2	G	501	LBN	P1-O2	4.76	1.78	1.59
2	E	502	LBN	P1-O2	4.76	1.78	1.59
2	A	501	LBN	P1-O2	4.76	1.78	1.59
2	C	503	LBN	P1-O2	4.76	1.78	1.59
2	B	503	LBN	P1-O2	4.76	1.78	1.59
2	G	503	LBN	P1-O2	4.75	1.78	1.59
2	C	501	LBN	P1-O2	4.75	1.78	1.59
2	F	501	LBN	P1-O2	4.75	1.78	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	505	LBN	P1-O2	4.75	1.78	1.59
2	G	505	LBN	P1-O2	4.74	1.78	1.59
2	B	501	LBN	P1-O2	4.74	1.78	1.59
2	D	501	LBN	P1-O2	4.73	1.78	1.59
2	E	507	LBN	C42-C5	4.23	1.56	1.31
2	D	505	LBN	C42-C5	4.21	1.56	1.31
2	G	506	LBN	C42-C5	4.21	1.56	1.31
2	F	505	LBN	C42-C5	4.21	1.56	1.31
2	A	503	LBN	C42-C5	4.21	1.56	1.31
2	C	505	LBN	C42-C5	4.21	1.56	1.31
2	B	505	LBN	C42-C5	4.20	1.56	1.31
2	B	504	LBN	C3-C2	3.76	1.60	1.51
2	A	502	LBN	C3-C2	3.74	1.60	1.51
2	E	501	LBN	C3-C2	3.73	1.60	1.51
2	G	504	LBN	C3-C2	3.73	1.60	1.51
2	F	504	LBN	C3-C2	3.72	1.60	1.51
2	C	504	LBN	C3-C2	3.72	1.60	1.51
2	E	506	LBN	C3-C2	3.71	1.60	1.51
2	F	502	LBN	C3-C2	3.19	1.60	1.50
2	C	502	LBN	C3-C2	3.15	1.60	1.50
2	D	502	LBN	C3-C2	3.15	1.60	1.50
2	E	503	LBN	C3-C2	3.14	1.60	1.50
2	G	502	LBN	C3-C2	3.14	1.60	1.50
2	B	502	LBN	C3-C2	3.14	1.60	1.50
2	A	506	LBN	C3-C2	3.14	1.60	1.50
2	D	504	LBN	C3-C2	3.12	1.60	1.50
2	F	503	LBN	C3-C2	3.11	1.60	1.50
2	B	501	LBN	C3-C2	3.10	1.60	1.50
2	E	505	LBN	C3-C2	3.10	1.60	1.50
2	C	503	LBN	C3-C2	3.10	1.60	1.50
2	E	502	LBN	C3-C2	3.10	1.60	1.50
2	A	501	LBN	C3-C2	3.10	1.60	1.50
2	G	505	LBN	C3-C2	3.09	1.60	1.50
2	B	503	LBN	C3-C2	3.09	1.60	1.50
2	C	501	LBN	C3-C2	3.09	1.60	1.50
2	G	501	LBN	C3-C2	3.08	1.60	1.50
2	F	501	LBN	C3-C2	3.08	1.60	1.50
2	G	503	LBN	C3-C2	3.07	1.60	1.50
2	D	501	LBN	C3-C2	3.06	1.60	1.50
2	B	501	LBN	P1-O1	3.03	1.71	1.59
2	D	501	LBN	P1-O1	3.02	1.71	1.59
2	G	501	LBN	P1-O1	3.02	1.71	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	LBN	P1-O1	3.02	1.71	1.59
2	E	502	LBN	P1-O1	3.02	1.71	1.59
2	F	501	LBN	P1-O1	3.02	1.71	1.59
2	G	505	LBN	P1-O1	3.01	1.71	1.59
2	G	504	LBN	P1-O1	2.99	1.71	1.59
2	D	502	LBN	P1-O1	2.99	1.71	1.59
2	F	502	LBN	P1-O1	2.99	1.71	1.59
2	E	506	LBN	P1-O1	2.99	1.71	1.59
2	C	502	LBN	P1-O1	2.98	1.71	1.59
2	G	502	LBN	P1-O1	2.98	1.71	1.59
2	E	501	LBN	P1-O1	2.98	1.71	1.59
2	B	504	LBN	P1-O1	2.98	1.71	1.59
2	A	506	LBN	P1-O1	2.98	1.71	1.59
2	C	504	LBN	P1-O1	2.98	1.71	1.59
2	A	502	LBN	P1-O1	2.97	1.71	1.59
2	F	504	LBN	P1-O1	2.97	1.71	1.59
2	B	502	LBN	P1-O1	2.97	1.71	1.59
2	E	503	LBN	P1-O1	2.97	1.71	1.59
2	G	503	LBN	P1-O1	2.96	1.71	1.59
2	C	503	LBN	P1-O1	2.96	1.71	1.59
2	F	503	LBN	P1-O1	2.96	1.71	1.59
2	A	501	LBN	P1-O1	2.95	1.71	1.59
2	D	504	LBN	P1-O1	2.95	1.71	1.59
2	B	503	LBN	P1-O1	2.95	1.71	1.59
2	E	505	LBN	P1-O1	2.94	1.71	1.59
2	E	502	LBN	O2-C9	-2.18	1.35	1.44
2	F	501	LBN	O2-C9	-2.18	1.35	1.44
2	G	505	LBN	O2-C9	-2.18	1.35	1.44
2	C	501	LBN	O2-C9	-2.17	1.35	1.44
2	A	501	LBN	O2-C9	-2.17	1.35	1.44
2	F	503	LBN	O2-C9	-2.17	1.35	1.44
2	E	501	LBN	O2-C9	-2.17	1.35	1.44
2	G	501	LBN	O2-C9	-2.17	1.35	1.44
2	G	503	LBN	O2-C9	-2.17	1.35	1.44
2	D	501	LBN	O2-C9	-2.17	1.35	1.44
2	B	501	LBN	O2-C9	-2.16	1.35	1.44
2	C	503	LBN	O2-C9	-2.16	1.35	1.44
2	E	505	LBN	O2-C9	-2.16	1.35	1.44
2	E	506	LBN	O2-C9	-2.16	1.35	1.44
2	F	504	LBN	O2-C9	-2.16	1.35	1.44
2	D	504	LBN	O2-C9	-2.15	1.35	1.44
2	B	504	LBN	O2-C9	-2.15	1.35	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	LBN	O2-C9	-2.15	1.35	1.44
2	B	503	LBN	O2-C9	-2.15	1.35	1.44
2	C	504	LBN	O2-C9	-2.14	1.36	1.44
2	G	504	LBN	O2-C9	-2.14	1.36	1.44
2	A	506	LBN	O2-C9	-2.14	1.36	1.44
2	D	502	LBN	O2-C9	-2.13	1.36	1.44
2	C	502	LBN	O2-C9	-2.13	1.36	1.44
2	C	506	LBN	O5-C25	2.13	1.37	1.30
2	E	503	LBN	O2-C9	-2.12	1.36	1.44
2	F	502	LBN	O2-C9	-2.12	1.36	1.44
2	G	502	LBN	O2-C9	-2.12	1.36	1.44
2	B	502	LBN	O2-C9	-2.12	1.36	1.44
2	D	506	LBN	O5-C25	2.12	1.37	1.30
2	A	505	LBN	O5-C25	2.12	1.37	1.30
2	B	507	LBN	O5-C25	2.11	1.37	1.30
2	F	507	LBN	O5-C25	2.11	1.37	1.30
2	G	508	LBN	O5-C25	2.10	1.37	1.30
2	E	509	LBN	O5-C25	2.10	1.37	1.30

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	LBN	O7-C34-C35	3.67	119.41	111.50
2	F	502	LBN	O7-C34-C35	3.67	119.41	111.50
2	B	502	LBN	O7-C34-C35	3.66	119.40	111.50
2	D	501	LBN	O7-C34-C35	3.66	119.39	111.50
2	E	503	LBN	O7-C34-C35	3.66	119.39	111.50
2	G	501	LBN	O7-C34-C35	3.66	119.38	111.50
2	B	501	LBN	O7-C34-C35	3.65	119.38	111.50
2	C	502	LBN	O7-C34-C35	3.65	119.38	111.50
2	E	502	LBN	O7-C34-C35	3.65	119.37	111.50
2	G	505	LBN	O7-C34-C35	3.65	119.36	111.50
2	D	502	LBN	O7-C34-C35	3.64	119.35	111.50
2	G	502	LBN	O7-C34-C35	3.63	119.31	111.50
2	C	501	LBN	O7-C34-C35	3.62	119.31	111.50
2	A	506	LBN	O7-C34-C35	3.62	119.31	111.50
2	G	503	LBN	O7-C34-C35	3.59	119.23	111.50
2	D	504	LBN	O7-C34-C35	3.58	119.22	111.50
2	E	505	LBN	O7-C34-C35	3.58	119.21	111.50
2	F	503	LBN	O7-C34-C35	3.57	119.20	111.50
2	C	503	LBN	O7-C34-C35	3.57	119.20	111.50
2	B	503	LBN	O7-C34-C35	3.57	119.19	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	LBN	O7-C34-C35	3.55	119.16	111.50
2	A	502	LBN	O7-C34-C35	3.54	119.14	111.50
2	E	506	LBN	O7-C34-C35	3.54	119.13	111.50
2	G	504	LBN	O7-C34-C35	3.54	119.12	111.50
2	E	501	LBN	O7-C34-C35	3.54	119.12	111.50
2	B	504	LBN	O7-C34-C35	3.54	119.12	111.50
2	F	504	LBN	O7-C34-C35	3.53	119.10	111.50
2	C	504	LBN	O7-C34-C35	3.52	119.10	111.50
2	G	501	LBN	O5-C3-C2	2.93	116.96	108.43
2	G	505	LBN	O5-C3-C2	2.92	116.95	108.43
2	F	501	LBN	O5-C3-C2	2.92	116.94	108.43
2	E	502	LBN	O5-C3-C2	2.92	116.93	108.43
2	D	501	LBN	O5-C3-C2	2.91	116.90	108.43
2	B	501	LBN	O5-C3-C2	2.90	116.89	108.43
2	C	501	LBN	O5-C3-C2	2.90	116.88	108.43
2	E	502	LBN	O5-C25-C26	2.85	120.86	111.91
2	G	501	LBN	O5-C25-C26	2.85	120.85	111.91
2	F	501	LBN	O5-C25-C26	2.85	120.84	111.91
2	G	505	LBN	O5-C25-C26	2.84	120.83	111.91
2	C	501	LBN	O5-C25-C26	2.84	120.83	111.91
2	A	506	LBN	O5-C3-C2	2.83	116.68	108.43
2	B	501	LBN	O5-C25-C26	2.83	120.79	111.91
2	D	501	LBN	O5-C25-C26	2.83	120.79	111.91
2	G	502	LBN	O5-C3-C2	2.82	116.65	108.43
2	D	502	LBN	O5-C3-C2	2.82	116.64	108.43
2	C	502	LBN	O5-C3-C2	2.82	116.63	108.43
2	F	502	LBN	O5-C3-C2	2.82	116.63	108.43
2	B	502	LBN	O5-C3-C2	2.81	116.62	108.43
2	E	503	LBN	O5-C3-C2	2.80	116.60	108.43
2	C	503	LBN	O5-C25-C26	2.76	120.58	111.91
2	G	503	LBN	O5-C25-C26	2.76	120.57	111.91
2	B	503	LBN	O5-C25-C26	2.75	120.54	111.91
2	F	503	LBN	O5-C25-C26	2.75	120.54	111.91
2	A	501	LBN	O5-C25-C26	2.74	120.52	111.91
2	D	504	LBN	O5-C25-C26	2.74	120.52	111.91
2	E	505	LBN	O5-C25-C26	2.74	120.52	111.91
2	B	502	LBN	O5-C25-C26	2.73	120.46	111.91
2	F	502	LBN	O5-C25-C26	2.72	120.45	111.91
2	G	502	LBN	O5-C25-C26	2.72	120.45	111.91
2	G	503	LBN	O5-C3-C2	2.72	116.35	108.43
2	D	504	LBN	O5-C3-C2	2.72	116.35	108.43
2	E	505	LBN	O5-C3-C2	2.72	116.35	108.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	LBN	O5-C25-C26	2.72	120.43	111.91
2	C	503	LBN	O5-C3-C2	2.71	116.33	108.43
2	C	502	LBN	O5-C25-C26	2.71	120.42	111.91
2	A	506	LBN	O5-C25-C26	2.71	120.42	111.91
2	E	503	LBN	O5-C25-C26	2.71	120.41	111.91
2	B	503	LBN	O5-C3-C2	2.71	116.31	108.43
2	A	501	LBN	O5-C3-C2	2.70	116.31	108.43
2	F	503	LBN	O5-C3-C2	2.70	116.31	108.43
2	D	501	LBN	O7-C34-O8	-2.42	117.86	123.70
2	G	501	LBN	O7-C34-O8	-2.41	117.88	123.70
2	F	501	LBN	O7-C34-O8	-2.41	117.88	123.70
2	F	503	LBN	O7-C34-O8	-2.41	117.88	123.70
2	G	505	LBN	O7-C34-O8	-2.40	117.89	123.70
2	G	503	LBN	O7-C34-O8	-2.40	117.91	123.70
2	B	503	LBN	O7-C34-O8	-2.39	117.92	123.70
2	C	503	LBN	O7-C34-O8	-2.39	117.92	123.70
2	E	502	LBN	O7-C34-O8	-2.39	117.92	123.70
2	B	501	LBN	O7-C34-O8	-2.39	117.92	123.70
2	C	502	LBN	O7-C34-O8	-2.39	117.92	123.70
2	E	503	LBN	O7-C34-O8	-2.39	117.93	123.70
2	D	504	LBN	O7-C34-O8	-2.39	117.93	123.70
2	E	505	LBN	O7-C34-O8	-2.39	117.93	123.70
2	C	501	LBN	O7-C34-O8	-2.39	117.93	123.70
2	F	502	LBN	O7-C34-O8	-2.39	117.94	123.70
2	B	502	LBN	O7-C34-O8	-2.38	117.95	123.70
2	A	501	LBN	O7-C34-O8	-2.38	117.95	123.70
2	D	502	LBN	O7-C34-O8	-2.37	117.98	123.70
2	A	506	LBN	O7-C34-O8	-2.36	117.99	123.70
2	G	502	LBN	O7-C34-O8	-2.36	118.01	123.70
2	G	504	LBN	O7-C34-O8	-2.35	118.03	123.70
2	A	502	LBN	O7-C34-O8	-2.34	118.04	123.70
2	E	506	LBN	O7-C34-O8	-2.34	118.04	123.70
2	B	504	LBN	O7-C34-O8	-2.33	118.06	123.70
2	F	504	LBN	O7-C34-O8	-2.33	118.08	123.70
2	C	504	LBN	O7-C34-O8	-2.32	118.09	123.70
2	E	501	LBN	O7-C34-O8	-2.31	118.11	123.70
2	G	503	LBN	O5-C25-O6	-2.19	118.07	123.59
2	G	505	LBN	O5-C25-O6	-2.19	118.07	123.59
2	E	502	LBN	O5-C25-O6	-2.19	118.08	123.59
2	F	501	LBN	O5-C25-O6	-2.18	118.09	123.59
2	C	503	LBN	O5-C25-O6	-2.18	118.10	123.59
2	B	502	LBN	O5-C25-O6	-2.18	118.10	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	LBN	O5-C25-O6	-2.17	118.11	123.59
2	B	503	LBN	O5-C25-O6	-2.17	118.12	123.59
2	E	505	LBN	O5-C25-O6	-2.17	118.12	123.59
2	A	501	LBN	O5-C25-O6	-2.17	118.12	123.59
2	D	504	LBN	O5-C25-O6	-2.16	118.13	123.59
2	F	503	LBN	O5-C25-O6	-2.16	118.13	123.59
2	F	502	LBN	O5-C25-O6	-2.16	118.13	123.59
2	G	502	LBN	O5-C25-O6	-2.16	118.14	123.59
2	A	506	LBN	O5-C25-O6	-2.16	118.14	123.59
2	D	501	LBN	O5-C25-O6	-2.16	118.14	123.59
2	G	501	LBN	O5-C25-O6	-2.16	118.15	123.59
2	B	501	LBN	O5-C25-O6	-2.16	118.15	123.59
2	C	502	LBN	O5-C25-O6	-2.15	118.16	123.59
2	E	503	LBN	O5-C25-O6	-2.14	118.19	123.59
2	D	502	LBN	O5-C25-O6	-2.13	118.20	123.59
2	E	509	LBN	O5-C25-O6	-2.07	118.15	123.30
2	D	504	LBN	O3-P1-O4	2.06	122.43	112.24
2	G	503	LBN	O3-P1-O4	2.06	122.43	112.24
2	A	501	LBN	O3-P1-O4	2.06	122.43	112.24
2	B	503	LBN	O3-P1-O4	2.06	122.42	112.24
2	C	503	LBN	O3-P1-O4	2.06	122.41	112.24
2	E	505	LBN	O3-P1-O4	2.06	122.41	112.24
2	B	507	LBN	O5-C25-O6	-2.05	118.18	123.30
2	F	503	LBN	O3-P1-O4	2.05	122.39	112.24
2	D	506	LBN	O5-C25-O6	-2.05	118.19	123.30
2	D	502	LBN	O3-P1-O4	2.05	122.36	112.24
2	C	502	LBN	O3-P1-O4	2.05	122.35	112.24
2	G	508	LBN	O5-C25-O6	-2.04	118.21	123.30
2	F	502	LBN	O3-P1-O4	2.04	122.33	112.24
2	C	504	LBN	O3-P1-O4	2.04	122.32	112.24
2	B	502	LBN	O3-P1-O4	2.04	122.32	112.24
2	A	505	LBN	O5-C25-O6	-2.04	118.22	123.30
2	C	506	LBN	O5-C25-O6	-2.04	118.22	123.30
2	G	502	LBN	O3-P1-O4	2.04	122.31	112.24
2	A	506	LBN	O3-P1-O4	2.04	122.31	112.24
2	G	504	LBN	O3-P1-O4	2.04	122.31	112.24
2	F	507	LBN	O5-C25-O6	-2.03	118.23	123.30
2	E	501	LBN	O3-P1-O4	2.03	122.30	112.24
2	F	504	LBN	O3-P1-O4	2.03	122.29	112.24
2	E	503	LBN	O3-P1-O4	2.03	122.29	112.24
2	B	504	LBN	O3-P1-O4	2.03	122.28	112.24
2	E	506	LBN	O3-P1-O4	2.03	122.27	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	LBN	O3-P1-O4	2.03	122.27	112.24
2	F	501	LBN	O3-P1-O4	2.02	122.24	112.24
2	G	501	LBN	O3-P1-O4	2.02	122.22	112.24
2	E	502	LBN	O3-P1-O4	2.02	122.22	112.24
2	B	501	LBN	O3-P1-O4	2.02	122.22	112.24
2	D	501	LBN	O3-P1-O4	2.02	122.22	112.24
2	C	501	LBN	O3-P1-O4	2.02	122.21	112.24
2	G	505	LBN	O3-P1-O4	2.01	122.19	112.24

There are no chirality outliers.

All (574) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LBN	C1-O1-P1-O4
2	A	501	LBN	N1-C6-C9-O2
2	A	501	LBN	C35-C34-O7-C2
2	A	502	LBN	C1-O1-P1-O3
2	A	502	LBN	C1-C2-C3-O5
2	A	502	LBN	O7-C2-C3-O5
2	A	502	LBN	N1-C6-C9-O2
2	A	502	LBN	C35-C34-O7-C2
2	A	502	LBN	O8-C34-O7-C2
2	A	506	LBN	N1-C6-C9-O2
2	B	501	LBN	C1-O1-P1-O3
2	B	502	LBN	N1-C6-C9-O2
2	B	503	LBN	C1-O1-P1-O4
2	B	503	LBN	N1-C6-C9-O2
2	B	503	LBN	C35-C34-O7-C2
2	B	504	LBN	C1-O1-P1-O3
2	B	504	LBN	C1-C2-C3-O5
2	B	504	LBN	O7-C2-C3-O5
2	B	504	LBN	N1-C6-C9-O2
2	B	504	LBN	C35-C34-O7-C2
2	B	504	LBN	O8-C34-O7-C2
2	C	501	LBN	C1-O1-P1-O3
2	C	502	LBN	N1-C6-C9-O2
2	C	503	LBN	C1-O1-P1-O4
2	C	503	LBN	N1-C6-C9-O2
2	C	503	LBN	C35-C34-O7-C2
2	C	504	LBN	C1-O1-P1-O3
2	C	504	LBN	C1-C2-C3-O5
2	C	504	LBN	O7-C2-C3-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	504	LBN	N1-C6-C9-O2
2	C	504	LBN	C35-C34-O7-C2
2	C	504	LBN	O8-C34-O7-C2
2	D	501	LBN	C1-O1-P1-O3
2	D	502	LBN	N1-C6-C9-O2
2	D	504	LBN	C1-O1-P1-O4
2	D	504	LBN	N1-C6-C9-O2
2	D	504	LBN	C35-C34-O7-C2
2	E	501	LBN	C1-O1-P1-O3
2	E	501	LBN	C1-C2-C3-O5
2	E	501	LBN	O7-C2-C3-O5
2	E	501	LBN	N1-C6-C9-O2
2	E	501	LBN	C35-C34-O7-C2
2	E	501	LBN	O8-C34-O7-C2
2	E	502	LBN	C1-O1-P1-O3
2	E	503	LBN	N1-C6-C9-O2
2	E	505	LBN	C1-O1-P1-O4
2	E	505	LBN	N1-C6-C9-O2
2	E	505	LBN	C35-C34-O7-C2
2	E	506	LBN	C1-O1-P1-O3
2	E	506	LBN	C1-C2-C3-O5
2	E	506	LBN	O7-C2-C3-O5
2	E	506	LBN	N1-C6-C9-O2
2	E	506	LBN	C35-C34-O7-C2
2	E	506	LBN	O8-C34-O7-C2
2	F	501	LBN	C1-O1-P1-O3
2	F	502	LBN	N1-C6-C9-O2
2	F	503	LBN	C1-O1-P1-O4
2	F	503	LBN	N1-C6-C9-O2
2	F	503	LBN	C35-C34-O7-C2
2	F	504	LBN	C1-O1-P1-O3
2	F	504	LBN	C1-C2-C3-O5
2	F	504	LBN	O7-C2-C3-O5
2	F	504	LBN	N1-C6-C9-O2
2	F	504	LBN	C35-C34-O7-C2
2	F	504	LBN	O8-C34-O7-C2
2	G	501	LBN	C1-O1-P1-O3
2	G	502	LBN	N1-C6-C9-O2
2	G	503	LBN	C1-O1-P1-O4
2	G	503	LBN	N1-C6-C9-O2
2	G	503	LBN	C35-C34-O7-C2
2	G	504	LBN	C1-O1-P1-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	504	LBN	C1-C2-C3-O5
2	G	504	LBN	O7-C2-C3-O5
2	G	504	LBN	N1-C6-C9-O2
2	G	504	LBN	C35-C34-O7-C2
2	G	504	LBN	O8-C34-O7-C2
2	G	505	LBN	C1-O1-P1-O3
2	A	501	LBN	O8-C34-O7-C2
2	B	503	LBN	O8-C34-O7-C2
2	C	503	LBN	O8-C34-O7-C2
2	D	504	LBN	O8-C34-O7-C2
2	E	505	LBN	O8-C34-O7-C2
2	F	503	LBN	O8-C34-O7-C2
2	G	503	LBN	O8-C34-O7-C2
2	A	506	LBN	C35-C34-O7-C2
2	B	502	LBN	C35-C34-O7-C2
2	C	502	LBN	C35-C34-O7-C2
2	D	502	LBN	C35-C34-O7-C2
2	E	503	LBN	C35-C34-O7-C2
2	F	502	LBN	C35-C34-O7-C2
2	G	502	LBN	C35-C34-O7-C2
2	B	501	LBN	C36-C37-C38-C39
2	C	501	LBN	C36-C37-C38-C39
2	D	501	LBN	C36-C37-C38-C39
2	E	502	LBN	C36-C37-C38-C39
2	F	501	LBN	C36-C37-C38-C39
2	G	501	LBN	C36-C37-C38-C39
2	G	505	LBN	C36-C37-C38-C39
2	A	501	LBN	C26-C25-O5-C3
2	B	503	LBN	C26-C25-O5-C3
2	C	503	LBN	C26-C25-O5-C3
2	D	504	LBN	C26-C25-O5-C3
2	E	505	LBN	C26-C25-O5-C3
2	F	503	LBN	C26-C25-O5-C3
2	G	503	LBN	C26-C25-O5-C3
2	B	501	LBN	C26-C27-C28-C29
2	C	501	LBN	C26-C27-C28-C29
2	D	501	LBN	C26-C27-C28-C29
2	E	502	LBN	C26-C27-C28-C29
2	F	501	LBN	C26-C27-C28-C29
2	G	501	LBN	C26-C27-C28-C29
2	G	505	LBN	C26-C27-C28-C29
2	A	501	LBN	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	503	LBN	C26-C27-C28-C29
2	C	503	LBN	C26-C27-C28-C29
2	D	504	LBN	C26-C27-C28-C29
2	E	505	LBN	C26-C27-C28-C29
2	F	503	LBN	C26-C27-C28-C29
2	G	503	LBN	C26-C27-C28-C29
2	A	506	LBN	O8-C34-O7-C2
2	B	502	LBN	O8-C34-O7-C2
2	C	502	LBN	O8-C34-O7-C2
2	D	502	LBN	O8-C34-O7-C2
2	E	503	LBN	O8-C34-O7-C2
2	F	502	LBN	O8-C34-O7-C2
2	G	502	LBN	O8-C34-O7-C2
2	A	501	LBN	O6-C25-O5-C3
2	B	503	LBN	O6-C25-O5-C3
2	C	503	LBN	O6-C25-O5-C3
2	D	504	LBN	O6-C25-O5-C3
2	E	505	LBN	O6-C25-O5-C3
2	F	503	LBN	O6-C25-O5-C3
2	G	503	LBN	O6-C25-O5-C3
2	A	501	LBN	C1-O1-P1-O2
2	A	502	LBN	C1-O1-P1-O2
2	A	502	LBN	C9-O2-P1-O1
2	A	506	LBN	C9-O2-P1-O1
2	B	501	LBN	C1-O1-P1-O2
2	B	501	LBN	C9-O2-P1-O1
2	B	502	LBN	C9-O2-P1-O1
2	B	503	LBN	C1-O1-P1-O2
2	B	504	LBN	C1-O1-P1-O2
2	B	504	LBN	C9-O2-P1-O1
2	C	501	LBN	C1-O1-P1-O2
2	C	501	LBN	C9-O2-P1-O1
2	C	502	LBN	C9-O2-P1-O1
2	C	503	LBN	C1-O1-P1-O2
2	C	504	LBN	C1-O1-P1-O2
2	C	504	LBN	C9-O2-P1-O1
2	D	501	LBN	C1-O1-P1-O2
2	D	501	LBN	C9-O2-P1-O1
2	D	502	LBN	C9-O2-P1-O1
2	D	504	LBN	C1-O1-P1-O2
2	E	501	LBN	C1-O1-P1-O2
2	E	501	LBN	C9-O2-P1-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	502	LBN	C1-O1-P1-O2
2	E	502	LBN	C9-O2-P1-O1
2	E	503	LBN	C9-O2-P1-O1
2	E	505	LBN	C1-O1-P1-O2
2	E	506	LBN	C1-O1-P1-O2
2	E	506	LBN	C9-O2-P1-O1
2	F	501	LBN	C1-O1-P1-O2
2	F	501	LBN	C9-O2-P1-O1
2	F	502	LBN	C9-O2-P1-O1
2	F	503	LBN	C1-O1-P1-O2
2	F	504	LBN	C1-O1-P1-O2
2	F	504	LBN	C9-O2-P1-O1
2	G	501	LBN	C1-O1-P1-O2
2	G	501	LBN	C9-O2-P1-O1
2	G	502	LBN	C9-O2-P1-O1
2	G	503	LBN	C1-O1-P1-O2
2	G	504	LBN	C1-O1-P1-O2
2	G	504	LBN	C9-O2-P1-O1
2	G	505	LBN	C1-O1-P1-O2
2	G	505	LBN	C9-O2-P1-O1
2	B	501	LBN	C9-C6-N1-C12
2	B	501	LBN	C9-C6-N1-C15
2	B	501	LBN	C9-C6-N1-C18
2	C	501	LBN	C9-C6-N1-C12
2	C	501	LBN	C9-C6-N1-C15
2	C	501	LBN	C9-C6-N1-C18
2	D	501	LBN	C9-C6-N1-C12
2	D	501	LBN	C9-C6-N1-C15
2	D	501	LBN	C9-C6-N1-C18
2	E	502	LBN	C9-C6-N1-C12
2	E	502	LBN	C9-C6-N1-C15
2	E	502	LBN	C9-C6-N1-C18
2	F	501	LBN	C9-C6-N1-C12
2	F	501	LBN	C9-C6-N1-C15
2	F	501	LBN	C9-C6-N1-C18
2	G	501	LBN	C9-C6-N1-C12
2	G	501	LBN	C9-C6-N1-C15
2	G	501	LBN	C9-C6-N1-C18
2	G	505	LBN	C9-C6-N1-C12
2	G	505	LBN	C9-C6-N1-C15
2	G	505	LBN	C9-C6-N1-C18
2	A	505	LBN	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	507	LBN	C26-C27-C28-C29
2	C	506	LBN	C26-C27-C28-C29
2	D	506	LBN	C26-C27-C28-C29
2	E	509	LBN	C26-C27-C28-C29
2	F	507	LBN	C26-C27-C28-C29
2	G	508	LBN	C26-C27-C28-C29
2	B	501	LBN	C35-C34-O7-C2
2	C	501	LBN	C35-C34-O7-C2
2	D	501	LBN	C35-C34-O7-C2
2	E	502	LBN	C35-C34-O7-C2
2	F	501	LBN	C35-C34-O7-C2
2	G	501	LBN	C35-C34-O7-C2
2	G	505	LBN	C35-C34-O7-C2
2	E	506	LBN	C34-C35-C36-C37
2	G	504	LBN	C34-C35-C36-C37
2	A	502	LBN	C34-C35-C36-C37
2	B	504	LBN	C34-C35-C36-C37
2	C	504	LBN	C34-C35-C36-C37
2	E	501	LBN	C34-C35-C36-C37
2	F	504	LBN	C34-C35-C36-C37
2	C	501	LBN	C1-C2-C3-O5
2	A	503	LBN	C38-C39-C40-C41
2	B	505	LBN	C38-C39-C40-C41
2	C	505	LBN	C38-C39-C40-C41
2	D	505	LBN	C38-C39-C40-C41
2	E	507	LBN	C38-C39-C40-C41
2	F	505	LBN	C38-C39-C40-C41
2	G	506	LBN	C38-C39-C40-C41
2	A	506	LBN	C31-C32-C33-C4
2	B	501	LBN	C29-C30-C31-C32
2	C	501	LBN	C29-C30-C31-C32
2	D	501	LBN	C29-C30-C31-C32
2	E	502	LBN	C29-C30-C31-C32
2	E	503	LBN	C31-C32-C33-C4
2	F	501	LBN	C29-C30-C31-C32
2	G	501	LBN	C29-C30-C31-C32
2	G	502	LBN	C31-C32-C33-C4
2	G	505	LBN	C29-C30-C31-C32
2	B	502	LBN	C31-C32-C33-C4
2	C	502	LBN	C31-C32-C33-C4
2	D	502	LBN	C31-C32-C33-C4
2	F	502	LBN	C31-C32-C33-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	507	LBN	C13-C10-C7-C4
2	C	506	LBN	C13-C10-C7-C4
2	D	506	LBN	C13-C10-C7-C4
2	E	509	LBN	C13-C10-C7-C4
2	F	507	LBN	C13-C10-C7-C4
2	G	508	LBN	C13-C10-C7-C4
2	A	505	LBN	C13-C10-C7-C4
2	B	501	LBN	C39-C40-C41-C42
2	C	501	LBN	C39-C40-C41-C42
2	D	501	LBN	C39-C40-C41-C42
2	E	502	LBN	C39-C40-C41-C42
2	F	501	LBN	C39-C40-C41-C42
2	G	501	LBN	C39-C40-C41-C42
2	G	505	LBN	C39-C40-C41-C42
2	B	501	LBN	O8-C34-O7-C2
2	C	501	LBN	O8-C34-O7-C2
2	D	501	LBN	O8-C34-O7-C2
2	E	502	LBN	O8-C34-O7-C2
2	F	501	LBN	O8-C34-O7-C2
2	G	501	LBN	O8-C34-O7-C2
2	G	505	LBN	O8-C34-O7-C2
2	B	501	LBN	C31-C32-C33-C4
2	C	501	LBN	C31-C32-C33-C4
2	D	501	LBN	C31-C32-C33-C4
2	E	501	LBN	C35-C36-C37-C38
2	E	502	LBN	C31-C32-C33-C4
2	F	501	LBN	C31-C32-C33-C4
2	G	501	LBN	C31-C32-C33-C4
2	G	505	LBN	C31-C32-C33-C4
2	A	502	LBN	C35-C36-C37-C38
2	B	504	LBN	C35-C36-C37-C38
2	C	504	LBN	C35-C36-C37-C38
2	E	506	LBN	C35-C36-C37-C38
2	F	504	LBN	C35-C36-C37-C38
2	G	504	LBN	C35-C36-C37-C38
2	E	505	LBN	C31-C32-C33-C4
2	A	501	LBN	C31-C32-C33-C4
2	B	503	LBN	C31-C32-C33-C4
2	C	503	LBN	C31-C32-C33-C4
2	D	504	LBN	C31-C32-C33-C4
2	F	503	LBN	C31-C32-C33-C4
2	G	503	LBN	C31-C32-C33-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	501	LBN	C30-C31-C32-C33
2	B	503	LBN	C30-C31-C32-C33
2	C	503	LBN	C30-C31-C32-C33
2	D	504	LBN	C30-C31-C32-C33
2	E	505	LBN	C30-C31-C32-C33
2	G	503	LBN	C30-C31-C32-C33
2	F	503	LBN	C30-C31-C32-C33
2	A	501	LBN	C13-C10-C7-C4
2	B	503	LBN	C13-C10-C7-C4
2	C	503	LBN	C13-C10-C7-C4
2	D	504	LBN	C13-C10-C7-C4
2	E	505	LBN	C13-C10-C7-C4
2	F	503	LBN	C13-C10-C7-C4
2	G	503	LBN	C13-C10-C7-C4
2	B	501	LBN	C1-C2-C3-O5
2	D	501	LBN	C1-C2-C3-O5
2	E	502	LBN	C1-C2-C3-O5
2	F	501	LBN	C1-C2-C3-O5
2	G	501	LBN	C1-C2-C3-O5
2	G	505	LBN	C1-C2-C3-O5
2	E	509	LBN	C31-C32-C33-C4
2	A	505	LBN	C31-C32-C33-C4
2	B	507	LBN	C31-C32-C33-C4
2	C	506	LBN	C31-C32-C33-C4
2	D	506	LBN	C31-C32-C33-C4
2	F	507	LBN	C31-C32-C33-C4
2	G	508	LBN	C31-C32-C33-C4
2	A	502	LBN	C39-C40-C41-C42
2	B	504	LBN	C39-C40-C41-C42
2	C	504	LBN	C39-C40-C41-C42
2	E	501	LBN	C39-C40-C41-C42
2	E	506	LBN	C39-C40-C41-C42
2	F	504	LBN	C39-C40-C41-C42
2	G	504	LBN	C39-C40-C41-C42
2	A	502	LBN	O1-C1-C2-O7
2	A	506	LBN	O1-C1-C2-O7
2	B	502	LBN	O1-C1-C2-O7
2	B	504	LBN	O1-C1-C2-O7
2	C	502	LBN	O1-C1-C2-O7
2	C	504	LBN	O1-C1-C2-O7
2	D	502	LBN	O1-C1-C2-O7
2	E	501	LBN	O1-C1-C2-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	503	LBN	O1-C1-C2-O7
2	E	506	LBN	O1-C1-C2-O7
2	F	502	LBN	O1-C1-C2-O7
2	F	504	LBN	O1-C1-C2-O7
2	G	502	LBN	O1-C1-C2-O7
2	G	504	LBN	O1-C1-C2-O7
2	A	501	LBN	O7-C2-C3-O5
2	B	503	LBN	O7-C2-C3-O5
2	C	503	LBN	O7-C2-C3-O5
2	D	504	LBN	O7-C2-C3-O5
2	E	505	LBN	O7-C2-C3-O5
2	F	503	LBN	O7-C2-C3-O5
2	G	503	LBN	O7-C2-C3-O5
2	F	506	LBN	C26-C27-C28-C29
2	A	504	LBN	C26-C27-C28-C29
2	B	506	LBN	C26-C27-C28-C29
2	D	503	LBN	C26-C27-C28-C29
2	E	504	LBN	C26-C27-C28-C29
2	E	508	LBN	C26-C27-C28-C29
2	G	507	LBN	C26-C27-C28-C29
2	A	506	LBN	C3-C2-O7-C34
2	B	502	LBN	C3-C2-O7-C34
2	C	502	LBN	C3-C2-O7-C34
2	D	502	LBN	C3-C2-O7-C34
2	E	503	LBN	C3-C2-O7-C34
2	F	502	LBN	C3-C2-O7-C34
2	G	502	LBN	C3-C2-O7-C34
2	A	501	LBN	C1-C2-C3-O5
2	B	503	LBN	C1-C2-C3-O5
2	C	503	LBN	C1-C2-C3-O5
2	D	504	LBN	C1-C2-C3-O5
2	E	505	LBN	C1-C2-C3-O5
2	F	503	LBN	C1-C2-C3-O5
2	G	503	LBN	C1-C2-C3-O5
2	B	501	LBN	O1-C1-C2-O7
2	C	501	LBN	O1-C1-C2-O7
2	E	502	LBN	O1-C1-C2-O7
2	F	501	LBN	O1-C1-C2-O7
2	G	505	LBN	O1-C1-C2-O7
2	B	501	LBN	O7-C2-C3-O5
2	C	501	LBN	O7-C2-C3-O5
2	D	501	LBN	O7-C2-C3-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	502	LBN	O7-C2-C3-O5
2	F	501	LBN	O7-C2-C3-O5
2	G	501	LBN	O7-C2-C3-O5
2	G	505	LBN	O7-C2-C3-O5
2	A	501	LBN	C9-O2-P1-O1
2	B	503	LBN	C9-O2-P1-O1
2	C	503	LBN	C9-O2-P1-O1
2	D	504	LBN	C9-O2-P1-O1
2	E	505	LBN	C9-O2-P1-O1
2	F	503	LBN	C9-O2-P1-O1
2	G	503	LBN	C9-O2-P1-O1
2	A	504	LBN	C30-C31-C32-C33
2	B	506	LBN	C30-C31-C32-C33
2	D	503	LBN	C30-C31-C32-C33
2	E	508	LBN	C30-C31-C32-C33
2	G	507	LBN	C30-C31-C32-C33
2	A	502	LBN	C2-C1-O1-P1
2	A	506	LBN	C2-C1-O1-P1
2	B	502	LBN	C2-C1-O1-P1
2	B	504	LBN	C2-C1-O1-P1
2	C	502	LBN	C2-C1-O1-P1
2	C	504	LBN	C2-C1-O1-P1
2	D	502	LBN	C2-C1-O1-P1
2	E	501	LBN	C2-C1-O1-P1
2	E	503	LBN	C2-C1-O1-P1
2	E	506	LBN	C2-C1-O1-P1
2	F	502	LBN	C2-C1-O1-P1
2	F	504	LBN	C2-C1-O1-P1
2	G	502	LBN	C2-C1-O1-P1
2	G	504	LBN	C2-C1-O1-P1
2	E	504	LBN	C30-C31-C32-C33
2	F	506	LBN	C30-C31-C32-C33
2	A	501	LBN	C1-O1-P1-O3
2	A	502	LBN	C1-O1-P1-O4
2	A	502	LBN	C9-O2-P1-O3
2	A	506	LBN	C9-O2-P1-O3
2	B	501	LBN	C1-O1-P1-O4
2	B	501	LBN	C9-O2-P1-O4
2	B	502	LBN	C9-O2-P1-O3
2	B	503	LBN	C1-O1-P1-O3
2	B	504	LBN	C1-O1-P1-O4
2	B	504	LBN	C9-O2-P1-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	501	LBN	C1-O1-P1-O4
2	C	501	LBN	C9-O2-P1-O4
2	C	502	LBN	C9-O2-P1-O3
2	C	503	LBN	C1-O1-P1-O3
2	C	504	LBN	C1-O1-P1-O4
2	C	504	LBN	C9-O2-P1-O3
2	D	501	LBN	C1-O1-P1-O4
2	D	501	LBN	C9-O2-P1-O4
2	D	502	LBN	C9-O2-P1-O3
2	D	504	LBN	C1-O1-P1-O3
2	E	501	LBN	C1-O1-P1-O4
2	E	501	LBN	C9-O2-P1-O3
2	E	502	LBN	C1-O1-P1-O4
2	E	502	LBN	C9-O2-P1-O4
2	E	503	LBN	C9-O2-P1-O3
2	E	505	LBN	C1-O1-P1-O3
2	E	506	LBN	C1-O1-P1-O4
2	E	506	LBN	C9-O2-P1-O3
2	F	501	LBN	C1-O1-P1-O4
2	F	501	LBN	C9-O2-P1-O4
2	F	502	LBN	C9-O2-P1-O3
2	F	503	LBN	C1-O1-P1-O3
2	F	504	LBN	C1-O1-P1-O4
2	F	504	LBN	C9-O2-P1-O3
2	G	501	LBN	C1-O1-P1-O4
2	G	501	LBN	C9-O2-P1-O4
2	G	502	LBN	C9-O2-P1-O3
2	G	503	LBN	C1-O1-P1-O3
2	G	504	LBN	C1-O1-P1-O4
2	G	504	LBN	C9-O2-P1-O3
2	G	505	LBN	C1-O1-P1-O4
2	G	505	LBN	C9-O2-P1-O4
2	B	501	LBN	O1-C1-C2-C3
2	C	501	LBN	O1-C1-C2-C3
2	D	501	LBN	O1-C1-C2-C3
2	E	502	LBN	O1-C1-C2-C3
2	F	501	LBN	O1-C1-C2-C3
2	G	501	LBN	O1-C1-C2-C3
2	G	505	LBN	O1-C1-C2-C3
2	D	501	LBN	O1-C1-C2-O7
2	G	501	LBN	O1-C1-C2-O7
2	G	508	LBN	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	505	LBN	C28-C29-C30-C31
2	B	507	LBN	C28-C29-C30-C31
2	D	506	LBN	C28-C29-C30-C31
2	F	507	LBN	C28-C29-C30-C31
2	C	506	LBN	C28-C29-C30-C31
2	E	509	LBN	C28-C29-C30-C31
2	A	506	LBN	C1-O1-P1-O2
2	B	502	LBN	C1-O1-P1-O2
2	C	502	LBN	C1-O1-P1-O2
2	D	502	LBN	C1-O1-P1-O2
2	E	503	LBN	C1-O1-P1-O2
2	F	502	LBN	C1-O1-P1-O2
2	G	502	LBN	C1-O1-P1-O2
2	E	508	LBN	C25-C26-C27-C28
2	F	506	LBN	C25-C26-C27-C28
2	A	504	LBN	C25-C26-C27-C28
2	B	506	LBN	C25-C26-C27-C28
2	D	503	LBN	C25-C26-C27-C28
2	G	507	LBN	C25-C26-C27-C28
2	B	501	LBN	C2-C1-O1-P1
2	C	501	LBN	C2-C1-O1-P1
2	D	501	LBN	C2-C1-O1-P1
2	E	502	LBN	C2-C1-O1-P1
2	F	501	LBN	C2-C1-O1-P1
2	G	501	LBN	C2-C1-O1-P1
2	G	505	LBN	C2-C1-O1-P1
2	E	504	LBN	C25-C26-C27-C28
2	A	504	LBN	C28-C29-C30-C31
2	B	506	LBN	C28-C29-C30-C31
2	D	503	LBN	C28-C29-C30-C31
2	E	504	LBN	C28-C29-C30-C31
2	G	507	LBN	C28-C29-C30-C31
2	E	508	LBN	C28-C29-C30-C31
2	F	506	LBN	C28-C29-C30-C31
2	C	501	LBN	C27-C28-C29-C30
2	E	502	LBN	C27-C28-C29-C30
2	G	501	LBN	C27-C28-C29-C30
2	B	501	LBN	C27-C28-C29-C30
2	B	501	LBN	C37-C38-C39-C40
2	C	501	LBN	C37-C38-C39-C40
2	D	501	LBN	C37-C38-C39-C40
2	E	502	LBN	C37-C38-C39-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	501	LBN	C27-C28-C29-C30
2	F	501	LBN	C37-C38-C39-C40
2	G	501	LBN	C37-C38-C39-C40
2	G	505	LBN	C27-C28-C29-C30
2	A	506	LBN	O1-C1-C2-C3
2	B	502	LBN	O1-C1-C2-C3
2	C	502	LBN	O1-C1-C2-C3
2	D	502	LBN	O1-C1-C2-C3
2	E	503	LBN	O1-C1-C2-C3
2	E	506	LBN	O1-C1-C2-C3
2	F	502	LBN	O1-C1-C2-C3
2	G	502	LBN	O1-C1-C2-C3
2	G	505	LBN	C37-C38-C39-C40
2	D	501	LBN	C27-C28-C29-C30
2	D	503	LBN	C27-C28-C29-C30
2	E	504	LBN	C27-C28-C29-C30
2	G	507	LBN	C27-C28-C29-C30
2	A	504	LBN	C27-C28-C29-C30
2	B	506	LBN	C27-C28-C29-C30
2	E	508	LBN	C27-C28-C29-C30
2	F	506	LBN	C27-C28-C29-C30
2	A	502	LBN	O1-C1-C2-C3
2	B	504	LBN	O1-C1-C2-C3
2	C	504	LBN	O1-C1-C2-C3
2	E	501	LBN	O1-C1-C2-C3
2	F	504	LBN	O1-C1-C2-C3
2	G	504	LBN	O1-C1-C2-C3
2	C	502	LBN	C35-C36-C37-C38
2	B	502	LBN	C35-C36-C37-C38
2	F	502	LBN	C35-C36-C37-C38
2	D	502	LBN	C35-C36-C37-C38
2	D	505	LBN	C36-C37-C38-C39
2	A	506	LBN	C35-C36-C37-C38
2	C	505	LBN	C36-C37-C38-C39
2	E	503	LBN	C35-C36-C37-C38
2	G	502	LBN	C35-C36-C37-C38
2	G	506	LBN	C36-C37-C38-C39
2	A	503	LBN	C36-C37-C38-C39
2	B	504	LBN	C36-C37-C38-C39
2	B	505	LBN	C36-C37-C38-C39
2	E	506	LBN	C36-C37-C38-C39
2	C	504	LBN	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

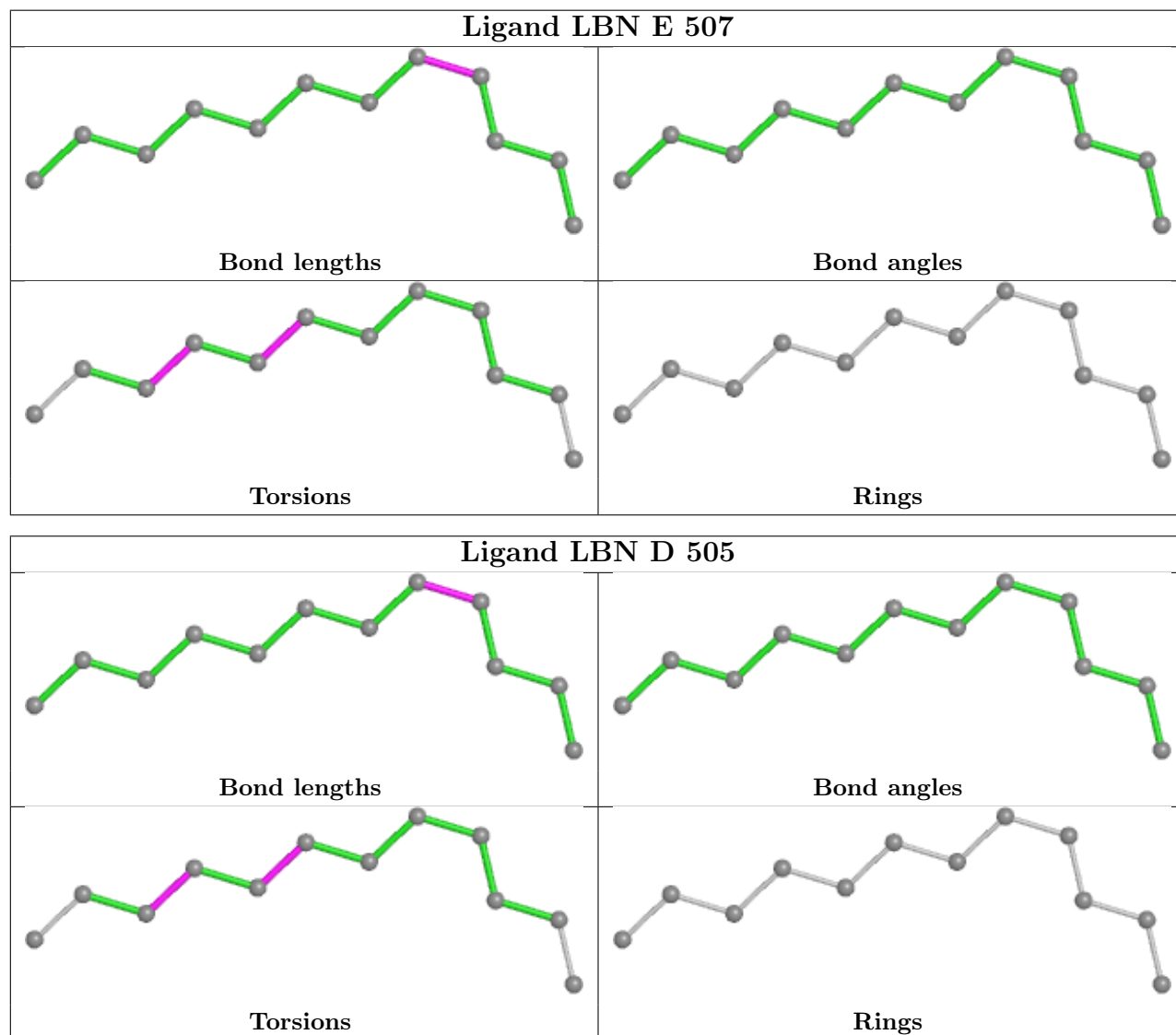
Mol	Chain	Res	Type	Atoms
2	F	504	LBN	C36-C37-C38-C39
2	F	505	LBN	C36-C37-C38-C39
2	E	501	LBN	C36-C37-C38-C39
2	E	507	LBN	C36-C37-C38-C39
2	G	504	LBN	C36-C37-C38-C39
2	A	502	LBN	C36-C37-C38-C39
2	D	502	LBN	C32-C33-C4-C7
2	E	503	LBN	C32-C33-C4-C7
2	G	502	LBN	C32-C33-C4-C7
2	B	502	LBN	C32-C33-C4-C7
2	C	502	LBN	C32-C33-C4-C7
2	F	502	LBN	C32-C33-C4-C7
2	A	506	LBN	C32-C33-C4-C7
2	A	502	LBN	C6-C9-O2-P1
2	B	504	LBN	C6-C9-O2-P1
2	C	504	LBN	C6-C9-O2-P1
2	E	501	LBN	C6-C9-O2-P1
2	E	506	LBN	C6-C9-O2-P1
2	F	504	LBN	C6-C9-O2-P1
2	G	504	LBN	C6-C9-O2-P1
2	A	506	LBN	O5-C25-C26-C27
2	B	502	LBN	O5-C25-C26-C27
2	C	502	LBN	O5-C25-C26-C27
2	D	502	LBN	O5-C25-C26-C27
2	E	503	LBN	O5-C25-C26-C27
2	F	502	LBN	O5-C25-C26-C27
2	G	502	LBN	O5-C25-C26-C27
2	A	505	LBN	C32-C33-C4-C7
2	C	506	LBN	C32-C33-C4-C7
2	E	509	LBN	C32-C33-C4-C7
2	F	507	LBN	C32-C33-C4-C7
2	D	506	LBN	C32-C33-C4-C7
2	G	508	LBN	C32-C33-C4-C7
2	B	507	LBN	C32-C33-C4-C7
2	G	502	LBN	O6-C25-C26-C27
2	A	506	LBN	O6-C25-C26-C27
2	B	502	LBN	O6-C25-C26-C27
2	C	502	LBN	O6-C25-C26-C27
2	D	502	LBN	O6-C25-C26-C27
2	E	503	LBN	O6-C25-C26-C27
2	F	502	LBN	O6-C25-C26-C27

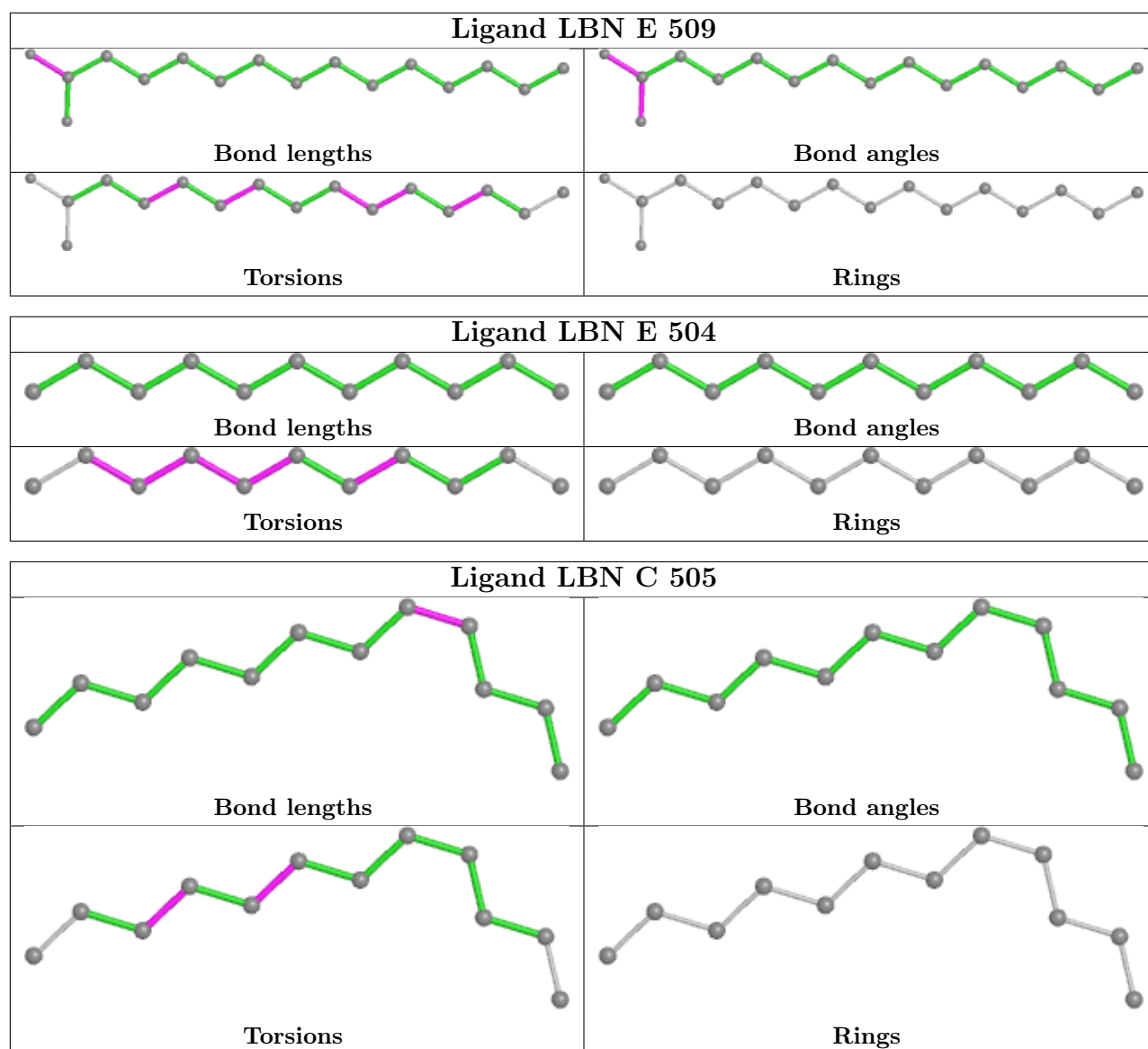
There are no ring outliers.

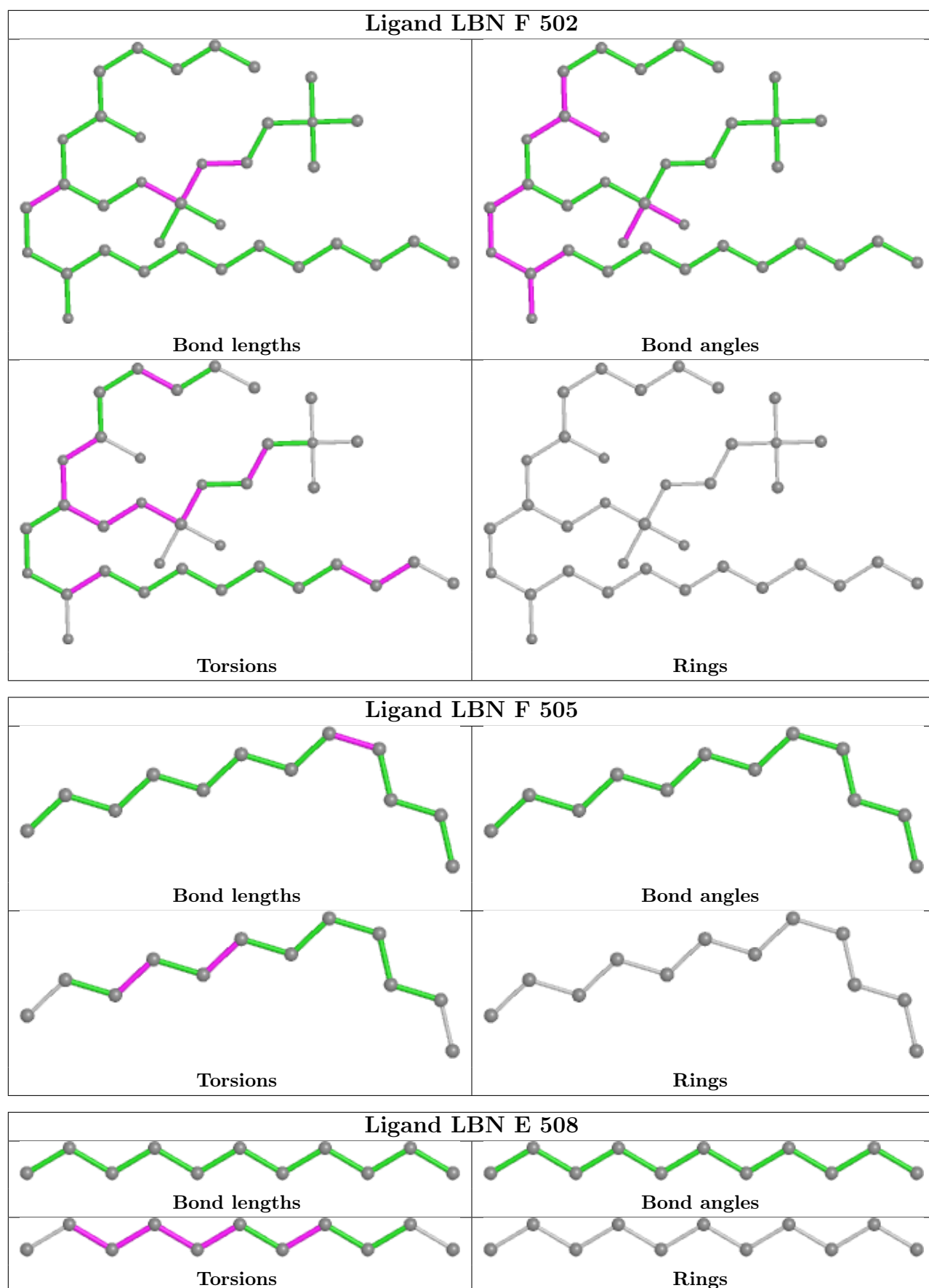
1 monomer is involved in 1 short contact:

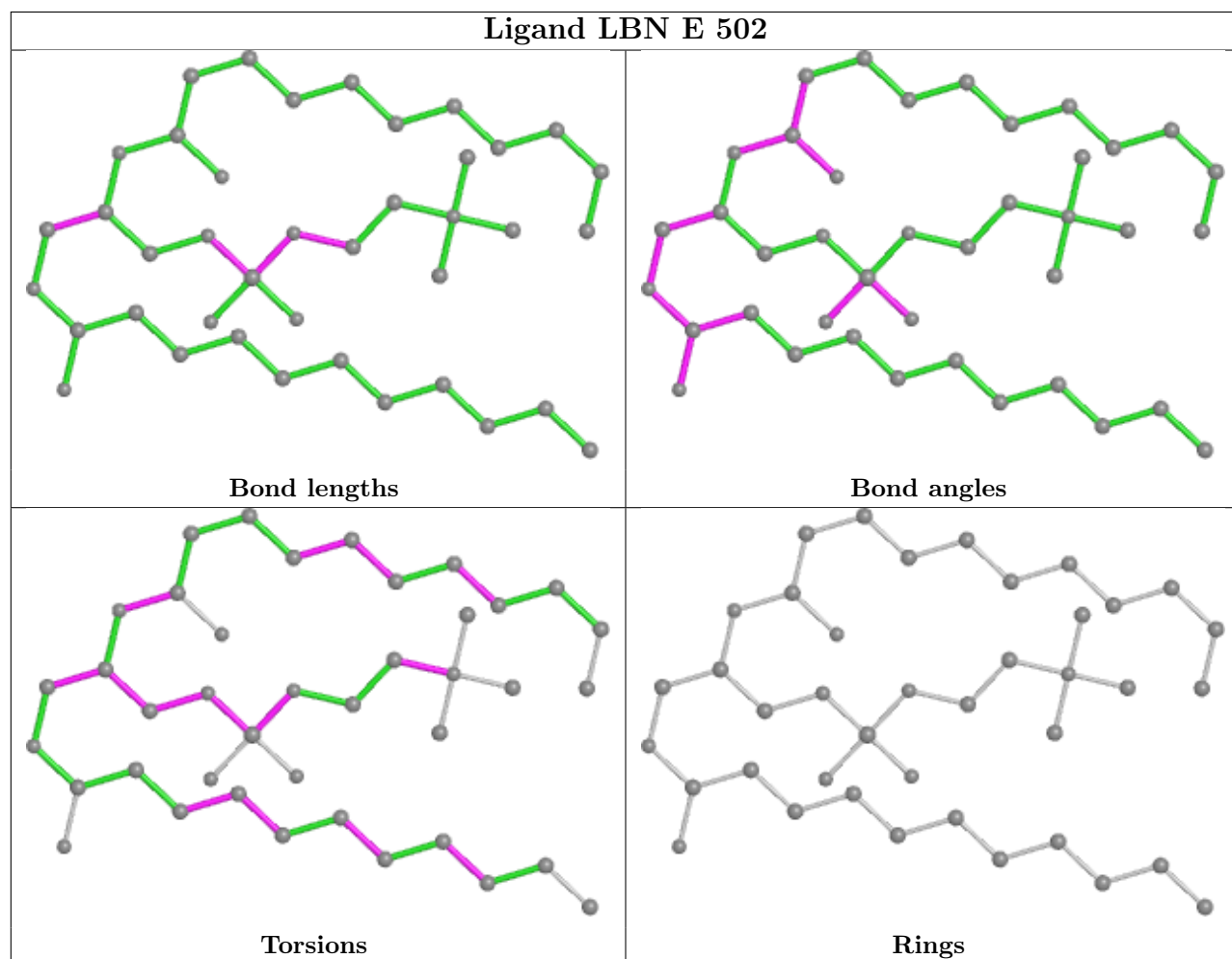
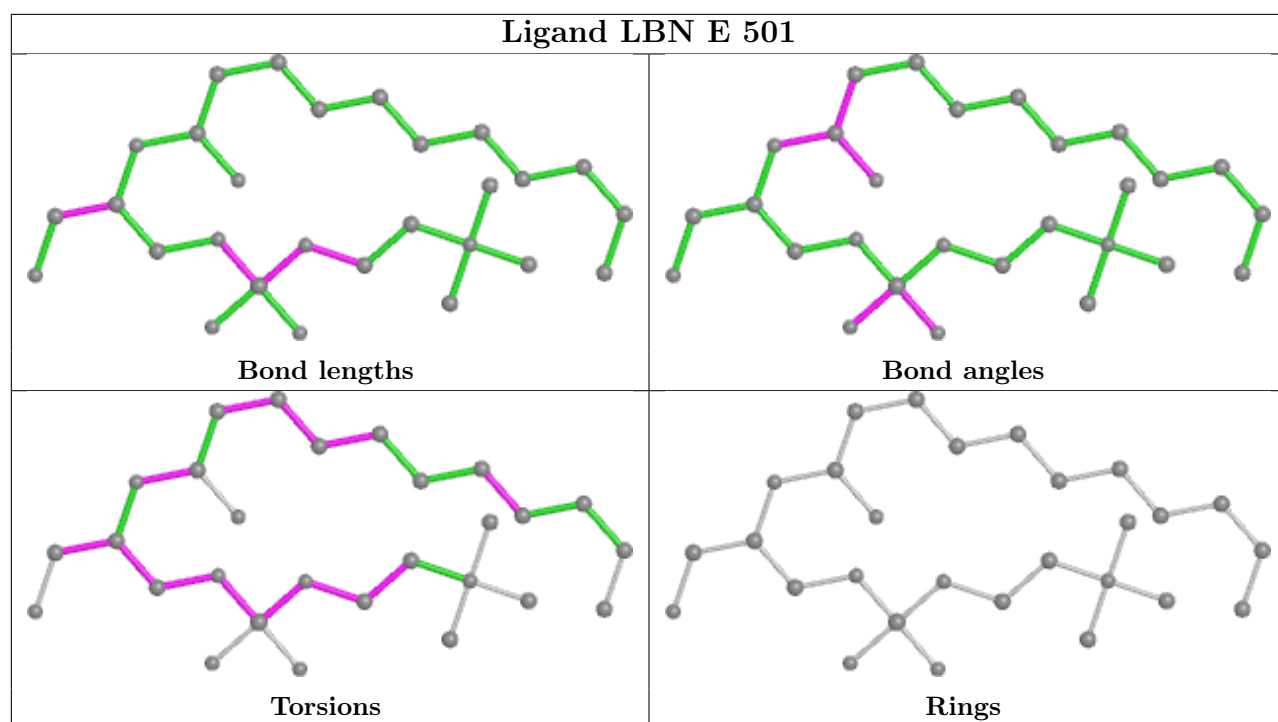
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	502	LBN	1	0

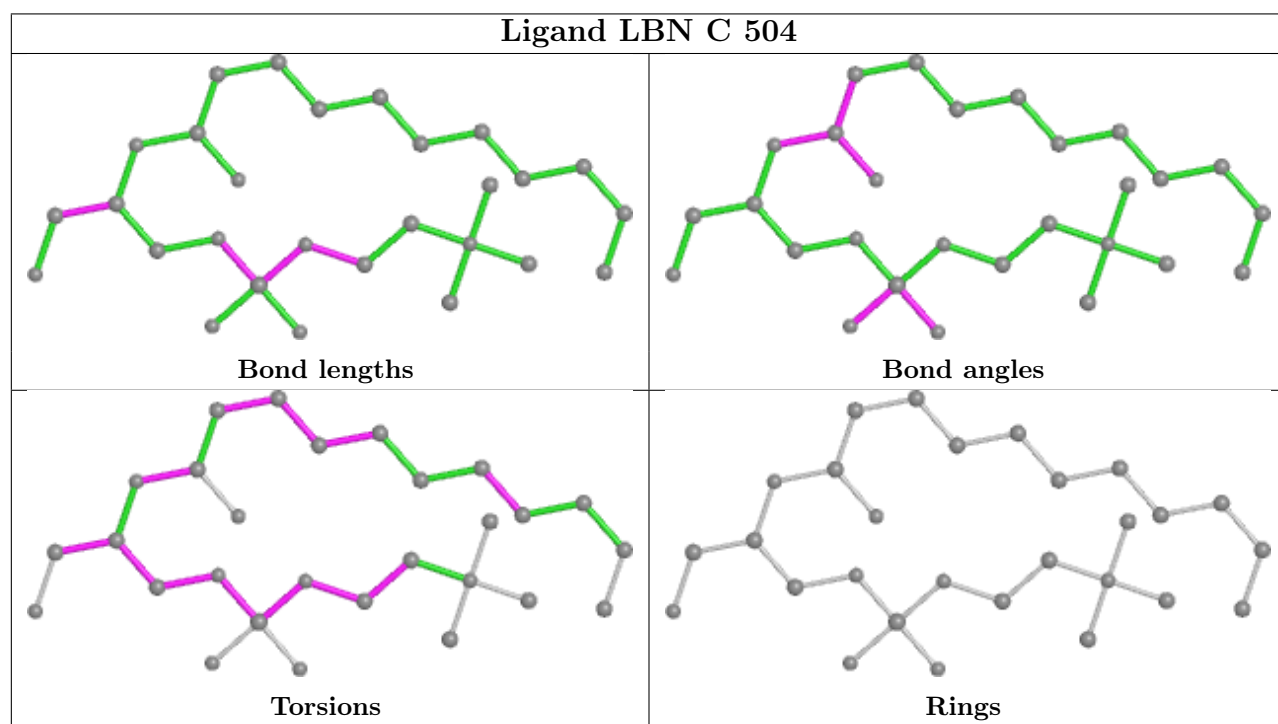
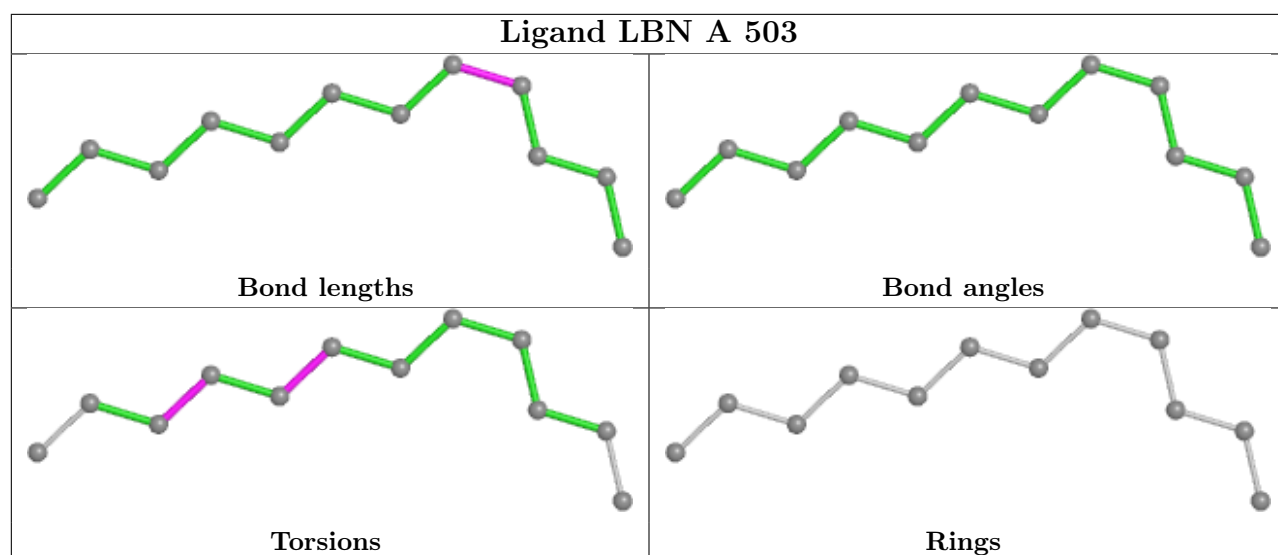
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



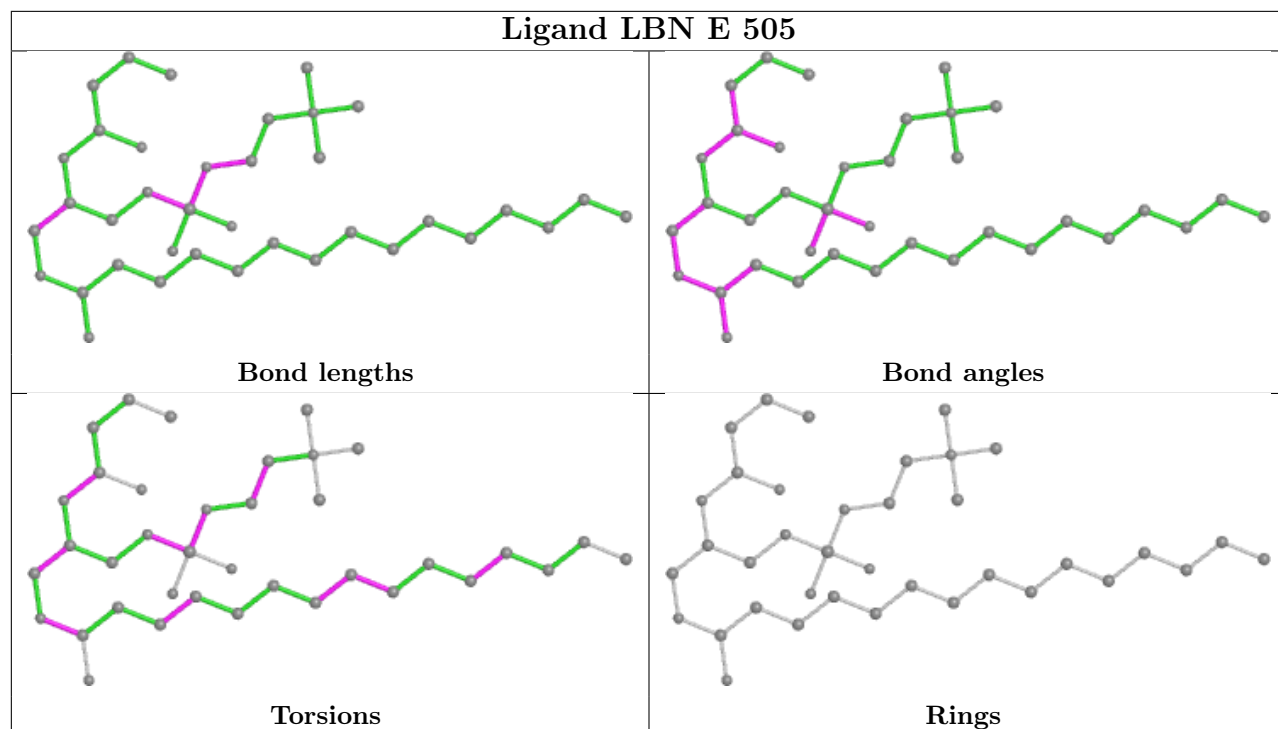




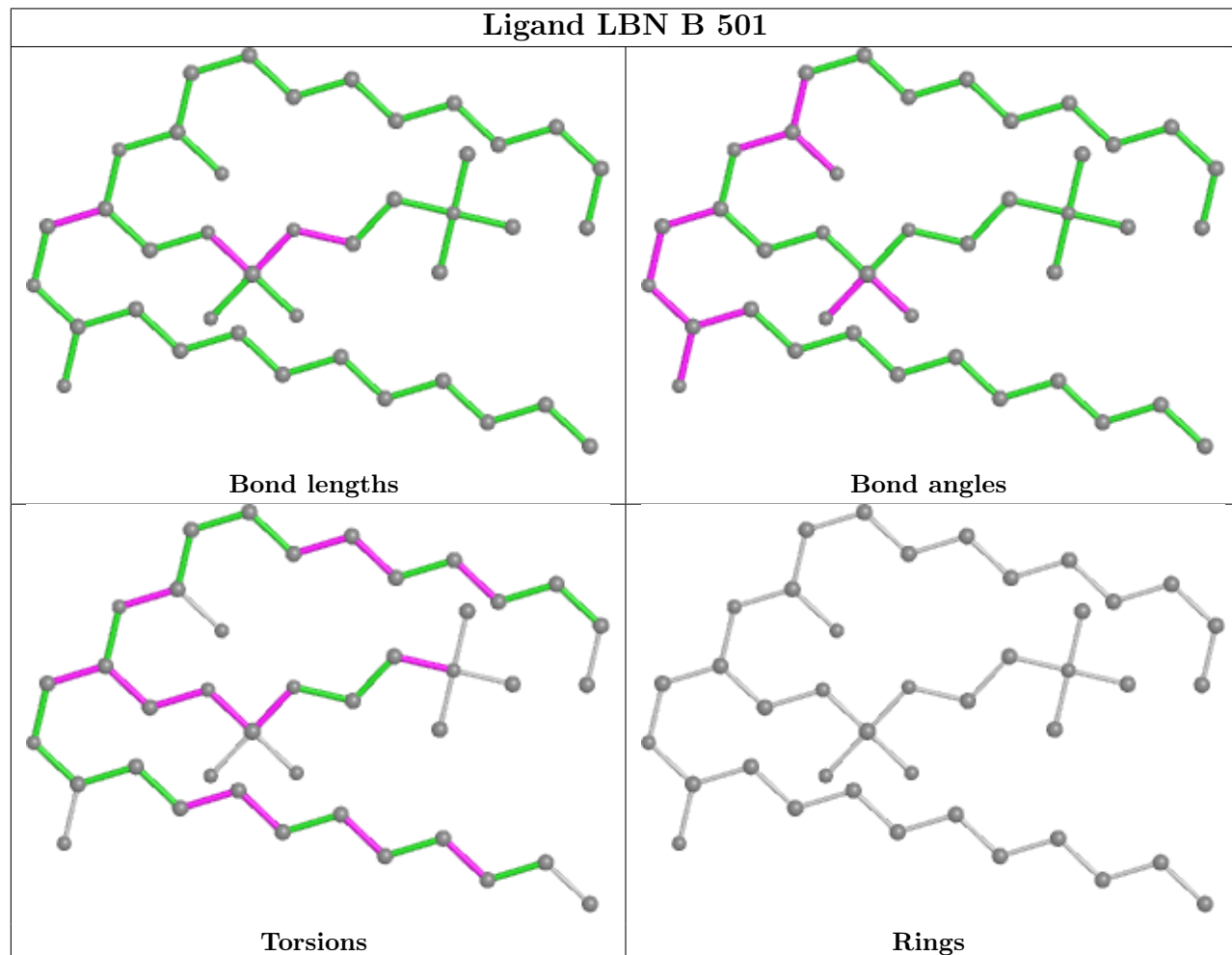


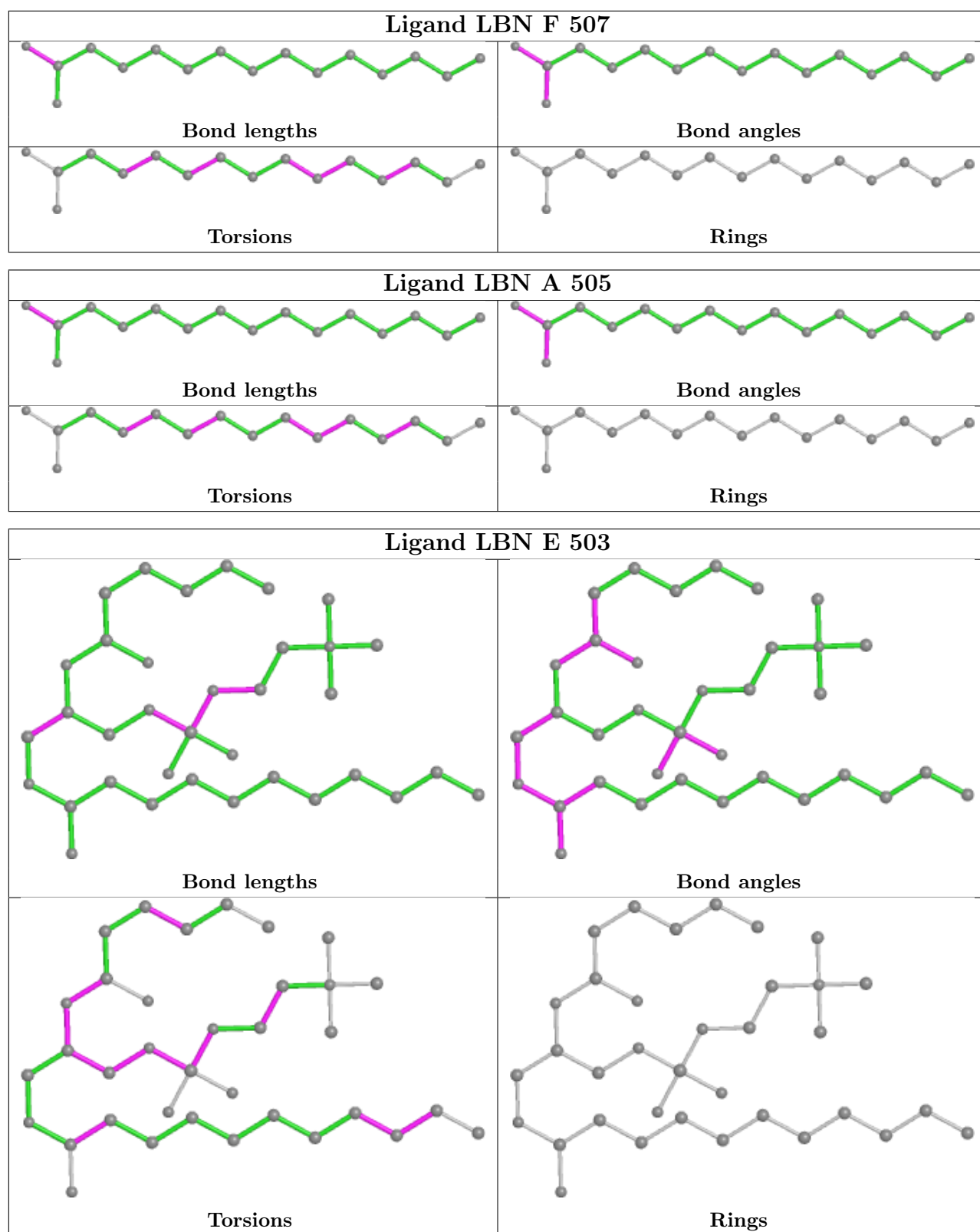


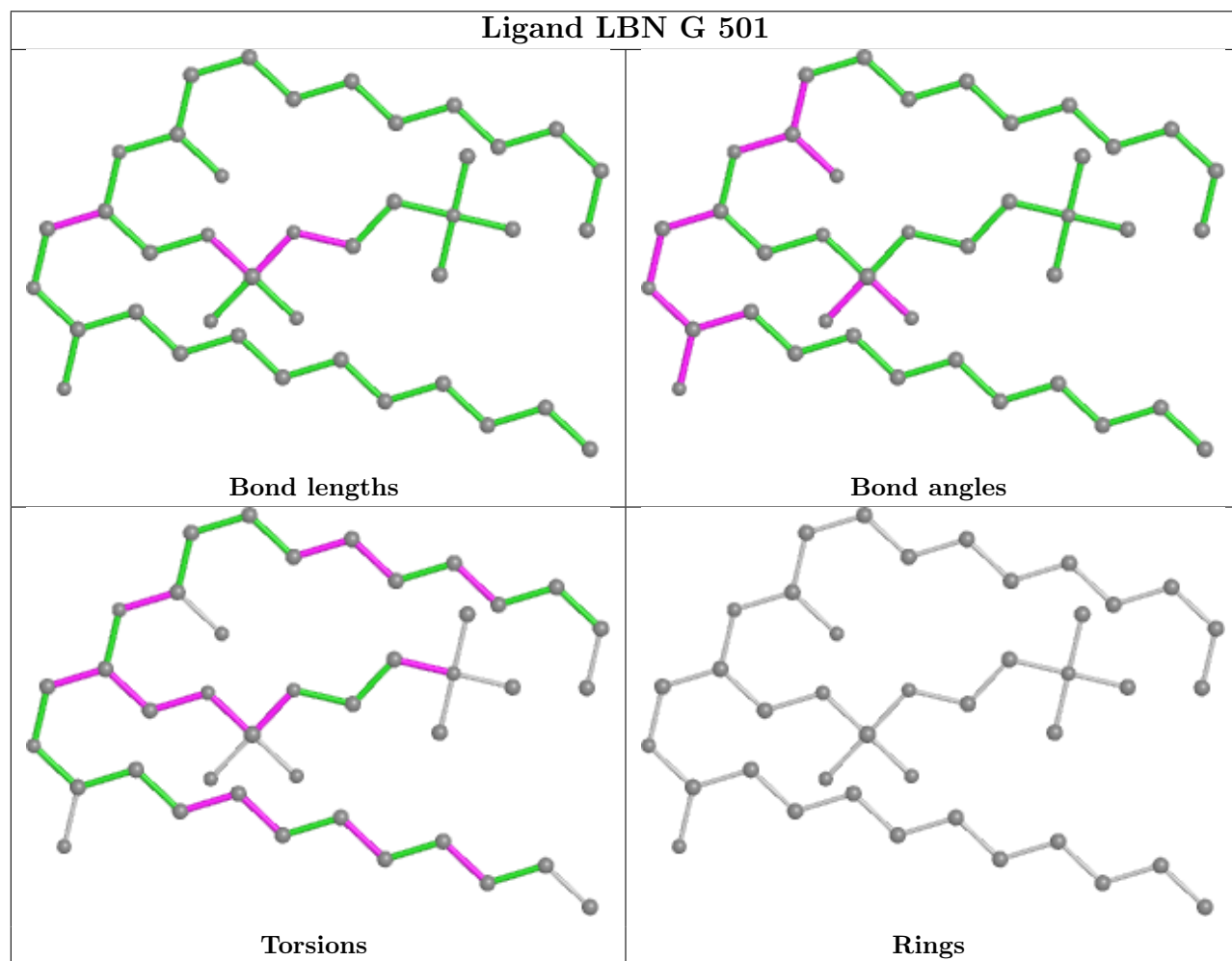
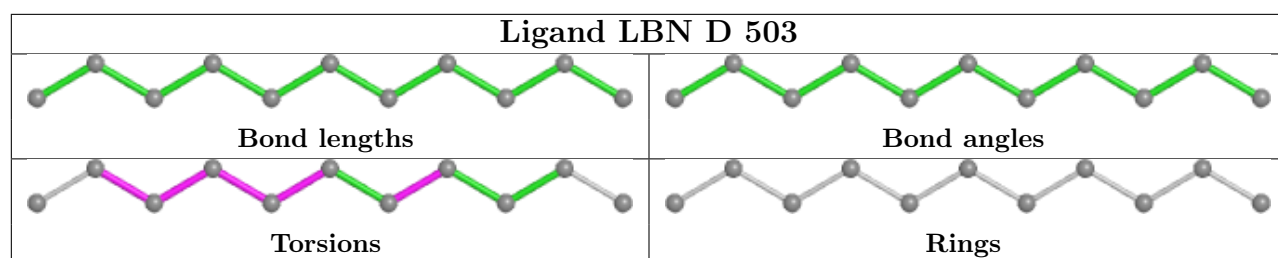
Ligand LBN E 505



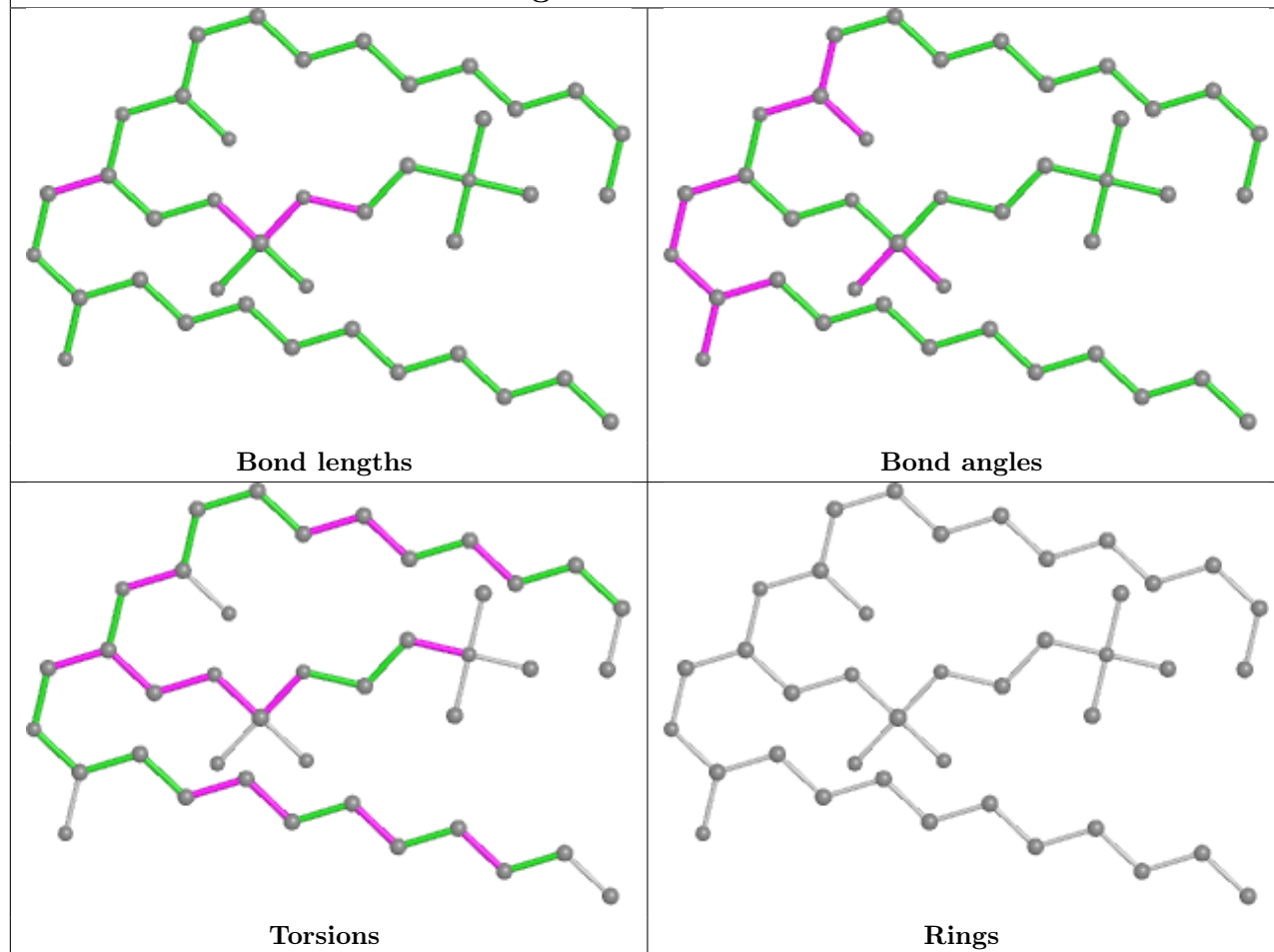
Ligand LBN B 501



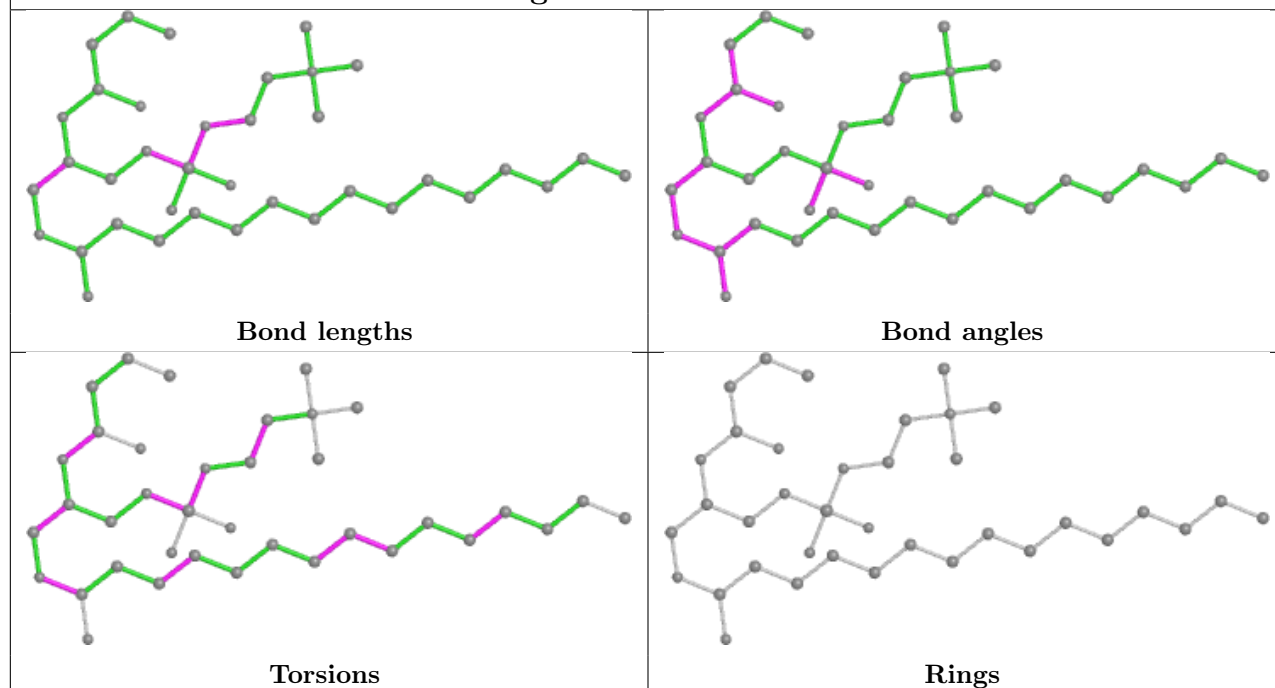


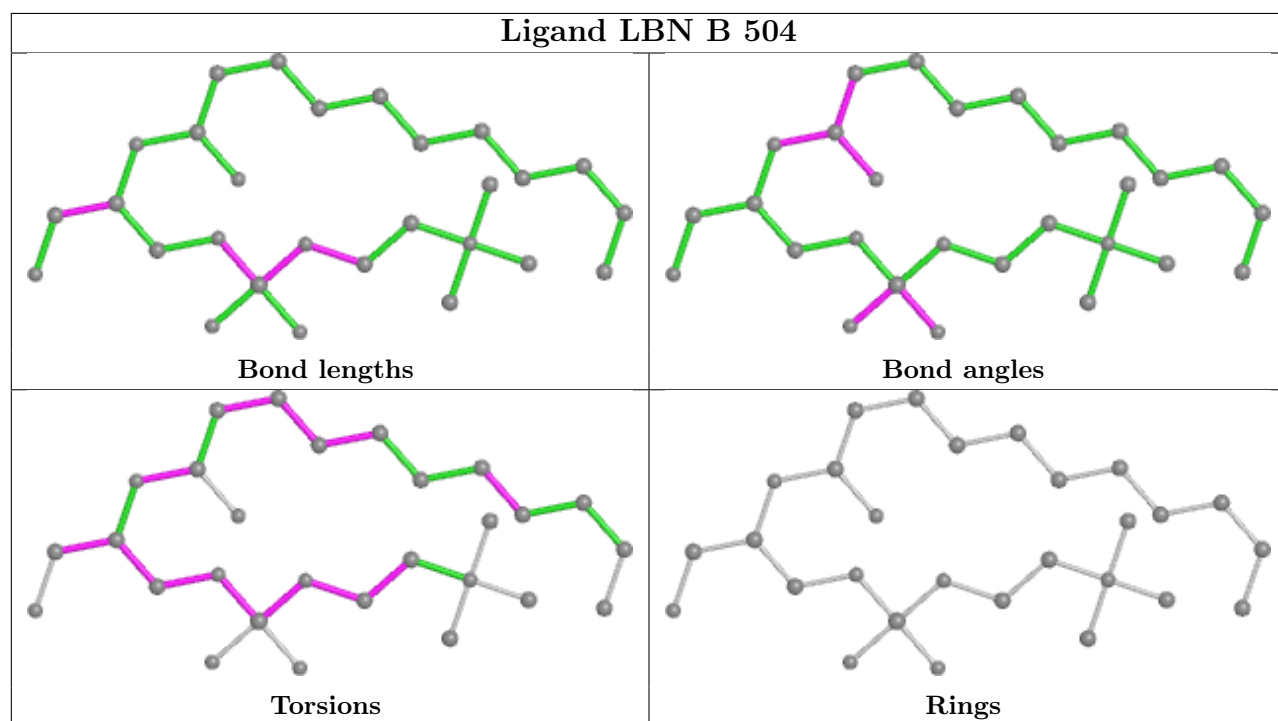
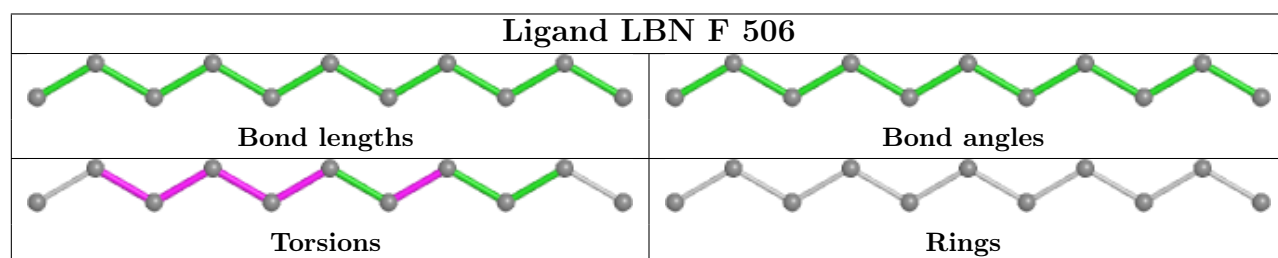
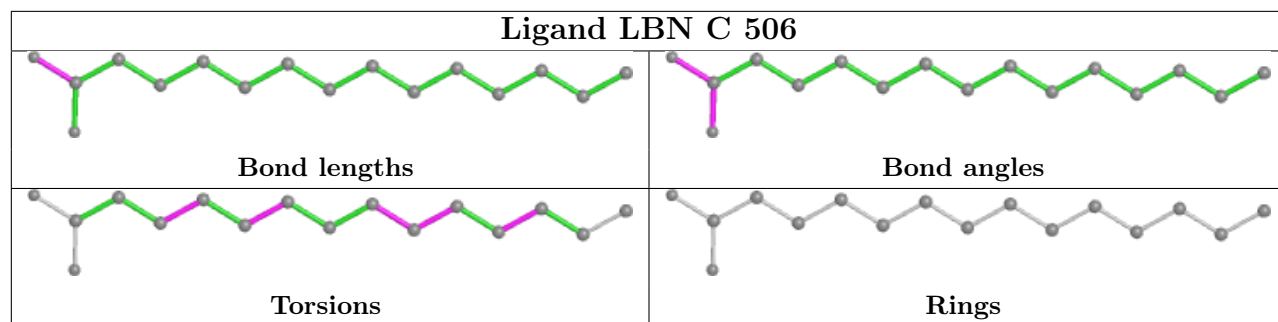


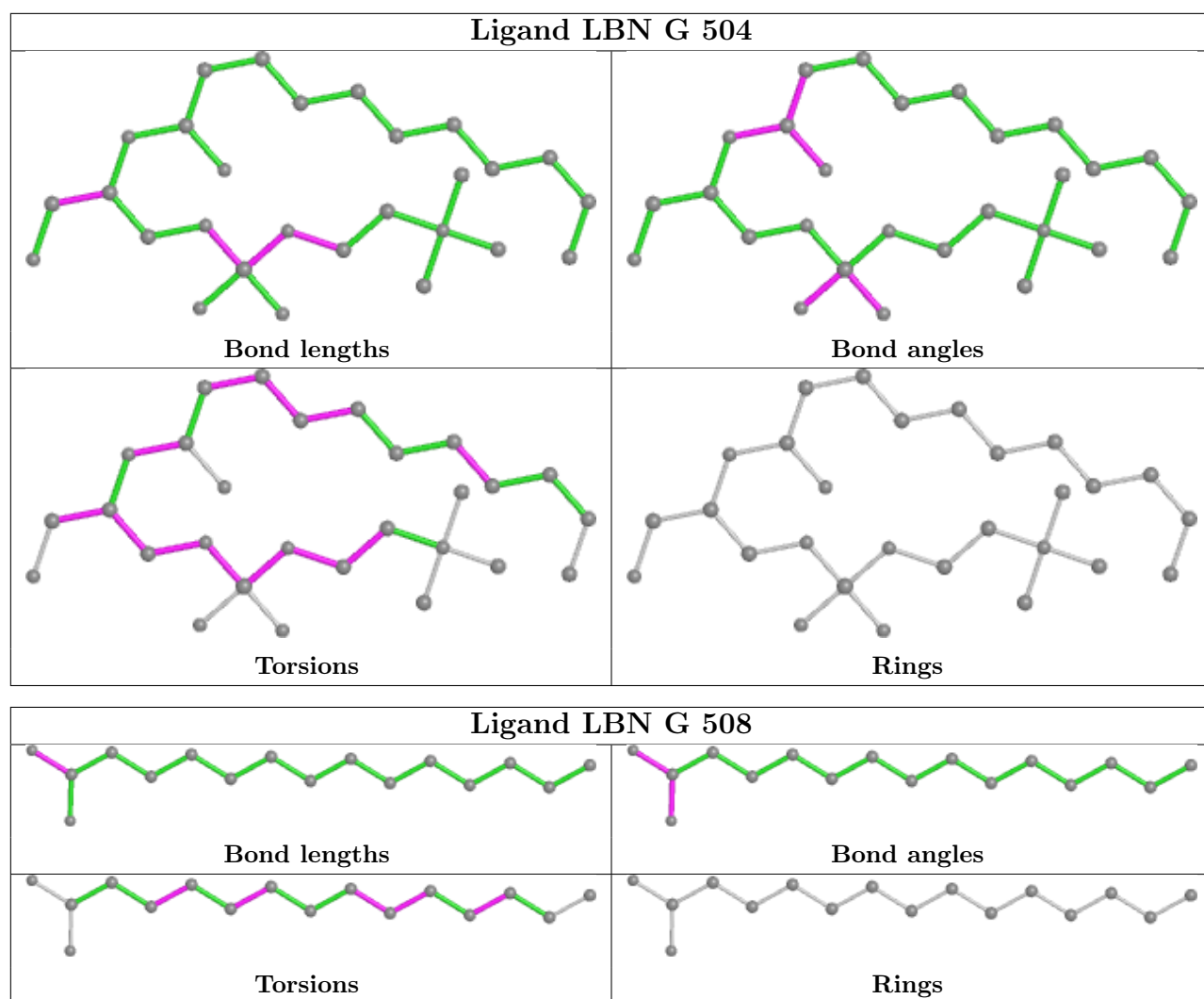
Ligand LBN F 501

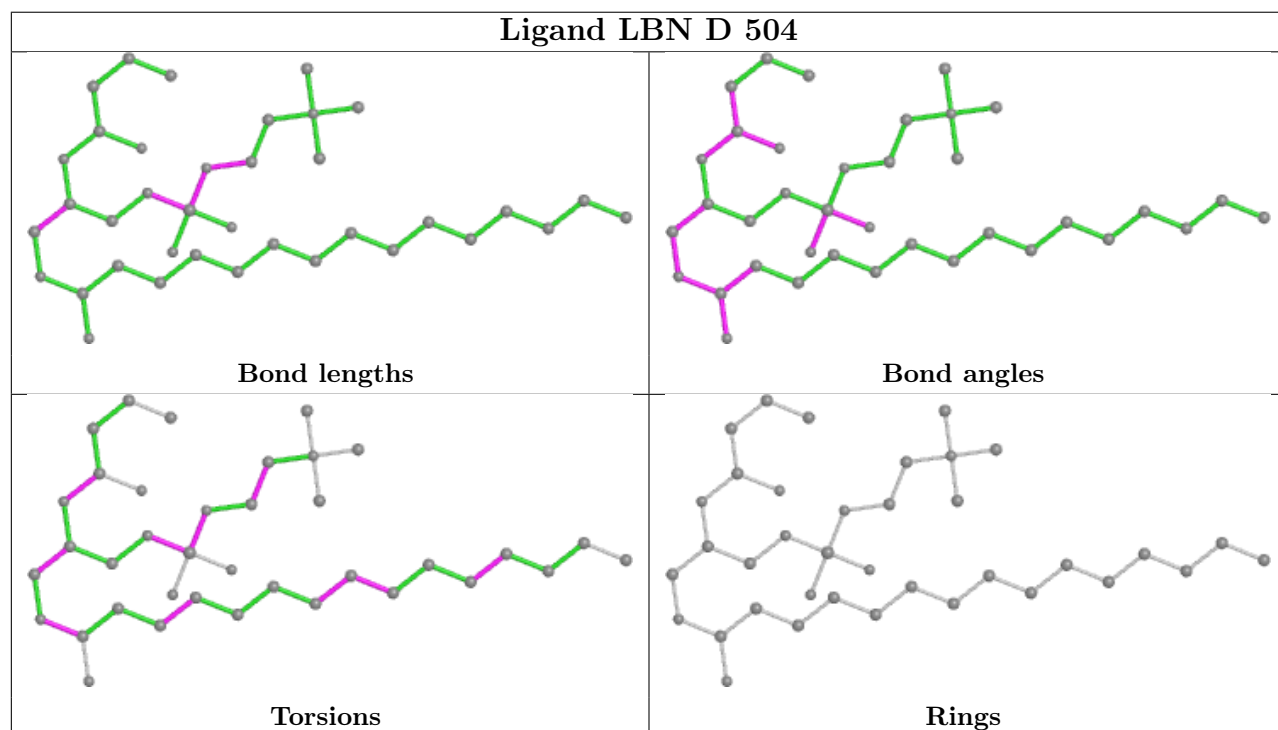
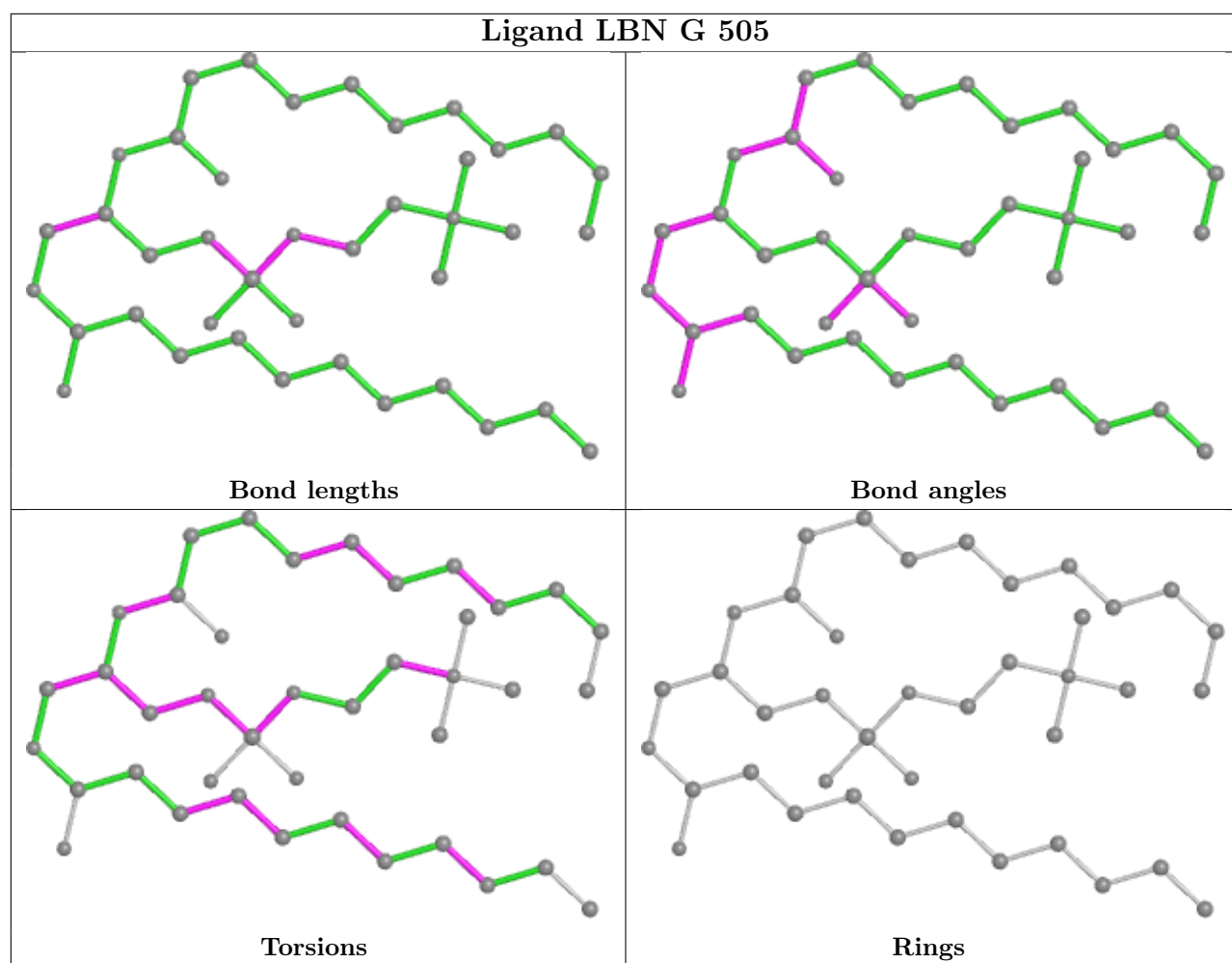


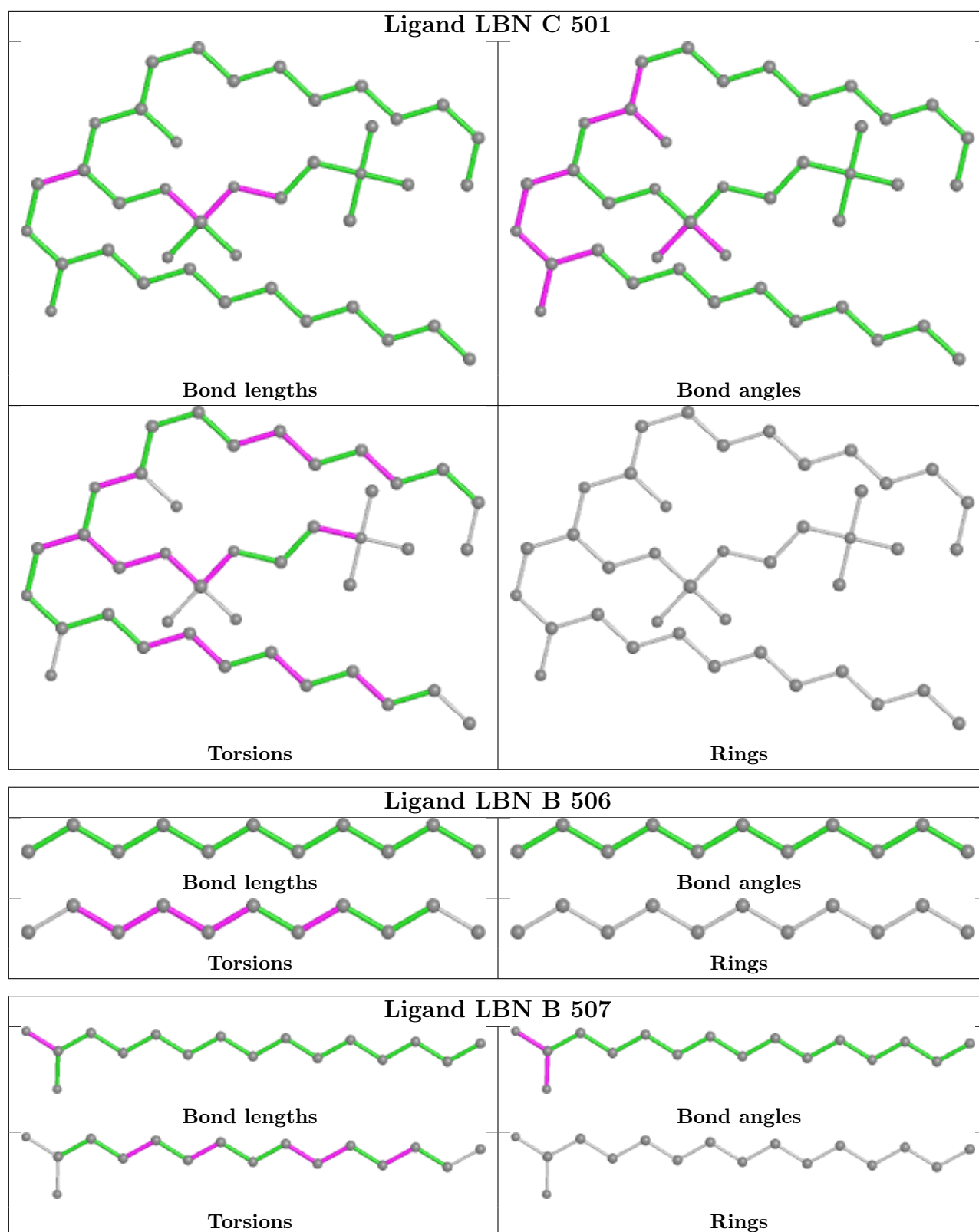
Ligand LBN A 501



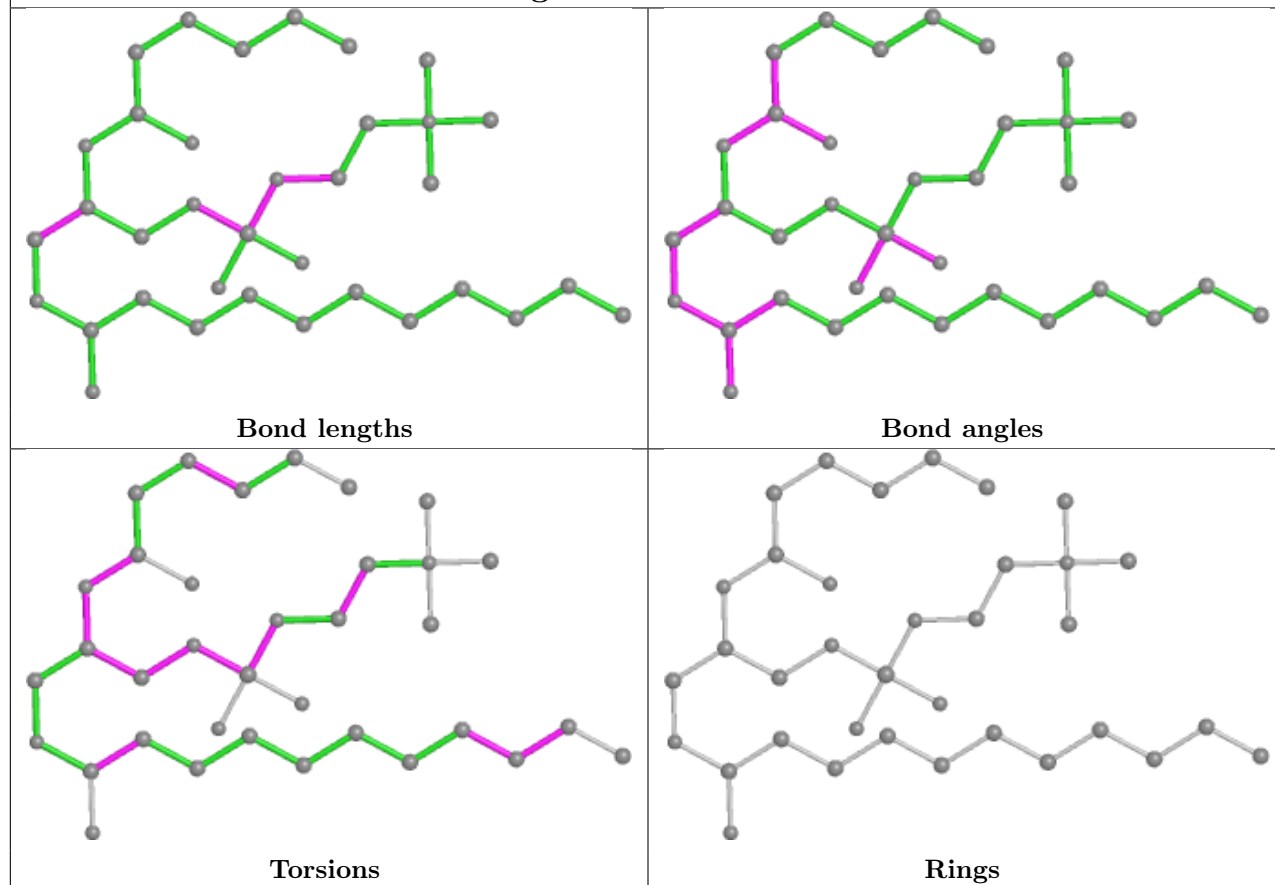




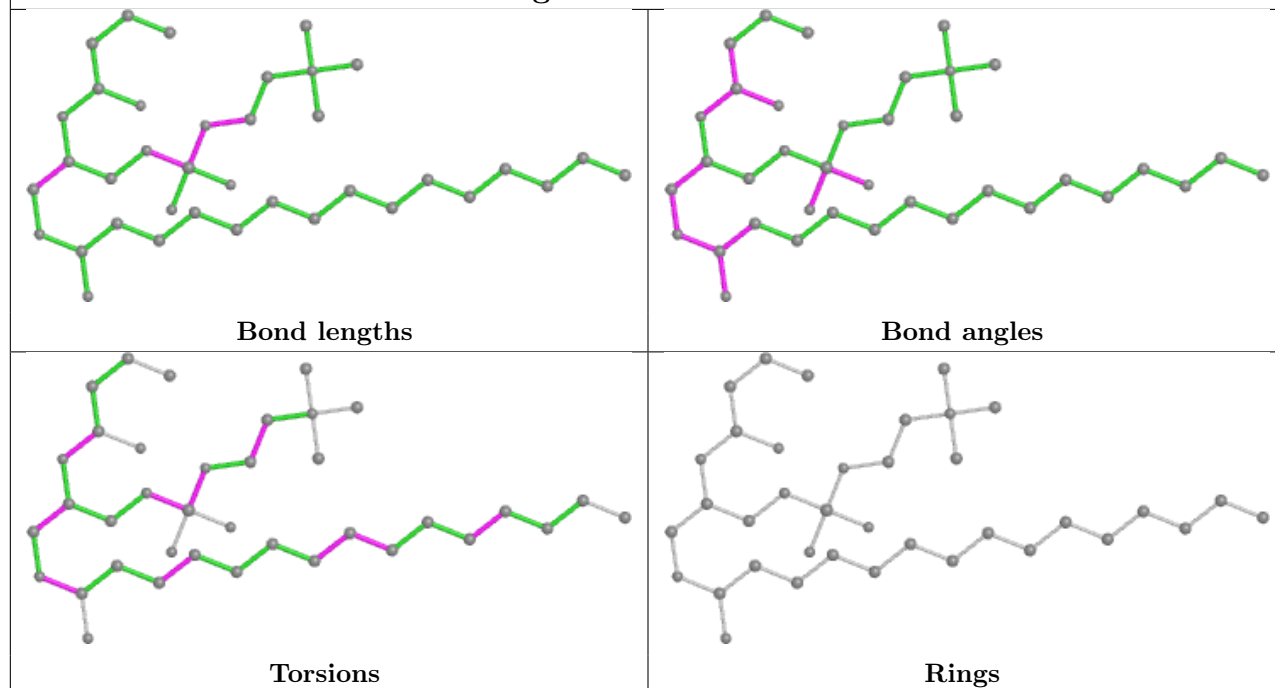


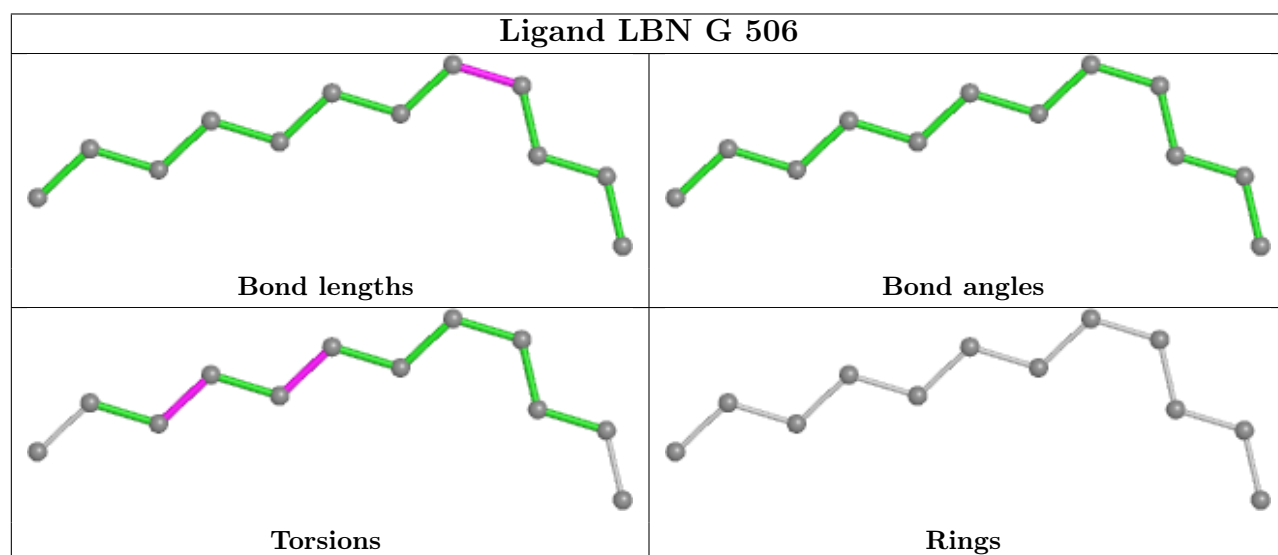
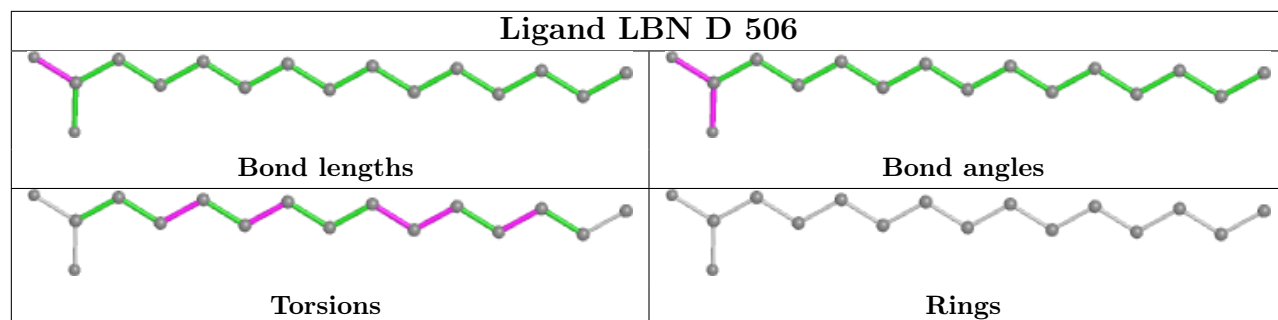


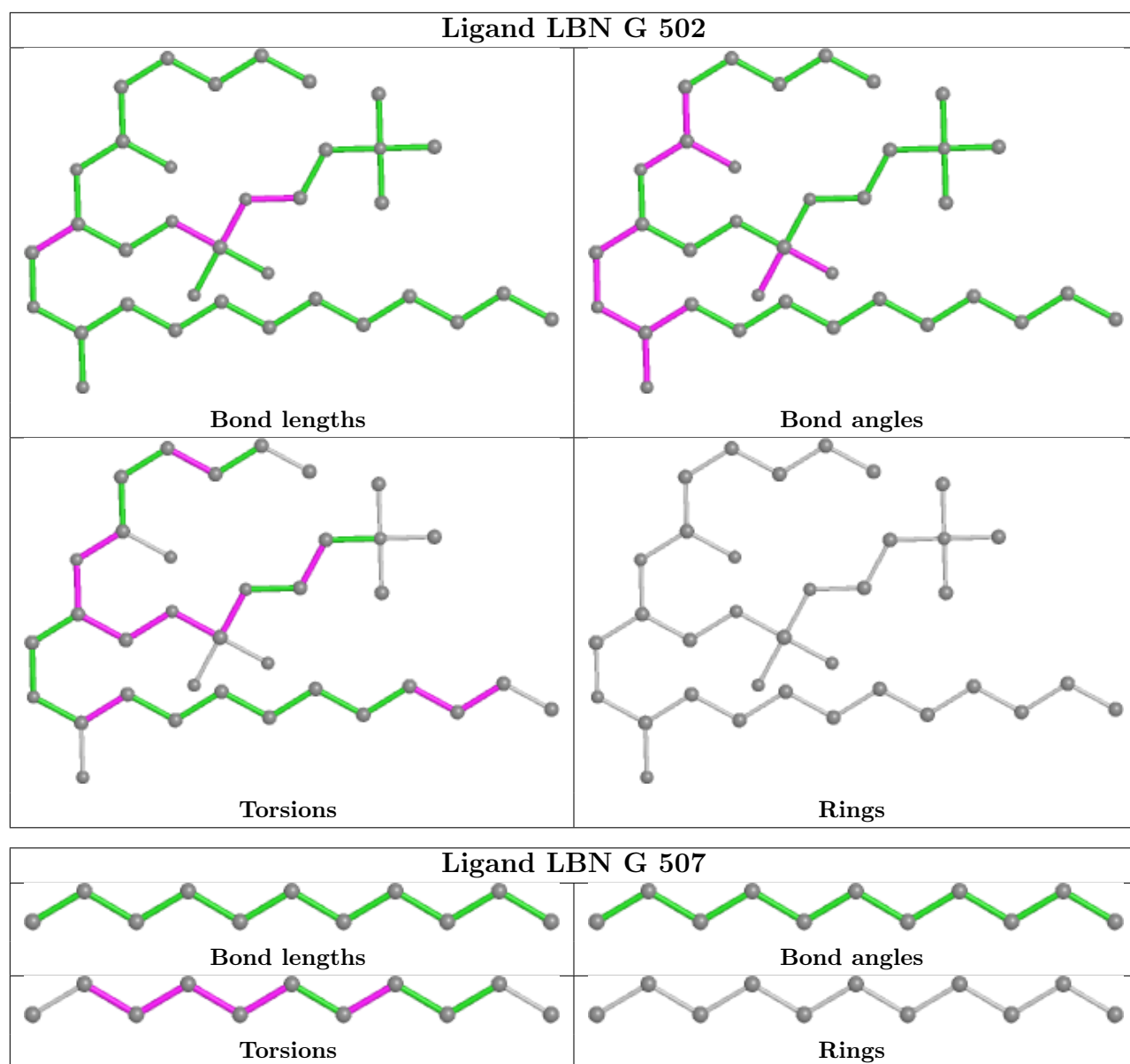
Ligand LBN C 502



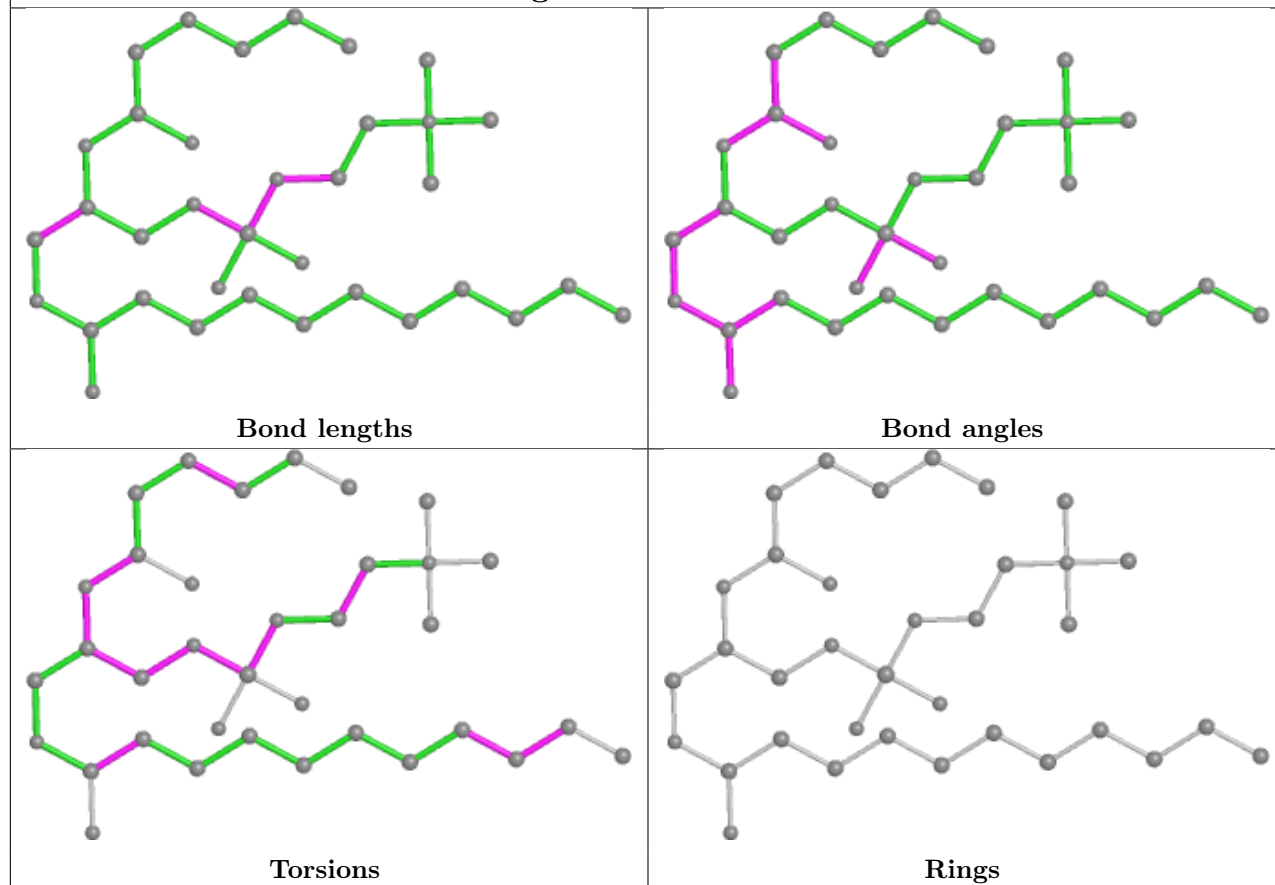
Ligand LBN F 503



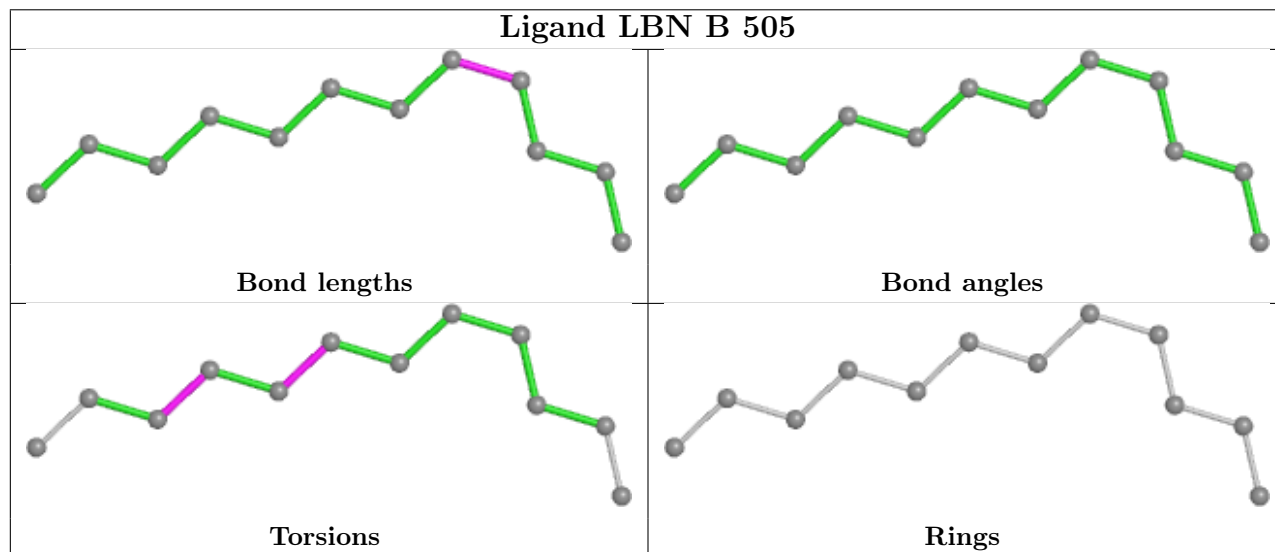


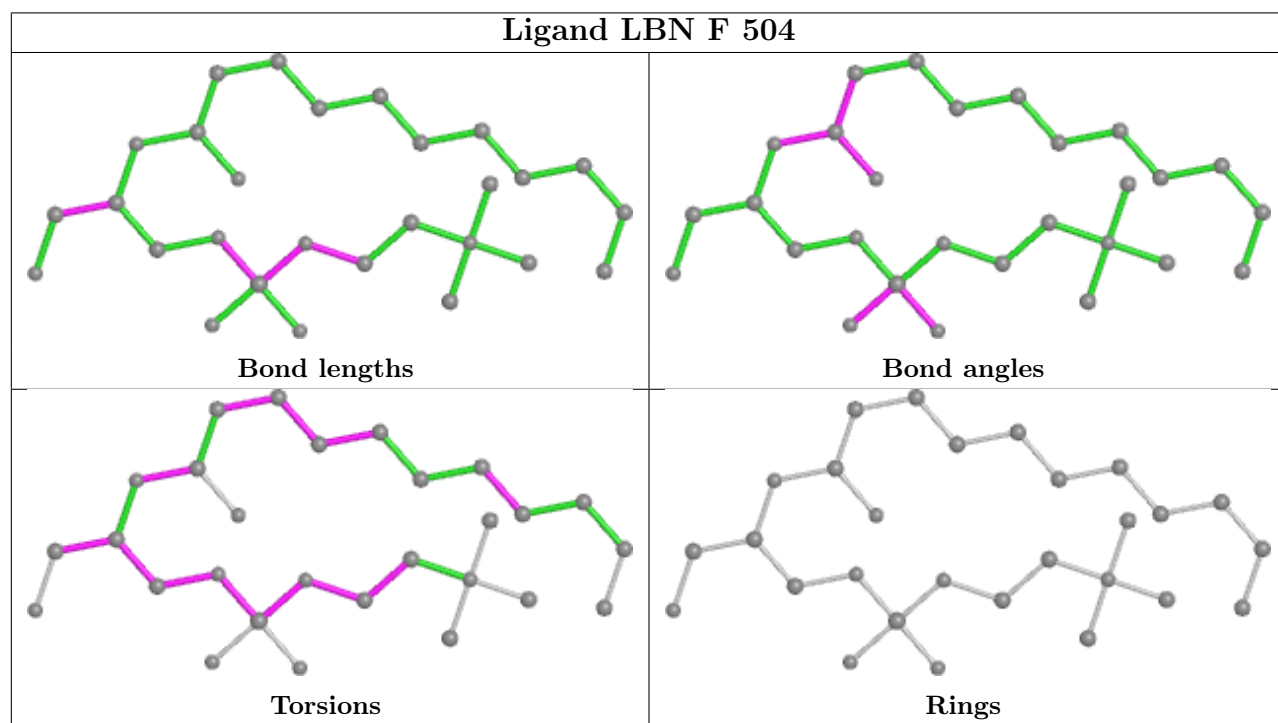
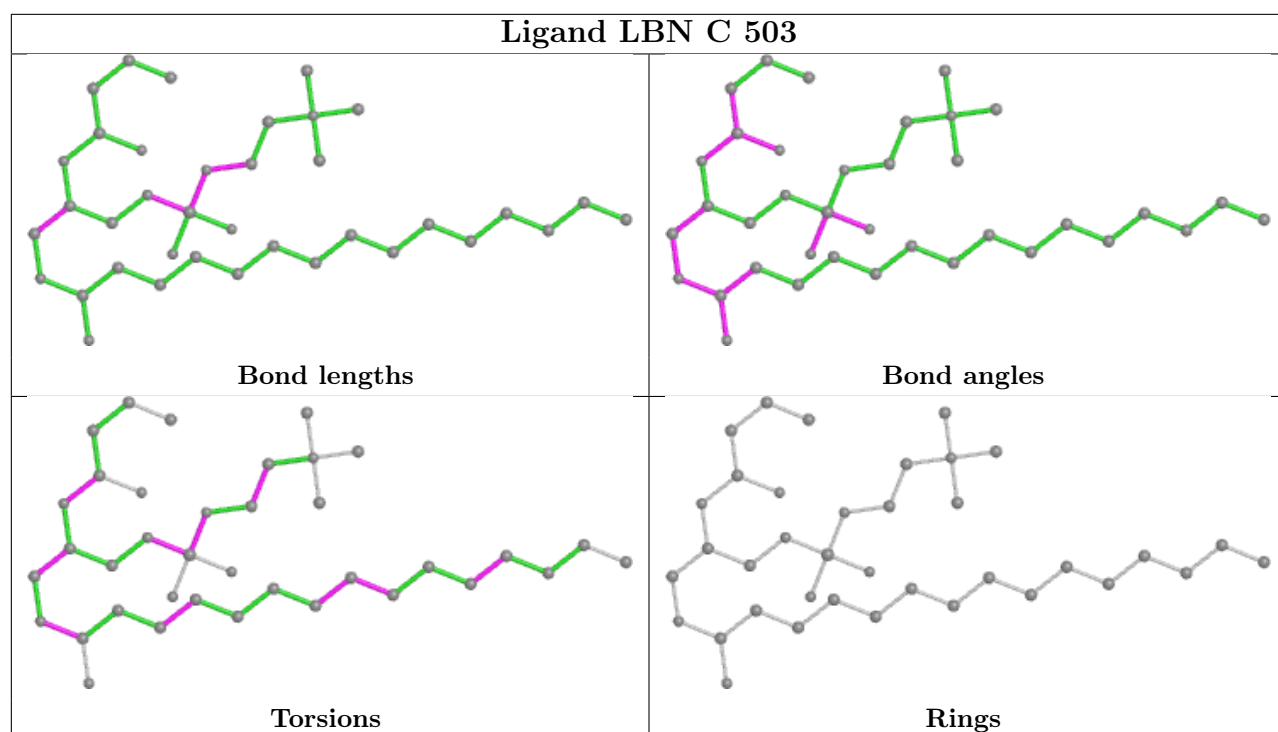


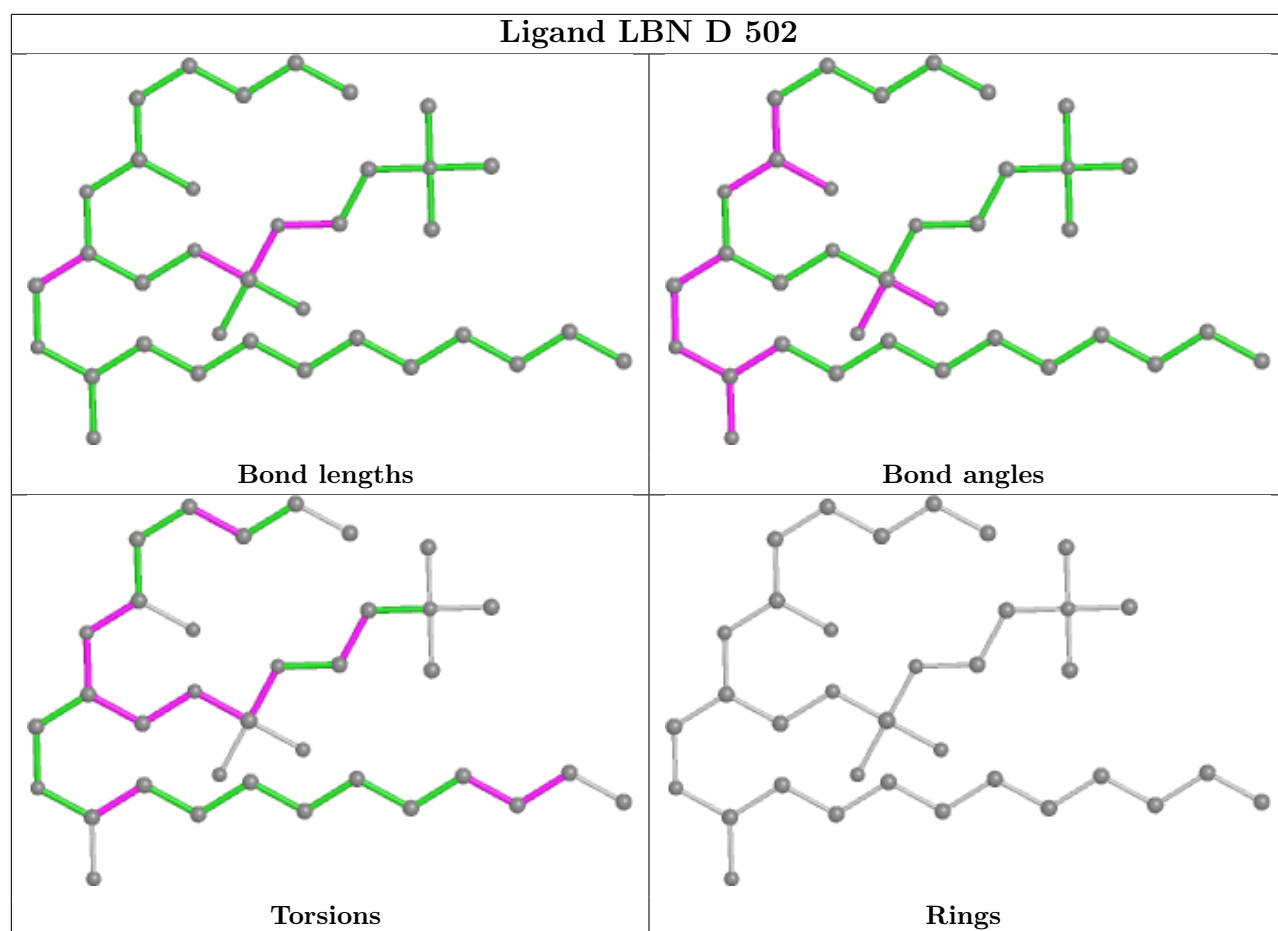
Ligand LBN B 502



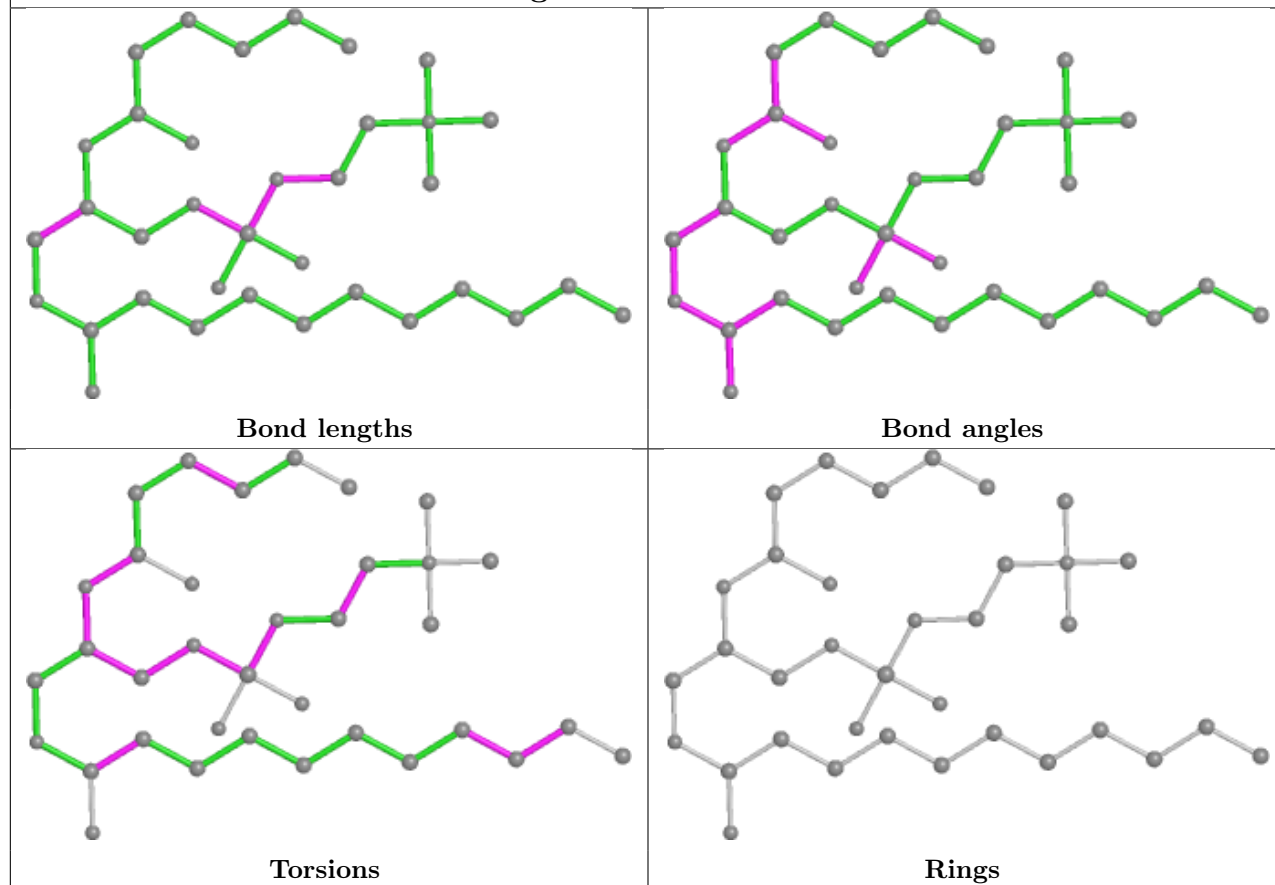
Ligand LBN B 505



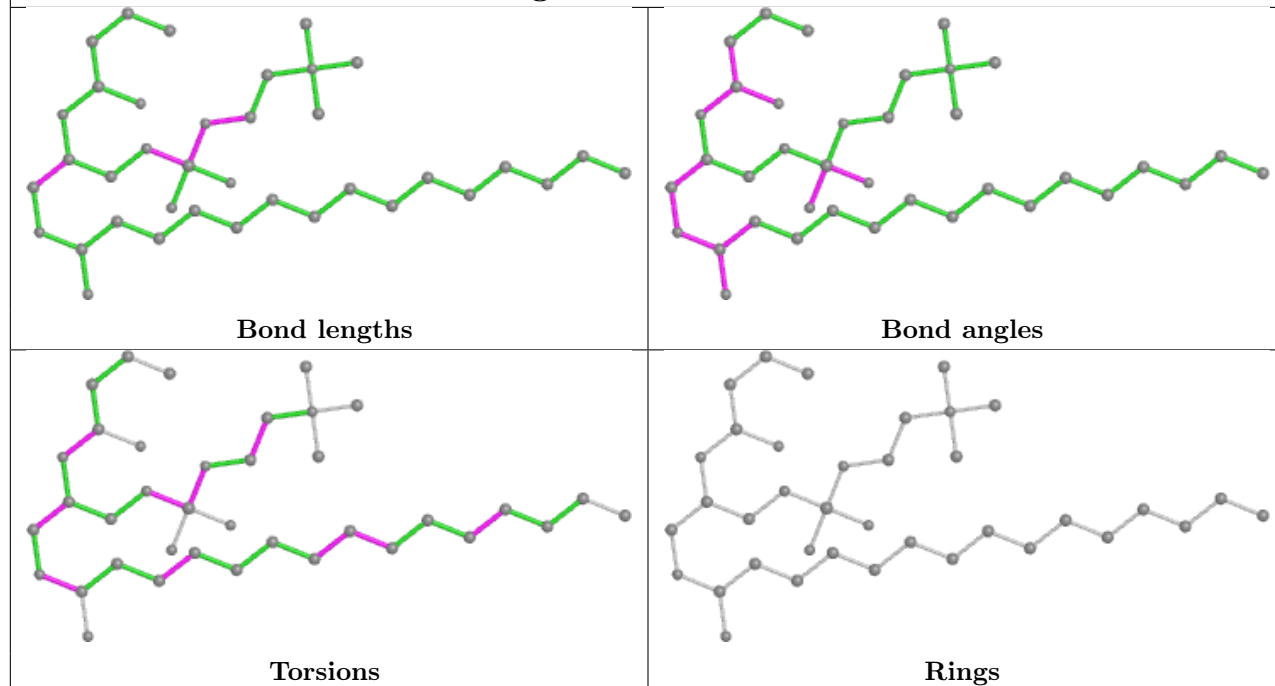


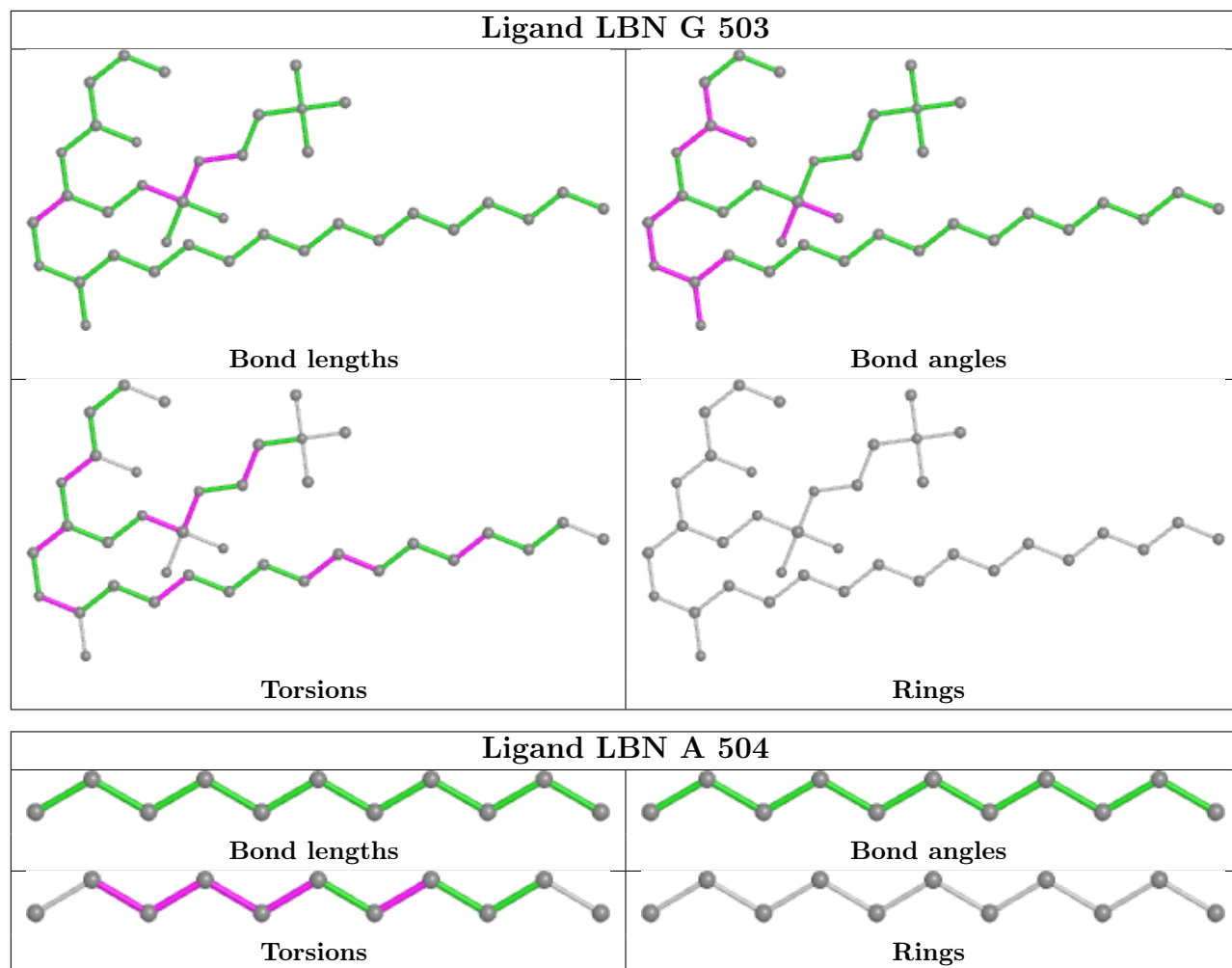


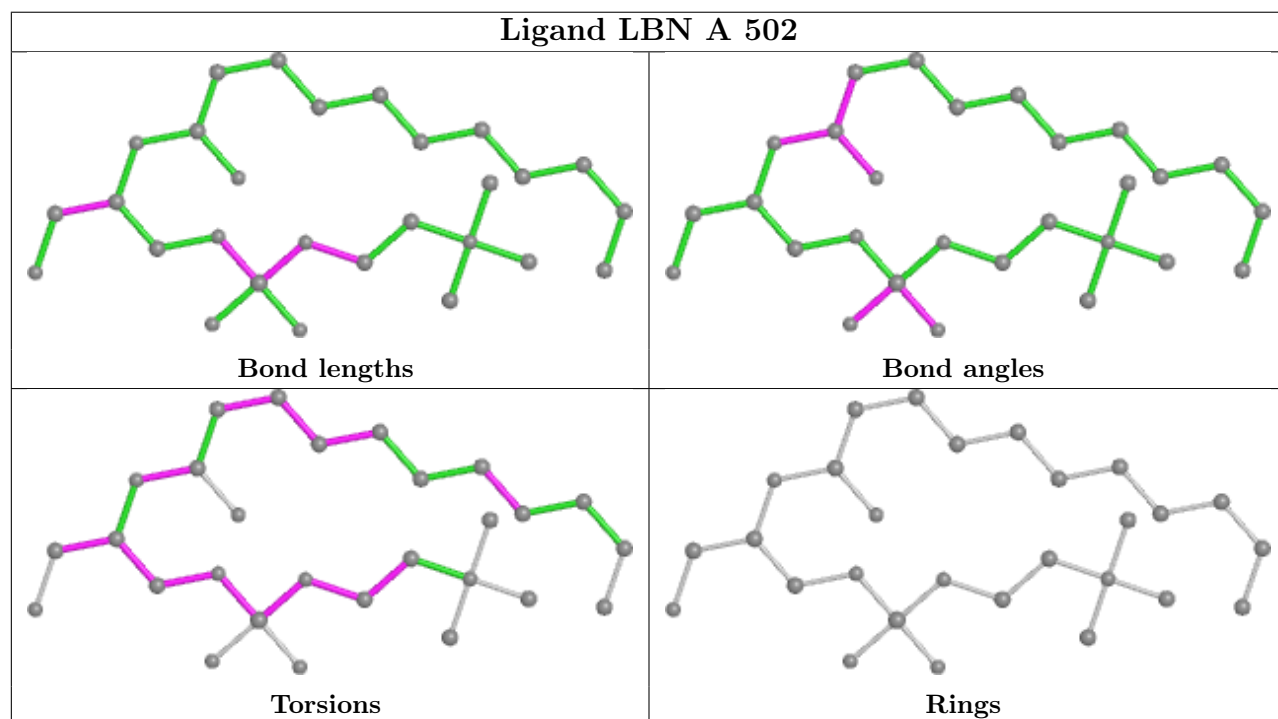
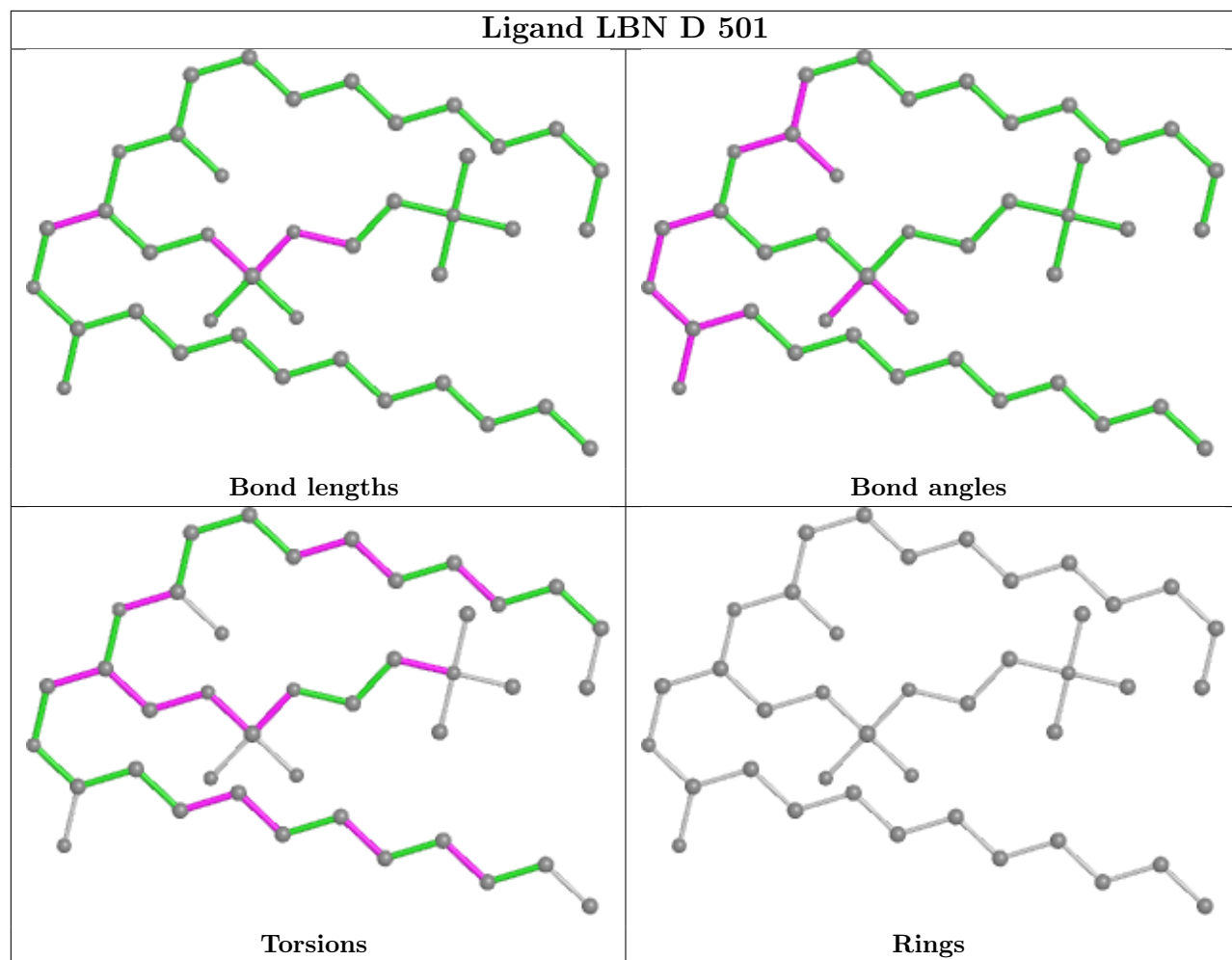
Ligand LBN A 506

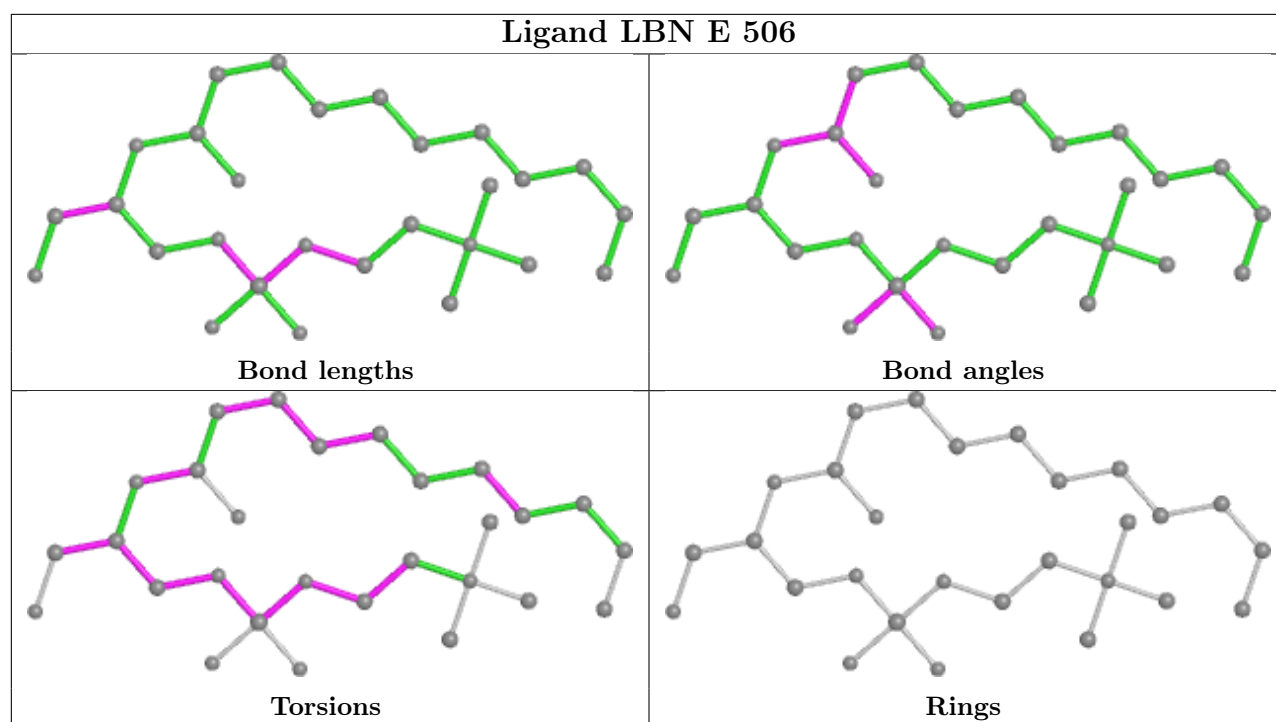


Ligand LBN B 503









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.

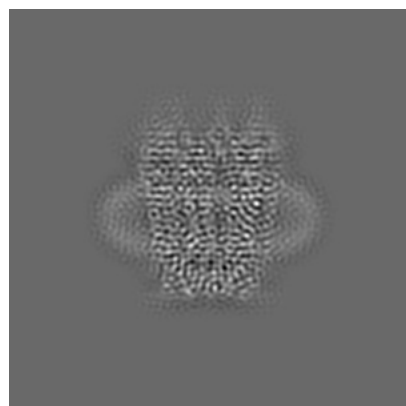
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31490. These allow visual inspection of the internal detail of the map and identification of artifacts.

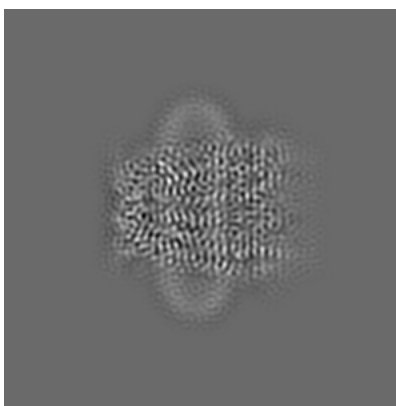
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

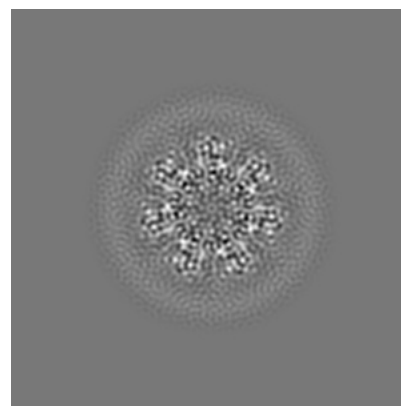
6.1.1 Primary map



X

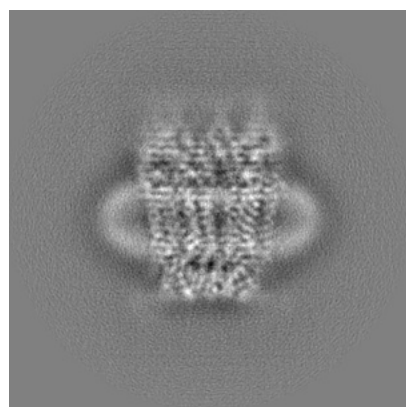


Y

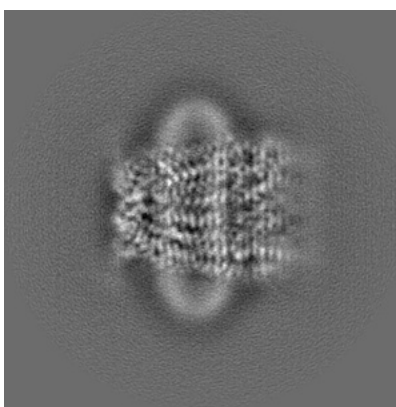


Z

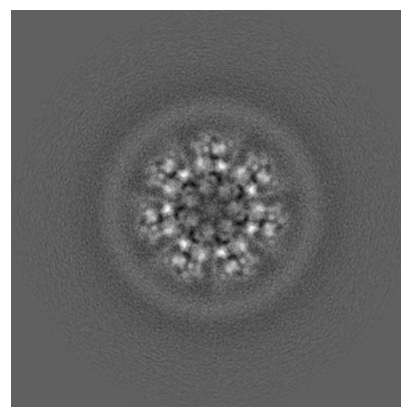
6.1.2 Raw map



X



Y



Z

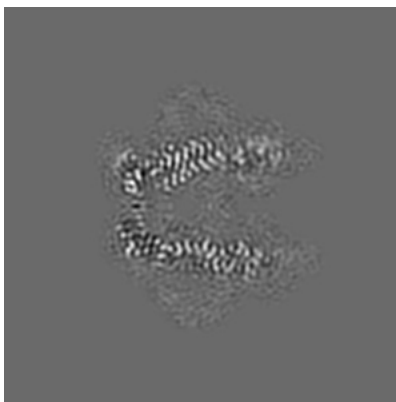
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

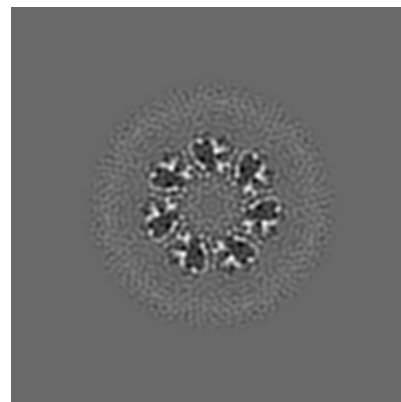
6.2.1 Primary map



X Index: 140

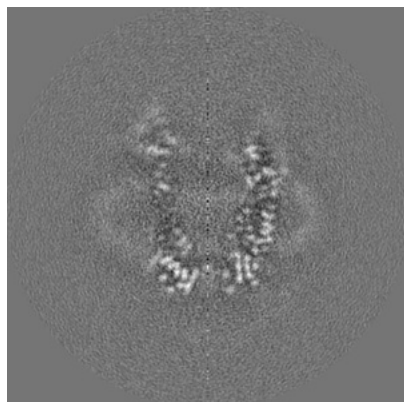


Y Index: 140

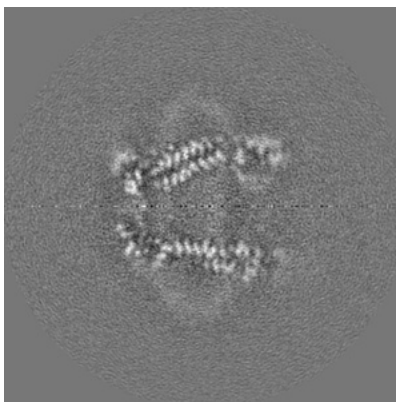


Z Index: 140

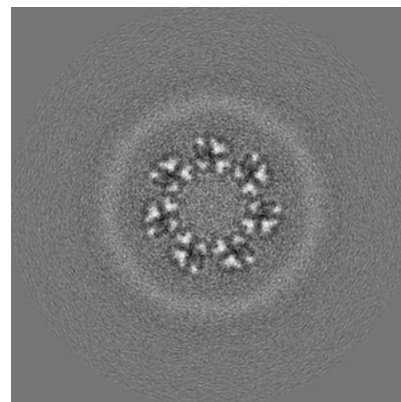
6.2.2 Raw map



X Index: 140



Y Index: 140



Z Index: 140

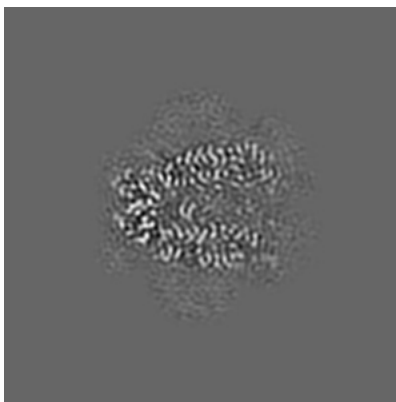
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

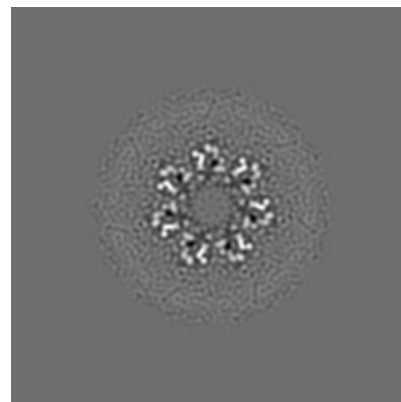
6.3.1 Primary map



X Index: 167

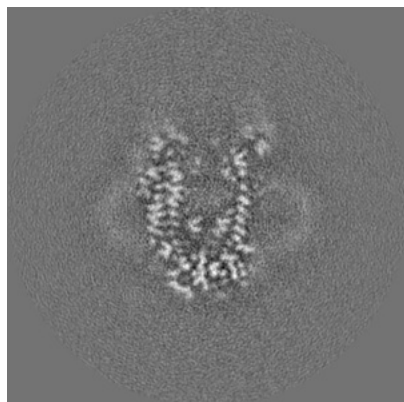


Y Index: 163

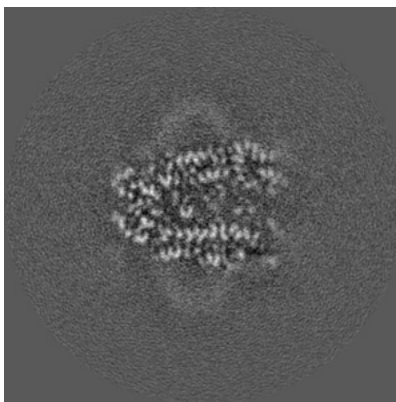


Z Index: 121

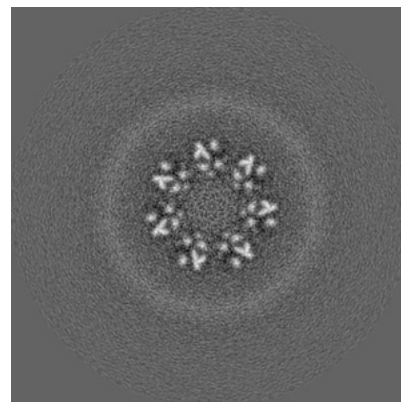
6.3.2 Raw map



X Index: 119



Y Index: 164

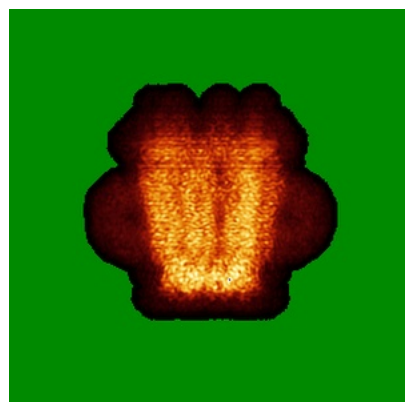


Z Index: 132

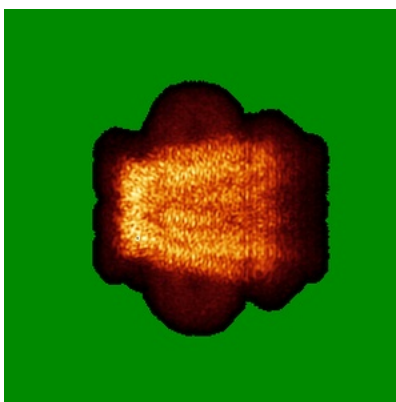
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

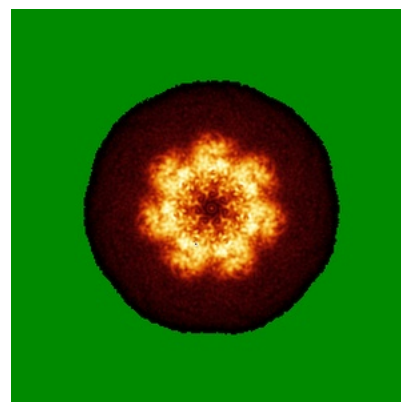
6.4.1 Primary map



X

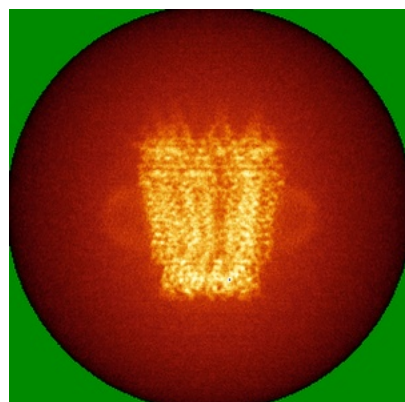


Y

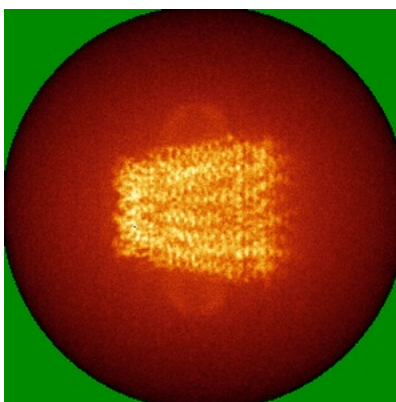


Z

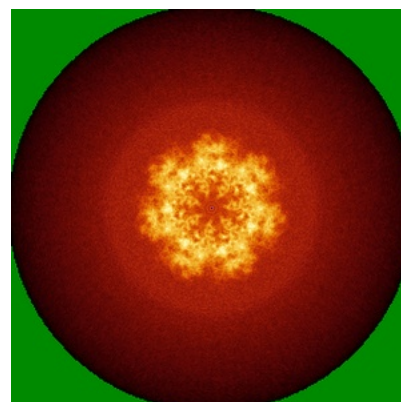
6.4.2 Raw map



X



Y

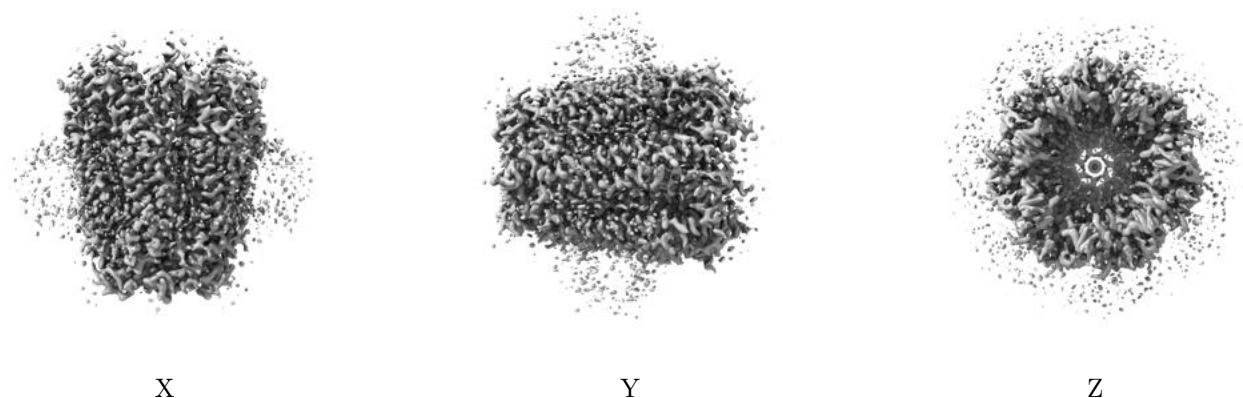


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

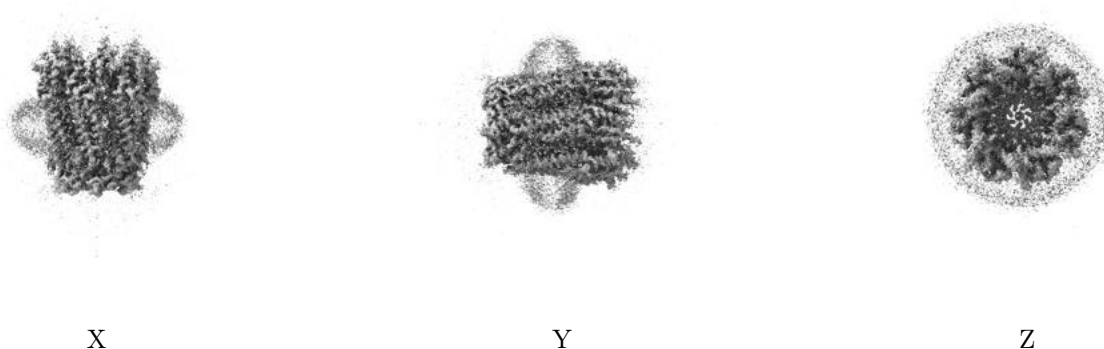
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

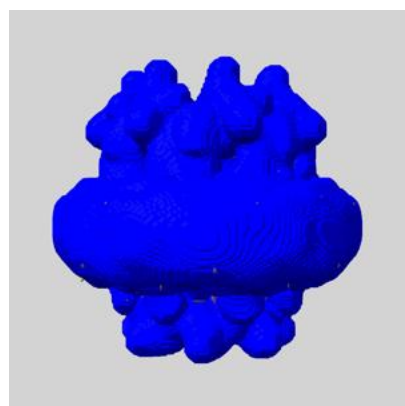
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

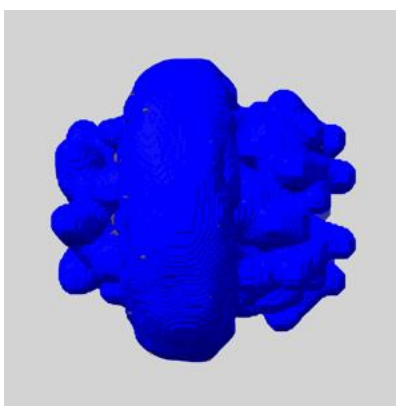
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

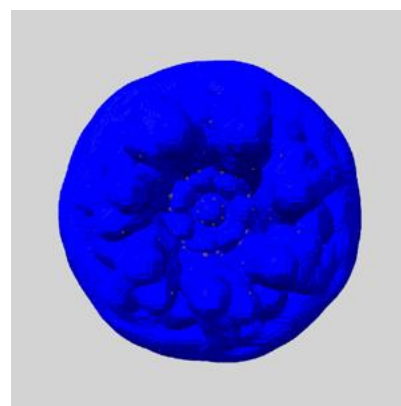
6.6.1 emd_31490_msk_1.map [i](#)



X



Y

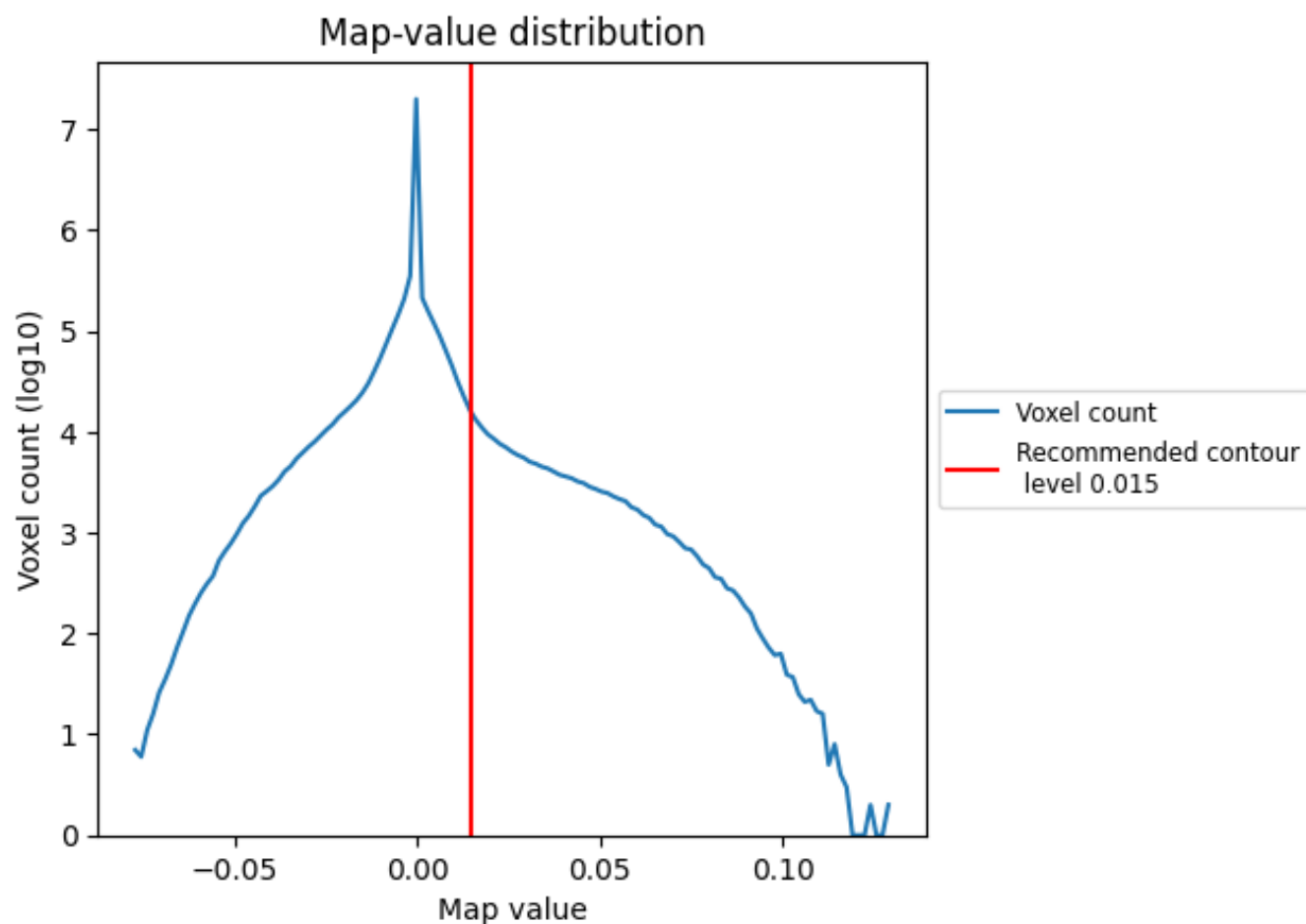


Z

7 Map analysis [i](#)

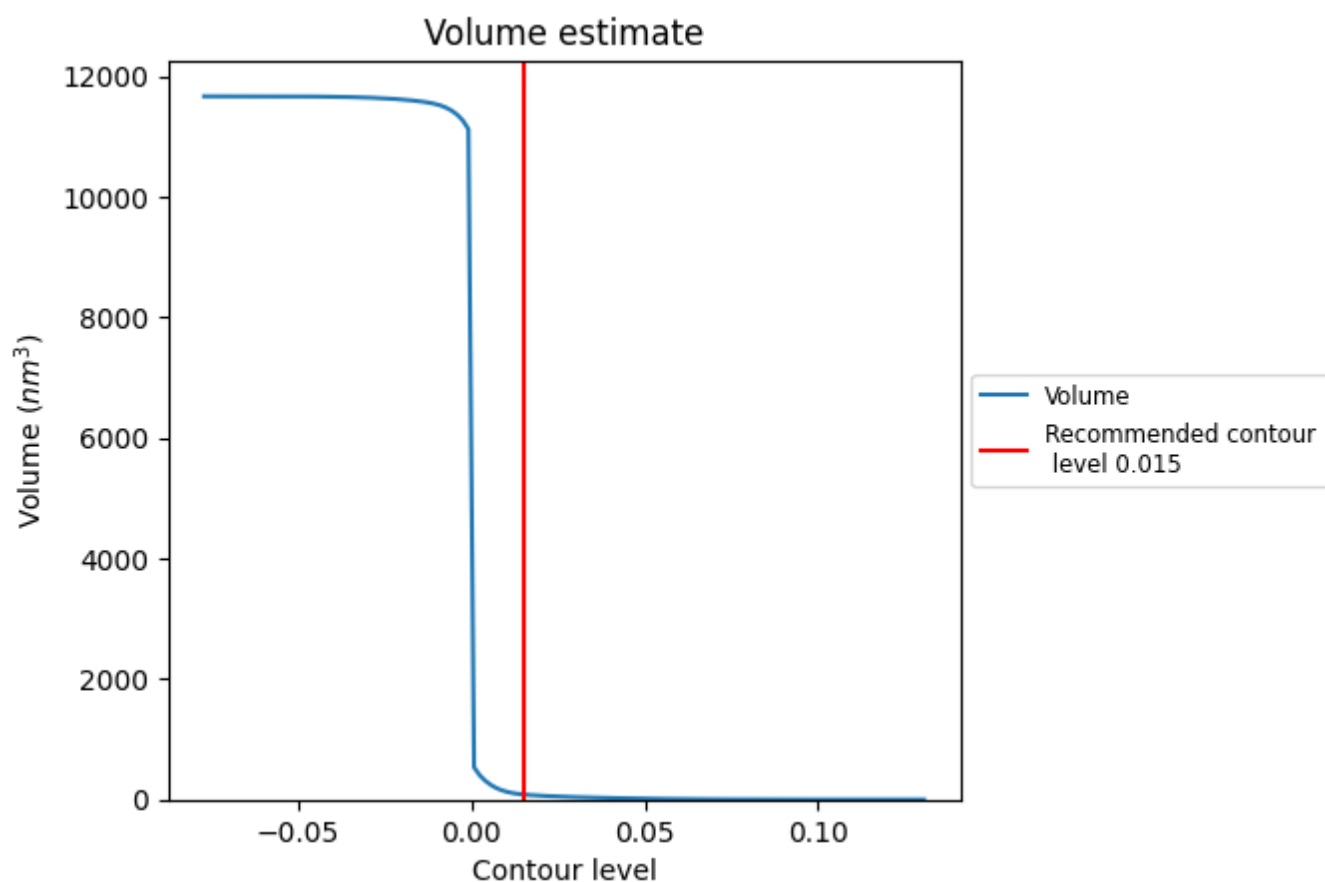
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

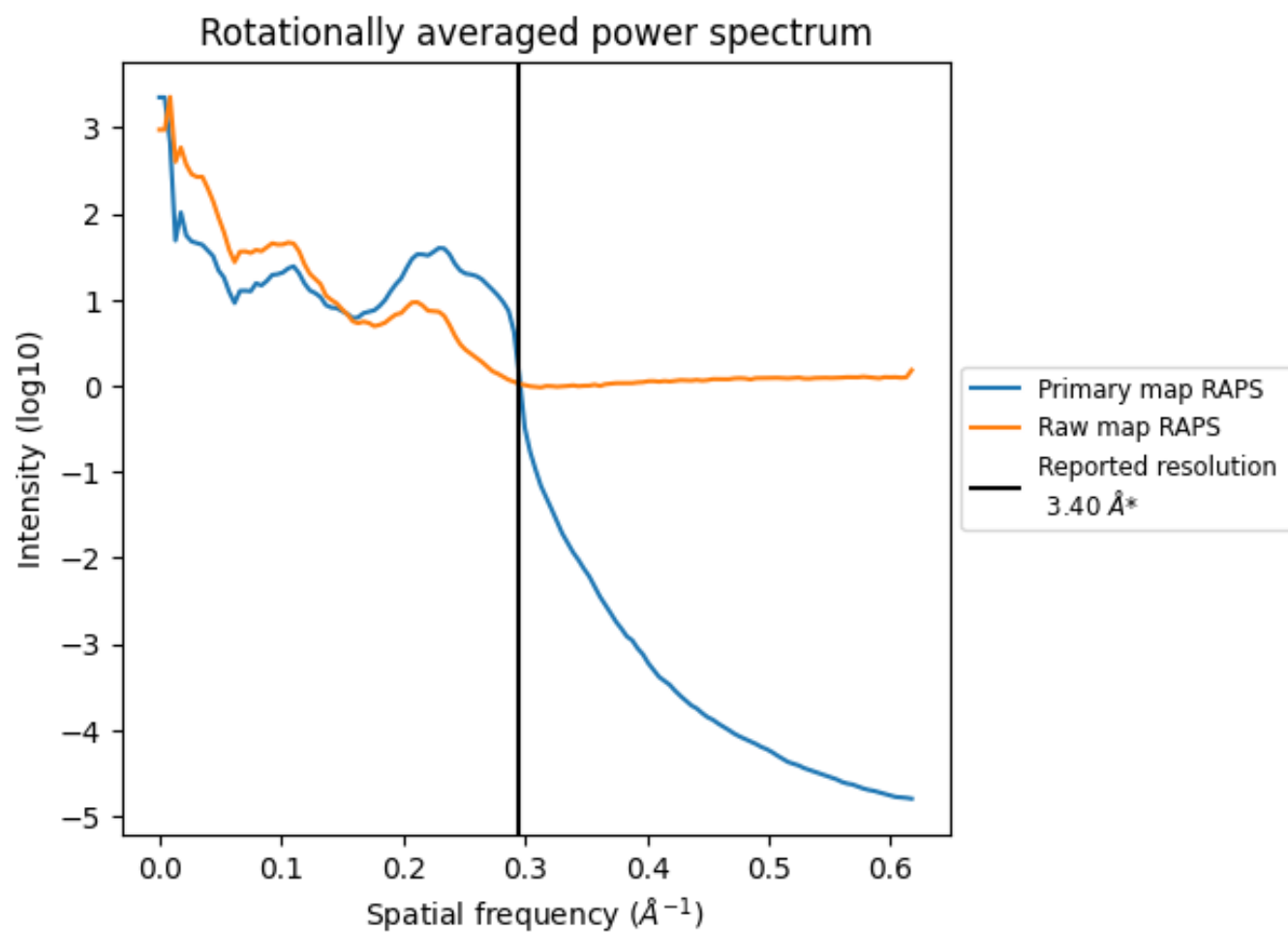
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm³; this corresponds to an approximate mass of 76 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

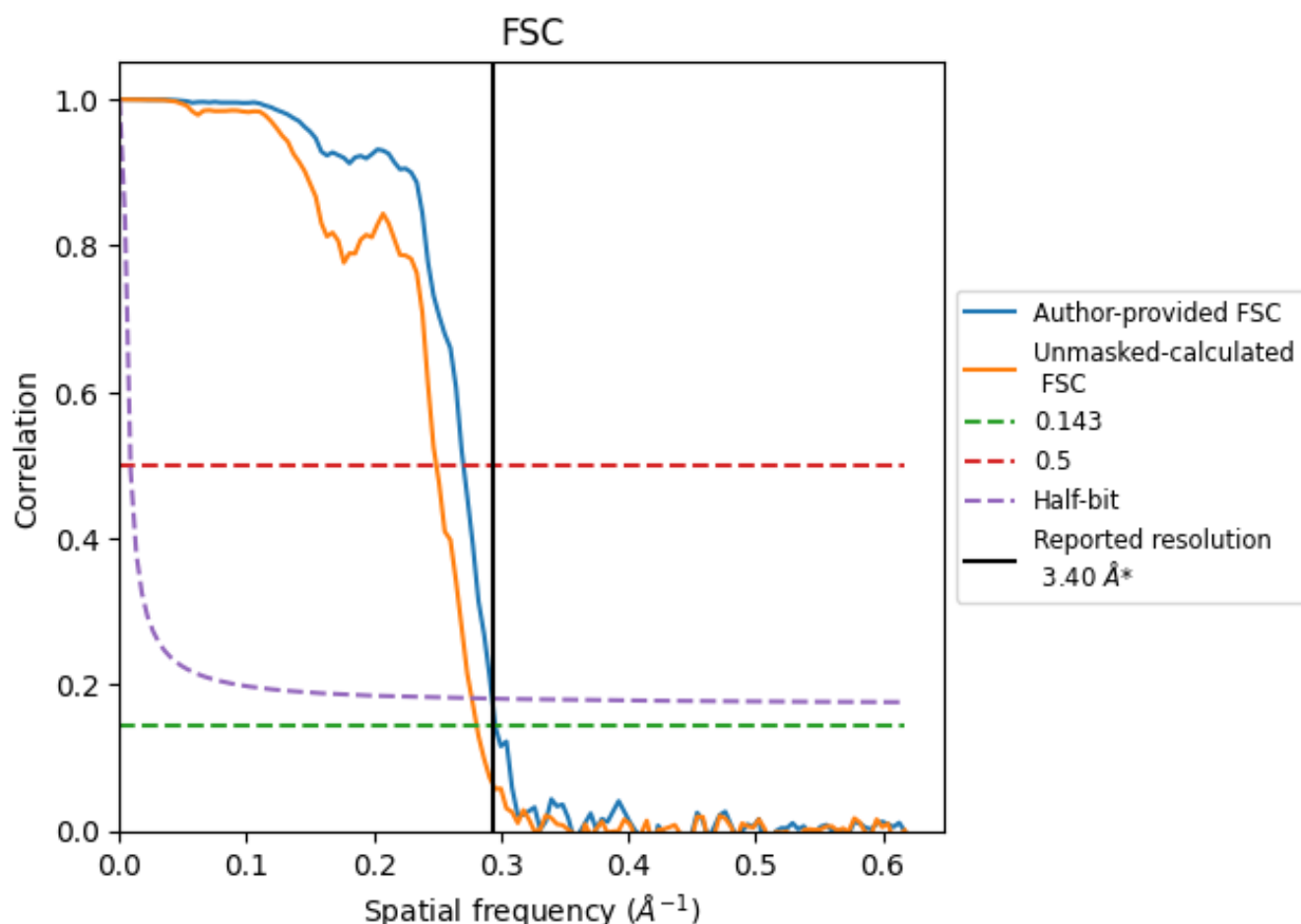


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

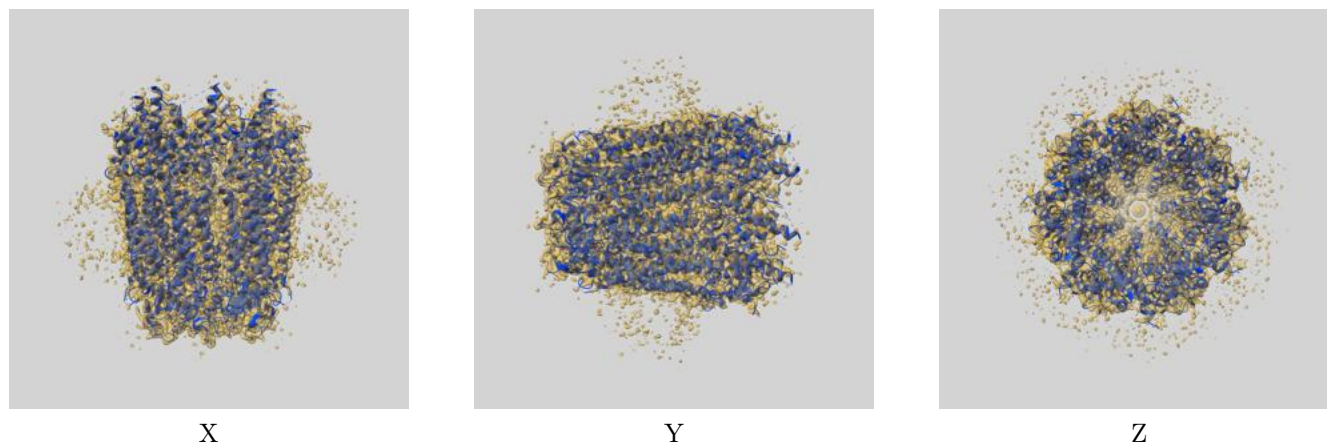
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.70	3.41
Unmasked-calculated*	3.56	4.01	3.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

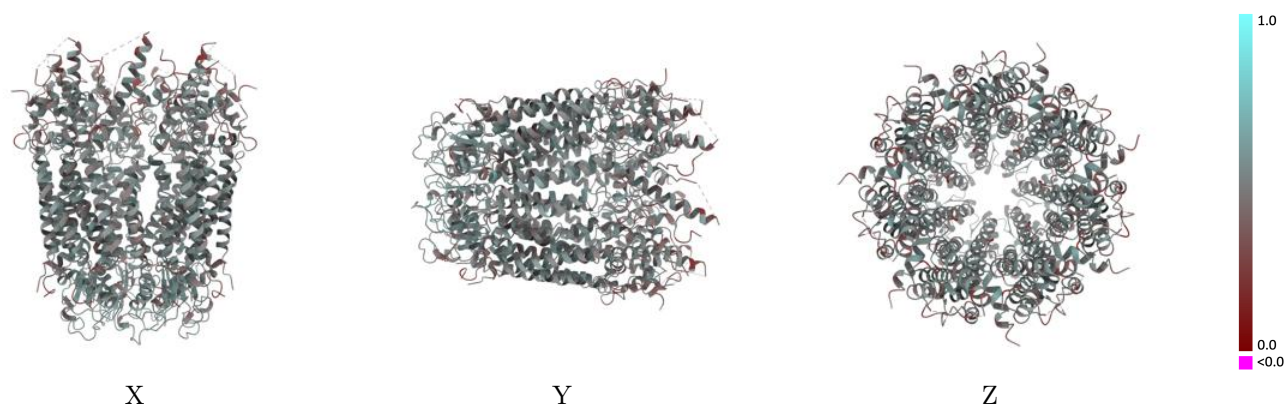
This section contains information regarding the fit between EMDB map EMD-31490 and PDB model 7F8N. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



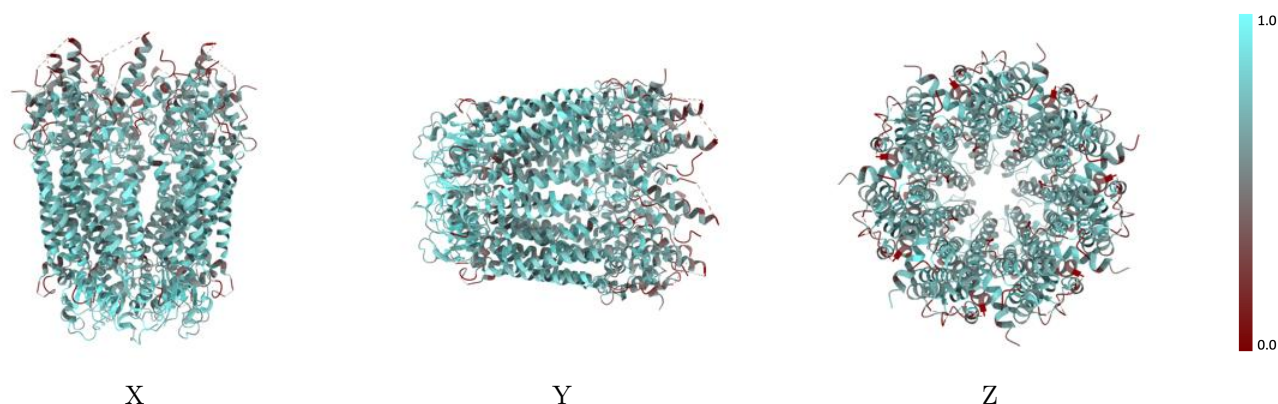
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



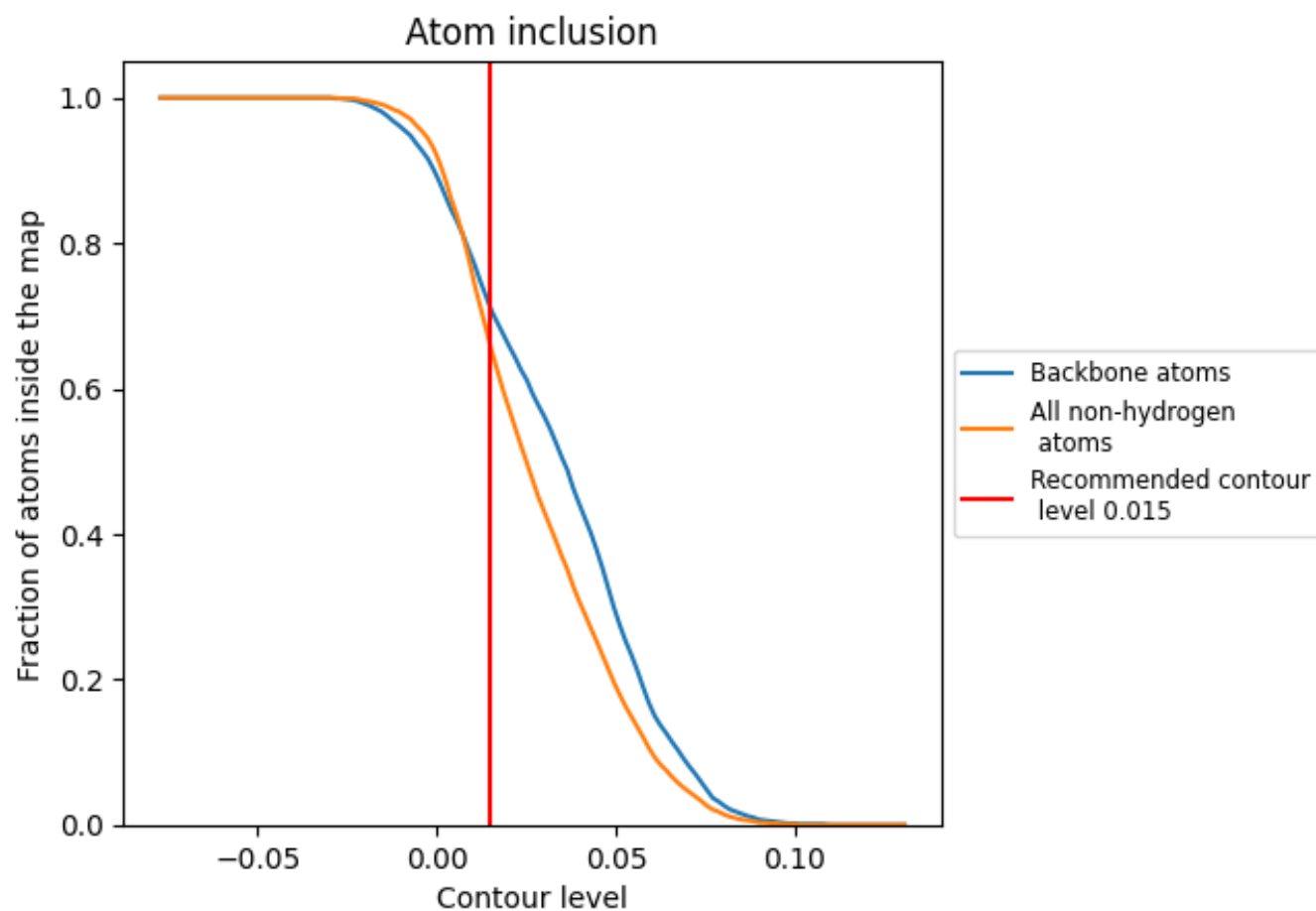
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6570	<div><div></div></div> 0.4880
A	<div><div></div></div> 0.6650	<div><div></div></div> 0.4890
B	<div><div></div></div> 0.6620	<div><div></div></div> 0.4920
C	<div><div></div></div> 0.6590	<div><div></div></div> 0.4880
D	<div><div></div></div> 0.6520	<div><div></div></div> 0.4860
E	<div><div></div></div> 0.6490	<div><div></div></div> 0.4880
F	<div><div></div></div> 0.6600	<div><div></div></div> 0.4920
G	<div><div></div></div> 0.6550	<div><div></div></div> 0.4840

1.0

0.0

<0.0