



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:57 AM UTC

PDB ID : 7W9P / pdb_00007w9p
EMDB ID : EMD-32371
Title : Cryo-EM structure of human Nav1.7(E406K) in complex with auxiliary beta subunits, huwentoxin-IV and saxitoxin (S6IV pi helix conformer)
Authors : Yan, N.; Huang, G.; Liu, D.; Wei, P.; Shen, H.
Deposited on : 2021-12-10
Resolution : 2.90 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

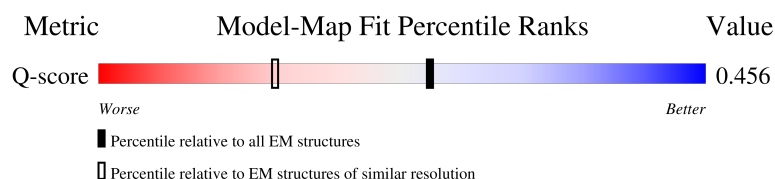
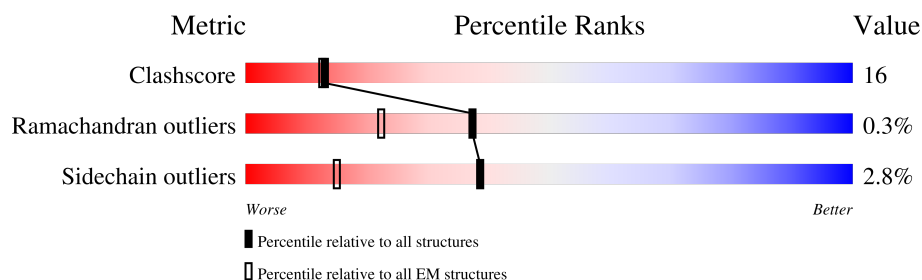
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	2031	11% 50% 19% 30%
2	B	218	56% 22% 21%
3	C	215	44% 48% 7% 45%
4	D	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	E	2	 100%
4	F	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	Y01	A	2006	-	-	X	-
9	LPE	A	2014	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 14817 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 Sodium channel protein type 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1413	Total	C	N	O	S	0	0
			11367	7504	1789	1989	85		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	expression tag	UNP Q15858
A	-41	ALA	-	expression tag	UNP Q15858
A	-40	SER	-	expression tag	UNP Q15858
A	-39	TRP	-	expression tag	UNP Q15858
A	-38	SER	-	expression tag	UNP Q15858
A	-37	HIS	-	expression tag	UNP Q15858
A	-36	PRO	-	expression tag	UNP Q15858
A	-35	GLN	-	expression tag	UNP Q15858
A	-34	PHE	-	expression tag	UNP Q15858
A	-33	GLU	-	expression tag	UNP Q15858
A	-32	LYS	-	expression tag	UNP Q15858
A	-31	GLY	-	expression tag	UNP Q15858
A	-30	GLY	-	expression tag	UNP Q15858
A	-29	GLY	-	expression tag	UNP Q15858
A	-28	ALA	-	expression tag	UNP Q15858
A	-27	ARG	-	expression tag	UNP Q15858
A	-26	GLY	-	expression tag	UNP Q15858
A	-25	GLY	-	expression tag	UNP Q15858
A	-24	SER	-	expression tag	UNP Q15858
A	-23	GLY	-	expression tag	UNP Q15858
A	-22	GLY	-	expression tag	UNP Q15858
A	-21	GLY	-	expression tag	UNP Q15858
A	-20	SER	-	expression tag	UNP Q15858
A	-19	TRP	-	expression tag	UNP Q15858
A	-18	SER	-	expression tag	UNP Q15858
A	-17	HIS	-	expression tag	UNP Q15858
A	-16	PRO	-	expression tag	UNP Q15858
A	-15	GLN	-	expression tag	UNP Q15858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP Q15858
A	-13	GLU	-	expression tag	UNP Q15858
A	-12	LYS	-	expression tag	UNP Q15858
A	-11	GLY	-	expression tag	UNP Q15858
A	-10	PHE	-	expression tag	UNP Q15858
A	-9	ASP	-	expression tag	UNP Q15858
A	-8	TYR	-	expression tag	UNP Q15858
A	-7	LYS	-	expression tag	UNP Q15858
A	-6	ASP	-	expression tag	UNP Q15858
A	-5	ASP	-	expression tag	UNP Q15858
A	-4	ASP	-	expression tag	UNP Q15858
A	-3	ASP	-	expression tag	UNP Q15858
A	-2	LYS	-	expression tag	UNP Q15858
A	-1	GLY	-	expression tag	UNP Q15858
A	0	THR	-	expression tag	UNP Q15858
A	406	LYS	GLU	engineered mutation	UNP Q15858

- Molecule 2 is a protein called Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	173	Total	C	N	O	S	0	0
			1416	902	232	272	10		

- Molecule 3 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	119	Total	C	N	O	S	4	0
			980	615	172	183	10		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



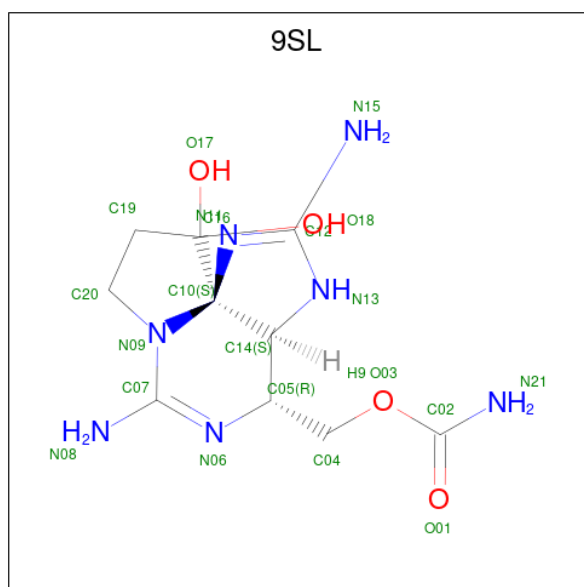
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	F	2	28	16	2	10	0	0

- Molecule 5 is [(3aS,4R,10aS)-2,6-diamino-10,10-dihydroxy-3a,4,9,10-tetrahydro-3H,8H-pyrrolo[1,2-c]purin-4-yl]methyl carbamate (CCD ID: 9SL) (formula: C₁₀H₁₇N₇O₄) (labeled as "Ligand of Interest" by depositor).



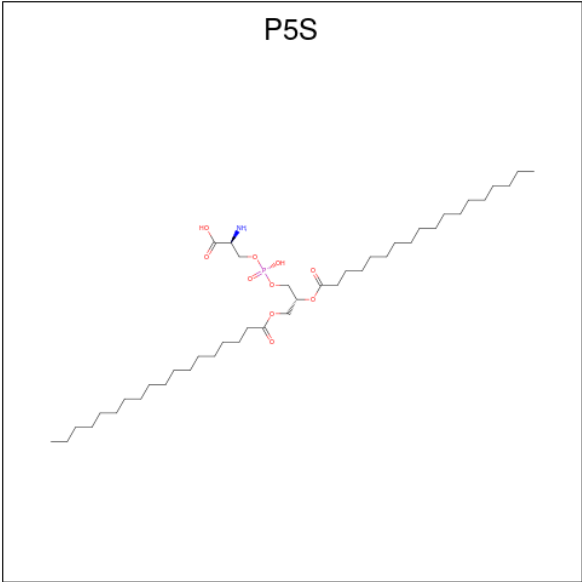
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	21	10	7	4	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



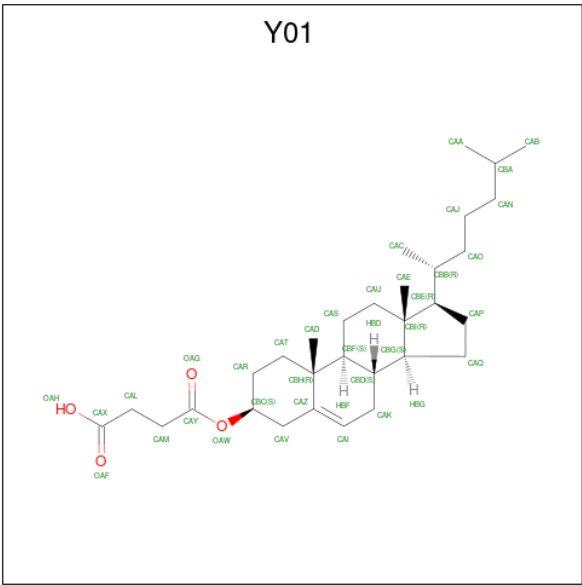
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			35	24	1	9	1	
7	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
7	A	1	Total	C	N	O	P	0
			34	22	1	10	1	

- Molecule 8 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



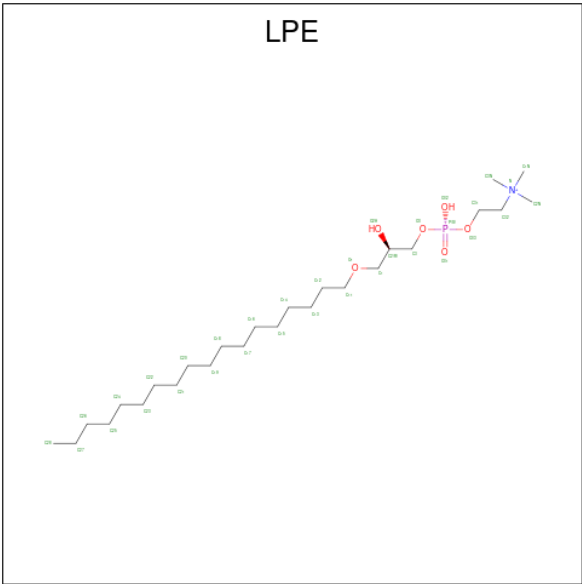
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			35	31	4	

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Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	

- Molecule 9 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: LPE) (formula: C₂₆H₅₇NO₆P).



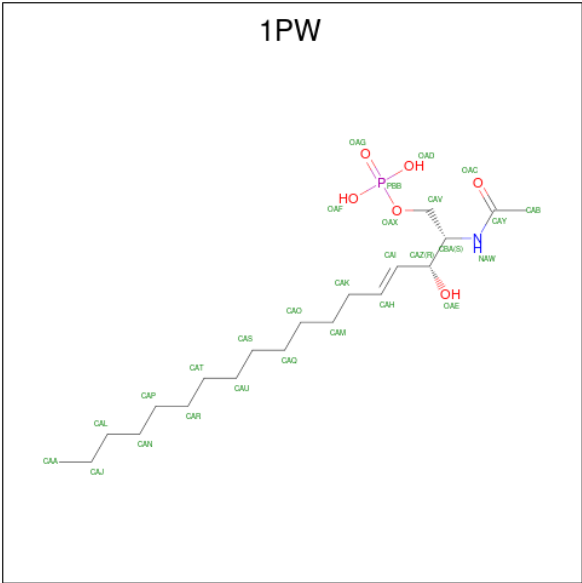
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
9	A	1	Total	C	N	O	P	0
			20	12	1	6	1	
9	A	1	Total	C	N	O	P	0
			22	14	1	6	1	
9	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
9	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
9	A	1	Total	C	N	O	P	0
			25	17	1	6	1	

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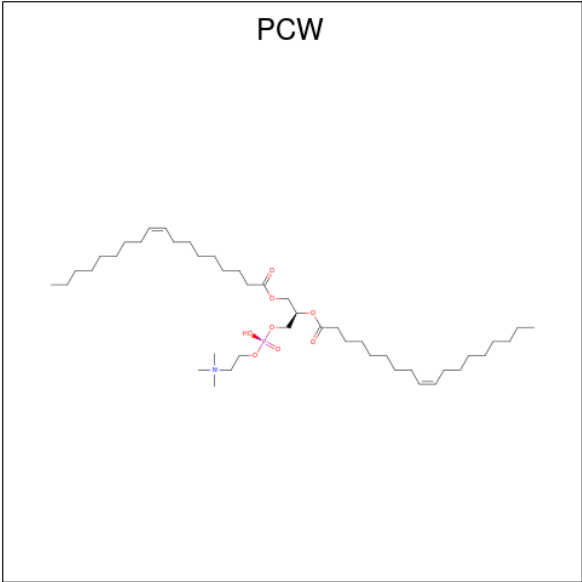
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
9	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
9	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
9	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
9	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
9	A	1	Total	C	N	O	P	0
			17	9	1	6	1	
9	B	1	Total	C	N	O	P	0
			17	9	1	6	1	

- Molecule 10 is (2S,3R,4E)-2-(acetylamino)-3-hydroxyoctadec-4-en-1-yl dihydrogen phosphate (CCD ID: 1PW) (formula: C₂₀H₄₀NO₆P).



Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	O	P	0
			24	18	5	1	

- Molecule 11 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).

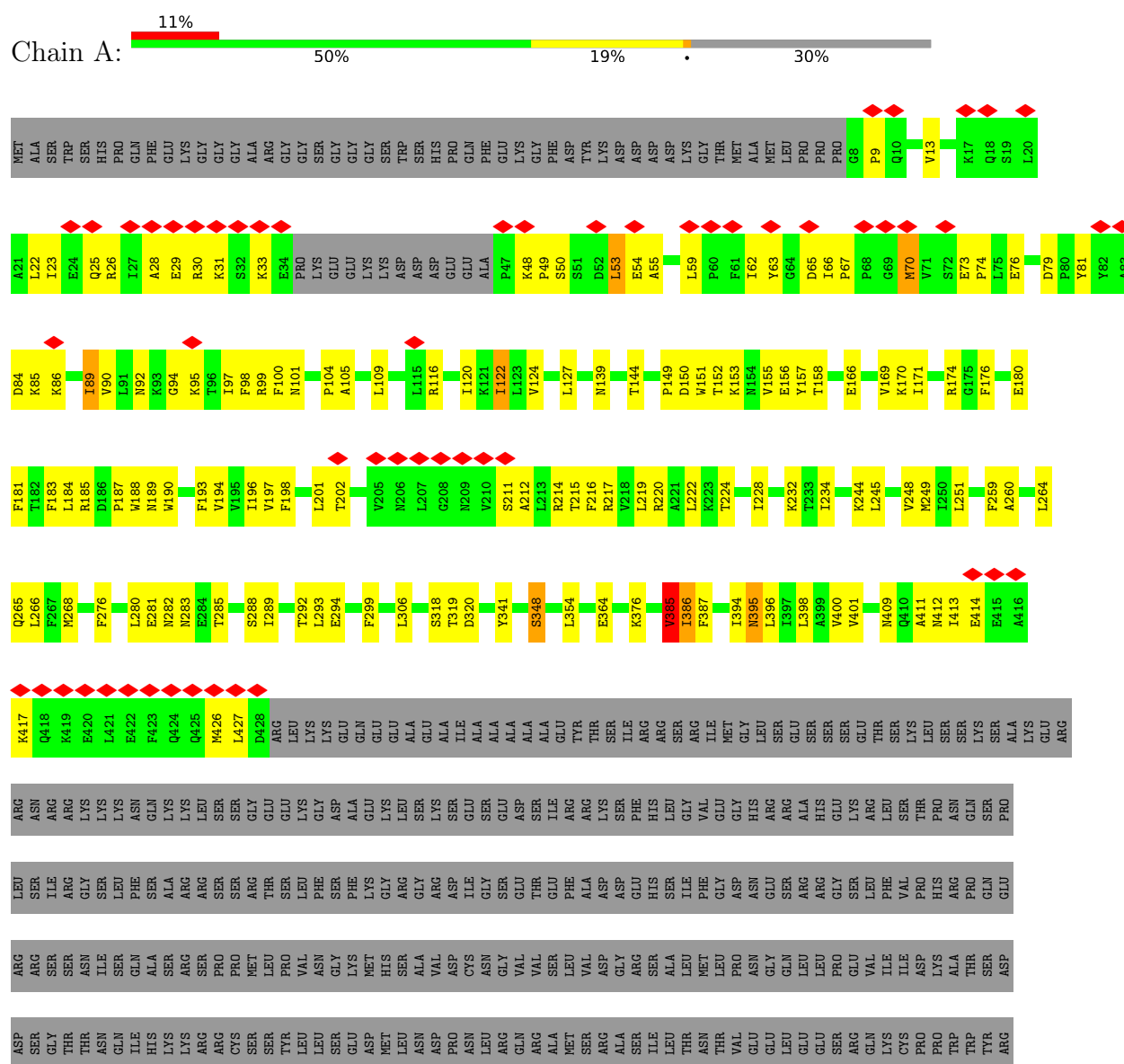


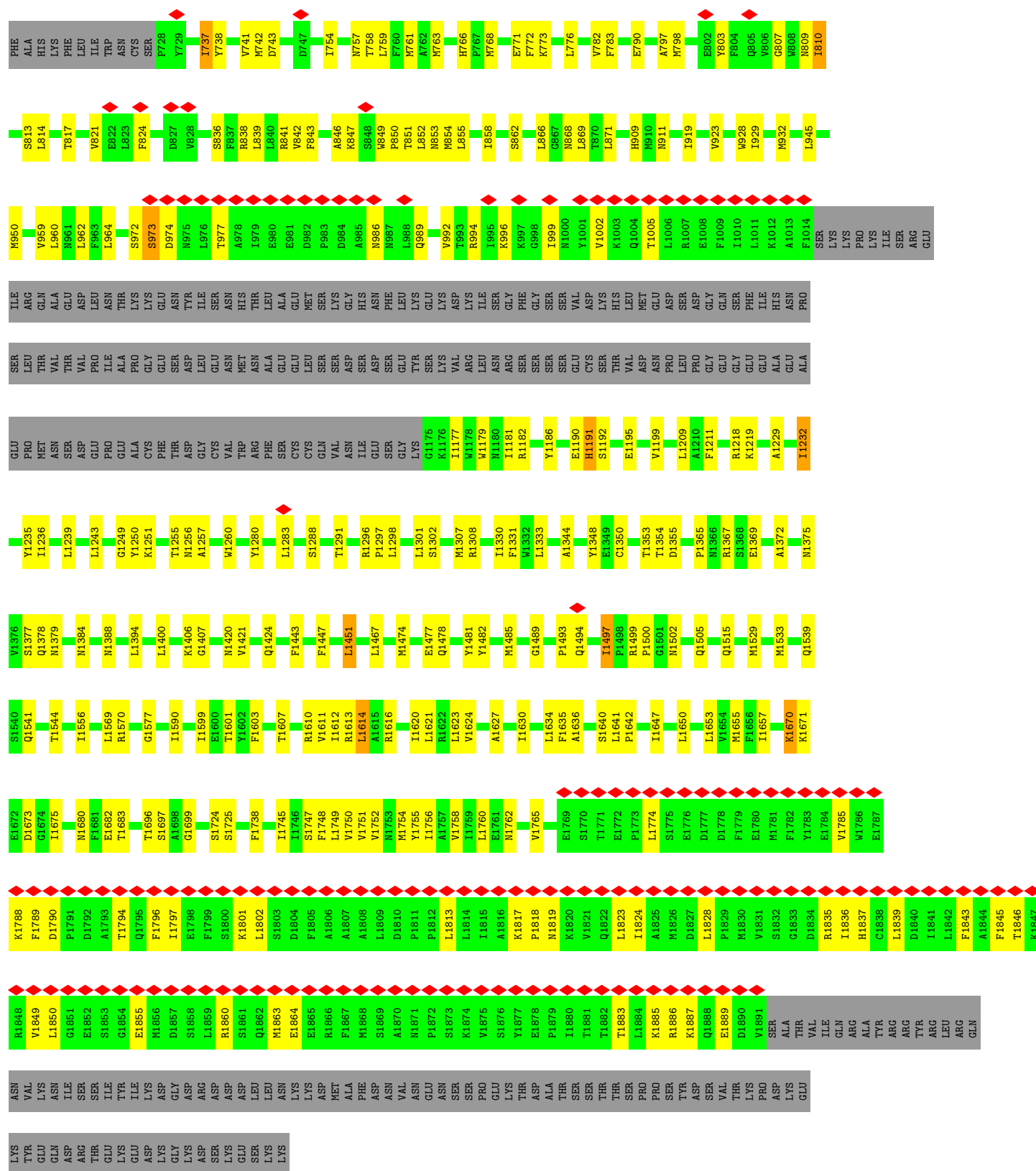
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
11	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	

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.

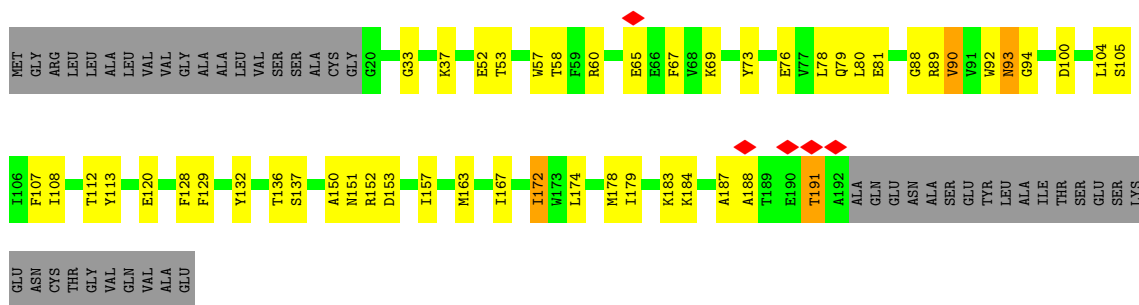
- Molecule 1: Sodium channel protein type 9 subunit alpha



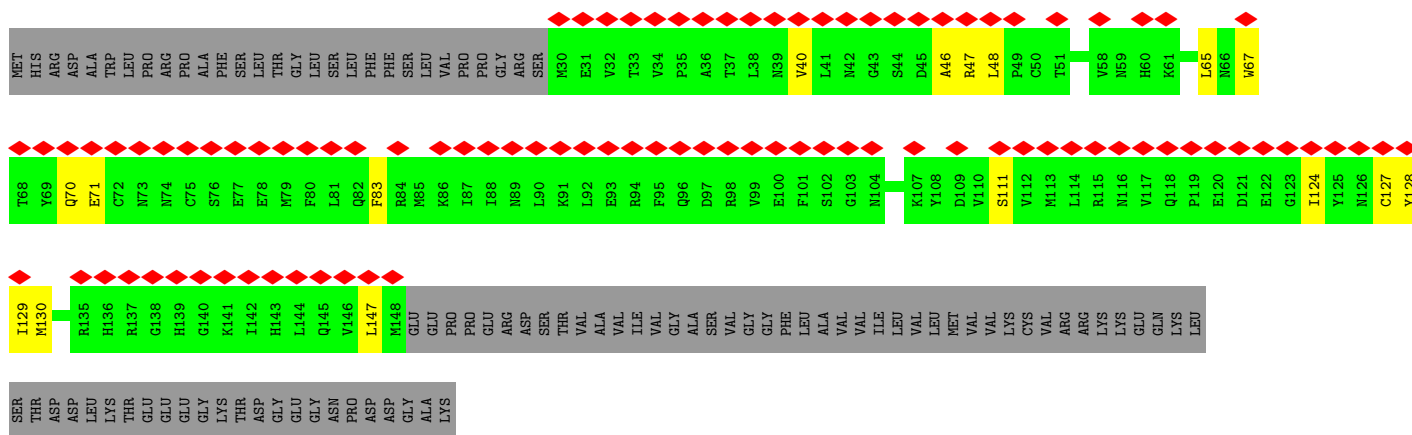
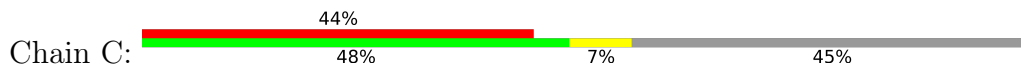


• Molecule 2: Sodium channel subunit beta-1

Chain B: 56% 22% 21%



- Molecule 3: Sodium channel subunit beta-2



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	194430	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.929	Depositor
Minimum map value	-2.041	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.120	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	261.84, 261.84, 261.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: P5S, Y01, 1PW, NAG, PCW, LPE, 9SL

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	0.56	4/11641 (0.0%)	0.63	10/15767 (0.1%)
2	B	0.53	0/1442	0.65	3/1949 (0.2%)
3	C	0.36	0/1011	0.57	0/1367
All	All	0.55	4/14094 (0.0%)	0.63	13/19083 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1407	GLY	C-O	-6.22	1.16	1.24
1	A	385	VAL	C-O	-6.20	1.16	1.24
1	A	1406	LYS	C-O	-6.00	1.17	1.23
1	A	1420	ASN	C-O	-5.40	1.18	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1670	LYS	N-CA-C	9.11	122.19	111.71
1	A	1344	ALA	N-CA-C	7.91	119.69	111.14
1	A	1601	THR	N-CA-C	7.11	118.82	111.14
1	A	1603	PHE	N-CA-C	-6.46	99.33	108.96
1	A	1755	TYR	N-CA-C	-6.39	104.31	111.28
1	A	1367	ARG	N-CA-C	5.53	118.23	111.82
1	A	1477	GLU	CB-CG-CD	5.30	121.62	112.60
2	B	105	SER	N-CA-C	5.25	117.50	110.35
2	B	53	THR	N-CA-C	5.20	117.97	110.28
1	A	395	ASN	CA-C-N	-5.17	113.35	120.28
1	A	395	ASN	C-N-CA	-5.17	113.35	120.28
2	B	100	ASP	N-CA-C	-5.07	98.60	107.73
1	A	1421	VAL	N-CA-C	5.01	115.23	110.42

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	11367	0	11565	393	0
2	B	1416	0	1379	37	0
3	C	980	0	935	6	0
4	D	28	0	25	6	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
5	A	21	0	0	2	0
6	A	28	0	26	2	0
6	B	42	0	39	4	0
7	A	110	0	130	16	0
8	A	210	0	294	68	0
9	A	287	0	391	57	0
9	B	17	0	19	0	0
10	A	24	0	33	5	0
11	A	231	0	318	27	0
All	All	14817	0	15204	492	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 16.

All (492) 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:1738:PHE:CE2	9:A:2014:LPE:H1N2	1.15	1.61
1:A:843:PHE:CD1	1:A:852:LEU:HD11	1.03	1.54
1:A:53:LEU:HD23	1:A:79:ASP:CB	1.14	1.52
1:A:843:PHE:CD1	1:A:852:LEU:CD1	1.92	1.49
1:A:768:MET:SD	1:A:772:PHE:CD2	2.07	1.45
1:A:53:LEU:CD2	1:A:79:ASP:CB	1.96	1.43
1:A:53:LEU:CD2	1:A:79:ASP:HB2	1.48	1.40
1:A:843:PHE:HB3	1:A:852:LEU:CD2	1.53	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:MET:SD	1:A:772:PHE:CE2	2.20	1.34
1:A:1738:PHE:CE2	9:A:2014:LPE:C1N	2.09	1.31
1:A:1738:PHE:HE2	9:A:2014:LPE:C1N	1.40	1.28
1:A:843:PHE:CE1	1:A:852:LEU:HD11	1.73	1.24
1:A:1355:ASP:OD1	4:D:1:NAG:H62	1.37	1.23
1:A:53:LEU:CD2	1:A:79:ASP:CA	2.17	1.21
1:A:1738:PHE:CD2	9:A:2014:LPE:H1N2	1.76	1.20
1:A:843:PHE:CG	1:A:852:LEU:HD21	1.76	1.19
1:A:843:PHE:CG	1:A:852:LEU:HD11	1.78	1.18
2:B:112:THR:HG21	6:B:303:NAG:H82	1.25	1.17
1:A:1355:ASP:OD1	4:D:1:NAG:C6	1.94	1.16
1:A:194:VAL:HG13	1:A:198:PHE:CZ	1.79	1.16
1:A:847:LYS:HE3	8:A:2006:Y01:CAM	1.74	1.15
1:A:194:VAL:CG1	1:A:198:PHE:CZ	2.31	1.15
1:A:843:PHE:HB3	1:A:852:LEU:HD22	1.15	1.14
1:A:843:PHE:CB	1:A:852:LEU:HD21	1.81	1.11
1:A:843:PHE:CB	1:A:852:LEU:CD2	2.30	1.10
1:A:194:VAL:HG12	1:A:198:PHE:CE2	1.85	1.10
1:A:1570:ARG:O	7:A:2029:P5S:H2	1.51	1.09
1:A:1653:LEU:HD23	9:A:2014:LPE:C16	1.84	1.06
1:A:53:LEU:HD21	1:A:79:ASP:CA	1.82	1.06
1:A:843:PHE:HB3	1:A:852:LEU:HD21	1.36	1.06
1:A:53:LEU:HD21	1:A:79:ASP:HA	1.34	1.05
1:A:194:VAL:CG1	1:A:198:PHE:CE2	2.40	1.05
11:A:2013:PCW:H371	8:A:2030:Y01:CAQ	1.86	1.04
11:A:2013:PCW:H371	8:A:2030:Y01:HAQ1	1.41	1.01
1:A:1301:LEU:HD21	9:A:2014:LPE:H152	1.38	1.01
1:A:1235:TYR:CE2	1:A:1239:LEU:HD11	1.97	1.00
1:A:1301:LEU:HD11	9:A:2014:LPE:H151	1.43	0.99
1:A:53:LEU:CD2	1:A:79:ASP:HA	1.85	0.99
1:A:847:LYS:CE	8:A:2006:Y01:HAM1	1.92	0.99
9:A:2014:LPE:O32	9:A:2015:LPE:H201	1.61	0.97
1:A:1738:PHE:HD2	9:A:2014:LPE:H2N3	1.28	0.97
1:A:1653:LEU:CD2	9:A:2014:LPE:C16	2.44	0.94
1:A:768:MET:SD	1:A:772:PHE:HD2	1.67	0.94
1:A:843:PHE:CG	1:A:852:LEU:CD2	2.51	0.94
9:A:2012:LPE:H112	8:A:2030:Y01:HAO1	1.47	0.94
1:A:843:PHE:HD1	1:A:852:LEU:HD11	1.32	0.93
1:A:847:LYS:HE3	8:A:2006:Y01:HAM1	0.97	0.93
1:A:821:VAL:O	1:A:824:PHE:HB2	1.69	0.92
1:A:53:LEU:HD23	1:A:79:ASP:CA	1.90	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:HD12	1:A:293:LEU:O	1.70	0.91
9:A:2012:LPE:H112	8:A:2030:Y01:CAO	2.00	0.91
7:A:2003:P5S:H42	9:A:2026:LPE:O32	1.69	0.91
11:A:2013:PCW:C37	8:A:2030:Y01:HAQ2	2.00	0.91
11:A:2013:PCW:C37	8:A:2030:Y01:CAQ	2.49	0.90
1:A:1355:ASP:OD2	4:D:1:NAG:O5	1.89	0.90
1:A:1235:TYR:CZ	1:A:1239:LEU:HD11	2.05	0.90
1:A:843:PHE:CD2	1:A:852:LEU:HD21	2.07	0.89
1:A:763:MET:O	1:A:772:PHE:HZ	1.55	0.89
9:A:2012:LPE:C11	8:A:2030:Y01:HAO1	2.03	0.87
1:A:1330:ILE:HD12	8:A:2006:Y01:HAA3	1.56	0.87
1:A:768:MET:SD	1:A:772:PHE:HE2	1.92	0.85
1:A:768:MET:CG	1:A:772:PHE:CD2	2.60	0.84
1:A:846:ALA:HB1	1:A:849:TRP:HB2	1.59	0.83
1:A:843:PHE:CB	1:A:852:LEU:HD22	2.03	0.83
2:B:136:THR:HG22	2:B:137:SER:N	1.94	0.81
1:A:170:LYS:NZ	1:A:189:ASN:OD1	2.13	0.81
1:A:53:LEU:CD2	1:A:79:ASP:CG	2.55	0.80
1:A:1599:ILE:HD11	1:A:1612:ILE:HD12	1.62	0.80
1:A:1330:ILE:HD12	8:A:2006:Y01:CAA	2.13	0.79
1:A:1577:GLY:H	11:A:2018:PCW:H63	1.45	0.79
1:A:48:LYS:NZ	1:A:49:PRO:O	2.12	0.78
1:A:763:MET:O	1:A:772:PHE:CZ	2.37	0.78
2:B:33:GLY:O	6:B:302:NAG:H82	1.83	0.78
1:A:1301:LEU:HD21	9:A:2014:LPE:C15	2.12	0.77
1:A:759:LEU:HD11	8:A:2030:Y01:CAC	2.15	0.77
1:A:843:PHE:HD1	1:A:852:LEU:CD1	1.82	0.77
11:A:2013:PCW:H81	8:A:2030:Y01:OAF	1.85	0.77
1:A:413:ILE:HG22	1:A:417:LYS:HE3	1.67	0.77
1:A:1301:LEU:HD11	9:A:2014:LPE:C15	2.13	0.77
1:A:1789:PHE:HB3	1:A:1801:LYS:HD3	1.65	0.77
1:A:973:SER:O	1:A:977:THR:HG23	1.83	0.77
1:A:1400:LEU:HD22	11:A:2013:PCW:H221	1.65	0.76
1:A:1330:ILE:CD1	8:A:2006:Y01:HAA3	2.16	0.76
1:A:1333:LEU:HD23	8:A:2006:Y01:HAB3	1.65	0.75
1:A:862:SER:O	1:A:866:LEU:O	2.05	0.75
1:A:414:GLU:HA	1:A:417:LYS:HD2	1.70	0.74
1:A:53:LEU:HD23	1:A:79:ASP:CG	2.07	0.74
1:A:909:HIS:HD2	1:A:911:ASN:H	1.36	0.74
1:A:1738:PHE:CD2	9:A:2014:LPE:H2N3	2.17	0.74
1:A:1624:VAL:HG21	7:A:2017:P5S:H28	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1211:PHE:CE2	9:A:2023:LPE:H2N2	2.23	0.73
1:A:341:TYR:CE1	11:A:2016:PCW:H62	2.25	0.71
2:B:60:ARG:HD2	2:B:65:GLU:HA	1.72	0.70
1:A:1738:PHE:HD2	9:A:2014:LPE:C2N	2.03	0.70
1:A:1235:TYR:CE2	1:A:1239:LEU:CD1	2.75	0.70
1:A:1355:ASP:OD1	4:D:1:NAG:O6	2.10	0.70
1:A:65:ASP:OD1	1:A:66:ILE:N	2.23	0.69
1:A:222:LEU:HD11	8:A:2007:Y01:HAN1	1.74	0.69
1:A:847:LYS:HE2	8:A:2006:Y01:OAW	1.93	0.69
1:A:222:LEU:HD21	8:A:2007:Y01:HAN1	1.75	0.69
8:A:2005:Y01:CAC	9:A:2026:LPE:C11	2.70	0.69
1:A:341:TYR:CE1	11:A:2016:PCW:C6	2.75	0.69
1:A:1474:MET:HE2	1:A:1642:PRO:HB2	1.75	0.69
1:A:1758:VAL:O	1:A:1762:ASN:ND2	2.26	0.68
2:B:136:THR:HG22	2:B:137:SER:H	1.58	0.68
11:A:2013:PCW:H372	8:A:2030:Y01:HAQ2	1.77	0.67
1:A:1570:ARG:HB3	7:A:2029:P5S:H3	1.75	0.67
1:A:950:MET:HE1	8:A:2007:Y01:HAC1	1.76	0.67
1:A:1301:LEU:CD1	9:A:2014:LPE:H151	2.21	0.67
1:A:1493:PRO:O	1:A:1494:GLN:NE2	2.27	0.67
1:A:401:VAL:HG21	1:A:960:LEU:HD23	1.77	0.67
1:A:847:LYS:CE	8:A:2006:Y01:CAM	2.63	0.66
1:A:768:MET:HE3	1:A:773:LYS:HG2	1.77	0.66
1:A:1802:LEU:HG	1:A:1823:LEU:HD21	1.76	0.65
9:A:2010:LPE:H21	11:A:2013:PCW:H131	1.78	0.65
1:A:289:ILE:HG22	1:A:293:LEU:HD21	1.79	0.65
1:A:53:LEU:HD21	1:A:79:ASP:N	2.11	0.65
1:A:843:PHE:CG	1:A:852:LEU:CD1	2.53	0.65
1:A:139:ASN:HD21	1:A:220:ARG:HH11	1.44	0.65
1:A:149:PRO:O	1:A:152:THR:OG1	2.11	0.65
1:A:1750:VAL:HG23	1:A:1751:VAL:H	1.63	0.64
1:A:1307:MET:CE	9:A:2023:LPE:C19	2.76	0.64
1:A:1653:LEU:CG	9:A:2014:LPE:C16	2.76	0.64
1:A:53:LEU:HD22	1:A:79:ASP:CG	2.23	0.64
1:A:843:PHE:CD1	1:A:852:LEU:HD13	2.20	0.64
1:A:809:ASN:O	1:A:813:SER:OG	2.10	0.64
2:B:136:THR:CG2	2:B:137:SER:N	2.59	0.63
1:A:1250:TYR:CE2	7:A:2003:P5S:C49	2.82	0.63
2:B:136:THR:CG2	2:B:137:SER:H	2.11	0.63
1:A:289:ILE:CG2	1:A:293:LEU:HD21	2.29	0.63
1:A:81:TYR:O	1:A:85:LYS:NZ	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1394:LEU:HG	11:A:2013:PCW:H121	1.80	0.62
1:A:234:ILE:HG13	1:A:868:ASN:HB3	1.81	0.62
1:A:1752:VAL:O	1:A:1756:ILE:HD13	1.99	0.62
10:A:2011:1PW:H21	11:A:2013:PCW:H262	1.80	0.62
1:A:1250:TYR:CE2	7:A:2003:P5S:H49	2.35	0.62
1:A:101:ASN:HD21	1:A:181:PHE:HD2	1.48	0.61
1:A:1653:LEU:HG	9:A:2014:LPE:C16	2.30	0.61
1:A:1365:PRO:HD2	1:A:1369:GLU:HG3	1.82	0.61
1:A:737:ILE:HG22	1:A:797:ALA:HB2	1.82	0.61
1:A:1002:VAL:HA	1:A:1005:THR:HG22	1.81	0.61
1:A:1627:ALA:HA	9:A:2024:LPE:H1N2	1.82	0.61
9:A:2012:LPE:H112	8:A:2030:Y01:HAO2	1.80	0.61
2:B:37:LYS:HB2	2:B:107:PHE:HD2	1.66	0.61
1:A:150:ASP:O	1:A:153:LYS:N	2.33	0.61
1:A:1539:GLN:HE21	1:A:1544:THR:HG22	1.66	0.61
8:A:2005:Y01:HAE2	8:A:2005:Y01:HAC1	1.84	0.60
7:A:2003:P5S:C42	9:A:2026:LPE:O32	2.47	0.60
1:A:98:PHE:HB3	1:A:100:PHE:HE2	1.67	0.60
8:A:2004:Y01:HAC1	8:A:2004:Y01:HAE2	1.84	0.60
1:A:1683:THR:HG21	9:A:2022:LPE:H32	1.84	0.59
8:A:2007:Y01:HAC1	8:A:2007:Y01:HAE2	1.84	0.59
1:A:1443:PHE:HA	1:A:1447:PHE:HD2	1.67	0.59
1:A:1377:SER:OG	1:A:1378:GLN:N	2.35	0.59
11:A:2018:PCW:H381	11:A:2027:PCW:H382	1.83	0.59
1:A:1849:VAL:HG13	1:A:1850:LEU:HD12	1.84	0.59
1:A:66:ILE:HD11	1:A:70:MET:HB2	1.83	0.59
8:A:2006:Y01:HAC1	8:A:2006:Y01:HAE2	1.83	0.59
8:A:2009:Y01:HAC1	8:A:2009:Y01:HAE2	1.84	0.59
1:A:1673:ASP:C	1:A:1675:ILE:H	2.11	0.58
1:A:853:ASN:ND2	1:A:854:MET:SD	2.76	0.58
8:A:2005:Y01:HAB1	9:A:2025:LPE:H181	1.86	0.58
1:A:1738:PHE:CD2	9:A:2014:LPE:C1N	2.61	0.58
1:A:289:ILE:HG23	1:A:293:LEU:HD23	1.84	0.58
1:A:1724:SER:OG	1:A:1725:SER:N	2.37	0.57
1:A:1307:MET:HE1	9:A:2023:LPE:C19	2.34	0.57
1:A:55:ALA:HA	1:A:97:ILE:HB	1.86	0.57
7:A:2017:P5S:C35	7:A:2017:P5S:C46	2.83	0.57
11:A:2013:PCW:C37	8:A:2030:Y01:HAQ1	2.20	0.57
1:A:1655:MET:HE1	9:A:2021:LPE:H161	1.86	0.57
1:A:401:VAL:HG21	1:A:960:LEU:CD2	2.34	0.57
1:A:289:ILE:CG2	1:A:293:LEU:CD2	2.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1499:ARG:HG2	1:A:1500:PRO:HD2	1.87	0.57
1:A:855:LEU:HB2	1:A:1451:LEU:HD11	1.85	0.57
1:A:1288:SER:O	1:A:1291:THR:OG1	2.22	0.57
2:B:58:THR:HG22	2:B:69:LYS:HA	1.86	0.56
1:A:260:ALA:CA	1:A:354:LEU:HD12	2.35	0.56
2:B:129:PHE:HB2	2:B:132:TYR:HB3	1.87	0.56
1:A:1384:ASN:OD1	1:A:1388:ASN:ND2	2.38	0.56
1:A:1250:TYR:CE2	7:A:2003:P5S:H49A	2.41	0.56
2:B:153:ASP:OD1	2:B:153:ASP:N	2.37	0.56
1:A:810:ILE:O	1:A:814:LEU:HG	2.06	0.56
1:A:1860:ARG:HD3	1:A:1864:GLU:HG3	1.88	0.56
1:A:187:PRO:O	1:A:190:TRP:HB2	2.05	0.55
1:A:1641:LEU:HB3	9:A:2019:LPE:H11	1.87	0.55
1:A:1817:LYS:HE3	1:A:1818:PRO:HA	1.88	0.55
1:A:66:ILE:HD12	1:A:67:PRO:HD2	1.87	0.55
1:A:1297:PRO:HB2	1:A:1653:LEU:HD11	1.87	0.55
1:A:1256:ASN:OD1	1:A:1257:ALA:N	2.40	0.55
1:A:216:PHE:O	1:A:219:LEU:HG	2.07	0.55
1:A:260:ALA:HA	1:A:354:LEU:HD12	1.89	0.55
1:A:1541:GLN:O	1:A:1544:THR:OG1	2.23	0.55
1:A:1577:GLY:N	11:A:2018:PCW:H51	2.21	0.55
2:B:78:LEU:HD21	2:B:80:LEU:HD13	1.88	0.55
1:A:259:PHE:C	1:A:354:LEU:HD11	2.32	0.55
1:A:1219:LYS:NZ	9:A:2022:LPE:H3N3	2.23	0.54
1:A:166:GLU:O	1:A:169:VAL:HG12	2.07	0.54
1:A:1680:ASN:ND2	1:A:1682:GLU:OE1	2.41	0.54
1:A:28:ALA:HA	1:A:31:LYS:HE2	1.90	0.54
1:A:54:GLU:HA	1:A:99:ARG:HH12	1.73	0.54
1:A:260:ALA:N	1:A:354:LEU:CD1	2.71	0.54
1:A:289:ILE:HG23	1:A:293:LEU:CD2	2.38	0.54
1:A:224:THR:HB	1:A:228:ILE:HD12	1.90	0.54
1:A:1529:MET:HG2	1:A:1533:MET:HE3	1.90	0.54
1:A:1497:ILE:HG21	1:A:1569:LEU:HD22	1.90	0.53
9:A:2012:LPE:C11	8:A:2030:Y01:CAO	2.75	0.53
2:B:112:THR:CG2	6:B:303:NAG:H82	2.18	0.53
1:A:26:ARG:O	1:A:29:GLU:HG2	2.08	0.53
1:A:854:MET:O	1:A:858:ILE:HG12	2.08	0.53
1:A:1785:VAL:HA	1:A:1788:LYS:HD2	1.90	0.53
1:A:1813:LEU:HD22	1:A:1845:PHE:HD2	1.74	0.53
1:A:1577:GLY:H	11:A:2018:PCW:H51	1.73	0.53
1:A:1219:LYS:HE3	9:A:2023:LPE:H3N1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:LEU:HD23	8:A:2006:Y01:CAB	2.37	0.52
1:A:994:ARG:O	1:A:994:ARG:NH2	2.42	0.52
2:B:52:GLU:HG3	2:B:128:PHE:HE2	1.74	0.52
1:A:1333:LEU:CD2	8:A:2006:Y01:CAB	2.87	0.52
1:A:9:PRO:HA	1:A:63:TYR:HA	1.92	0.52
1:A:266:LEU:O	1:A:1610:ARG:NH2	2.42	0.52
1:A:293:LEU:HD12	1:A:293:LEU:C	2.34	0.52
2:B:93:ASN:OD1	6:B:301:NAG:N2	2.43	0.52
1:A:843:PHE:CE1	1:A:852:LEU:CD1	2.57	0.52
1:A:1355:ASP:CG	4:D:1:NAG:O6	2.52	0.52
1:A:839:LEU:C	1:A:839:LEU:HD12	2.35	0.52
1:A:1251:LYS:HE2	9:A:2026:LPE:H1N3	1.92	0.51
9:A:2012:LPE:H111	8:A:2030:Y01:HAO1	1.89	0.51
1:A:53:LEU:HD23	1:A:79:ASP:HB2	0.53	0.51
1:A:1355:ASP:CG	4:D:1:NAG:O5	2.53	0.51
1:A:53:LEU:HD22	1:A:79:ASP:OD2	2.10	0.51
1:A:766:HIS:O	1:A:768:MET:N	2.43	0.51
1:A:1250:TYR:OH	7:A:2003:P5S:H51A	2.11	0.51
1:A:798:MET:HE3	1:A:803:TYR:HD1	1.76	0.51
1:A:1607:THR:O	1:A:1611:VAL:HG23	2.09	0.51
2:B:65:GLU:OE2	2:B:65:GLU:N	2.43	0.51
1:A:807:GLY:O	1:A:810:ILE:HG13	2.10	0.51
3:C:47:ARG:NH2	3:C:111[B]:SER:OG	2.43	0.51
8:A:2004:Y01:HAE2	8:A:2004:Y01:CAC	2.41	0.51
1:A:1533:MET:HE1	9:A:2024:LPE:H122	1.93	0.50
1:A:986:ASN:O	1:A:989:GLN:HG2	2.11	0.50
1:A:26:ARG:O	1:A:30:ARG:HG2	2.11	0.50
1:A:1307:MET:HE3	9:A:2023:LPE:C19	2.40	0.50
1:A:737:ILE:O	1:A:738:TYR:C	2.54	0.50
1:A:98:PHE:HB3	1:A:100:PHE:CE2	2.46	0.50
8:A:2006:Y01:HAE2	8:A:2006:Y01:CAC	2.41	0.50
1:A:251:LEU:HB2	1:A:1630:ILE:HD12	1.94	0.50
1:A:1372:ALA:O	1:A:1375:ASN:HB3	2.12	0.50
1:A:152:THR:HA	1:A:155:VAL:HG22	1.94	0.50
1:A:211:SER:O	1:A:215:THR:OG1	2.29	0.50
1:A:1577:GLY:H	11:A:2018:PCW:C6	2.19	0.50
1:A:341:TYR:CD1	11:A:2016:PCW:C6	2.94	0.50
1:A:1307:MET:HE1	9:A:2023:LPE:C18	2.42	0.50
1:A:754:ILE:O	1:A:758:THR:HG23	2.12	0.49
1:A:843:PHE:CG	1:A:852:LEU:CG	2.95	0.49
1:A:1745:ILE:HG21	10:A:2011:1PW:H13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1785:VAL:HG22	1:A:1789:PHE:HE1	1.76	0.49
1:A:759:LEU:HD11	8:A:2030:Y01:HAC1	1.93	0.49
1:A:1794:THR:HG23	1:A:1796:PHE:H	1.77	0.49
1:A:153:LYS:O	1:A:156:GLU:HG3	2.13	0.49
1:A:364:GLU:OE2	5:A:2001:9SL:N11	2.45	0.49
1:A:972:SER:O	1:A:974:ASP:N	2.45	0.49
1:A:1182:ARG:NH2	7:A:2003:P5S:H46A	2.28	0.49
1:A:1748:PHE:HB2	10:A:2011:1PW:H28	1.95	0.49
8:A:2009:Y01:HAE2	8:A:2009:Y01:CAC	2.41	0.49
1:A:385:VAL:O	1:A:386:ILE:C	2.56	0.49
1:A:193:PHE:HA	1:A:196:ILE:HD12	1.93	0.49
1:A:850:PRO:CD	8:A:2006:Y01:HAL1	2.43	0.49
8:A:2007:Y01:HAE2	8:A:2007:Y01:CAC	2.41	0.49
1:A:771:GLU:OE2	1:A:771:GLU:N	2.25	0.49
1:A:869:LEU:HB3	1:A:962:LEU:HD13	1.95	0.48
1:A:1750:VAL:HG23	1:A:1751:VAL:N	2.26	0.48
1:A:283:ASN:HB2	6:A:2002:NAG:O7	2.13	0.48
1:A:1699:GLY:HA2	5:A:2001:9SL:O17	2.12	0.48
1:A:1250:TYR:HE2	7:A:2003:P5S:H49A	1.76	0.48
1:A:1195:GLU:O	1:A:1199:VAL:HG23	2.13	0.48
1:A:1260:TRP:CD1	8:A:2004:Y01:HAD3	2.48	0.48
8:A:2005:Y01:CAC	8:A:2005:Y01:HAE2	2.41	0.48
11:A:2016:PCW:H42	11:A:2016:PCW:H83	1.62	0.48
1:A:53:LEU:CD2	1:A:79:ASP:N	2.71	0.48
1:A:180:GLU:HA	1:A:185:ARG:NH2	2.29	0.48
1:A:248:VAL:HG21	1:A:400:VAL:HG21	1.94	0.48
2:B:152:ARG:NH1	2:B:157:ILE:HG12	2.29	0.48
1:A:84:ASP:OD1	1:A:84:ASP:N	2.47	0.48
1:A:320:ASP:OD1	1:A:320:ASP:N	2.47	0.48
1:A:348:SER:HB2	11:A:2016:PCW:H332	1.95	0.48
1:A:1350:CYS:H	1:A:1424:GLN:HE22	1.60	0.48
8:A:2005:Y01:HAC1	8:A:2005:Y01:HAU2	1.96	0.48
1:A:197:VAL:HG22	1:A:201:LEU:HD23	1.96	0.48
8:A:2006:Y01:HAC1	8:A:2006:Y01:HAU2	1.96	0.47
1:A:1738:PHE:CD2	9:A:2014:LPE:C2N	2.89	0.47
1:A:1333:LEU:CD2	8:A:2006:Y01:HAB3	2.40	0.47
1:A:1843:PHE:HB2	1:A:1860:ARG:NH2	2.30	0.47
8:A:2007:Y01:HAC1	8:A:2007:Y01:HAU2	1.96	0.47
11:A:2013:PCW:C38	8:A:2030:Y01:HAQ2	2.43	0.47
1:A:139:ASN:HD21	1:A:220:ARG:NH1	2.11	0.47
1:A:166:GLU:HA	1:A:169:VAL:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:PHE:CE1	1:A:174:ARG:HG2	2.48	0.47
1:A:187:PRO:HA	1:A:190:TRP:CD1	2.50	0.47
8:A:2006:Y01:HAV2	8:A:2006:Y01:OAG	2.14	0.47
1:A:92:ASN:HD22	1:A:94:GLY:N	2.13	0.47
1:A:320:ASP:HB3	9:A:2021:LPE:H1N2	1.97	0.47
1:A:1297:PRO:HG2	1:A:1657:ILE:HG12	1.97	0.47
1:A:1749:LEU:HD11	10:A:2011:1PW:H10	1.97	0.47
11:A:2027:PCW:H182	11:A:2027:PCW:H211	1.68	0.47
1:A:171:ILE:HG23	1:A:176:PHE:HB2	1.97	0.47
1:A:222:LEU:HD21	8:A:2007:Y01:HAB2	1.96	0.47
1:A:1301:LEU:CD2	9:A:2014:LPE:H152	2.27	0.47
8:A:2004:Y01:HAC1	8:A:2004:Y01:HAU2	1.96	0.47
8:A:2009:Y01:OAG	8:A:2009:Y01:HAV2	2.14	0.47
1:A:260:ALA:CA	1:A:354:LEU:CD1	2.92	0.47
1:A:260:ALA:HA	1:A:354:LEU:CD1	2.45	0.46
1:A:188:TRP:NE1	1:A:232:LYS:HE3	2.29	0.46
1:A:394:ILE:O	1:A:398:LEU:HD23	2.16	0.46
1:A:999:ILE:HA	1:A:1002:VAL:HG22	1.96	0.46
2:B:37:LYS:HB2	2:B:107:PHE:CD2	2.50	0.46
1:A:55:ALA:H	1:A:99:ARG:HH12	1.62	0.46
1:A:1738:PHE:HE2	9:A:2014:LPE:H1N2	0.68	0.46
8:A:2009:Y01:HAC1	8:A:2009:Y01:HAU2	1.96	0.46
1:A:1489:GLY:HA3	1:A:1635:PHE:CE1	2.50	0.46
1:A:53:LEU:CD2	1:A:79:ASP:OD2	2.63	0.46
8:A:2005:Y01:HAC3	9:A:2026:LPE:C11	2.46	0.46
2:B:150:ALA:C	2:B:151:ASN:HD22	2.23	0.46
2:B:163:MET:O	2:B:163:MET:HG2	2.16	0.46
1:A:1251:LYS:O	1:A:1255:THR:HG23	2.16	0.46
1:A:1623:LEU:HD23	1:A:1623:LEU:HA	1.77	0.46
1:A:1828:LEU:HD22	1:A:1836:ILE:HD11	1.98	0.46
1:A:1249:GLY:HA2	7:A:2003:P5S:H48A	1.98	0.46
1:A:1478:GLN:HE21	1:A:1642:PRO:HB3	1.81	0.46
8:A:2005:Y01:HAC1	9:A:2026:LPE:C11	2.45	0.45
2:B:188:ALA:O	2:B:191:THR:OG1	2.34	0.45
1:A:73:GLU:CD	1:A:74:PRO:HD2	2.41	0.45
1:A:761:MET:HE1	1:A:836:SER:HB3	1.98	0.45
1:A:989:GLN:HA	1:A:992:VAL:HG12	1.98	0.45
1:A:1191:HIS:CG	1:A:1192:SER:H	2.35	0.45
1:A:1886:ARG:HA	1:A:1886:ARG:HD3	1.81	0.45
1:A:376:LYS:HB2	9:A:2021:LPE:O32	2.16	0.45
1:A:1353:THR:OG1	1:A:1379:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1673:ASP:C	1:A:1675:ILE:N	2.74	0.45
1:A:1846:THR:HG22	1:A:1850:LEU:HD13	1.99	0.45
1:A:1375:ASN:ND2	6:A:2008:NAG:C7	2.78	0.45
1:A:1647:ILE:HG12	1:A:1754:MET:HE3	1.98	0.45
1:A:81:TYR:CE1	1:A:85:LYS:HE2	2.52	0.45
1:A:264:LEU:O	1:A:268:MET:HB2	2.17	0.45
2:B:69:LYS:O	2:B:81:GLU:HG3	2.17	0.45
1:A:62:ILE:HG22	1:A:426:MET:HE2	1.97	0.45
1:A:276:PHE:CZ	1:A:280:LEU:HD11	2.52	0.45
1:A:171:ILE:HG12	1:A:183:PHE:CG	2.52	0.45
1:A:411:ALA:O	1:A:414:GLU:HG3	2.17	0.45
1:A:838:ARG:O	1:A:841:ARG:HG3	2.17	0.45
1:A:29:GLU:O	1:A:33:LYS:NZ	2.41	0.45
1:A:212:ALA:HB1	8:A:2007:Y01:HAL1	1.99	0.45
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.78	0.45
1:A:398:LEU:HD13	1:A:960:LEU:HD11	1.99	0.45
1:A:929:ILE:HD12	1:A:932:MET:HE2	1.98	0.45
1:A:259:PHE:C	1:A:354:LEU:CD1	2.90	0.44
1:A:850:PRO:O	1:A:854:MET:CE	2.65	0.44
2:B:183:LYS:O	2:B:183:LYS:HD3	2.17	0.44
1:A:23:ILE:HG21	1:A:86:LYS:HA	1.99	0.44
1:A:972:SER:C	1:A:974:ASP:N	2.75	0.44
1:A:1177:ILE:O	1:A:1181:ILE:HG12	2.17	0.44
1:A:1485:MET:CE	9:A:2020:LPE:H132	2.47	0.44
2:B:178:MET:HE3	2:B:178:MET:HB2	1.74	0.44
1:A:1481:TYR:HE1	9:A:2020:LPE:H322	1.83	0.44
1:A:53:LEU:CG	1:A:79:ASP:HB2	2.37	0.44
1:A:170:LYS:HE3	1:A:183:PHE:HE1	1.82	0.44
1:A:1256:ASN:O	1:A:1260:TRP:HD1	2.01	0.44
1:A:1613:ARG:O	1:A:1616:ARG:HG2	2.17	0.44
1:A:1885:LYS:O	1:A:1889:GLU:HG3	2.18	0.44
1:A:1860:ARG:NH1	1:A:1863:MET:HB3	2.33	0.44
1:A:73:GLU:H	1:A:90:VAL:HG23	1.82	0.44
1:A:105:ALA:H	1:A:116:ARG:NH1	2.16	0.44
1:A:813:SER:O	1:A:817:THR:HG23	2.18	0.44
11:A:2013:PCW:C8	8:A:2030:Y01:OAF	2.60	0.44
7:A:2029:P5S:H1A	7:A:2029:P5S:H20A	1.74	0.44
1:A:122:ILE:HD13	1:A:122:ILE:HA	1.82	0.43
1:A:92:ASN:HD22	1:A:94:GLY:H	1.65	0.43
1:A:104:PRO:HA	1:A:109:LEU:O	2.17	0.43
1:A:945:LEU:HD12	11:A:2016:PCW:H152	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:TYR:O	1:A:1283:LEU:HD22	2.19	0.43
3:C:67:TRP:CZ2	3:C:127:CYS:HB3	2.53	0.43
3:C:128:TYR:C	3:C:129:ILE:HG13	2.43	0.43
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.78	0.43
1:A:850:PRO:O	1:A:854:MET:HE2	2.18	0.43
1:A:923:VAL:HG13	1:A:928:TRP:HB3	2.00	0.43
1:A:1824:ILE:HD12	1:A:1887:LYS:HG2	2.00	0.43
1:A:1331:PHE:CE2	1:A:1443:PHE:HB3	2.54	0.43
1:A:1348:TYR:CE2	1:A:1384:ASN:HB2	2.54	0.43
1:A:1400:LEU:HD22	11:A:2013:PCW:C22	2.41	0.43
1:A:1796:PHE:HB3	1:A:1835:ARG:HG2	2.00	0.43
1:A:150:ASP:OD1	1:A:151:TRP:N	2.50	0.43
1:A:850:PRO:HD3	8:A:2006:Y01:HAL1	2.01	0.43
1:A:1655:MET:HE1	9:A:2021:LPE:C19	2.48	0.43
1:A:214:ARG:HB3	1:A:217:ARG:NH1	2.33	0.43
1:A:1302:SER:O	1:A:1308:ARG:NH1	2.51	0.43
1:A:1636:ALA:O	1:A:1640:SER:OG	2.35	0.43
2:B:187:ALA:O	2:B:191:THR:HG23	2.18	0.43
2:B:73:TYR:HD1	2:B:78:LEU:HB2	1.83	0.43
1:A:22:LEU:O	1:A:25:GLN:HG3	2.19	0.43
8:A:2009:Y01:HAN2	8:A:2009:Y01:HAC3	2.00	0.43
1:A:294:GLU:OE1	1:A:294:GLU:N	2.52	0.42
8:A:2006:Y01:HAC3	8:A:2006:Y01:HAN2	2.00	0.42
8:A:2030:Y01:HBB	8:A:2030:Y01:HAE2	1.61	0.42
2:B:172:ILE:HD13	2:B:172:ILE:HA	1.77	0.42
1:A:120:ILE:O	1:A:124:VAL:HG12	2.19	0.42
1:A:293:LEU:CD1	1:A:299:PHE:CE1	3.03	0.42
1:A:318:SER:OG	1:A:319:THR:N	2.51	0.42
1:A:843:PHE:CD1	1:A:843:PHE:N	2.87	0.42
1:A:1502:ASN:HB2	1:A:1505:GLN:HB2	2.02	0.42
1:A:153:LYS:HE3	1:A:157:TYR:CZ	2.54	0.42
1:A:281:GLU:HG3	1:A:282:ASN:ND2	2.34	0.42
1:A:846:ALA:HB1	1:A:849:TRP:CB	2.41	0.42
1:A:1243:LEU:HA	1:A:1243:LEU:HD23	1.72	0.42
2:B:184:LYS:HE3	2:B:184:LYS:HB2	1.75	0.42
1:A:176:PHE:HE2	1:A:184:LEU:HB2	1.84	0.42
1:A:244:LYS:HB3	1:A:244:LYS:HE3	1.85	0.42
8:A:2030:Y01:HAO2	8:A:2030:Y01:HAP1	1.36	0.42
1:A:95:LYS:HE2	1:A:95:LYS:HB2	1.80	0.42
1:A:251:LEU:HD13	1:A:1630:ILE:HG23	1.99	0.42
1:A:757:ASN:HB2	1:A:783:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:TRP:O	1:A:851:THR:N	2.52	0.42
1:A:1747:SER:O	1:A:1751:VAL:HG12	2.18	0.42
1:A:13:VAL:HG23	1:A:76:GLU:HB2	2.00	0.42
1:A:116:ARG:NH2	1:A:174:ARG:O	2.53	0.42
1:A:212:ALA:CB	8:A:2007:Y01:HAL1	2.50	0.42
1:A:1671:LYS:HD3	1:A:1675:ILE:HG22	2.02	0.42
1:A:89:ILE:HG22	1:A:99:ARG:HG3	2.02	0.42
1:A:871:LEU:HD12	1:A:871:LEU:HA	1.77	0.42
1:A:395:ASN:N	1:A:395:ASN:HD22	2.17	0.42
1:A:771:GLU:H	1:A:771:GLU:CD	2.19	0.42
1:A:847:LYS:CE	8:A:2006:Y01:CAY	2.97	0.42
1:A:285:THR:O	1:A:289:ILE:HG12	2.20	0.42
2:B:76:GLU:OE1	2:B:76:GLU:N	2.53	0.42
1:A:50:SER:N	1:A:79:ASP:OD2	2.53	0.41
1:A:245:LEU:O	1:A:249:MET:HG2	2.20	0.41
1:A:1296:ARG:N	1:A:1297:PRO:HD2	2.35	0.41
8:A:2009:Y01:HAS2	8:A:2009:Y01:HAE1	1.81	0.41
8:A:2030:Y01:HAS2	8:A:2030:Y01:HAE1	1.81	0.41
1:A:341:TYR:CE1	11:A:2016:PCW:H63	2.55	0.41
9:A:2021:LPE:H2N3	9:A:2021:LPE:H311	1.78	0.41
9:A:2025:LPE:H2N2	9:A:2025:LPE:H312	1.81	0.41
2:B:88:GLY:O	2:B:90:VAL:HG12	2.21	0.41
1:A:427:LEU:HD23	1:A:427:LEU:HA	1.94	0.41
1:A:964:LEU:HD23	1:A:964:LEU:HA	1.91	0.41
1:A:1481:TYR:CE2	9:A:2019:LPE:H321	2.55	0.41
3:C:40:VAL:HG11	3:C:46:ALA:HB2	2.03	0.41
1:A:1797:ILE:HD12	1:A:1797:ILE:HA	1.84	0.41
1:A:265:GLN:HG2	1:A:1614:LEU:CD1	2.50	0.41
1:A:742:MET:O	1:A:743:ASP:C	2.64	0.41
1:A:1229:ALA:O	1:A:1232:ILE:HG22	2.21	0.41
1:A:396:LEU:HA	1:A:396:LEU:HD23	1.71	0.41
1:A:1179:TRP:CZ2	7:A:2003:P5S:O15	2.74	0.41
1:A:1650:LEU:HD11	9:A:2014:LPE:H132	2.03	0.41
1:A:1756:ILE:O	1:A:1760:LEU:HD23	2.20	0.41
1:A:409:ASN:HA	1:A:412:ASN:HD22	1.84	0.41
1:A:1298:LEU:HA	1:A:1298:LEU:HD23	1.82	0.41
1:A:1634:LEU:HB3	7:A:2017:P5S:H42	2.03	0.41
1:A:1696:THR:O	1:A:1697:SER:OG	2.33	0.41
8:A:2006:Y01:HAS2	8:A:2006:Y01:HAE1	1.81	0.41
2:B:89:ARG:O	2:B:108:ILE:HA	2.20	0.41
2:B:112:THR:HG22	2:B:113:TYR:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:O	1:A:33:LYS:HG3	2.20	0.41
1:A:65:ASP:OD1	1:A:66:ILE:HG22	2.21	0.41
1:A:67:PRO:HB2	1:A:70:MET:HG3	2.03	0.41
1:A:245:LEU:HA	1:A:245:LEU:HD23	1.82	0.41
1:A:768:MET:HG2	1:A:772:PHE:CD2	2.50	0.41
1:A:772:PHE:CZ	1:A:776:LEU:HD11	2.56	0.41
1:A:839:LEU:C	1:A:841:ARG:N	2.79	0.41
1:A:1474:MET:HE1	1:A:1482:TYR:CD1	2.55	0.41
1:A:1655:MET:HE1	9:A:2021:LPE:C16	2.50	0.41
1:A:1828:LEU:H	1:A:1883:THR:HG22	1.86	0.41
1:A:1837:HIS:CD2	1:A:1839:LEU:HB2	2.56	0.41
8:A:2005:Y01:HAE1	8:A:2005:Y01:HAS2	1.81	0.41
2:B:92:TRP:CD1	2:B:94:GLY:H	2.38	0.41
3:C:70:GLN:HG3	3:C:124:ILE:HB	2.02	0.41
1:A:972:SER:C	1:A:974:ASP:H	2.28	0.41
1:A:1209:LEU:HD23	1:A:1209:LEU:HA	1.90	0.41
1:A:59:LEU:N	1:A:95:LYS:O	2.36	0.40
1:A:288:SER:O	1:A:292:THR:HG23	2.21	0.40
1:A:1354:THR:OG1	1:A:1355:ASP:N	2.54	0.40
1:A:1670:LYS:HE2	1:A:1670:LYS:HB3	1.83	0.40
2:B:58:THR:HB	2:B:67:PHE:HB3	2.04	0.40
3:C:65:LEU:HB3	3:C:83:PHE:HB3	2.03	0.40
1:A:1817:LYS:HZ1	1:A:1819:ASN:H	1.69	0.40
2:B:57:TRP:HA	2:B:120:GLU:O	2.22	0.40
2:B:152:ARG:CZ	2:B:157:ILE:HG12	2.51	0.40
1:A:180:GLU:HA	1:A:185:ARG:HH22	1.85	0.40
1:A:1790:ASP:OD2	1:A:1794:THR:HG22	2.21	0.40
1:A:1855:GLU:O	1:A:1855:GLU:HG3	2.21	0.40
1:A:996:LYS:HA	1:A:999:ILE:HG22	2.02	0.40
2:B:179:ILE:HA	2:B:179:ILE:HD13	1.81	0.40
1:A:198:PHE:O	1:A:202:THR:HG22	2.21	0.40
1:A:1186:TYR:CE1	1:A:1190:GLU:HG3	2.57	0.40
1:A:1745:ILE:CG2	10:A:2011:1PW:H13	2.51	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	1405/2031 (69%)	1342 (96%)	58 (4%)	5 (0%)	30	59
2	B	171/218 (78%)	157 (92%)	14 (8%)	0	100	100
3	C	120/215 (56%)	117 (98%)	3 (2%)	0	100	100
All	All	1696/2464 (69%)	1616 (95%)	75 (4%)	5 (0%)	37	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	973	SER
1	A	1191	HIS
1	A	387	PHE
1	A	386	ILE
1	A	385	VAL

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	1257/1809 (70%)	1226 (98%)	31 (2%)	42	74
2	B	157/190 (83%)	149 (95%)	8 (5%)	21	53
3	C	114/193 (59%)	110 (96%)	4 (4%)	32	66
All	All	1528/2192 (70%)	1485 (97%)	43 (3%)	38	72

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	70	MET
1	A	89	ILE
1	A	122	ILE
1	A	127	LEU
1	A	144	THR
1	A	158	THR
1	A	306	LEU
1	A	348	SER
1	A	737	ILE
1	A	741	VAL
1	A	782	VAL
1	A	790	GLU
1	A	810	ILE
1	A	842	VAL
1	A	919	ILE
1	A	959	VAL
1	A	1218	ARG
1	A	1232	ILE
1	A	1236	ILE
1	A	1451	LEU
1	A	1467	LEU
1	A	1497	ILE
1	A	1515	GLN
1	A	1556	ILE
1	A	1590	ILE
1	A	1614	LEU
1	A	1620	ILE
1	A	1621	LEU
1	A	1765	VAL
1	A	1774	LEU
2	B	79	GLN
2	B	90	VAL
2	B	93	ASN
2	B	104	LEU
2	B	167	ILE
2	B	172	ILE
2	B	174	LEU
2	B	191	THR
3	C	48	LEU
3	C	71	GLU
3	C	130	MET
3	C	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	14	HIS
1	A	92	ASN
1	A	139	ASN
1	A	270	ASN
1	A	273	HIS
1	A	282	ASN
1	A	360	GLN
1	A	395	ASN
1	A	412	ASN
1	A	780	ASN
1	A	805	GLN
1	A	868	ASN
1	A	886	GLN
1	A	900	ASN
1	A	909	HIS
1	A	911	ASN
1	A	961	ASN
1	A	986	ASN
1	A	1000	ASN
1	A	1378	GLN
1	A	1461	ASN
1	A	1478	GLN
1	A	1515	GLN
1	A	1539	GLN
1	A	1541	GLN
1	A	1732	ASN
1	A	1753	ASN
1	A	1795	GLN
2	B	143	HIS
2	B	151	ASN
3	C	53	ASN
3	C	82	GLN
3	C	145	GLN

5.3.3 RNA ⓘ

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](#)

6 monosaccharides 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	$\# Z > 2$
4	NAG	D	1	4,1	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	D	2	4	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	E	1	4,1	14,14,15	0.18	0	17,19,21	0.48	0
4	NAG	E	2	4	14,14,15	0.45	0	17,19,21	0.68	0
4	NAG	F	1	4,2	14,14,15	0.55	0	17,19,21	1.18	2 (11%)
4	NAG	F	2	4	14,14,15	0.66	0	17,19,21	1.21	1 (5%)

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	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	2.79	115.92	112.19
4	F	1	NAG	C3-C4-C5	-2.61	105.50	110.23
4	F	2	NAG	C4-C3-C2	-2.41	107.49	111.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

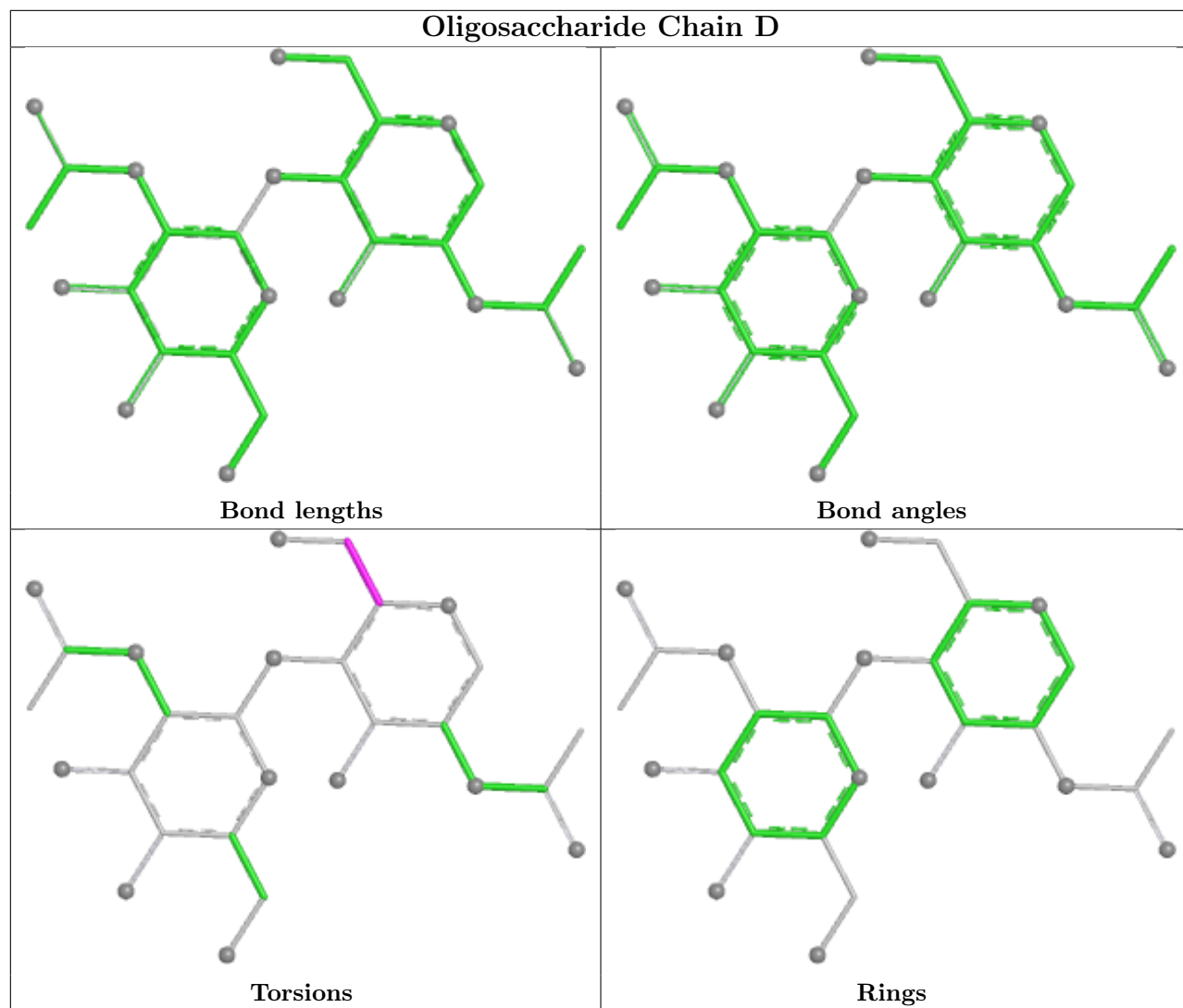
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6

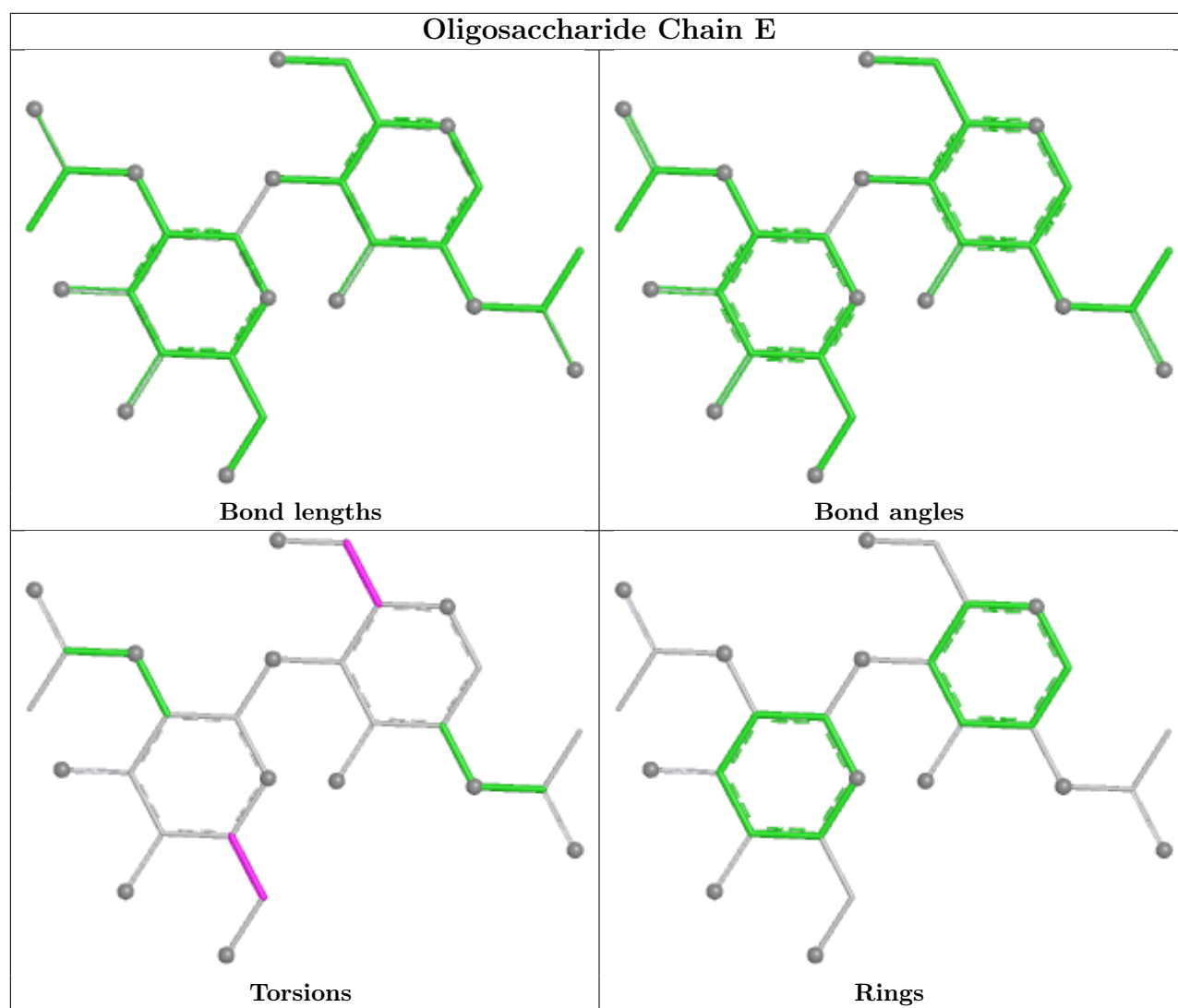
There are no ring outliers.

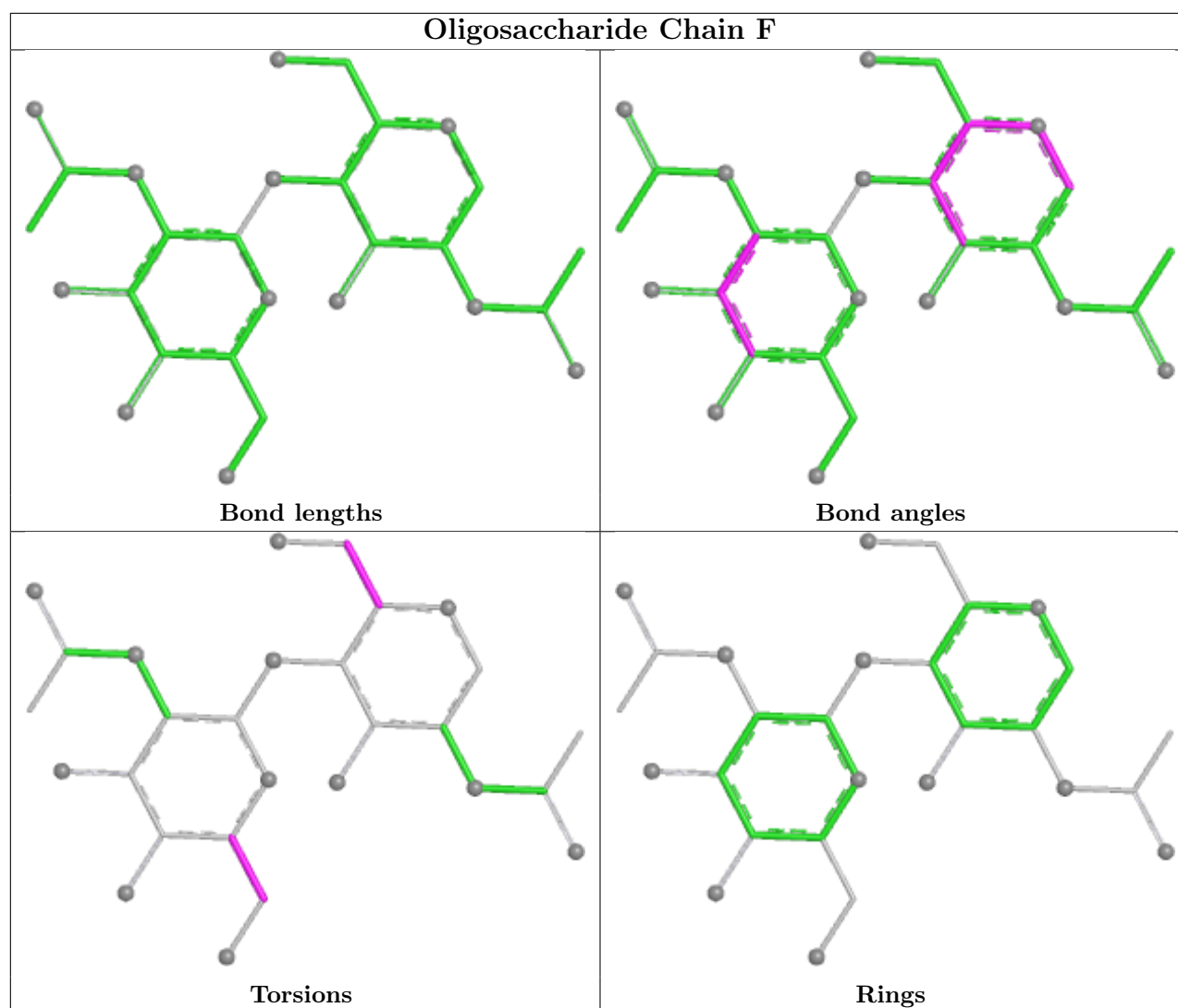
1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry [i](#)

34 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	$\# Z > 2$
9	LPE	A	2026	-	16,16,33	0.71	0	20,22,39	0.69	0
9	LPE	A	2021	-	24,24,33	0.55	0	28,30,39	0.69	1 (3%)
9	LPE	A	2025	-	24,24,33	0.56	0	28,30,39	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	LPE	A	2010	-	24,24,33	0.34	0	25,27,39	0.61	0
6	NAG	B	302	2	14,14,15	0.18	0	17,19,21	0.43	0
9	LPE	A	2020	-	24,24,33	0.88	0	28,30,39	0.91	1 (3%)
5	9SL	A	2001	-	17,23,23	3.66	9 (52%)	14,37,37	2.99	7 (50%)
8	Y01	A	2030	-	38,38,38	1.66	7 (18%)	57,57,57	1.68	12 (21%)
11	PCW	A	2028	-	43,43,53	0.99	2 (4%)	49,51,61	2.89	8 (16%)
6	NAG	A	2008	1	14,14,15	0.30	0	17,19,21	1.00	1 (5%)
10	1PW	A	2011	-	23,23,27	0.40	0	24,26,32	0.46	0
11	PCW	A	2027	-	43,43,53	1.04	2 (4%)	49,51,61	0.89	2 (4%)
7	P5S	A	2003	-	33,34,53	0.77	1 (3%)	34,40,60	1.81	4 (11%)
9	LPE	A	2023	-	24,24,33	0.54	0	28,30,39	0.54	0
11	PCW	A	2013	-	51,51,53	0.95	2 (3%)	57,59,61	0.99	2 (3%)
8	Y01	A	2005	-	38,38,38	0.68	1 (2%)	57,57,57	1.83	13 (22%)
9	LPE	A	2019	-	24,24,33	0.61	0	28,30,39	0.90	1 (3%)
7	P5S	A	2029	-	32,33,53	1.19	4 (12%)	34,40,60	1.02	2 (5%)
8	Y01	A	2007	-	38,38,38	0.69	1 (2%)	57,57,57	1.83	12 (21%)
9	LPE	A	2012	-	19,19,33	0.63	0	23,25,39	0.52	0
9	LPE	A	2015	-	27,27,33	0.55	0	31,33,39	0.62	0
7	P5S	A	2017	-	40,40,53	1.17	3 (7%)	43,45,60	1.38	3 (6%)
6	NAG	B	301	2	14,14,15	0.64	0	17,19,21	0.97	0
8	Y01	A	2004	-	38,38,38	0.69	1 (2%)	57,57,57	1.83	12 (21%)
11	PCW	A	2018	-	43,43,53	1.03	2 (4%)	49,51,61	1.13	5 (10%)
11	PCW	A	2016	-	46,46,53	1.00	3 (6%)	52,54,61	1.19	4 (7%)
9	LPE	A	2022	-	24,24,33	0.55	0	28,30,39	0.65	0
6	NAG	B	303	2	14,14,15	0.26	0	17,19,21	0.44	0
9	LPE	B	304	-	16,16,33	0.69	0	20,22,39	0.61	0
8	Y01	A	2009	-	38,38,38	1.17	4 (10%)	57,57,57	1.79	12 (21%)
9	LPE	A	2014	-	21,21,33	0.70	0	25,27,39	1.05	2 (8%)
6	NAG	A	2002	1	14,14,15	0.36	0	17,19,21	0.46	0
8	Y01	A	2006	-	38,38,38	1.17	4 (10%)	57,57,57	1.79	12 (21%)
9	LPE	A	2024	-	24,24,33	0.52	0	28,30,39	0.62	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
9	LPE	A	2026	-	-	6/17/17/34	-
9	LPE	A	2021	-	-	2/25/25/34	-
9	LPE	A	2025	-	-	10/25/25/34	-
9	LPE	A	2010	-	-	8/25/25/34	-
6	NAG	B	302	2	-	0/6/23/26	0/1/1/1
9	LPE	A	2020	-	-	11/25/25/34	-
5	9SL	A	2001	-	-	4/5/53/53	0/3/3/3
8	Y01	A	2030	-	-	7/19/77/77	0/4/4/4
11	PCW	A	2028	-	-	12/47/47/57	-
6	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
10	1PW	A	2011	-	-	2/22/22/29	-
11	PCW	A	2027	-	-	5/47/47/57	-
7	P5S	A	2003	-	-	27/39/39/59	-
9	LPE	A	2023	-	-	7/25/25/34	-
11	PCW	A	2013	-	-	16/55/55/57	-
8	Y01	A	2005	-	-	0/19/77/77	0/4/4/4
9	LPE	A	2019	-	-	5/25/25/34	-
7	P5S	A	2029	-	-	18/39/39/59	-
8	Y01	A	2007	-	-	0/19/77/77	0/4/4/4
9	LPE	A	2012	-	-	8/20/20/34	-
9	LPE	A	2015	-	-	8/28/28/34	-
7	P5S	A	2017	-	-	8/44/44/59	-
6	NAG	B	301	2	-	0/6/23/26	0/1/1/1
8	Y01	A	2004	-	-	0/19/77/77	0/4/4/4
11	PCW	A	2018	-	-	10/47/47/57	-
11	PCW	A	2016	-	-	12/50/50/57	-
9	LPE	A	2022	-	-	3/25/25/34	-
6	NAG	B	303	2	-	0/6/23/26	0/1/1/1
9	LPE	B	304	-	-	9/17/17/34	-
8	Y01	A	2009	-	-	4/19/77/77	0/4/4/4
9	LPE	A	2014	-	-	15/22/22/34	-
6	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
8	Y01	A	2006	-	-	4/19/77/77	0/4/4/4
9	LPE	A	2024	-	-	4/25/25/34	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2001	9SL	C12-N13	8.85	1.49	1.35
5	A	2001	9SL	C07-N08	6.31	1.45	1.34
5	A	2001	9SL	C02-N21	6.17	1.44	1.33
5	A	2001	9SL	C12-N15	4.65	1.45	1.34
8	A	2030	Y01	CBB-CBE	-4.49	1.46	1.54
7	A	2017	P5S	O37-C38	4.40	1.46	1.34
11	A	2027	PCW	O3-C11	4.34	1.46	1.33
11	A	2028	PCW	O3-C11	4.25	1.45	1.33
8	A	2030	Y01	CAR-CBC	-4.22	1.40	1.51
11	A	2013	PCW	O2-C31	4.21	1.46	1.34
11	A	2013	PCW	O3-C11	4.15	1.45	1.33
5	A	2001	9SL	C05-C14	4.12	1.60	1.52
11	A	2027	PCW	O2-C31	4.05	1.45	1.34
11	A	2028	PCW	O2-C31	4.04	1.45	1.34
11	A	2018	PCW	O2-C31	3.95	1.45	1.34
7	A	2017	P5S	O19-C17	3.91	1.44	1.33
11	A	2018	PCW	O3-C11	3.90	1.44	1.33
11	A	2016	PCW	O3-C11	3.87	1.44	1.33
7	A	2017	P5S	C28-C27	-3.80	1.32	1.51
8	A	2030	Y01	OAW-CAY	3.71	1.44	1.34
11	A	2016	PCW	O2-C31	3.67	1.44	1.34
8	A	2006	Y01	OAW-CAY	3.63	1.44	1.34
8	A	2009	Y01	OAW-CAY	3.63	1.44	1.34
7	A	2003	P5S	O37-C38	3.41	1.43	1.34
8	A	2030	Y01	CAV-CBC	3.14	1.59	1.52
5	A	2001	9SL	O01-C02	-2.85	1.17	1.22
5	A	2001	9SL	O03-C02	2.83	1.39	1.35
7	A	2029	P5S	O19-C17	2.75	1.41	1.33
7	A	2029	P5S	O37-C2	-2.68	1.40	1.46
5	A	2001	9SL	C05-N06	-2.62	1.43	1.47
8	A	2030	Y01	CAM-CAY	2.42	1.57	1.50
8	A	2006	Y01	CAM-CAY	2.41	1.57	1.50
8	A	2009	Y01	CAM-CAY	2.40	1.57	1.50
8	A	2004	Y01	CBH-CBF	-2.37	1.52	1.56
8	A	2006	Y01	CBH-CBF	-2.35	1.52	1.56
7	A	2029	P5S	O19-C1	-2.34	1.39	1.45
8	A	2007	Y01	CBH-CBF	-2.30	1.52	1.56
8	A	2030	Y01	CBH-CBF	-2.27	1.52	1.56
8	A	2009	Y01	CAL-CAX	2.27	1.55	1.50
7	A	2029	P5S	O37-C38	2.26	1.40	1.34
8	A	2005	Y01	CBH-CBF	-2.23	1.52	1.56
8	A	2009	Y01	CBH-CBF	-2.23	1.52	1.56
8	A	2006	Y01	CAL-CAX	2.22	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2030	Y01	CAL-CAX	2.21	1.55	1.50
11	A	2016	PCW	C6-N	-2.13	1.43	1.50
5	A	2001	9SL	C14-N13	-2.02	1.42	1.45

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	2028	PCW	C8-N-C6	-11.79	78.00	108.98
11	A	2028	PCW	C8-N-C7	-11.73	78.17	108.98
11	A	2028	PCW	C8-N-C5	-8.07	77.82	109.91
5	A	2001	9SL	O03-C02-N21	7.77	120.78	111.11
7	A	2003	P5S	OG-CB-CA	7.16	114.30	108.06
8	A	2005	Y01	CBI-CBE-CBB	-6.03	110.18	119.50
8	A	2009	Y01	CBI-CBE-CBB	-6.03	110.18	119.50
8	A	2007	Y01	CBI-CBE-CBB	-6.02	110.20	119.50
8	A	2004	Y01	CBI-CBE-CBB	-6.01	110.21	119.50
8	A	2006	Y01	CBI-CBE-CBB	-6.00	110.22	119.50
7	A	2017	P5S	O37-C38-C39	5.48	123.34	111.48
8	A	2007	Y01	CBI-CBG-CBD	-5.07	107.21	114.41
8	A	2005	Y01	CBI-CBG-CBD	-5.05	107.25	114.41
8	A	2009	Y01	CBI-CBG-CBD	-5.00	107.32	114.41
8	A	2030	Y01	CBI-CBG-CBD	-4.97	107.35	114.41
8	A	2004	Y01	CBI-CBG-CBD	-4.97	107.36	114.41
8	A	2006	Y01	CBI-CBG-CBD	-4.95	107.39	114.41
11	A	2016	PCW	O2-C31-C32	4.81	121.90	111.48
5	A	2001	9SL	O01-C02-N21	-4.50	118.48	125.58
8	A	2030	Y01	CBI-CBE-CBB	-4.19	113.02	119.50
7	A	2003	P5S	OXT-C-O	-4.07	114.85	124.08
8	A	2005	Y01	OAW-CAY-CAM	3.99	120.11	111.48
8	A	2004	Y01	OAW-CAY-CAM	3.93	119.99	111.48
8	A	2007	Y01	OAW-CAY-CAM	3.91	119.95	111.48
11	A	2028	PCW	O2-C31-C32	3.89	119.90	111.48
11	A	2013	PCW	O2-C31-C32	3.87	119.85	111.48
9	A	2020	LPE	C3N-N-C2N	3.84	119.06	108.98
8	A	2006	Y01	OAW-CAY-CAM	3.71	119.52	111.48
7	A	2003	P5S	O37-C38-C39	3.71	119.51	111.48
8	A	2009	Y01	OAW-CAY-CAM	3.71	119.51	111.48
8	A	2030	Y01	OAW-CAY-CAM	3.57	119.21	111.48
7	A	2029	P5S	O37-C38-C39	3.41	118.86	111.48
8	A	2030	Y01	CAS-CAU-CBI	-3.35	107.09	112.74
8	A	2004	Y01	CAS-CAU-CBI	-3.35	107.09	112.74
8	A	2005	Y01	CAS-CAU-CBI	-3.34	107.11	112.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2009	Y01	CAS-CAU-CBI	-3.33	107.12	112.74
8	A	2006	Y01	CAS-CAU-CBI	-3.33	107.13	112.74
8	A	2007	Y01	CAS-CAU-CBI	-3.31	107.15	112.74
5	A	2001	9SL	N09-C07-N06	-3.29	120.83	125.42
11	A	2016	PCW	O3-C11-C12	3.17	121.50	111.83
8	A	2004	Y01	CAD-CBH-CBF	-3.09	108.20	111.66
8	A	2009	Y01	CAD-CBH-CBF	-3.08	108.20	111.66
8	A	2005	Y01	CAD-CBH-CBF	-3.07	108.21	111.66
8	A	2007	Y01	CAD-CBH-CBF	-3.07	108.21	111.66
5	A	2001	9SL	N13-C12-N11	-3.06	107.66	115.62
8	A	2006	Y01	CAD-CBH-CBF	-3.06	108.22	111.66
8	A	2030	Y01	CAD-CBH-CBF	-3.04	108.25	111.66
11	A	2018	PCW	C3-C2-C1	-2.94	104.92	111.78
6	A	2008	NAG	C4-C3-C2	-2.94	106.71	111.02
9	A	2014	LPE	C3-C2-C1	-2.89	104.34	112.65
11	A	2018	PCW	O2-C31-C32	2.82	117.57	111.48
8	A	2030	Y01	CBG-CBI-CBE	2.79	103.30	100.10
8	A	2006	Y01	CBG-CBI-CBE	2.78	103.29	100.10
8	A	2004	Y01	CBG-CBI-CBE	2.77	103.28	100.10
11	A	2028	PCW	O3-C11-C12	2.75	120.23	111.83
8	A	2007	Y01	CBG-CBI-CBE	2.75	103.26	100.10
8	A	2009	Y01	CBG-CBI-CBE	2.74	103.25	100.10
8	A	2007	Y01	CAS-CBF-CBH	-2.72	109.73	113.08
8	A	2009	Y01	CAS-CBF-CBH	-2.71	109.74	113.08
8	A	2005	Y01	CAS-CBF-CBH	-2.71	109.74	113.08
8	A	2030	Y01	CAS-CBF-CBH	-2.70	109.75	113.08
8	A	2005	Y01	CBG-CBI-CBE	2.70	103.20	100.10
8	A	2004	Y01	CAS-CBF-CBH	-2.68	109.78	113.08
9	A	2014	LPE	C31-C32-N	-2.67	107.25	115.82
8	A	2006	Y01	CAS-CBF-CBH	-2.66	109.81	113.08
8	A	2009	Y01	CBD-CAK-CAI	-2.63	109.12	112.76
11	A	2027	PCW	O2-C31-C32	2.62	117.16	111.48
8	A	2006	Y01	CBD-CAK-CAI	-2.60	109.16	112.76
11	A	2018	PCW	O3-C11-C12	2.60	119.75	111.83
8	A	2004	Y01	CBD-CAK-CAI	-2.58	109.18	112.76
11	A	2028	PCW	C7-N-C6	2.57	115.72	108.98
8	A	2007	Y01	CBD-CAK-CAI	-2.56	109.21	112.76
11	A	2013	PCW	O3-C11-C12	2.55	119.61	111.83
8	A	2005	Y01	CBD-CAK-CAI	-2.54	109.24	112.76
8	A	2030	Y01	CBD-CAK-CAI	-2.54	109.25	112.76
5	A	2001	9SL	O03-C02-O01	-2.53	120.74	123.08
7	A	2029	P5S	O19-C17-C20	2.52	119.53	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2006	Y01	CBF-CBH-CAZ	2.52	113.34	109.65
8	A	2004	Y01	CBF-CBH-CAZ	2.51	113.32	109.65
8	A	2007	Y01	CBF-CBH-CAZ	2.48	113.29	109.65
8	A	2030	Y01	CBF-CBH-CAZ	2.46	113.26	109.65
8	A	2009	Y01	CBF-CBH-CAZ	2.43	113.21	109.65
8	A	2005	Y01	CBF-CBH-CAZ	2.41	113.19	109.65
11	A	2028	PCW	C2-O2-C31	-2.40	112.06	117.80
7	A	2003	P5S	C2-O37-C38	-2.36	112.14	117.80
7	A	2017	P5S	C41-C40-C39	-2.31	104.65	113.13
5	A	2001	9SL	O03-C04-C05	2.29	112.95	108.46
9	A	2021	LPE	C31-C32-N	-2.28	108.51	115.82
8	A	2007	Y01	CAC-CBB-CBE	-2.27	109.47	112.88
8	A	2004	Y01	CAC-CBB-CBE	-2.27	109.48	112.88
8	A	2005	Y01	CAC-CBB-CBE	-2.24	109.52	112.88
11	A	2027	PCW	C13-C12-C11	-2.24	105.50	113.69
8	A	2006	Y01	CAC-CBB-CBE	-2.23	109.54	112.88
9	A	2019	LPE	C31-C32-N	-2.22	108.70	115.82
8	A	2009	Y01	CAC-CBB-CBE	-2.21	109.56	112.88
7	A	2017	P5S	O15-P12-O13	2.20	122.68	112.44
11	A	2016	PCW	O2-C31-O31	-2.20	118.57	123.70
8	A	2006	Y01	CAQ-CBG-CBD	-2.16	115.65	119.10
8	A	2005	Y01	CAQ-CBG-CBD	-2.14	115.69	119.10
8	A	2004	Y01	CAQ-CBG-CBD	-2.12	115.72	119.10
5	A	2001	9SL	C14-C05-N06	2.11	116.99	111.22
8	A	2030	Y01	CAQ-CBG-CBD	-2.10	115.74	119.10
8	A	2009	Y01	CAQ-CBG-CBD	-2.10	115.75	119.10
8	A	2007	Y01	CAQ-CBG-CBD	-2.10	115.75	119.10
11	A	2018	PCW	O3-C3-C2	2.09	114.42	108.40
11	A	2018	PCW	C34-C33-C32	-2.09	105.45	113.13
8	A	2007	Y01	CBC-CAV-CAZ	-2.09	108.37	111.45
11	A	2016	PCW	O3-C11-O11	-2.07	118.44	123.63
11	A	2028	PCW	C4-C5-N	-2.06	109.22	115.82
8	A	2004	Y01	CBC-CAV-CAZ	-2.05	108.42	111.45
8	A	2006	Y01	CBC-CAV-CAZ	-2.05	108.42	111.45
8	A	2030	Y01	CAR-CBC-CAV	2.04	113.81	110.97
8	A	2009	Y01	CBC-CAV-CAZ	-2.04	108.44	111.45
8	A	2005	Y01	CBC-CAV-CAZ	-2.03	108.45	111.45
8	A	2030	Y01	CAT-CAR-CBC	2.02	113.62	110.33
8	A	2005	Y01	CAJ-CAO-CBB	-2.01	109.45	115.08

There are no chirality outliers.

All (229) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2001	9SL	O01-C02-O03-C04
5	A	2001	9SL	N21-C02-O03-C04
5	A	2001	9SL	O03-C04-C05-N06
5	A	2001	9SL	O03-C04-C05-C14
7	A	2003	P5S	C-CA-CB-OG
7	A	2003	P5S	N-CA-CB-OG
7	A	2003	P5S	CB-OG-P12-O13
7	A	2003	P5S	CB-OG-P12-O16
7	A	2003	P5S	C3-O16-P12-OG
7	A	2003	P5S	C3-O16-P12-O13
7	A	2003	P5S	C3-O16-P12-O15
7	A	2017	P5S	CB-OG-P12-O15
7	A	2017	P5S	C3-O16-P12-OG
7	A	2017	P5S	C3-O16-P12-O13
7	A	2017	P5S	C3-O16-P12-O15
7	A	2029	P5S	O-C-CA-CB
7	A	2029	P5S	OXT-C-CA-CB
7	A	2029	P5S	C3-O16-P12-O13
9	A	2010	LPE	C3-O3-P-O31
9	A	2010	LPE	C31-O33-P-O3
9	A	2012	LPE	C3-O3-P-O32
9	A	2012	LPE	C3-O3-P-O33
9	A	2012	LPE	C31-O33-P-O31
9	A	2014	LPE	O1-C1-C2-C3
9	A	2014	LPE	C3-O3-P-O32
9	A	2014	LPE	C3-O3-P-O33
9	A	2014	LPE	C31-O33-P-O3
9	A	2014	LPE	C31-O33-P-O31
9	A	2014	LPE	C32-C31-O33-P
9	A	2014	LPE	O33-C31-C32-N
9	A	2015	LPE	C3-O3-P-O32
9	A	2015	LPE	C3-O3-P-O33
9	A	2019	LPE	C31-O33-P-O31
9	A	2019	LPE	O33-C31-C32-N
9	A	2020	LPE	C31-O33-P-O31
9	A	2021	LPE	C31-O33-P-O31
9	A	2022	LPE	C3-O3-P-O31
9	A	2023	LPE	C31-O33-P-O3
9	A	2023	LPE	C31-O33-P-O32
9	A	2024	LPE	C31-O33-P-O31
9	A	2025	LPE	O1-C1-C2-C3
9	A	2025	LPE	C3-O3-P-O32
9	A	2025	LPE	C3-O3-P-O33

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Mol	Chain	Res	Type	Atoms
9	A	2025	LPE	C31-O33-P-O3
9	A	2025	LPE	C31-O33-P-O31
9	A	2025	LPE	C31-O33-P-O32
9	A	2026	LPE	C31-O33-P-O3
9	B	304	LPE	C3-O3-P-O31
9	B	304	LPE	C3-O3-P-O32
9	B	304	LPE	C3-O3-P-O33
9	B	304	LPE	C31-O33-P-O3
10	A	2011	1PW	CAH-CAI-CAZ-OAE
10	A	2011	1PW	CAH-CAI-CAZ-CBA
11	A	2013	PCW	C4-O4P-P-O3P
11	A	2016	PCW	O4P-C4-C5-N
11	A	2016	PCW	C4-O4P-P-O3P
11	A	2018	PCW	C32-C31-O2-C2
11	A	2018	PCW	C4-O4P-P-O3P
11	A	2027	PCW	C1-O3P-P-O2P
11	A	2027	PCW	C4-O4P-P-O2P
11	A	2028	PCW	C32-C31-O2-C2
11	A	2028	PCW	O31-C31-O2-C2
11	A	2028	PCW	C1-O3P-P-O1P
11	A	2028	PCW	C1-O3P-P-O2P
11	A	2028	PCW	C1-O3P-P-O4P
11	A	2028	PCW	C4-O4P-P-O2P
11	A	2028	PCW	C4-O4P-P-O3P
7	A	2029	P5S	O18-C17-O19-C1
7	A	2029	P5S	C20-C17-O19-C1
8	A	2030	Y01	CAC-CBB-CBE-CAP
8	A	2030	Y01	CAC-CBB-CBE-CBI
11	A	2018	PCW	O31-C31-O2-C2
8	A	2030	Y01	CAJ-CAO-CBB-CAC
8	A	2030	Y01	CAO-CBB-CBE-CBI
6	A	2002	NAG	O5-C5-C6-O6
9	A	2025	LPE	O1-C1-C2-O2H
8	A	2030	Y01	CAO-CBB-CBE-CAP
6	A	2002	NAG	C4-C5-C6-O6
11	A	2027	PCW	C12-C11-O3-C3
11	A	2027	PCW	O11-C11-O3-C3
11	A	2028	PCW	C12-C11-O3-C3
8	A	2006	Y01	CAR-CBC-OAW-CAY
9	A	2023	LPE	C31-C32-N-C2N
9	A	2023	LPE	C31-C32-N-C3N
11	A	2016	PCW	C4-C5-N-C8

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Mol	Chain	Res	Type	Atoms
11	A	2018	PCW	C4-C5-N-C7
8	A	2030	Y01	CAJ-CAO-CBB-CBE
6	A	2008	NAG	C8-C7-N2-C2
8	A	2009	Y01	CAR-CBC-OAW-CAY
9	A	2014	LPE	O1-C1-C2-O2H
11	A	2028	PCW	O11-C11-O3-C3
6	A	2008	NAG	O7-C7-N2-C2
9	A	2026	LPE	C31-C32-N-C3N
11	A	2016	PCW	C4-C5-N-C7
7	A	2003	P5S	C38-C39-C40-C41
9	A	2014	LPE	O1-C11-C12-C13
9	A	2020	LPE	O1-C1-C2-O2H
8	A	2006	Y01	CAV-CBC-OAW-CAY
8	A	2009	Y01	CAV-CBC-OAW-CAY
9	A	2014	LPE	C31-C32-N-C1N
9	A	2014	LPE	C31-C32-N-C2N
9	A	2014	LPE	C31-C32-N-C3N
11	A	2018	PCW	C4-C5-N-C6
11	A	2028	PCW	C4-C5-N-C8
9	A	2020	LPE	O1-C1-C2-C3
9	A	2023	LPE	C31-C32-N-C1N
9	A	2010	LPE	O1-C11-C12-C13
7	A	2029	P5S	C17-C20-C21-C22
7	A	2017	P5S	C25-C26-C27-C28
7	A	2003	P5S	C46-C48-C49-C50
7	A	2017	P5S	C27-C28-C29-C30
11	A	2016	PCW	C4-C5-N-C6
11	A	2018	PCW	C4-C5-N-C8
9	A	2020	LPE	C12-C13-C14-C15
11	A	2013	PCW	C32-C31-O2-C2
7	A	2003	P5S	C41-C42-C43-C44
7	A	2029	P5S	C42-C43-C44-C45
7	A	2003	P5S	C52-C53-C54-C55
7	A	2029	P5S	C21-C22-C23-C24
11	A	2013	PCW	C32-C33-C34-C35
9	A	2026	LPE	C31-C32-N-C1N
9	A	2026	LPE	C31-C32-N-C2N
7	A	2003	P5S	C39-C38-O37-C2
7	A	2003	P5S	C51-C52-C53-C54
9	A	2020	LPE	C14-C15-C16-C17
11	A	2013	PCW	O31-C31-O2-C2
7	A	2003	P5S	C48-C49-C50-C51

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Mol	Chain	Res	Type	Atoms
7	A	2029	P5S	C40-C41-C42-C43
7	A	2029	P5S	C43-C44-C45-C46
9	A	2024	LPE	C13-C14-C15-C16
7	A	2029	P5S	C38-C39-C40-C41
8	A	2030	Y01	CAN-CAJ-CAO-CBB
9	A	2010	LPE	C13-C14-C15-C16
11	A	2016	PCW	C35-C36-C37-C38
11	A	2016	PCW	C34-C35-C36-C37
9	A	2015	LPE	O1-C1-C2-O2H
9	B	304	LPE	C2-C3-O3-P
11	A	2013	PCW	C41-C42-C43-C44
7	A	2003	P5S	C1-C2-C3-O16
7	A	2003	P5S	O47-C38-O37-C2
7	A	2003	P5S	C2-C3-O16-P12
9	A	2026	LPE	C2-C1-O1-C11
11	A	2028	PCW	C32-C33-C34-C35
9	A	2020	LPE	C11-C12-C13-C14
9	A	2015	LPE	O1-C1-C2-C3
11	A	2013	PCW	C24-C25-C26-C27
9	A	2020	LPE	C16-C17-C18-C19
9	A	2019	LPE	C2-C1-O1-C11
9	B	304	LPE	C2-C1-O1-C11
8	A	2006	Y01	CAO-CAJ-CAN-CBA
8	A	2009	Y01	CAO-CAJ-CAN-CBA
7	A	2003	P5S	O37-C2-C3-O16
7	A	2029	P5S	C39-C38-O37-C2
9	A	2010	LPE	C32-C31-O33-P
9	B	304	LPE	C32-C31-O33-P
11	A	2013	PCW	C4-C5-N-C7
9	A	2020	LPE	C12-C11-O1-C1
9	A	2012	LPE	O33-C31-C32-N
9	A	2015	LPE	O33-C31-C32-N
9	A	2020	LPE	O33-C31-C32-N
9	A	2021	LPE	O33-C31-C32-N
9	A	2022	LPE	O33-C31-C32-N
9	A	2023	LPE	O33-C31-C32-N
9	A	2024	LPE	O33-C31-C32-N
9	A	2025	LPE	O33-C31-C32-N
9	B	304	LPE	O33-C31-C32-N
11	A	2027	PCW	O4P-C4-C5-N
11	A	2028	PCW	O4P-C4-C5-N
7	A	2003	P5S	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
7	A	2029	P5S	CA-CB-OG-P12
9	A	2012	LPE	C12-C11-O1-C1
11	A	2013	PCW	C4-C5-N-C6
7	A	2029	P5S	O47-C38-O37-C2
9	A	2014	LPE	C12-C11-O1-C1
9	A	2019	LPE	C12-C11-O1-C1
7	A	2003	P5S	CB-OG-P12-O15
7	A	2017	P5S	CB-OG-P12-O16
7	A	2029	P5S	C3-O16-P12-OG
7	A	2029	P5S	C3-O16-P12-O15
9	A	2010	LPE	C3-O3-P-O32
9	A	2010	LPE	C3-O3-P-O33
9	A	2010	LPE	C31-O33-P-O31
9	A	2012	LPE	C3-O3-P-O31
9	A	2015	LPE	C31-O33-P-O31
9	A	2019	LPE	C3-O3-P-O31
9	A	2020	LPE	C3-O3-P-O32
9	A	2022	LPE	C3-O3-P-O33
9	A	2023	LPE	C31-O33-P-O31
9	A	2025	LPE	C3-O3-P-O31
9	A	2026	LPE	C31-O33-P-O31
9	B	304	LPE	C31-O33-P-O31
11	A	2013	PCW	C4-C5-N-C8
11	A	2013	PCW	C4-O4P-P-O2P
11	A	2016	PCW	C1-O3P-P-O2P
11	A	2016	PCW	C4-O4P-P-O2P
11	A	2018	PCW	C1-O3P-P-O2P
11	A	2018	PCW	C4-O4P-P-O2P
9	A	2024	LPE	C2-C1-O1-C11
7	A	2029	P5S	C2-C3-O16-P12
11	A	2018	PCW	C2-C1-O3P-P
9	A	2014	LPE	C13-C14-C15-C16
7	A	2003	P5S	C50-C51-C52-C53
11	A	2016	PCW	C17-C18-C19-C20
11	A	2016	PCW	C37-C38-C39-C40
9	A	2015	LPE	C12-C11-O1-C1
9	A	2012	LPE	C2-C3-O3-P
9	A	2025	LPE	C2-C1-O1-C11
11	A	2013	PCW	C23-C24-C25-C26
9	A	2014	LPE	C11-C12-C13-C14
11	A	2013	PCW	C44-C45-C46-C47
7	A	2003	P5S	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
7	A	2003	P5S	O19-C1-C2-O37
7	A	2003	P5S	C39-C40-C41-C42
11	A	2013	PCW	C17-C18-C19-C20
7	A	2029	P5S	C41-C42-C43-C44
7	A	2003	P5S	C53-C54-C55-C56
9	A	2015	LPE	C2-C3-O3-P
11	A	2013	PCW	C13-C14-C15-C16
11	A	2016	PCW	C39-C40-C41-C42
11	A	2018	PCW	O3-C11-C12-C13
11	A	2013	PCW	C39-C40-C41-C42
11	A	2013	PCW	C19-C20-C21-C22
9	A	2020	LPE	C13-C14-C15-C16
7	A	2017	P5S	C39-C38-O37-C2
9	A	2012	LPE	C31-C32-N-C2N
8	A	2009	Y01	CAN-CAJ-CAO-CBB
8	A	2006	Y01	CAN-CAJ-CAO-CBB
7	A	2003	P5S	C49-C50-C51-C52
7	A	2003	P5S	O37-C38-C39-C40

There are no ring outliers.

32 monomers are involved in 158 short contacts:

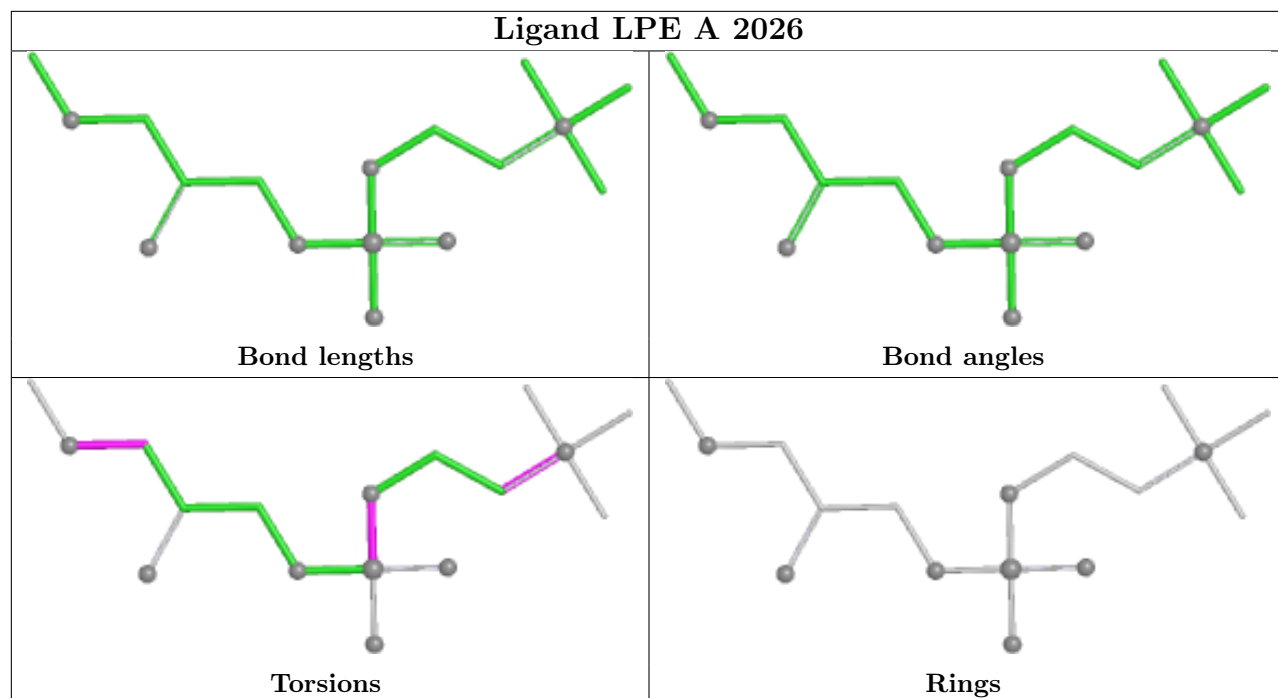
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2026	LPE	6	0
9	A	2021	LPE	6	0
9	A	2025	LPE	2	0
9	A	2010	LPE	1	0
6	B	302	NAG	1	0
9	A	2020	LPE	2	0
5	A	2001	9SL	2	0
8	A	2030	Y01	20	0
6	A	2008	NAG	1	0
10	A	2011	1PW	5	0
11	A	2027	PCW	2	0
7	A	2003	P5S	10	0
9	A	2023	LPE	6	0
11	A	2013	PCW	14	0
8	A	2005	Y01	8	0
9	A	2019	LPE	2	0
7	A	2029	P5S	3	0
8	A	2007	Y01	9	0
9	A	2012	LPE	6	0

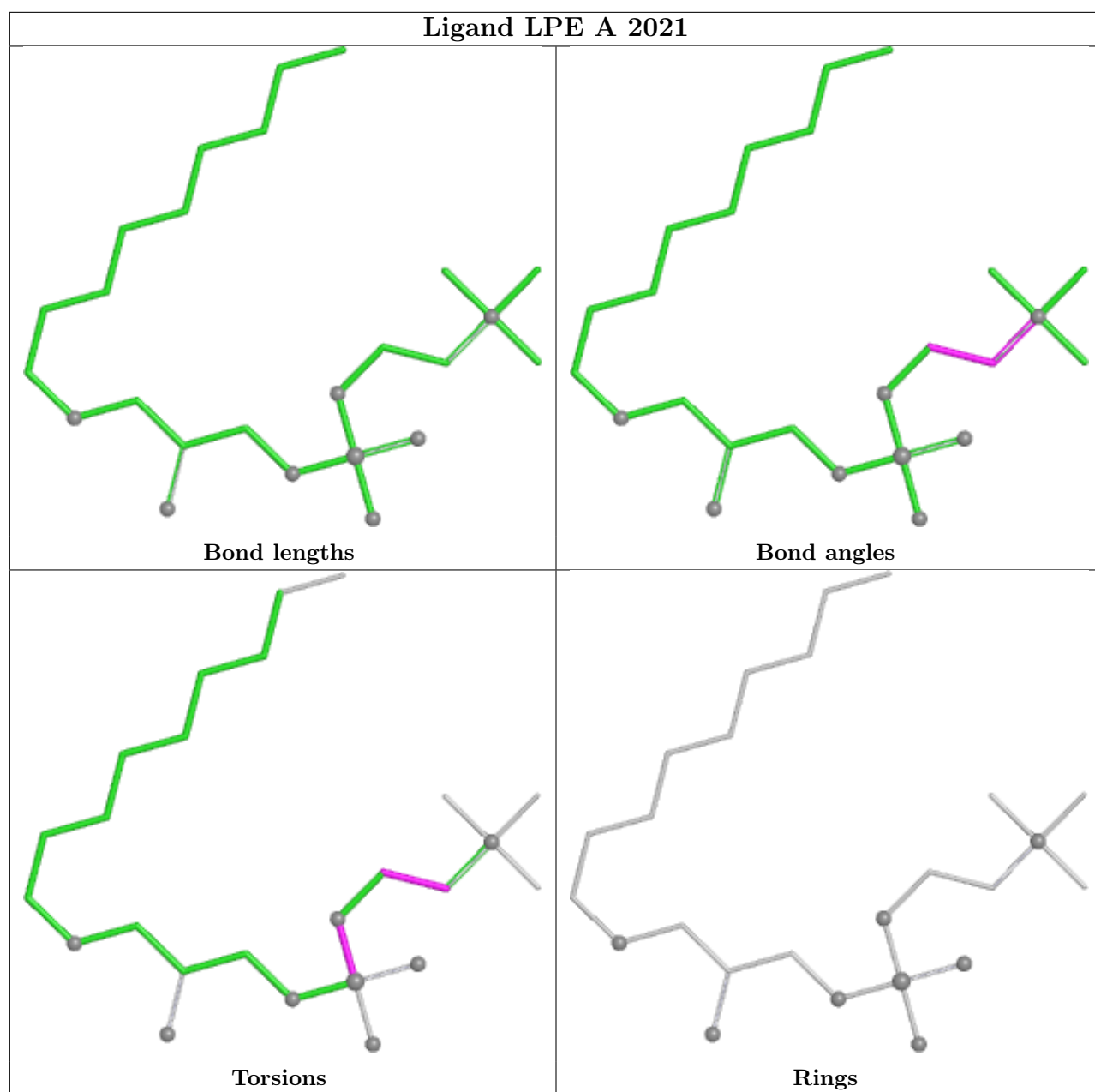
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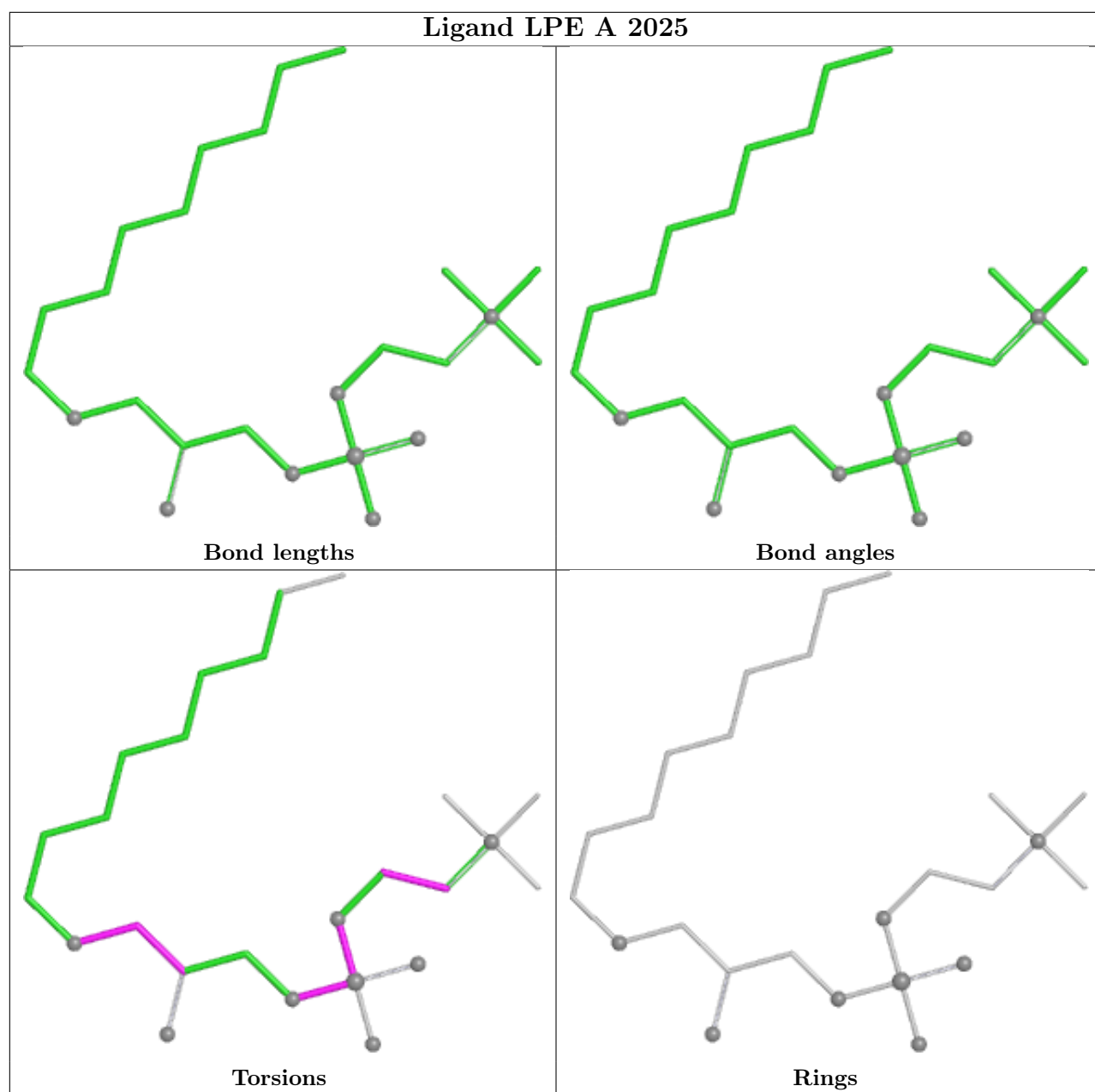
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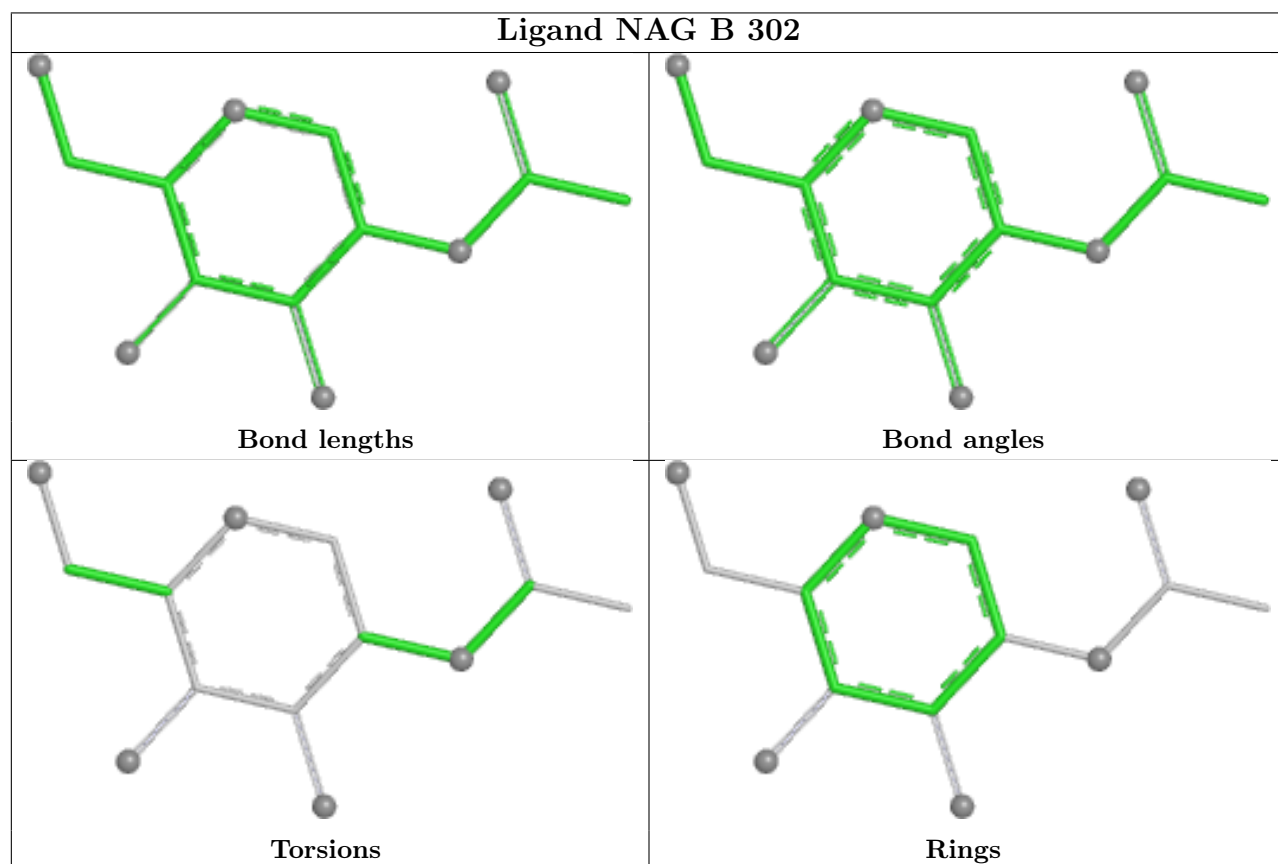
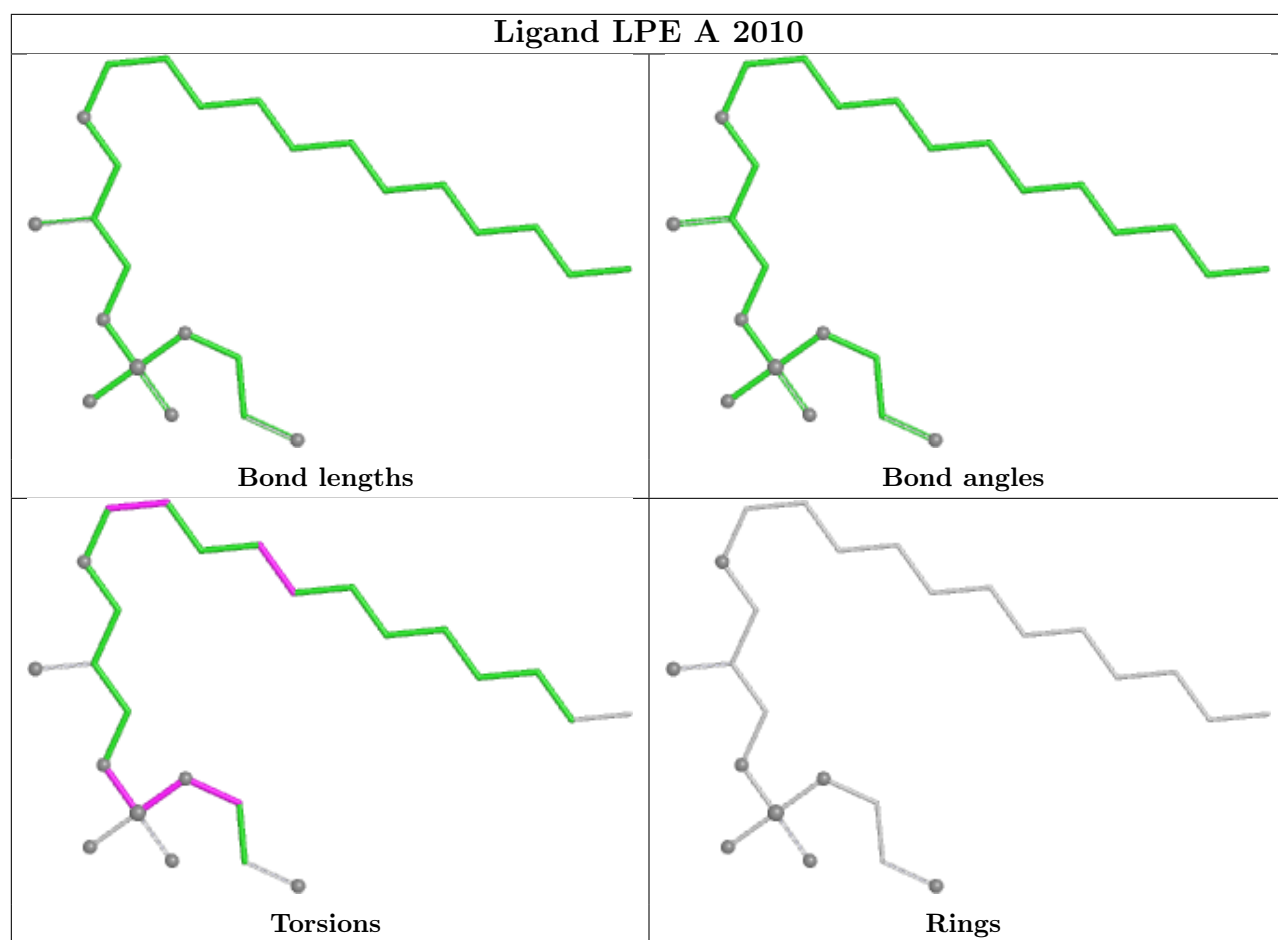
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2015	LPE	1	0
7	A	2017	P5S	3	0
6	B	301	NAG	1	0
8	A	2004	Y01	4	0
11	A	2018	PCW	5	0
11	A	2016	PCW	7	0
9	A	2022	LPE	2	0
6	B	303	NAG	2	0
8	A	2009	Y01	6	0
9	A	2014	LPE	22	0
6	A	2002	NAG	1	0
8	A	2006	Y01	21	0
9	A	2024	LPE	2	0

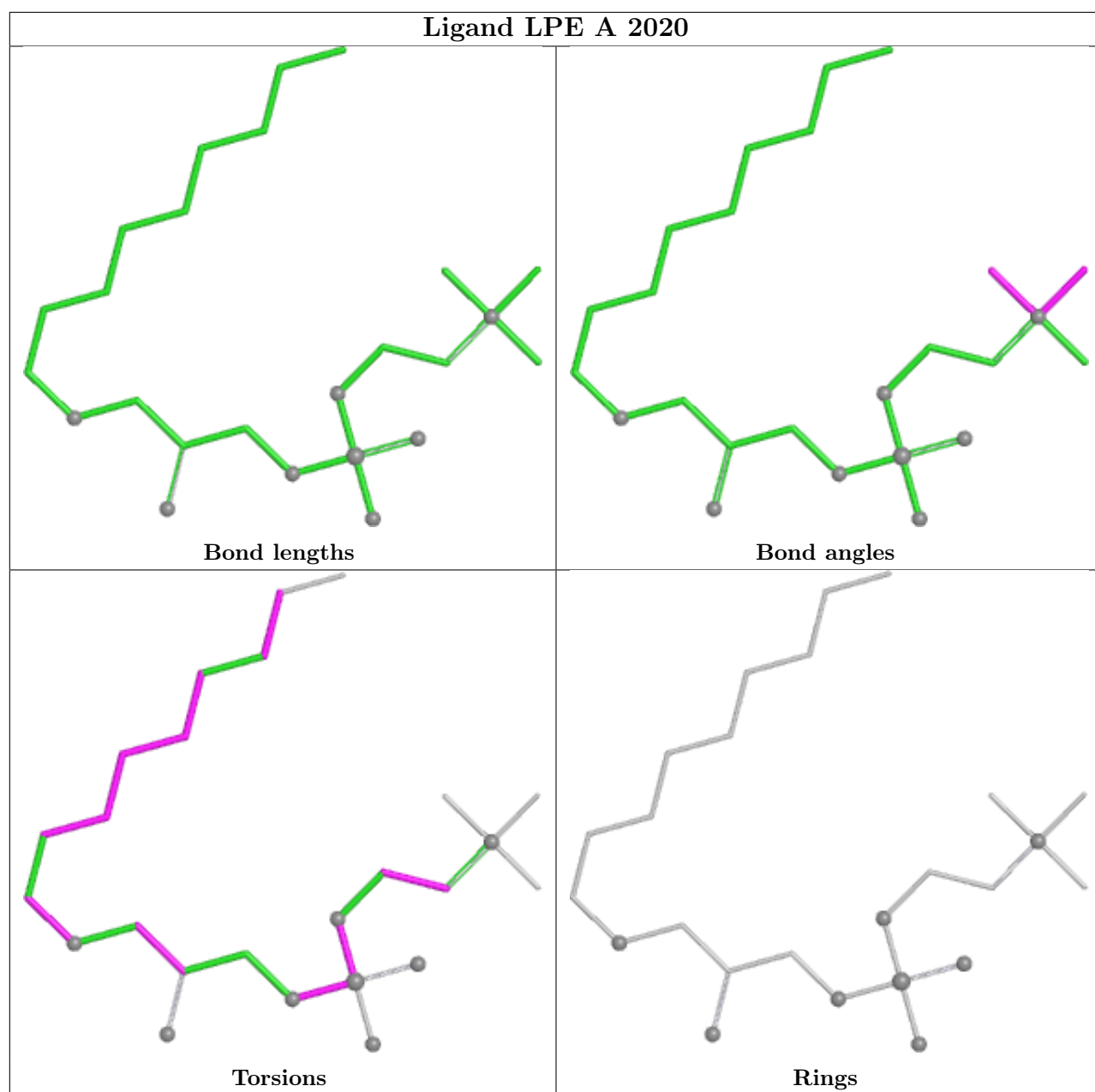
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

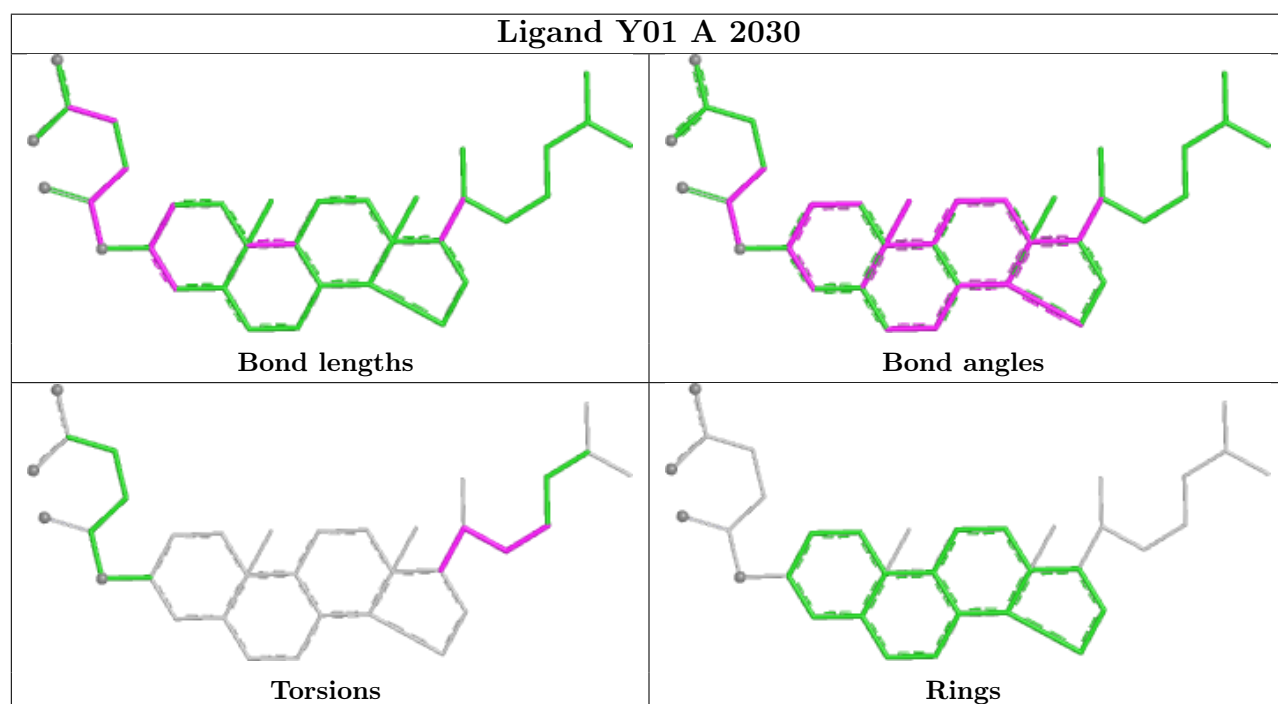
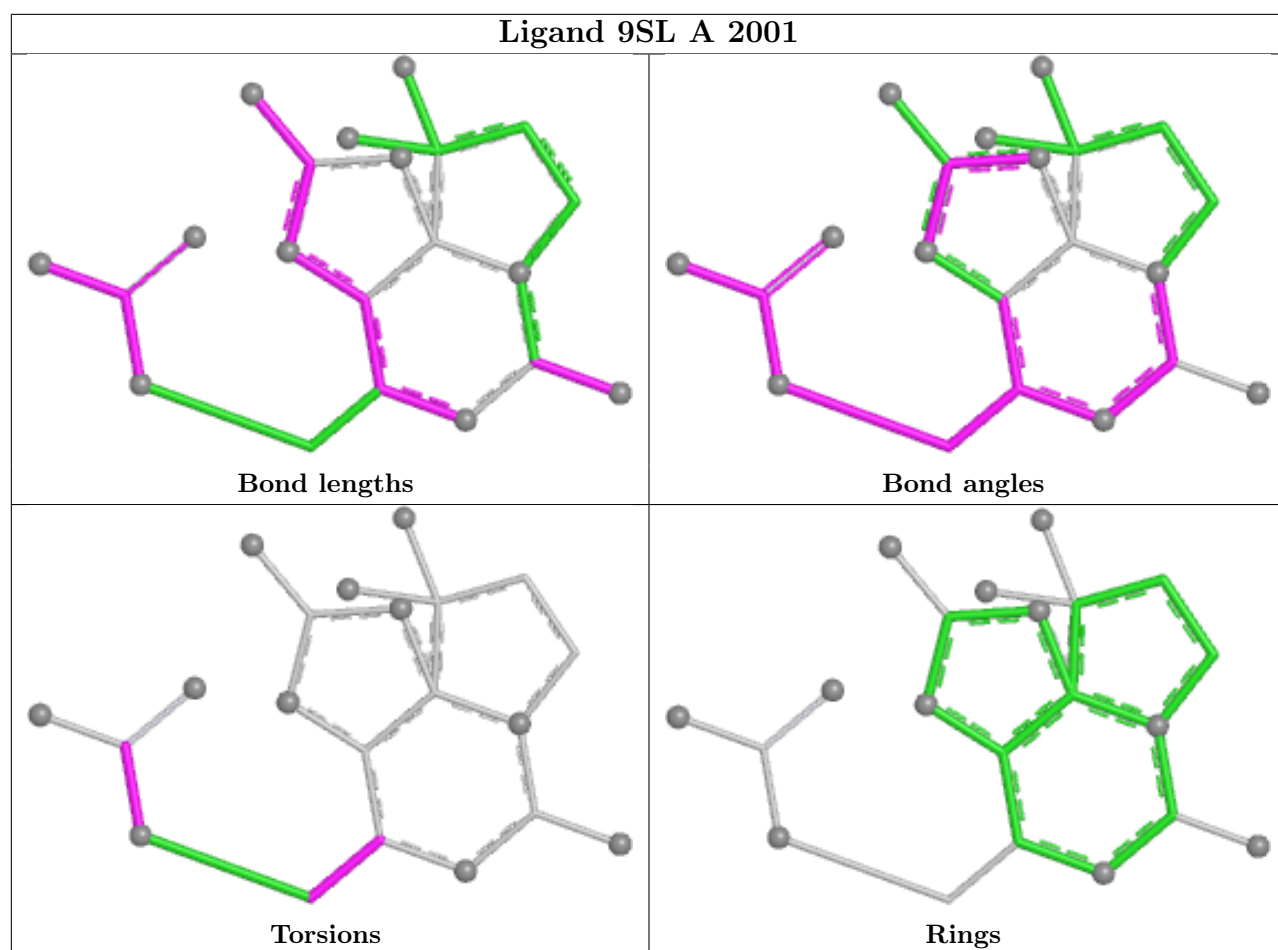


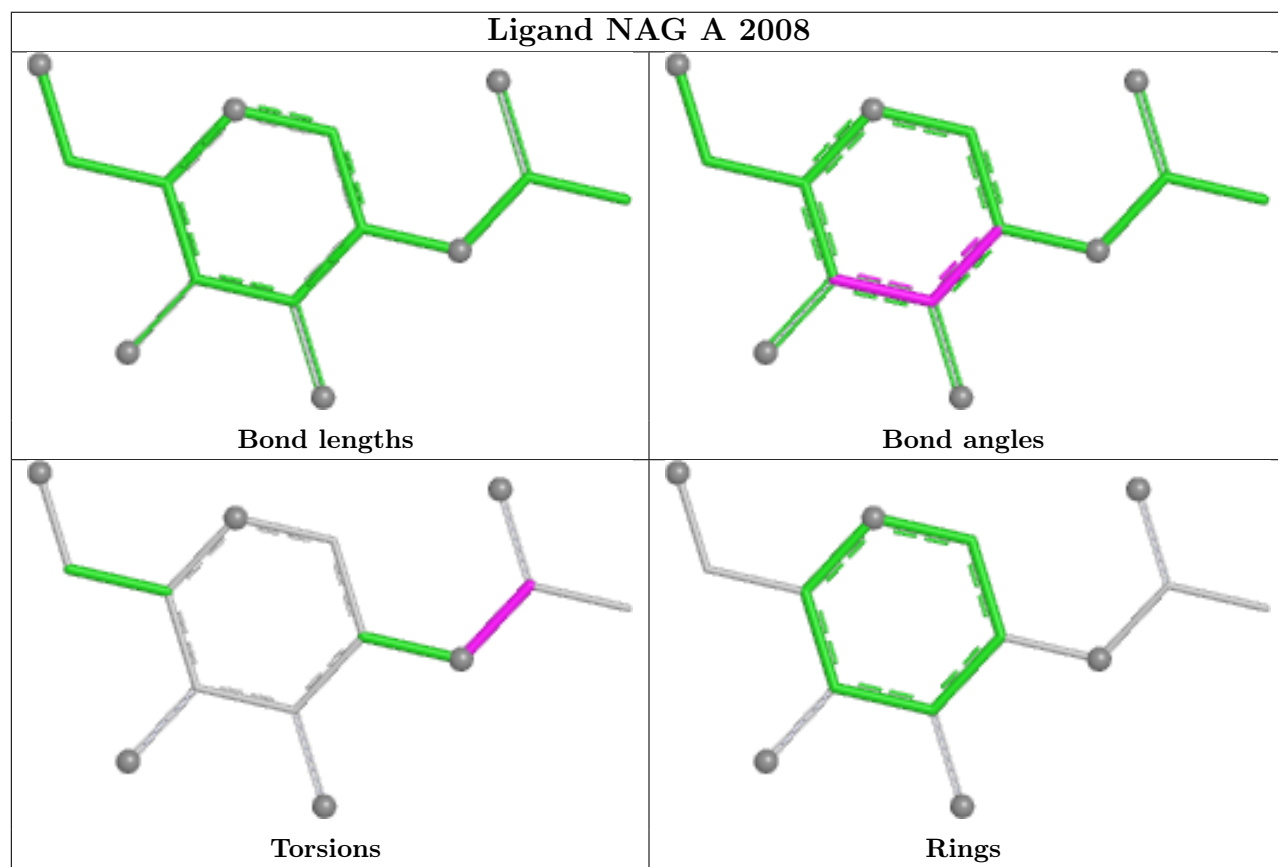
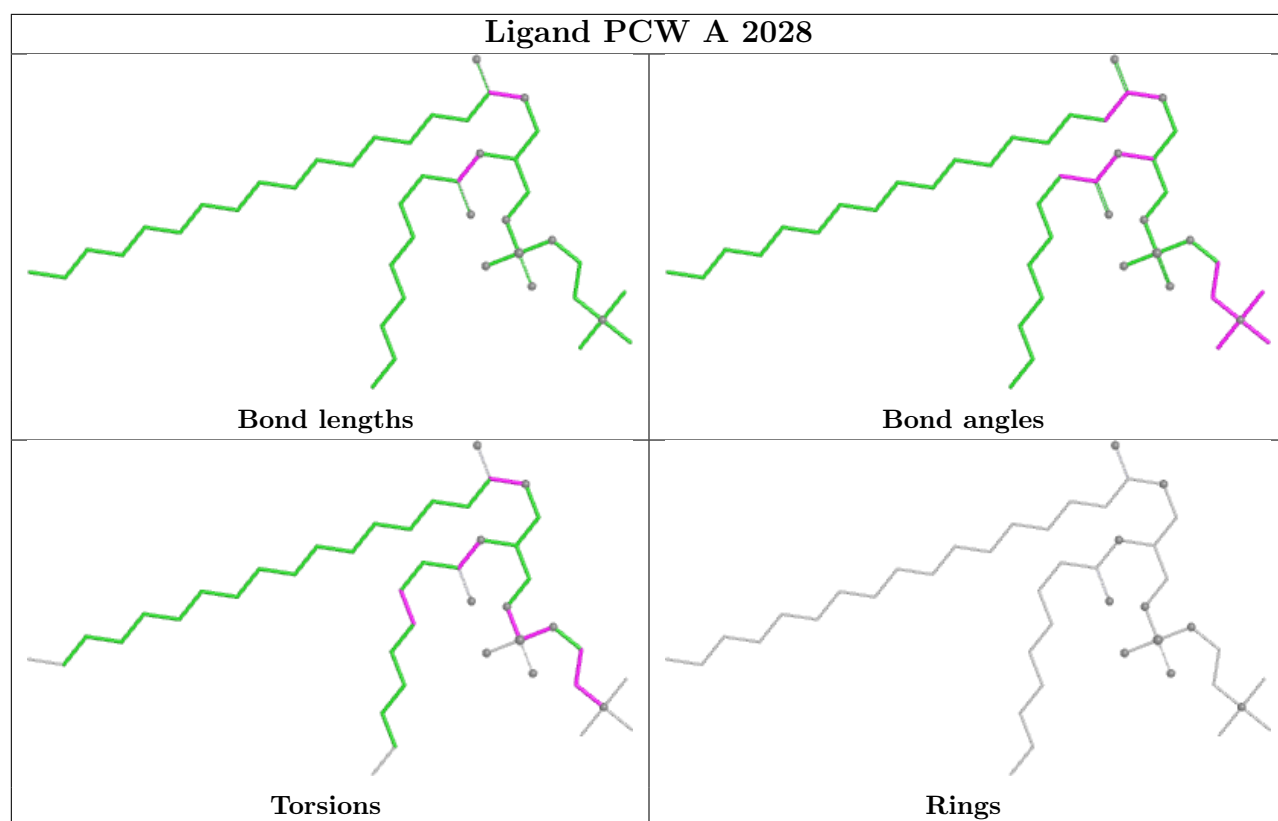


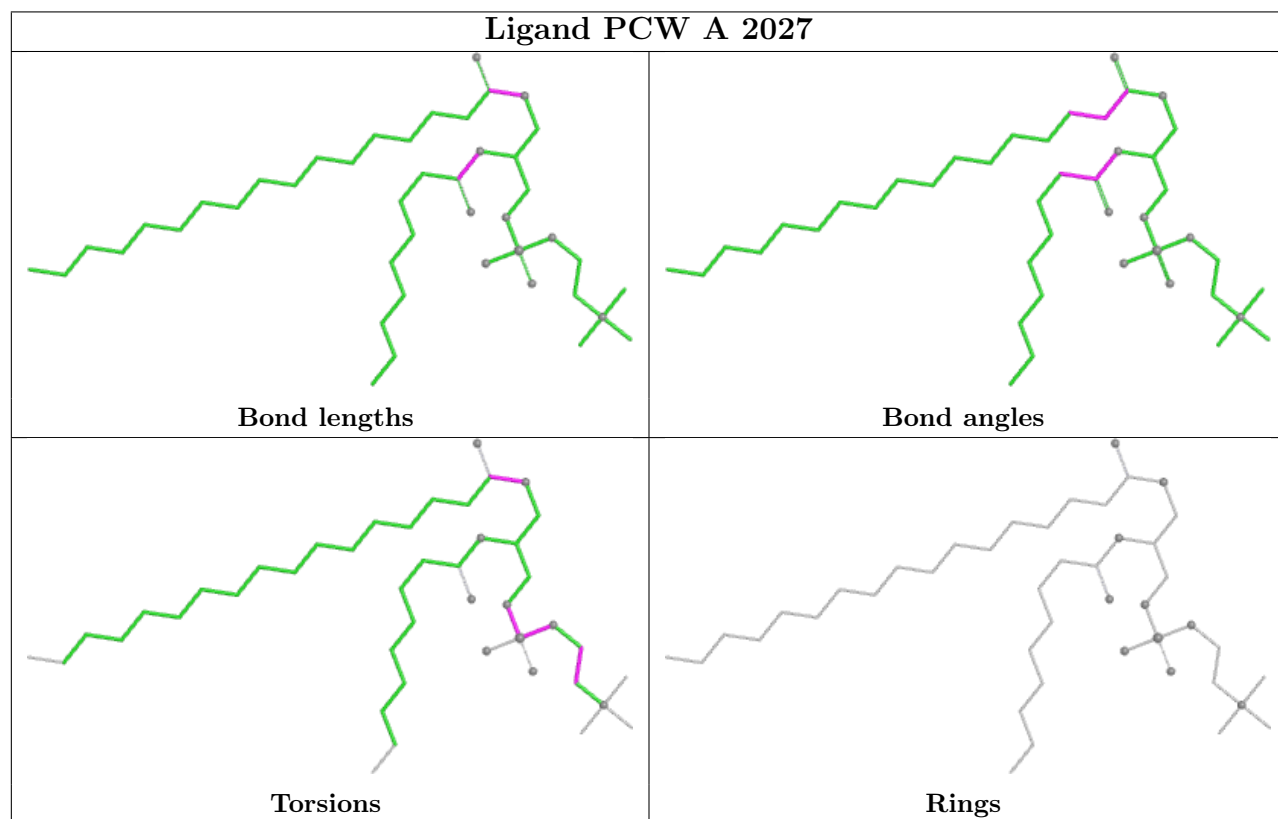
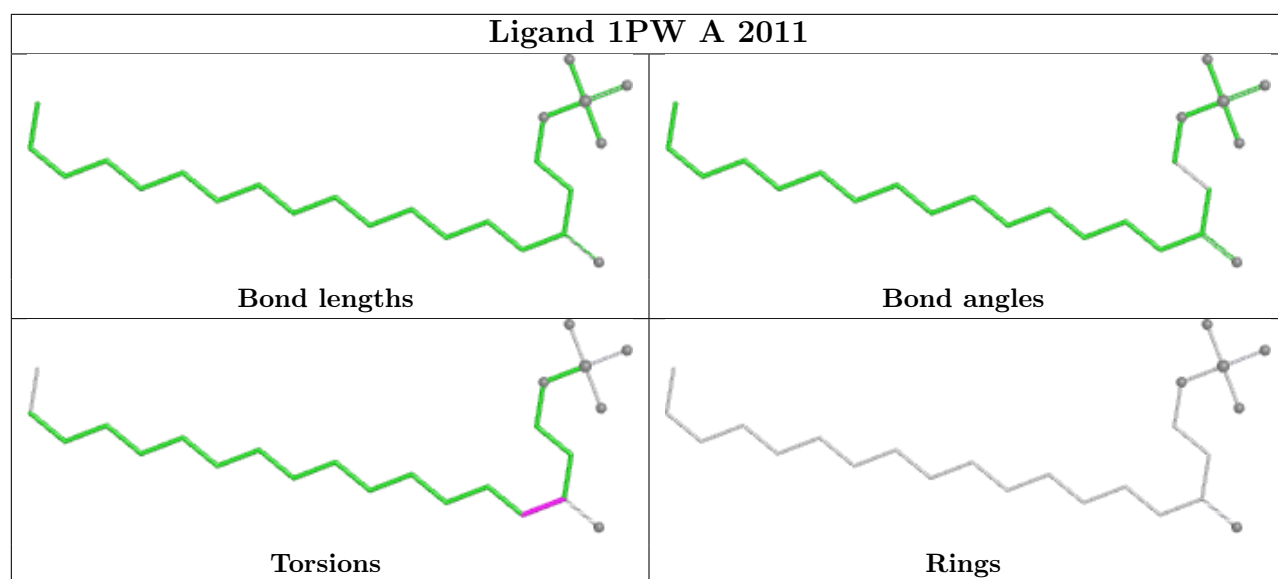


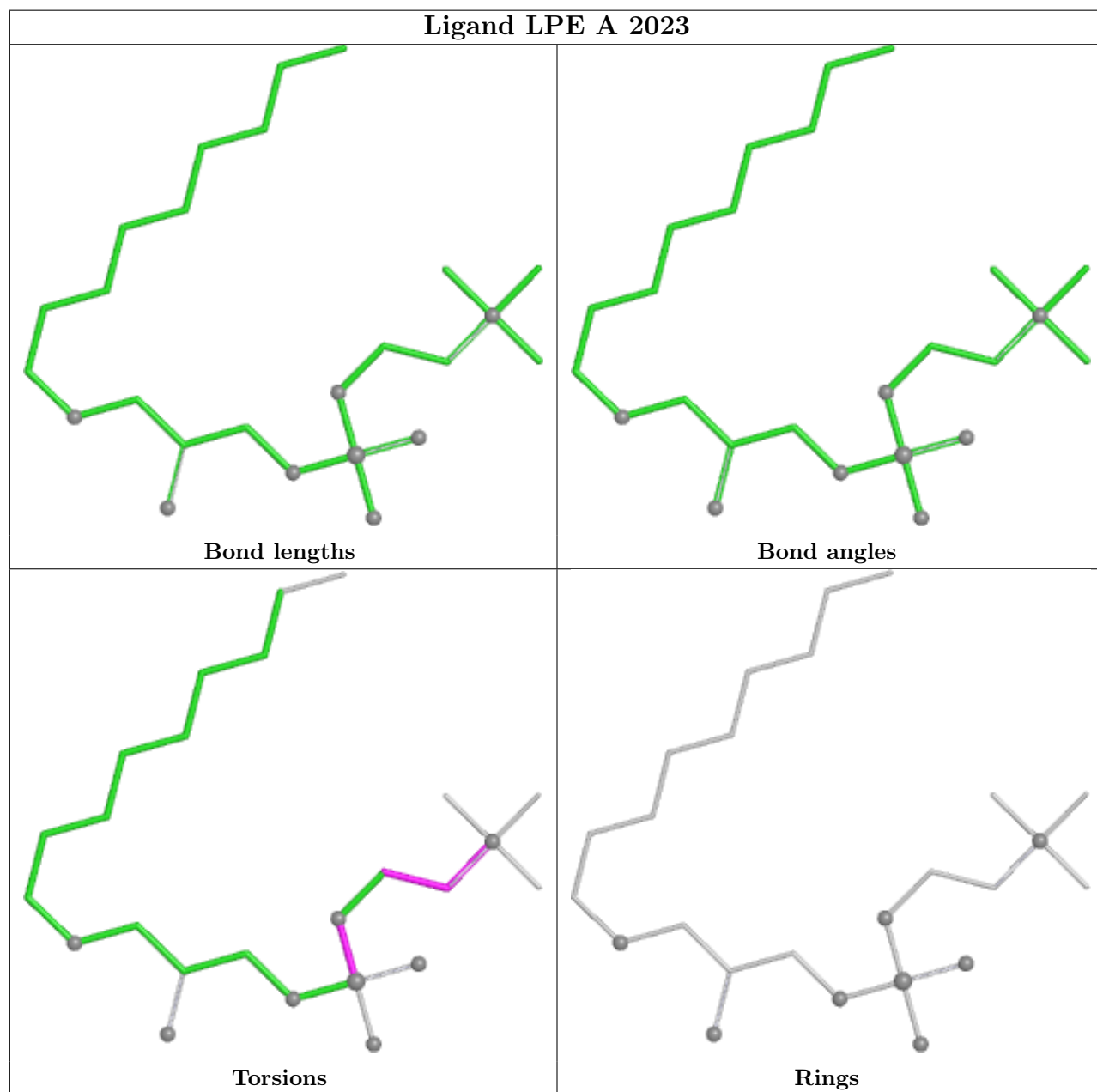
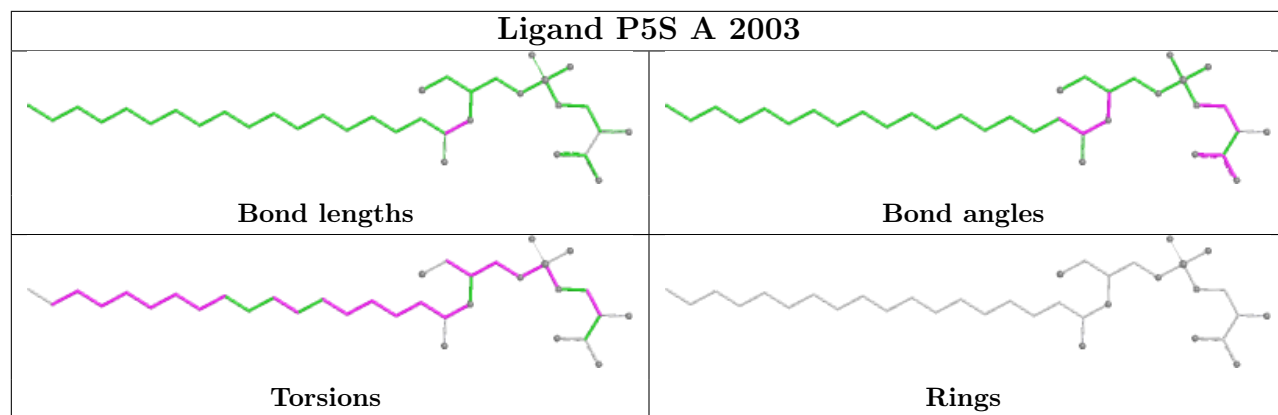


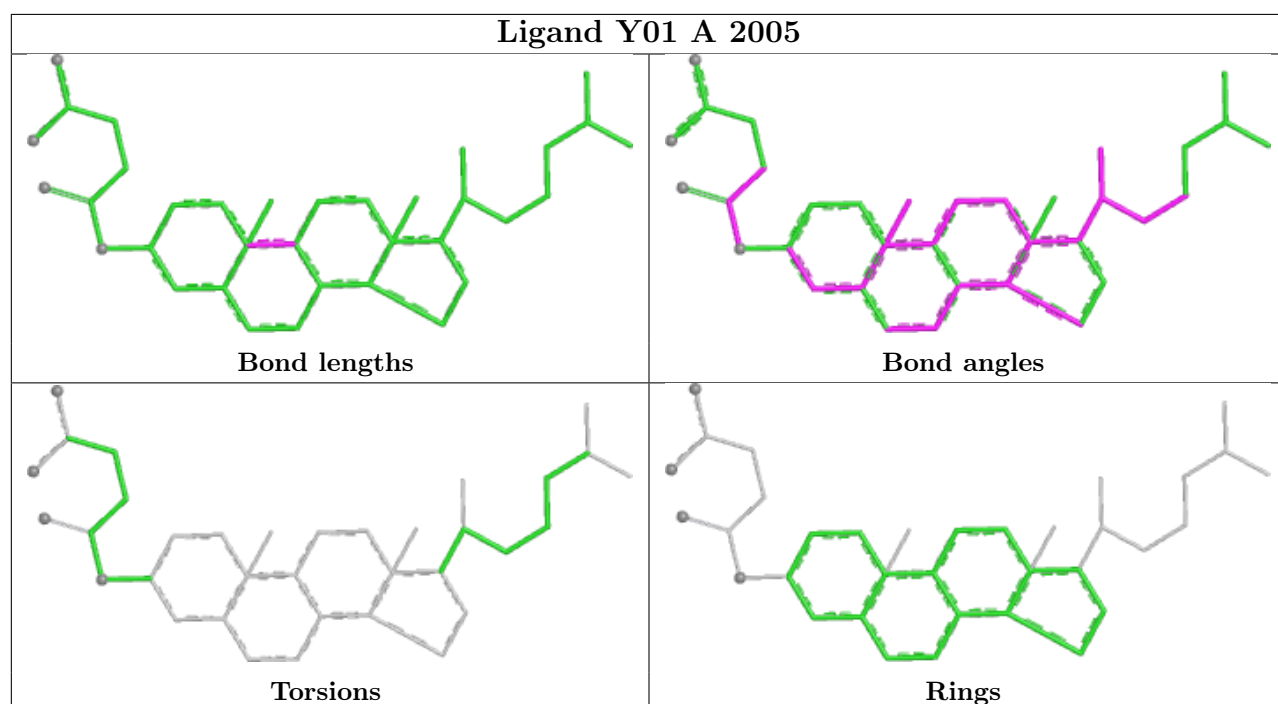
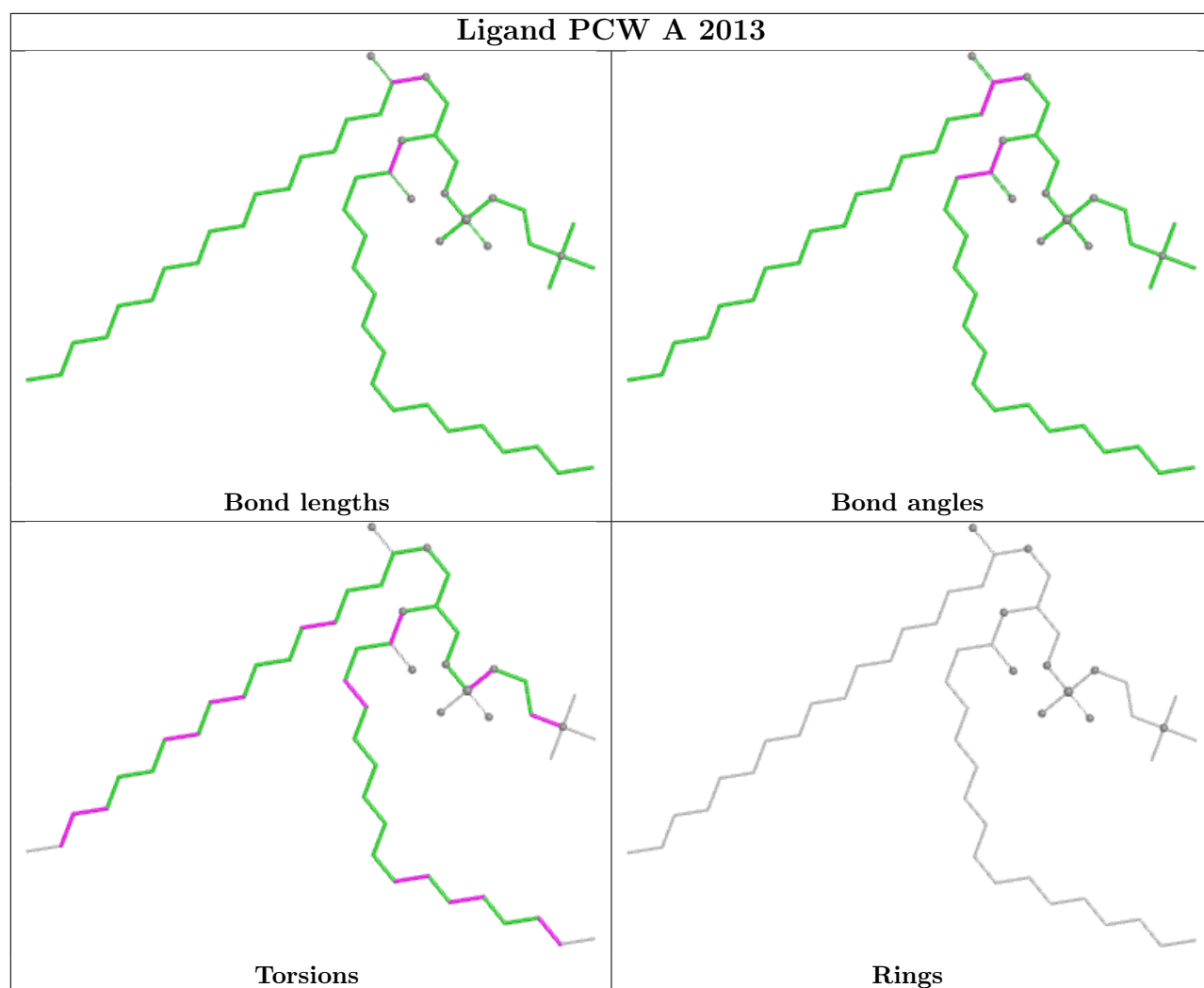


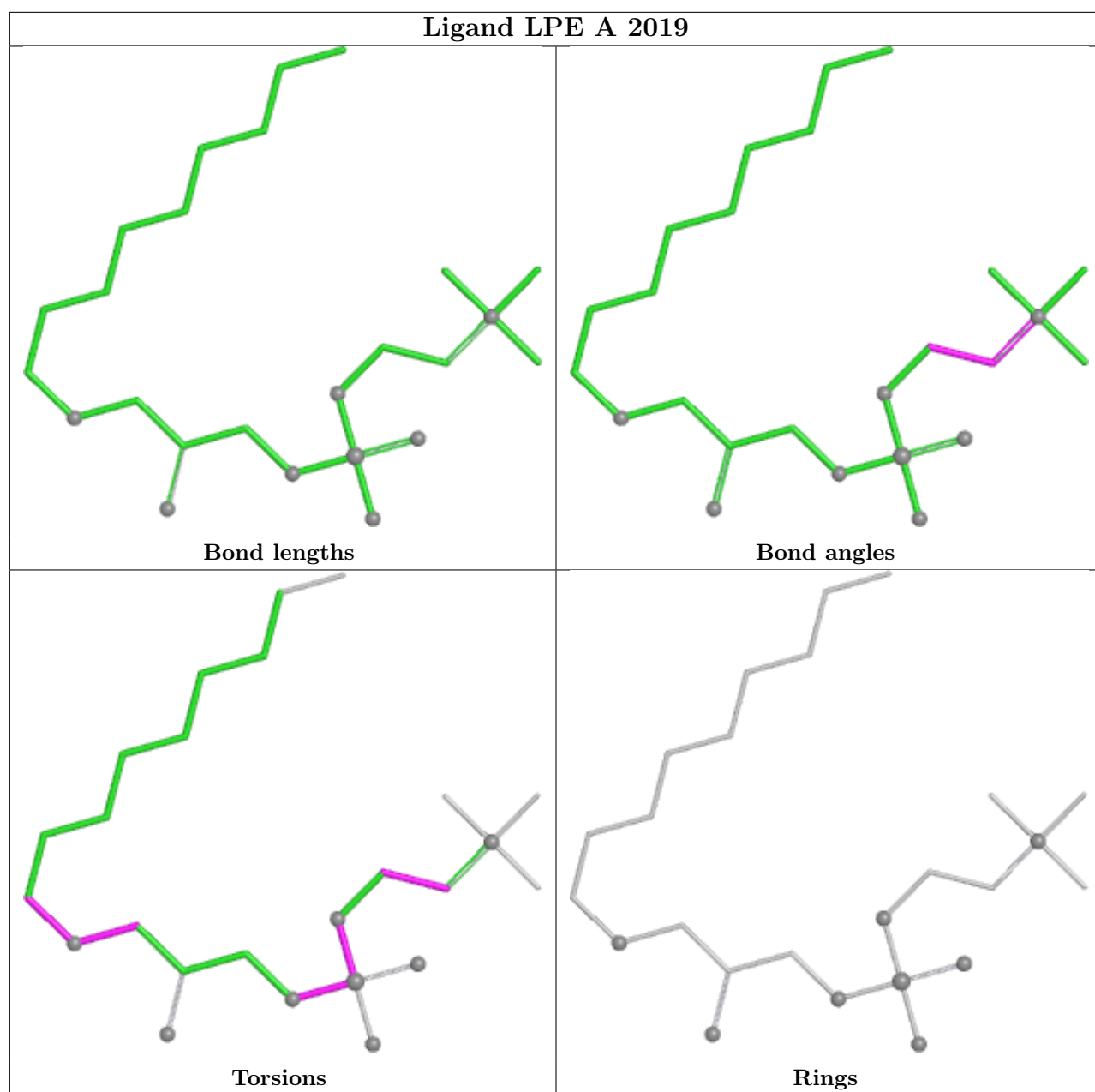


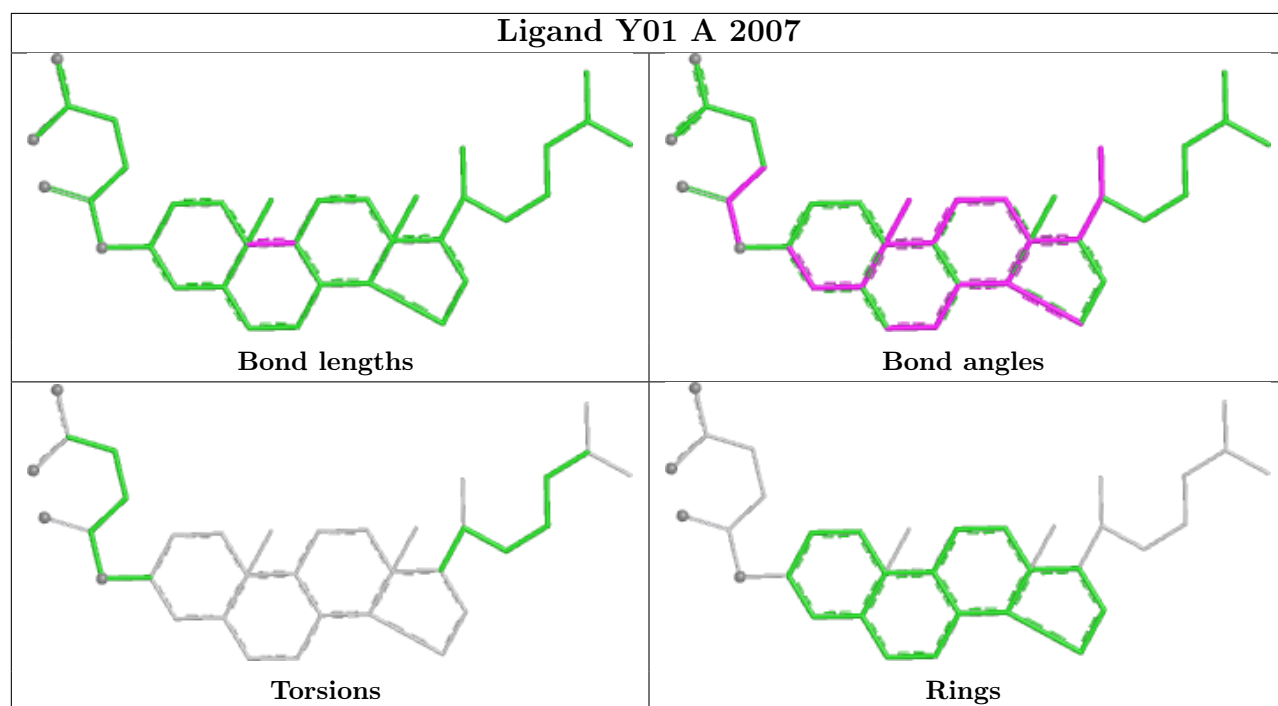
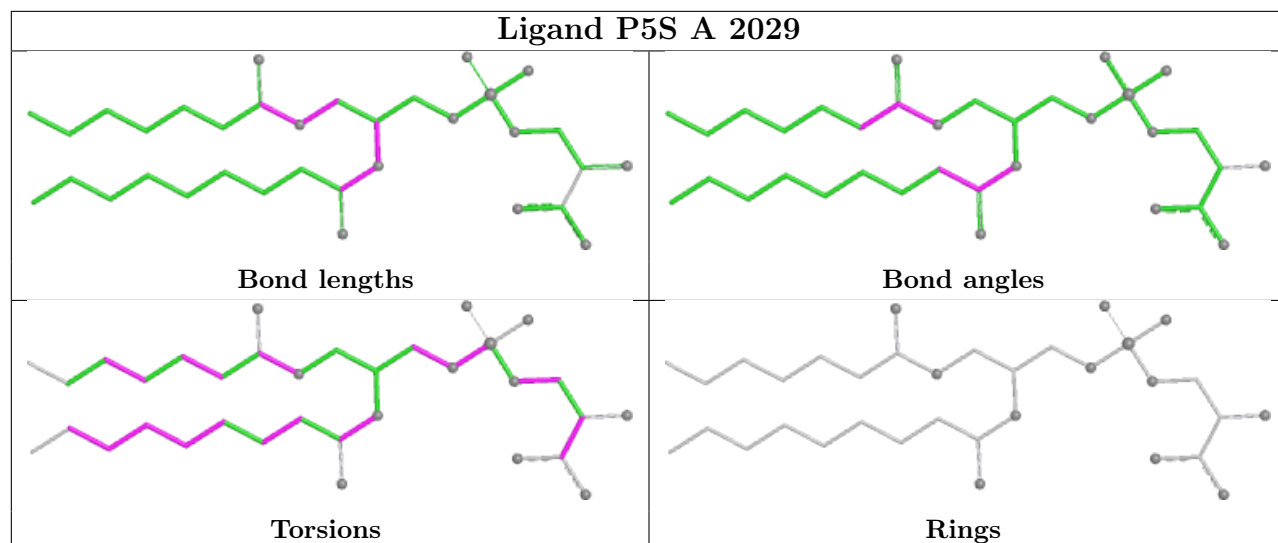


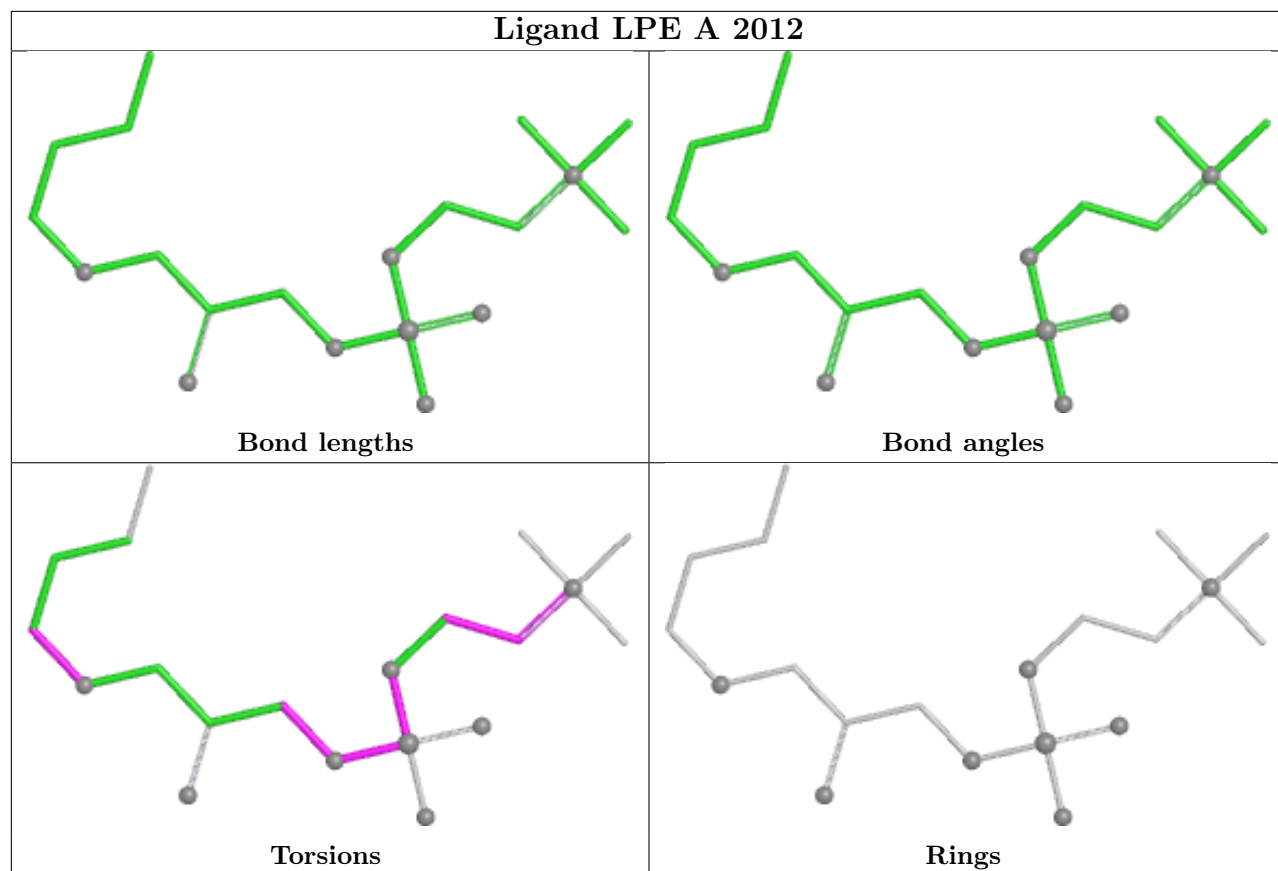


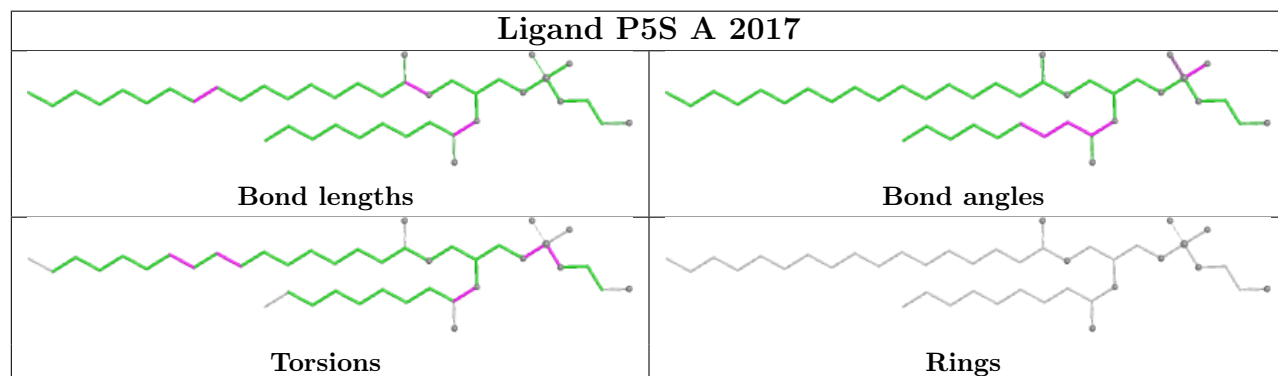
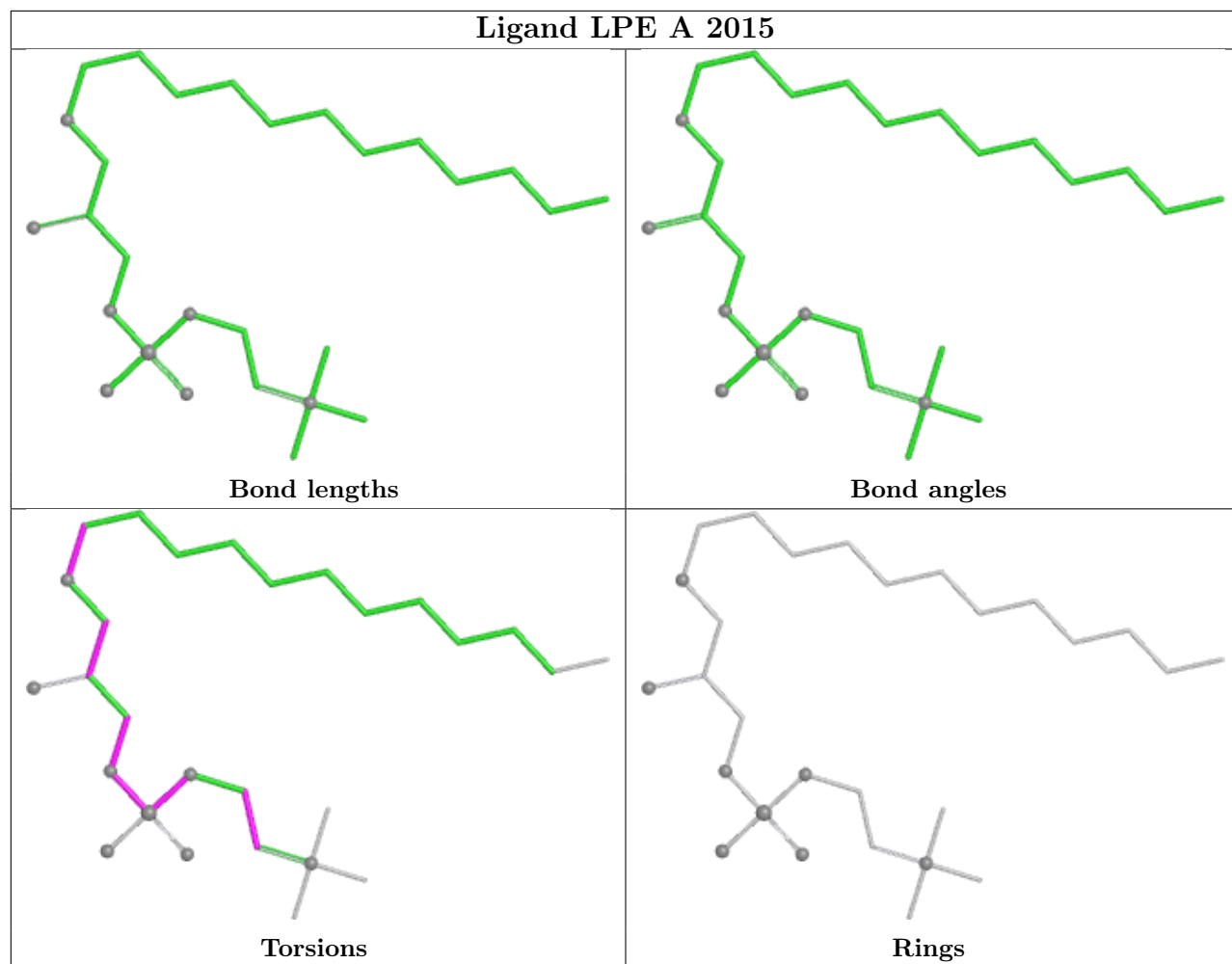


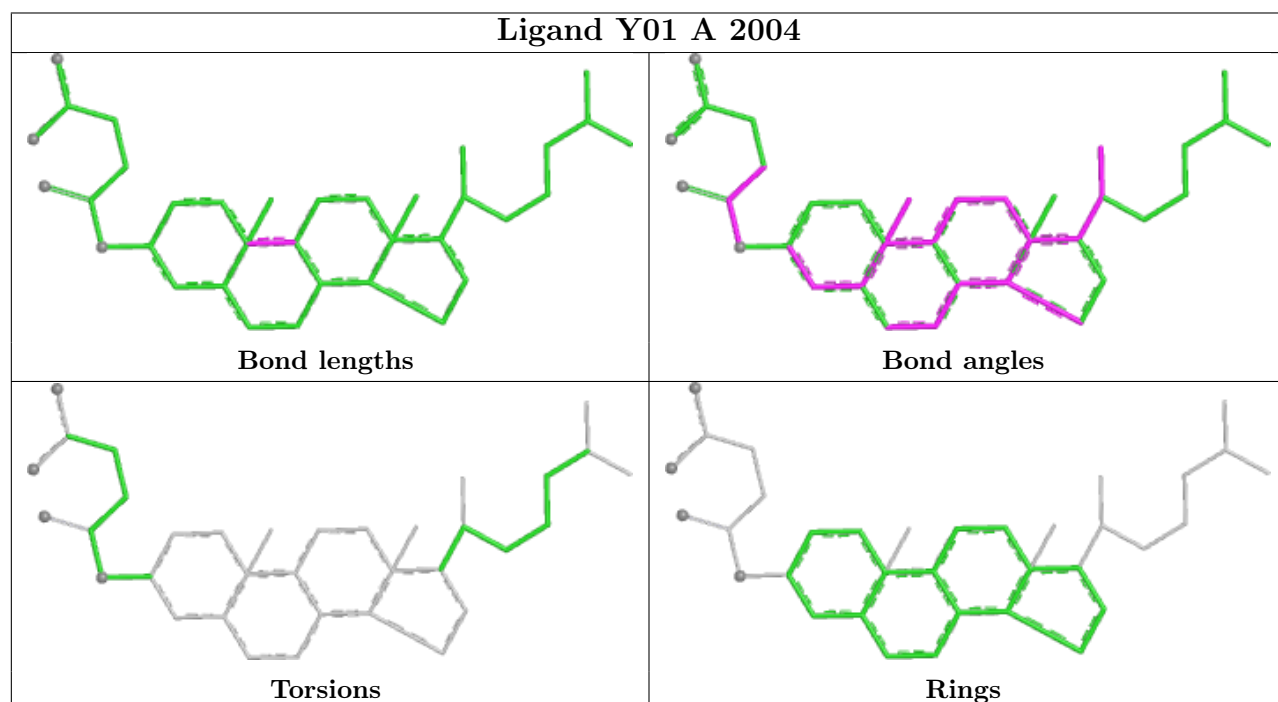
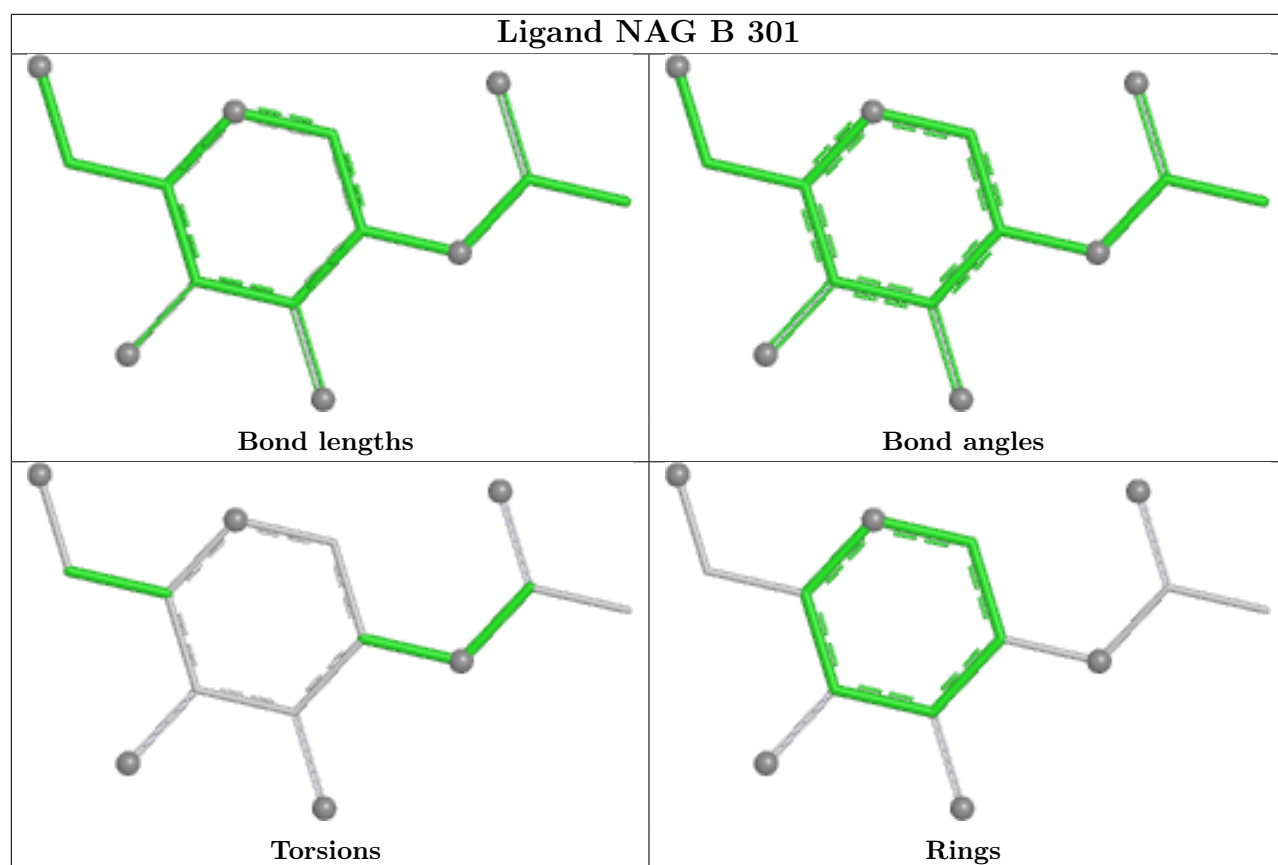


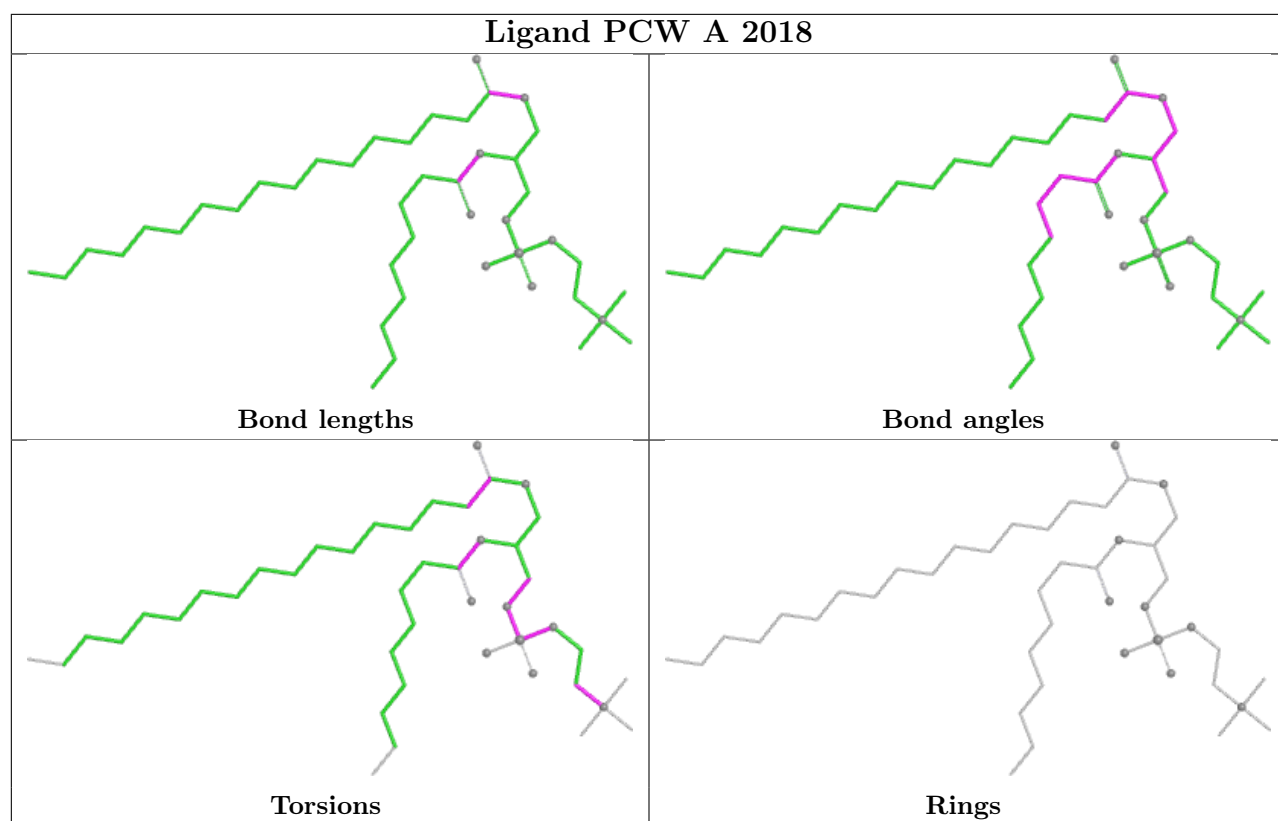


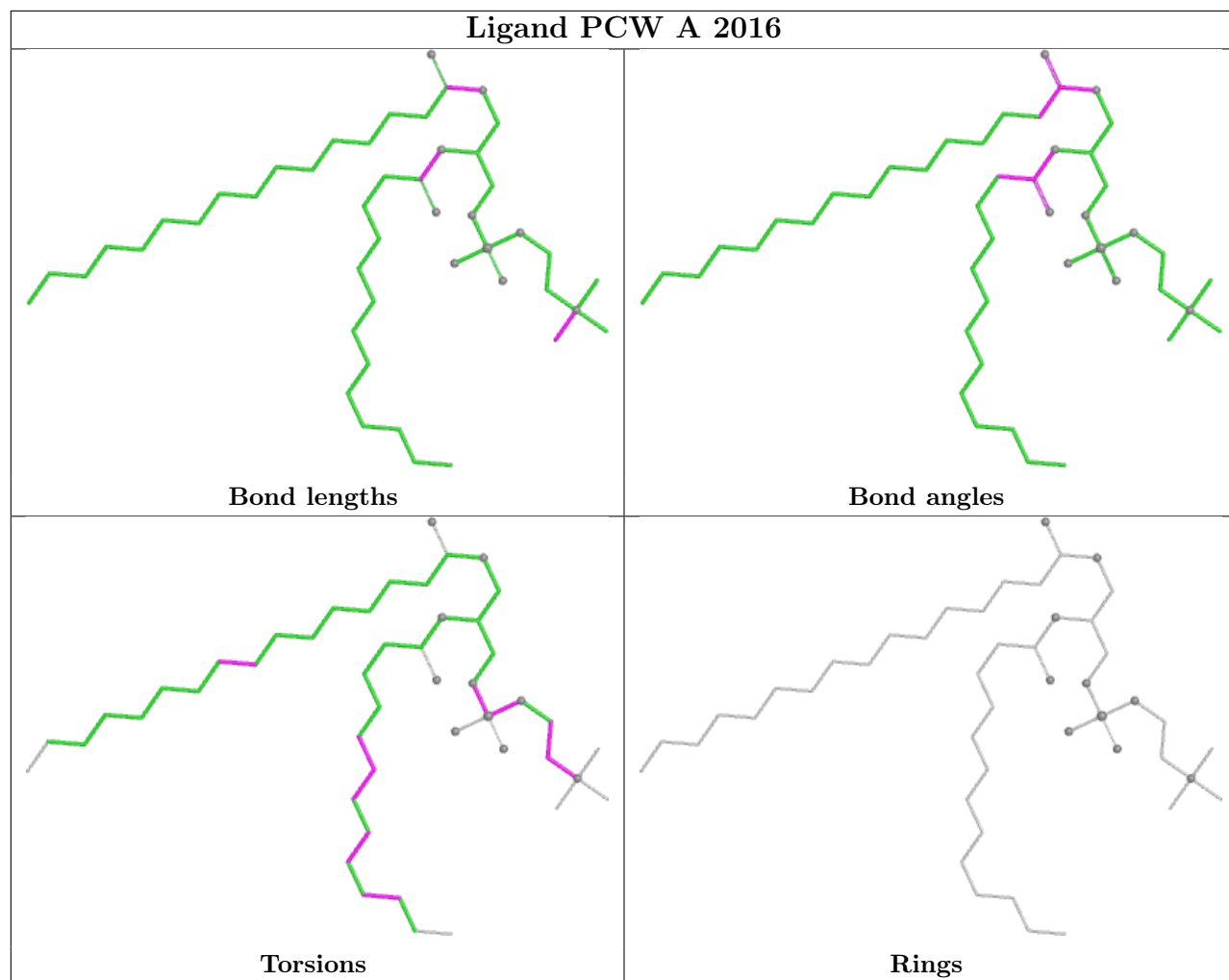


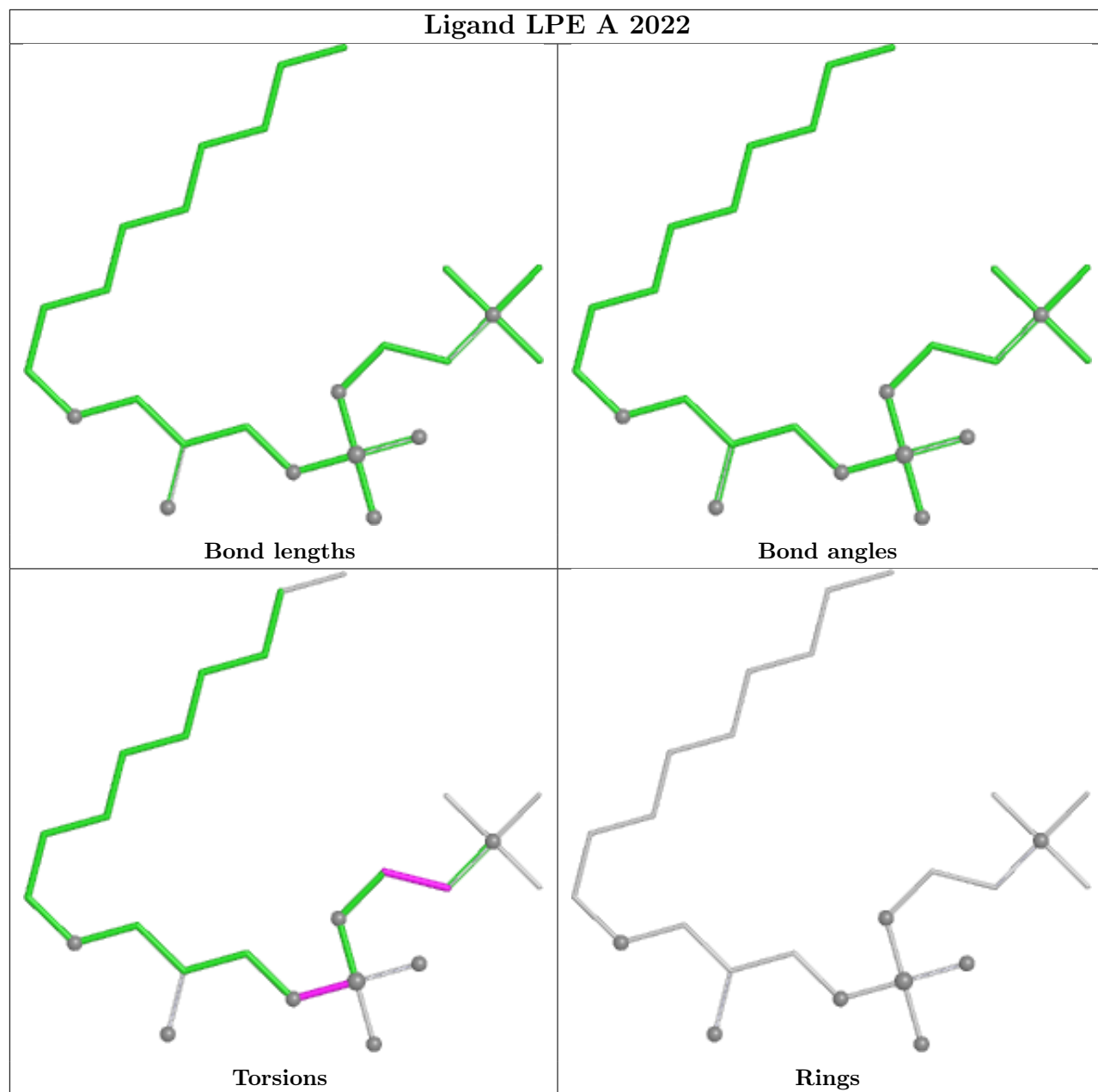


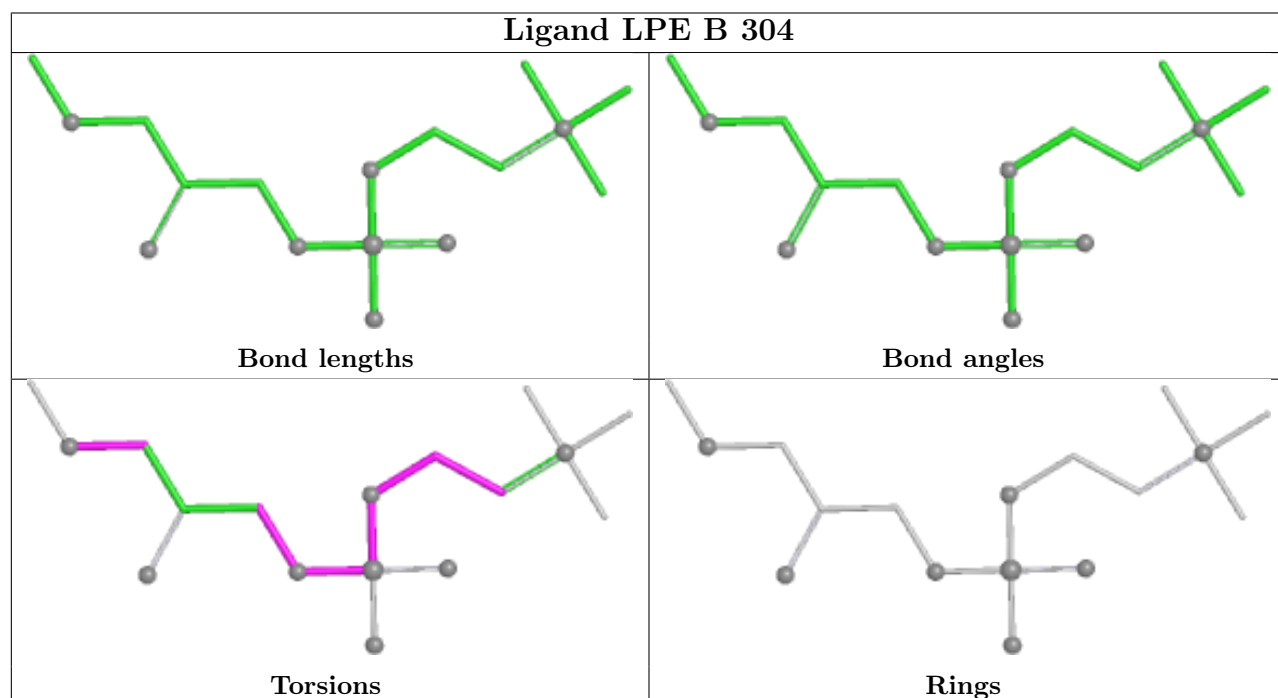
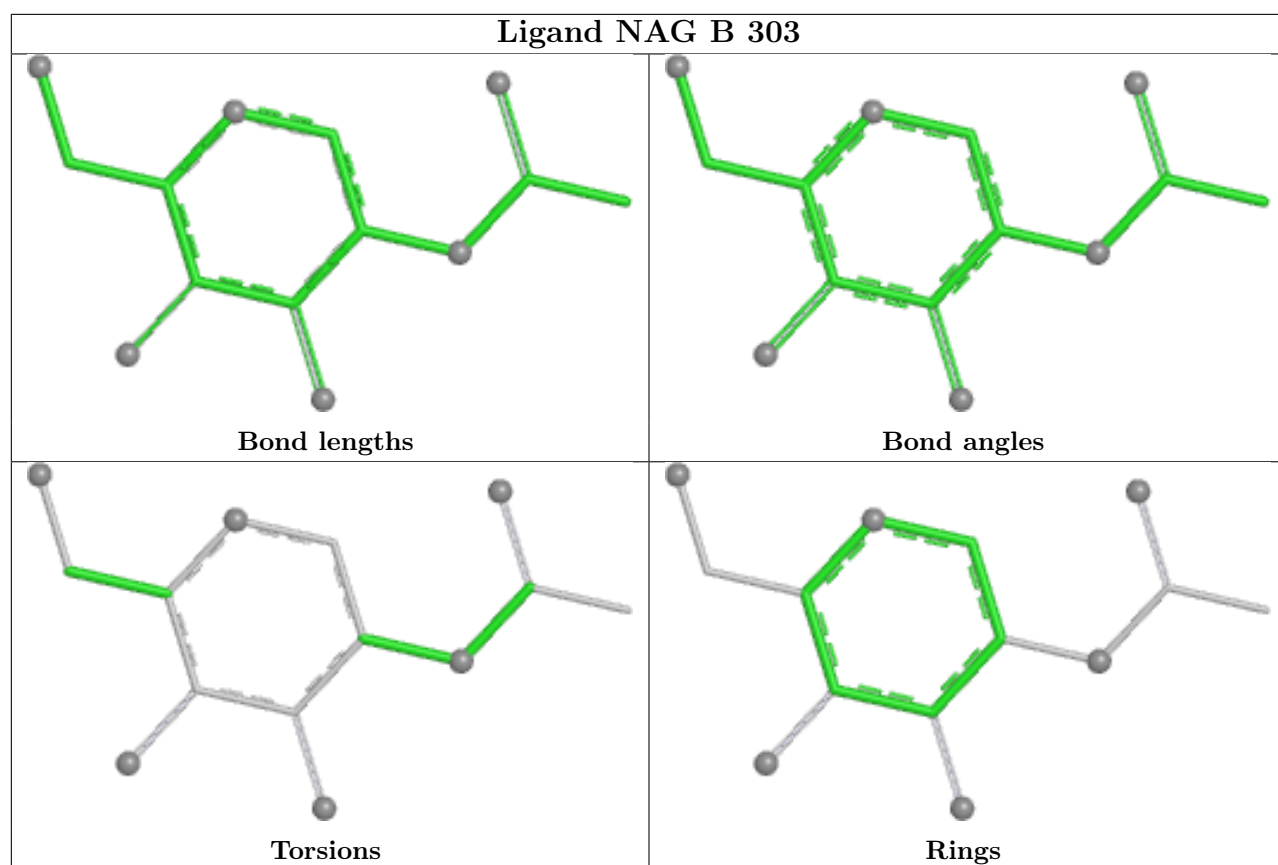


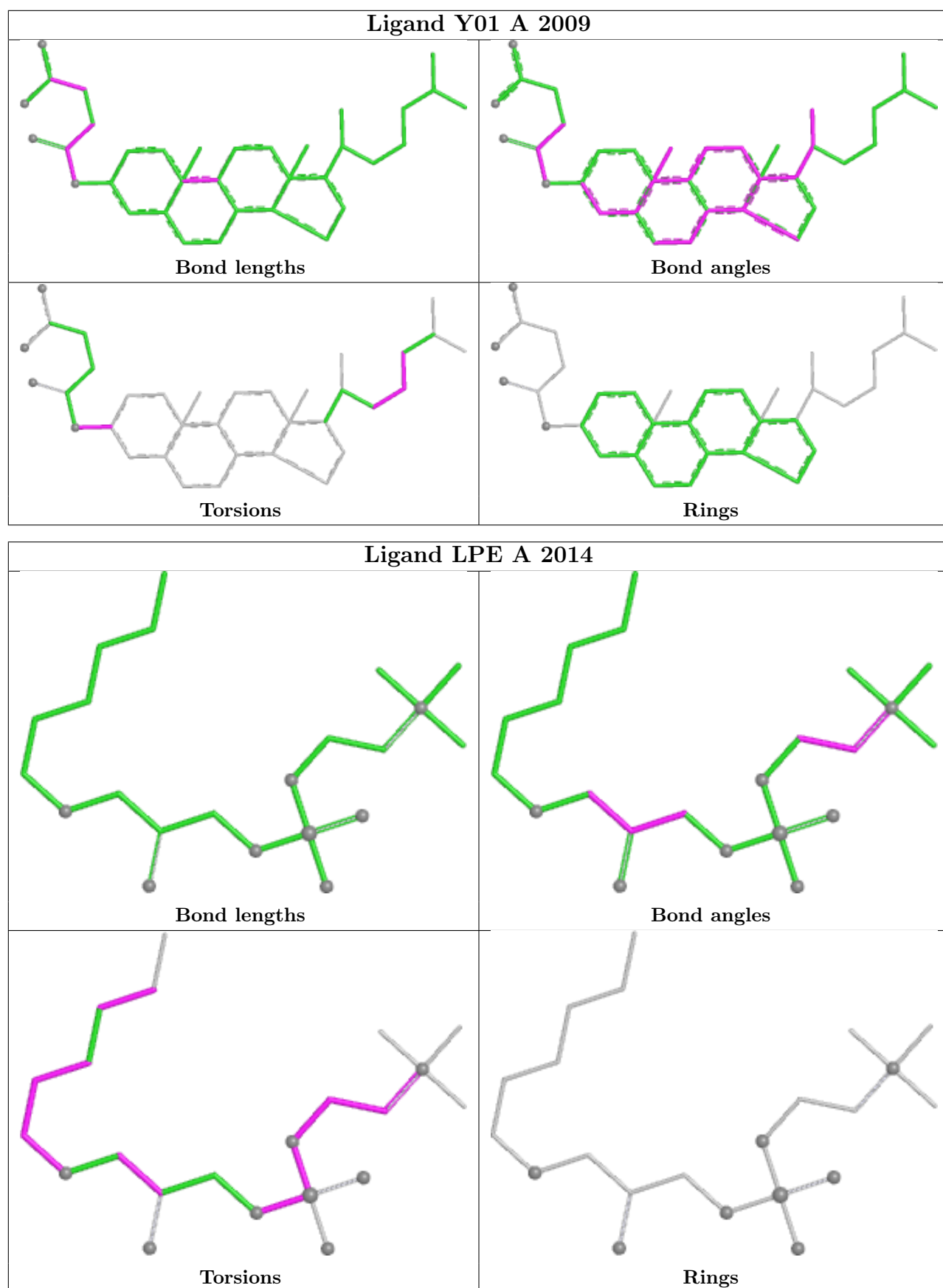




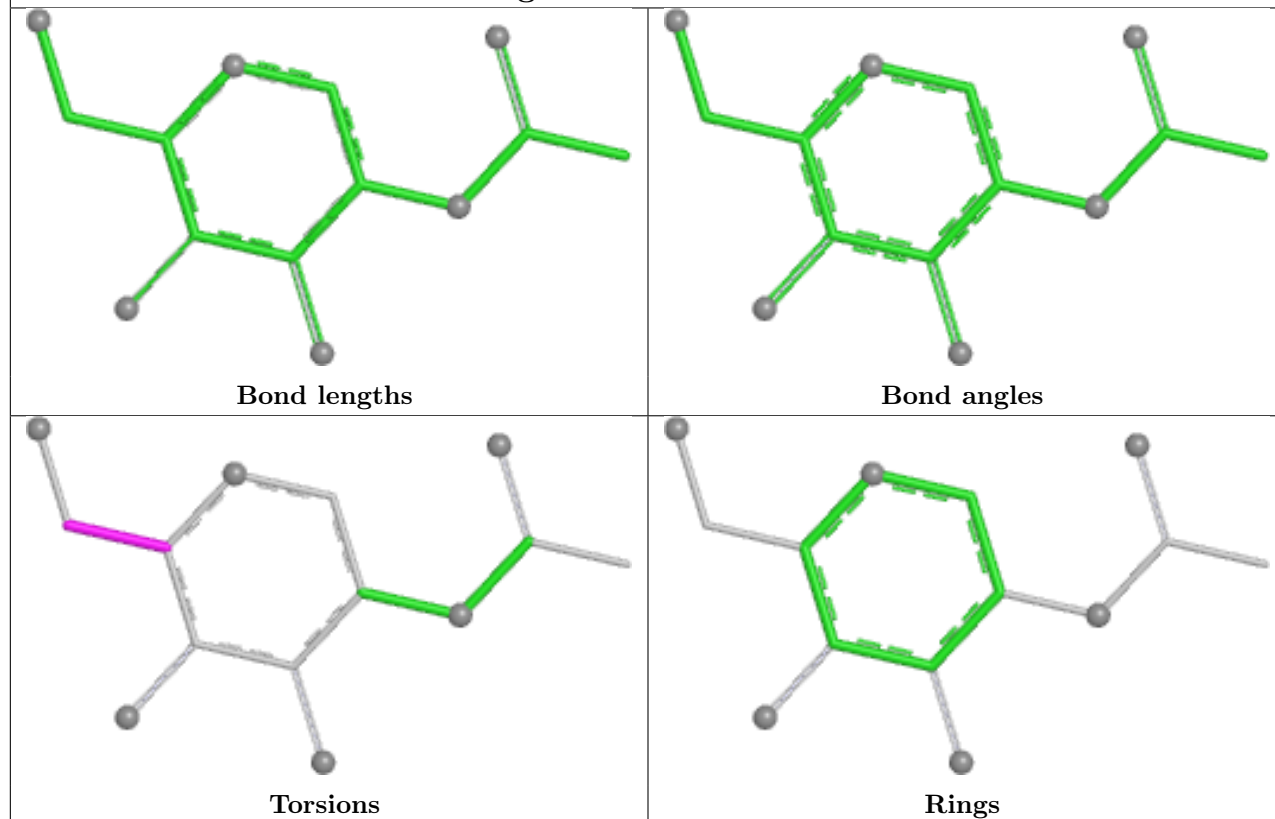




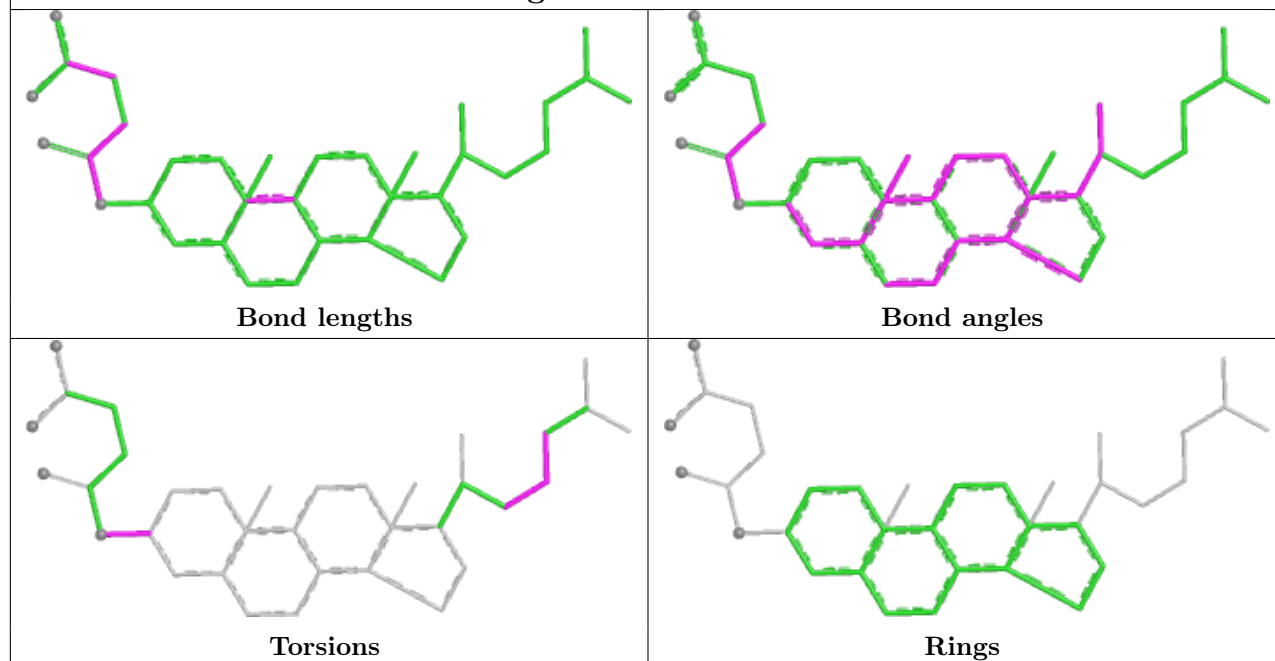


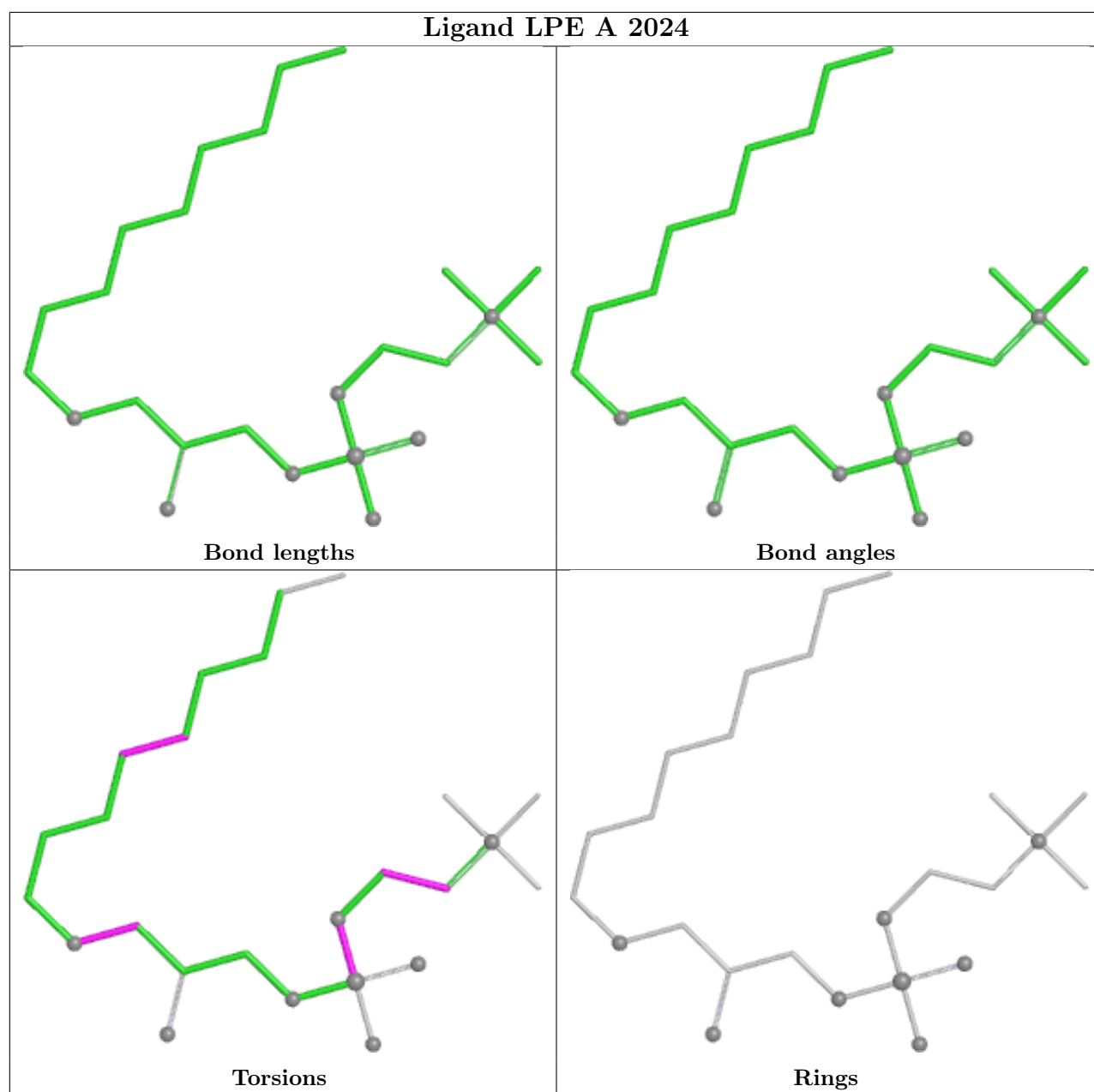


Ligand NAG A 2002



Ligand Y01 A 2006





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.

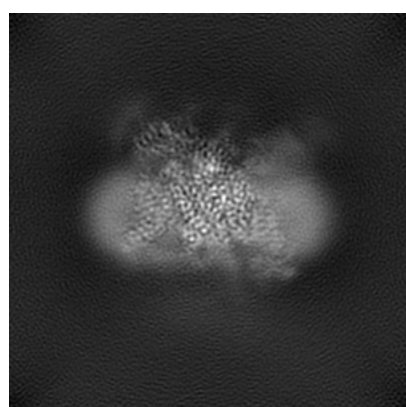
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32371. These allow visual inspection of the internal detail of the map and identification of artifacts.

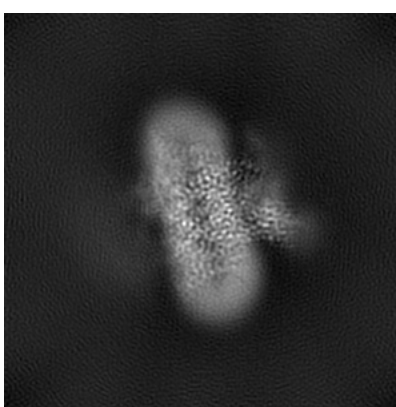
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

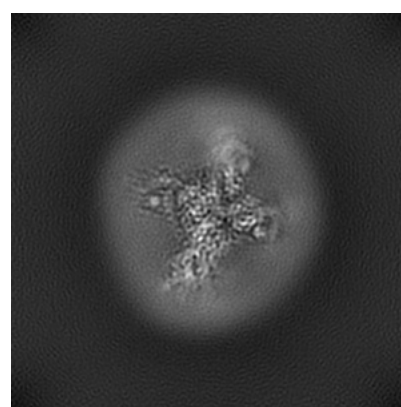
6.1.1 Primary map



X



Y

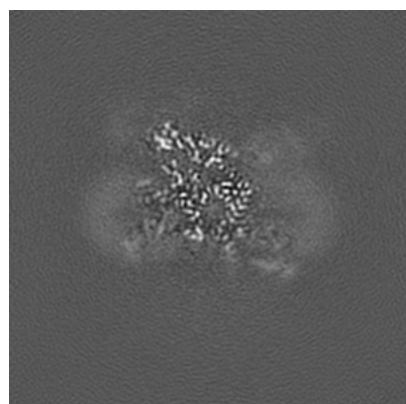


Z

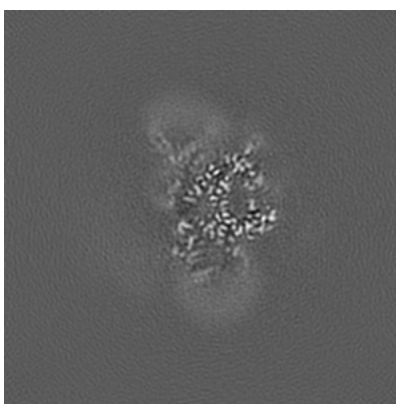
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

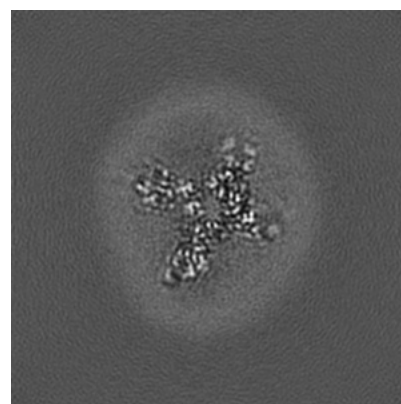
6.2.1 Primary map



X Index: 120



Y Index: 120

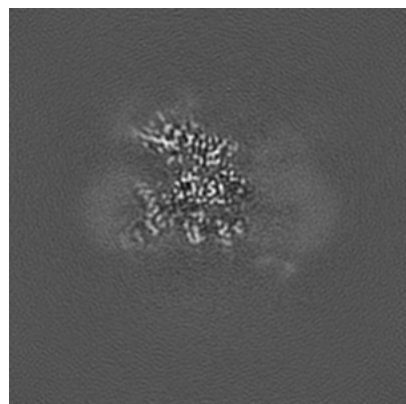


Z Index: 120

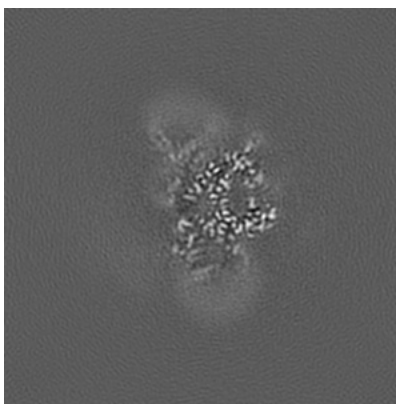
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

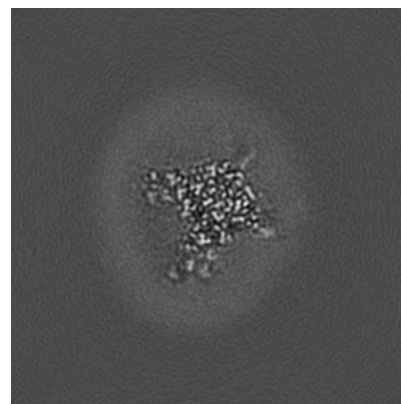
6.3.1 Primary map



X Index: 116



Y Index: 120

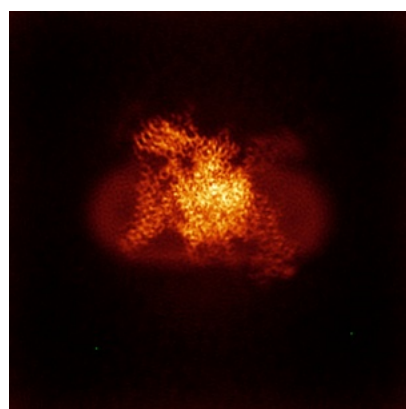


Z Index: 130

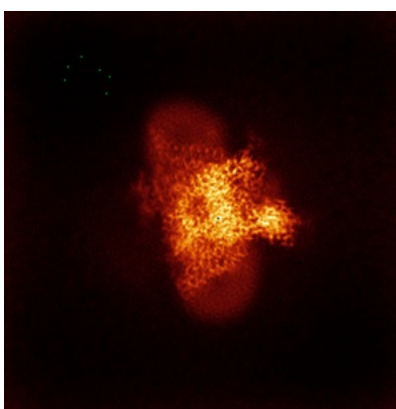
The images above show the largest variance slices of the map in three orthogonal directions.

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

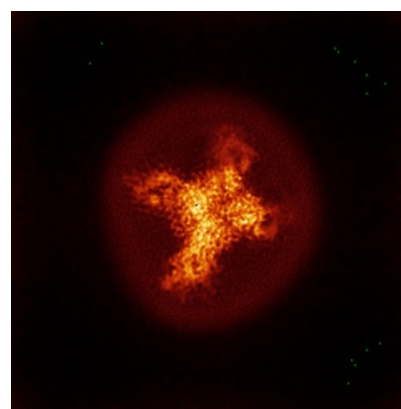
6.4.1 Primary map



X



Y



Z

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 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

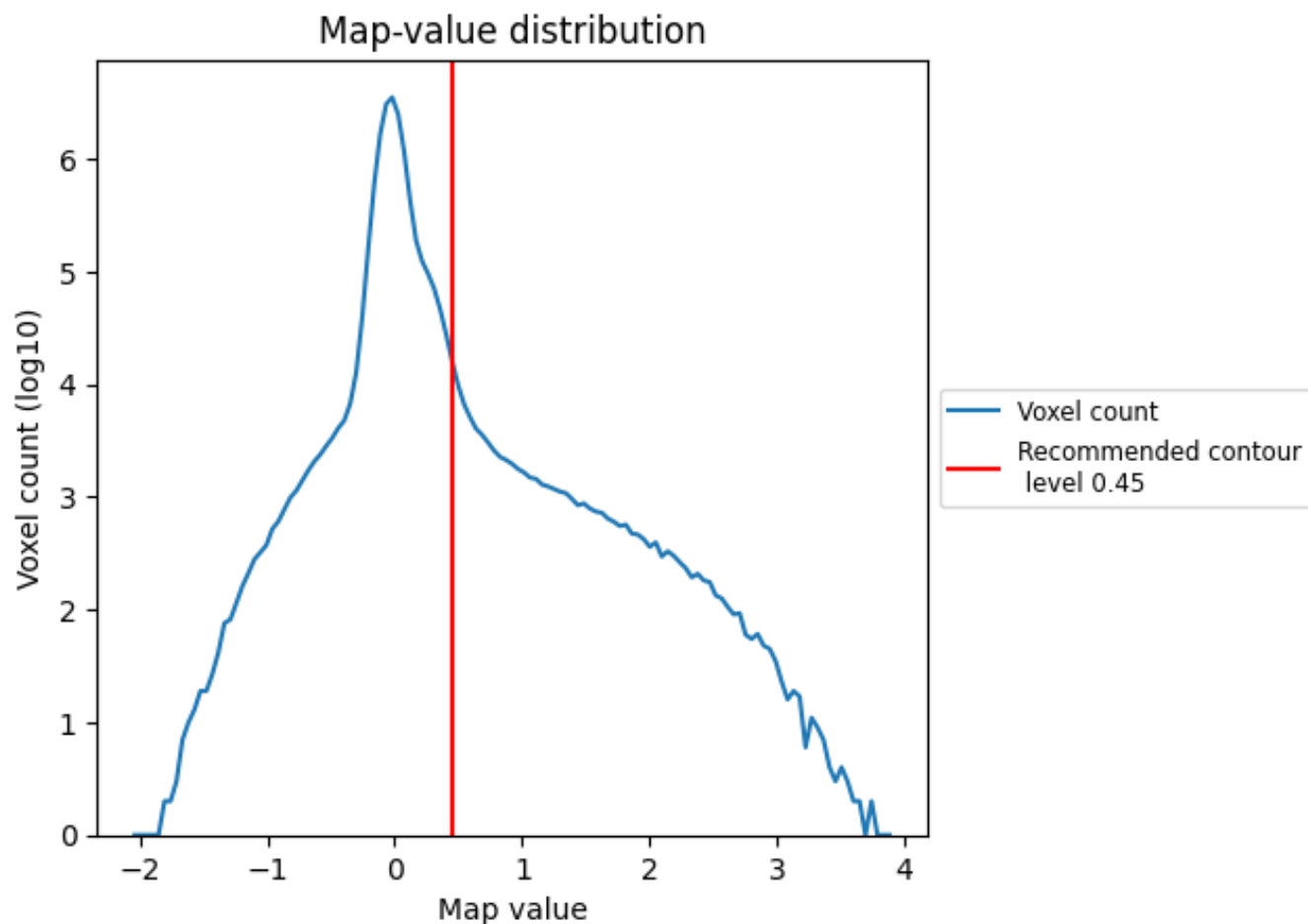
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

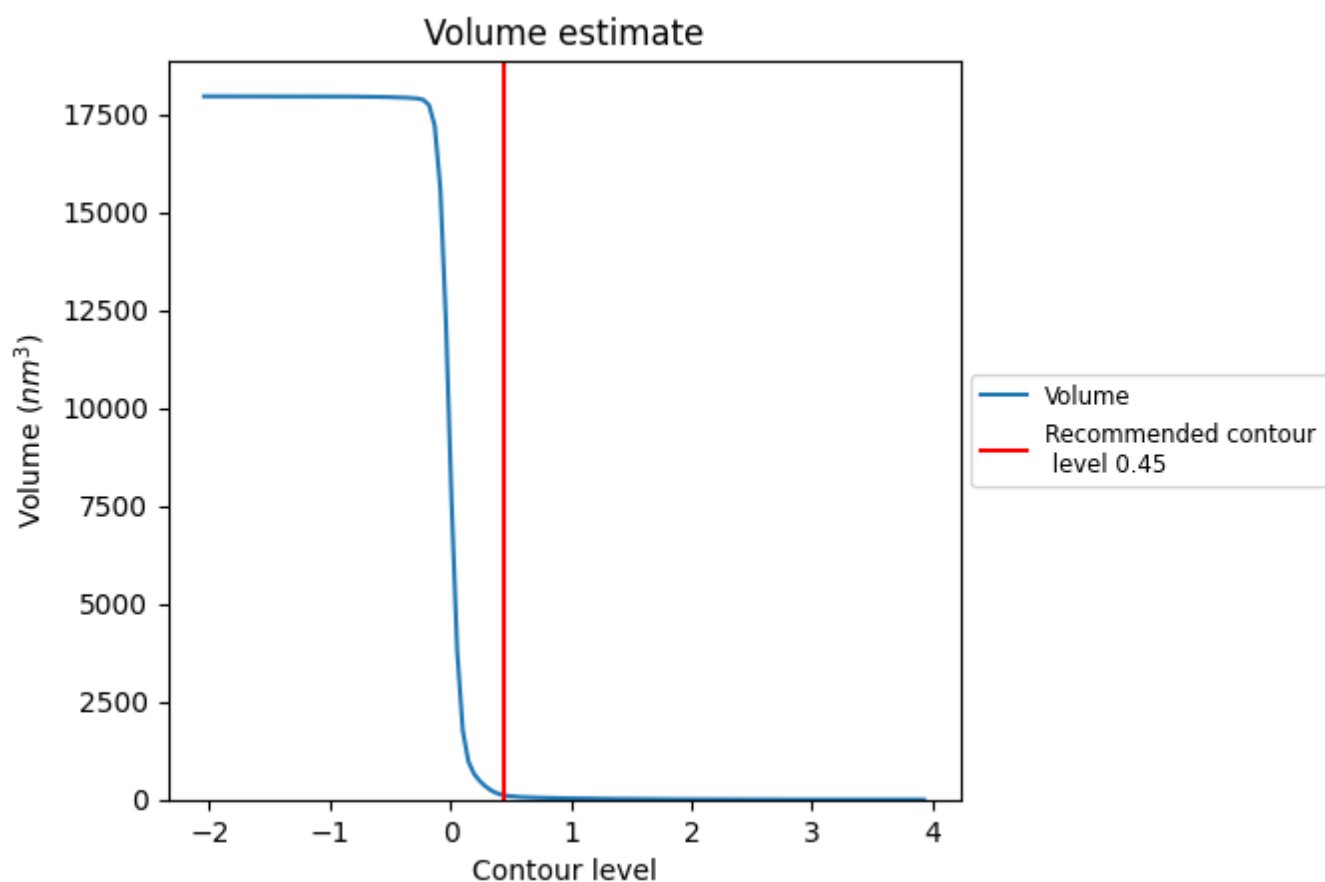
This section contains the results of statistical analysis of the map.

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.

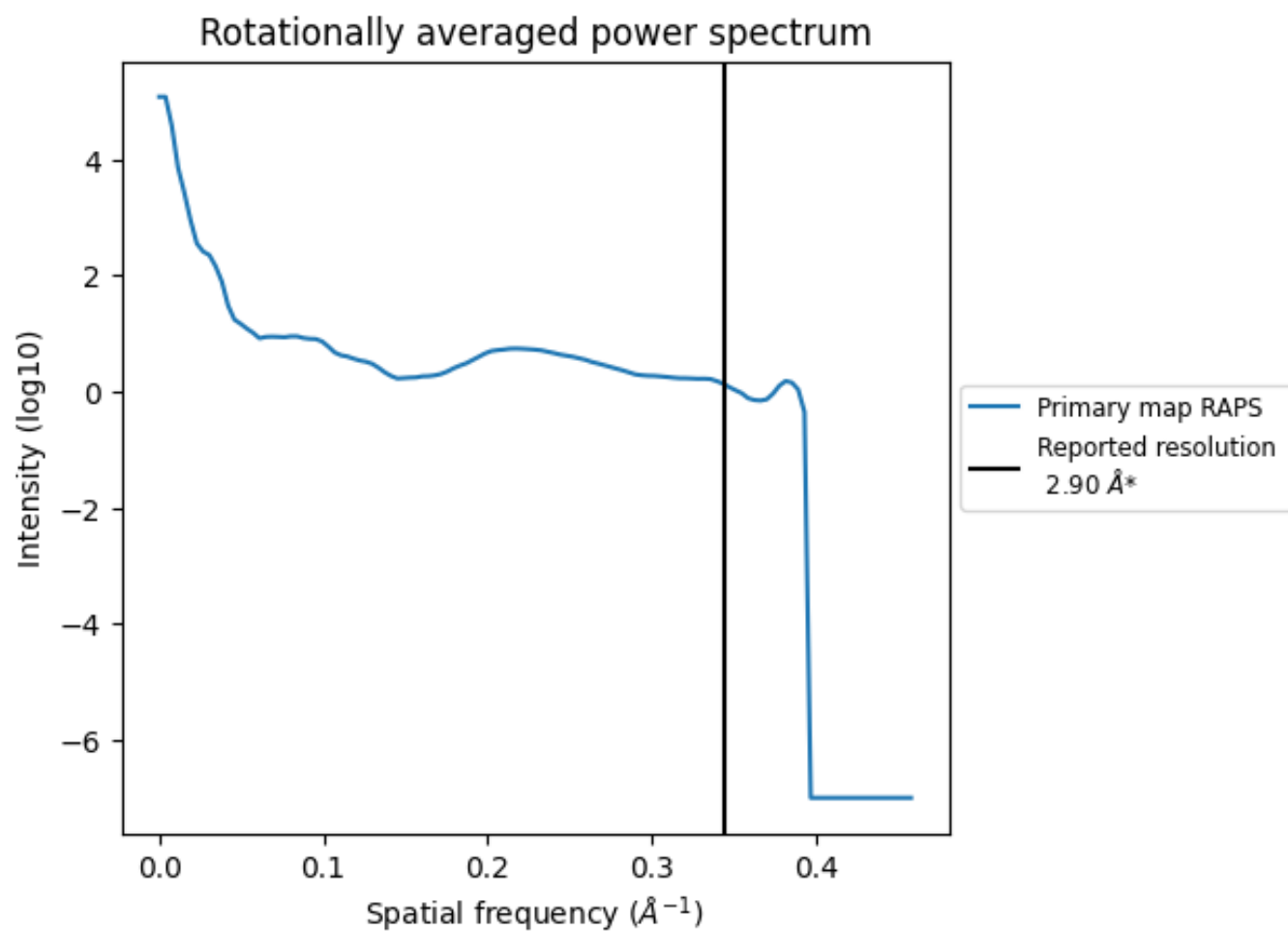
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm³; this corresponds to an approximate mass of 98 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

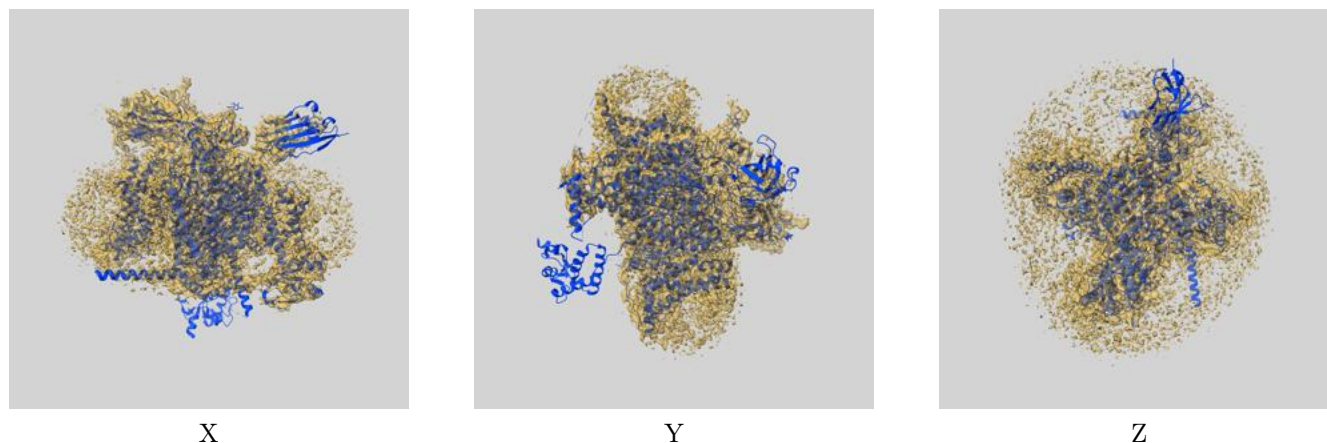
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

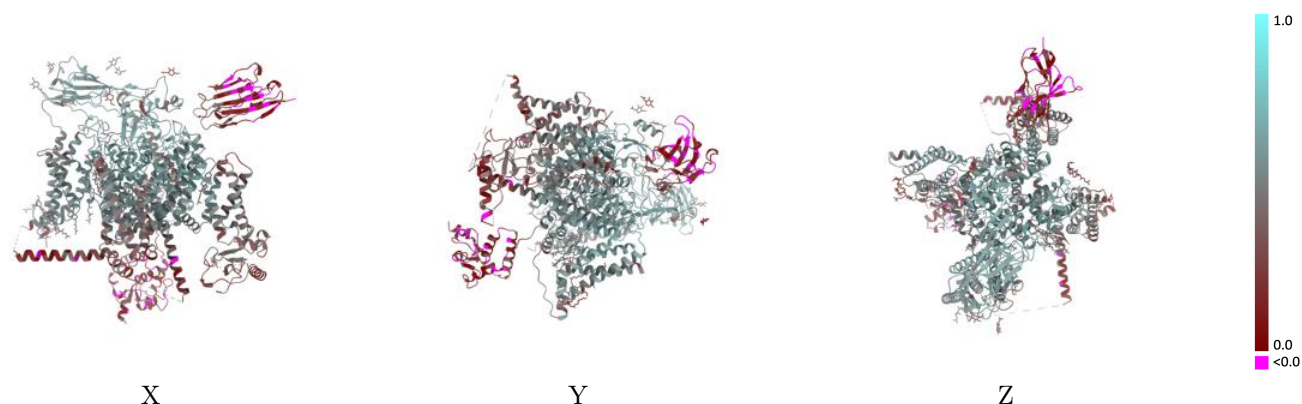
This section contains information regarding the fit between EMDB map EMD-32371 and PDB model 7W9P. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.45 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](#)

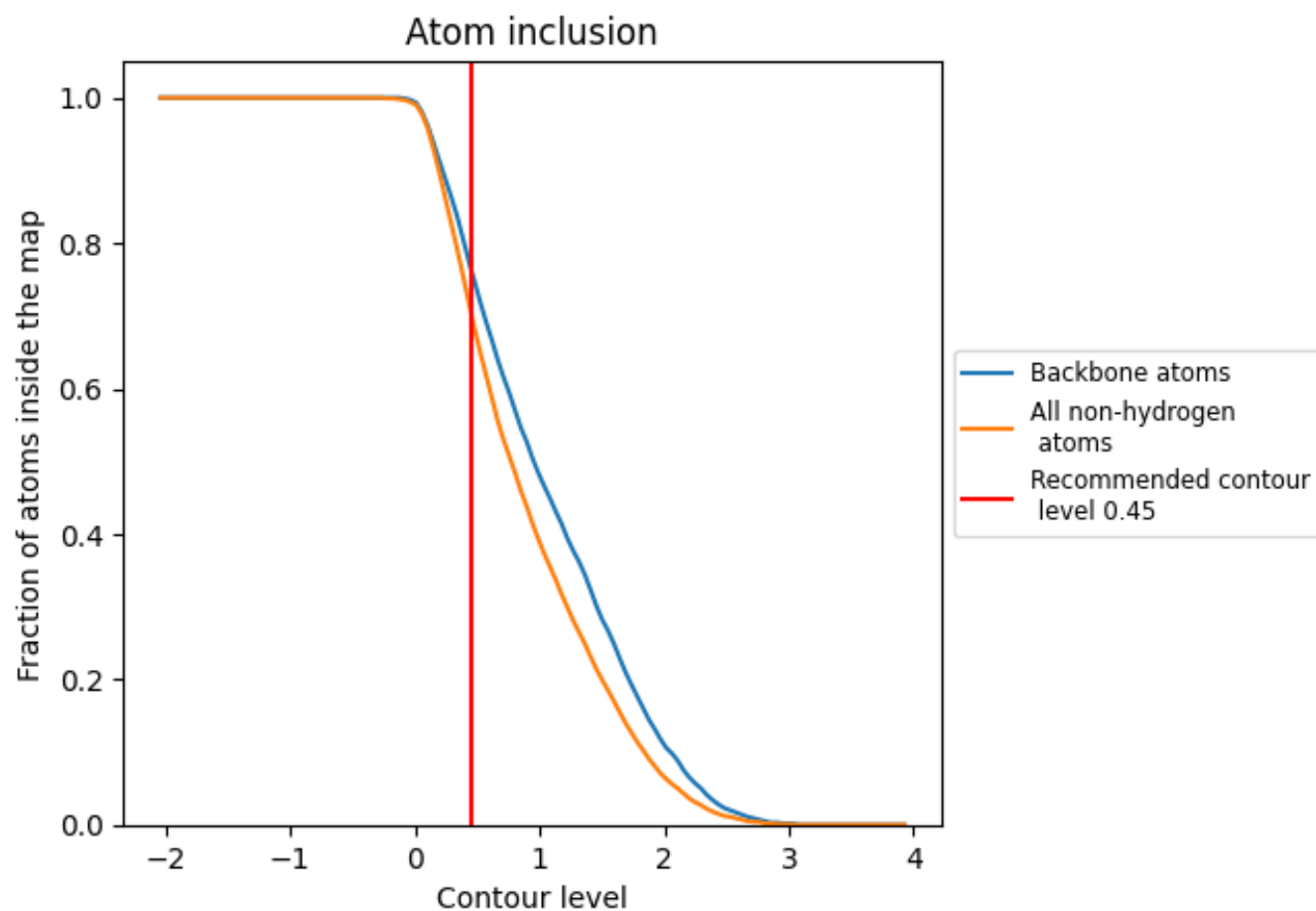


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7030	0.4560
A	0.7200	0.4710
B	0.8910	0.5480
C	0.1920	0.1320
D	0.8210	0.4690
E	0.6790	0.2970
F	0.8930	0.4960

1.0

0.0

<0.0