



Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 04:31 AM EDT

PDB ID : 8FE1
EMDB ID : EMD-29019
Title : Alpha1/BetaB Heteromeric Glycine Receptor in 1 mM Glycine 20 uM Ivermectin State
Authors : Gibbs, E.; Chakrapani, S.
Deposited on : 2022-12-05
Resolution : 3.00 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 : 2022.3.0, CSD as543be (2022)
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

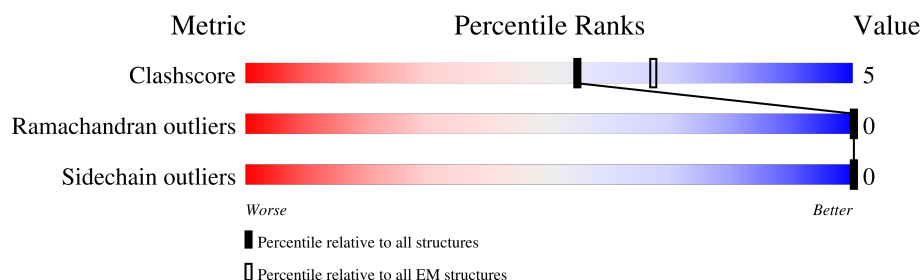
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	458	
1	B	458	
1	C	458	
1	D	458	
2	E	591	

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
3	GLY	A	501	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15445 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 Glycine receptor subunit alphaZ1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	355	Total	C	N	O	S	0	0
			2887	1877	474	517	19		
1	D	355	Total	C	N	O	S	0	0
			2886	1878	474	514	20		
1	C	356	Total	C	N	O	S	0	0
			2895	1883	475	517	20		
1	B	355	Total	C	N	O	S	0	0
			2887	1879	474	514	20		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	LEU	-	expression tag	UNP O93430
A	446	VAL	-	expression tag	UNP O93430
A	447	PRO	-	expression tag	UNP O93430
A	448	ARG	-	expression tag	UNP O93430
A	449	GLY	-	expression tag	UNP O93430
A	450	SER	-	expression tag	UNP O93430
A	451	HIS	-	expression tag	UNP O93430
A	452	HIS	-	expression tag	UNP O93430
A	453	HIS	-	expression tag	UNP O93430
A	454	HIS	-	expression tag	UNP O93430
A	455	HIS	-	expression tag	UNP O93430
A	456	HIS	-	expression tag	UNP O93430
A	457	HIS	-	expression tag	UNP O93430
A	458	HIS	-	expression tag	UNP O93430
D	445	LEU	-	expression tag	UNP O93430
D	446	VAL	-	expression tag	UNP O93430
D	447	PRO	-	expression tag	UNP O93430
D	448	ARG	-	expression tag	UNP O93430
D	449	GLY	-	expression tag	UNP O93430
D	450	SER	-	expression tag	UNP O93430
D	451	HIS	-	expression tag	UNP O93430
D	452	HIS	-	expression tag	UNP O93430

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Chain	Residue	Modelled	Actual	Comment	Reference
D	453	HIS	-	expression tag	UNP O93430
D	454	HIS	-	expression tag	UNP O93430
D	455	HIS	-	expression tag	UNP O93430
D	456	HIS	-	expression tag	UNP O93430
D	457	HIS	-	expression tag	UNP O93430
D	458	HIS	-	expression tag	UNP O93430
C	445	LEU	-	expression tag	UNP O93430
C	446	VAL	-	expression tag	UNP O93430
C	447	PRO	-	expression tag	UNP O93430
C	448	ARG	-	expression tag	UNP O93430
C	449	GLY	-	expression tag	UNP O93430
C	450	SER	-	expression tag	UNP O93430
C	451	HIS	-	expression tag	UNP O93430
C	452	HIS	-	expression tag	UNP O93430
C	453	HIS	-	expression tag	UNP O93430
C	454	HIS	-	expression tag	UNP O93430
C	455	HIS	-	expression tag	UNP O93430
C	456	HIS	-	expression tag	UNP O93430
C	457	HIS	-	expression tag	UNP O93430
C	458	HIS	-	expression tag	UNP O93430
B	445	LEU	-	expression tag	UNP O93430
B	446	VAL	-	expression tag	UNP O93430
B	447	PRO	-	expression tag	UNP O93430
B	448	ARG	-	expression tag	UNP O93430
B	449	GLY	-	expression tag	UNP O93430
B	450	SER	-	expression tag	UNP O93430
B	451	HIS	-	expression tag	UNP O93430
B	452	HIS	-	expression tag	UNP O93430
B	453	HIS	-	expression tag	UNP O93430
B	454	HIS	-	expression tag	UNP O93430
B	455	HIS	-	expression tag	UNP O93430
B	456	HIS	-	expression tag	UNP O93430
B	457	HIS	-	expression tag	UNP O93430
B	458	HIS	-	expression tag	UNP O93430

- Molecule 2 is a protein called Glycine receptor beta subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	346	Total	C	N	O	S	0	0
			2800	1827	449	507	17		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-80	MET	-	initiating methionine	UNP Q6DC22
E	-79	LYS	-	expression tag	UNP Q6DC22
E	-78	ALA	-	expression tag	UNP Q6DC22
E	-77	LEU	-	expression tag	UNP Q6DC22
E	-76	LYS	-	expression tag	UNP Q6DC22
E	-75	VAL	-	expression tag	UNP Q6DC22
E	-74	ILE	-	expression tag	UNP Q6DC22
E	-73	PHE	-	expression tag	UNP Q6DC22
E	-72	MET	-	expression tag	UNP Q6DC22
E	-71	LEU	-	expression tag	UNP Q6DC22
E	-70	LEU	-	expression tag	UNP Q6DC22
E	-69	ILE	-	expression tag	UNP Q6DC22
E	-68	ILE	-	expression tag	UNP Q6DC22
E	-67	CYS	-	expression tag	UNP Q6DC22
E	-66	LEU	-	expression tag	UNP Q6DC22
E	-65	TRP	-	expression tag	UNP Q6DC22
E	-64	MET	-	expression tag	UNP Q6DC22
E	-63	GLU	-	expression tag	UNP Q6DC22
E	-62	GLY	-	expression tag	UNP Q6DC22
E	-61	GLY	-	expression tag	UNP Q6DC22
E	-60	PHE	-	expression tag	UNP Q6DC22
E	-59	THR	-	expression tag	UNP Q6DC22
E	-58	LYS	-	expression tag	UNP Q6DC22
E	-57	GLU	-	expression tag	UNP Q6DC22
E	-56	LYS	-	expression tag	UNP Q6DC22
E	-55	SER	-	expression tag	UNP Q6DC22
E	-54	ALA	-	expression tag	UNP Q6DC22
E	-53	LYS	-	expression tag	UNP Q6DC22
E	-52	LYS	-	expression tag	UNP Q6DC22
E	-51	TRP	-	expression tag	UNP Q6DC22
E	-50	SER	-	expression tag	UNP Q6DC22
E	-49	HIS	-	expression tag	UNP Q6DC22
E	-48	PRO	-	expression tag	UNP Q6DC22
E	-47	GLN	-	expression tag	UNP Q6DC22
E	-46	PHE	-	expression tag	UNP Q6DC22
E	-45	GLU	-	expression tag	UNP Q6DC22
E	-44	LYS	-	expression tag	UNP Q6DC22
E	-43	GLY	-	expression tag	UNP Q6DC22
E	-42	GLY	-	expression tag	UNP Q6DC22
E	-41	GLY	-	expression tag	UNP Q6DC22
E	-40	SER	-	expression tag	UNP Q6DC22
E	-39	GLY	-	expression tag	UNP Q6DC22
E	-38	GLY	-	expression tag	UNP Q6DC22

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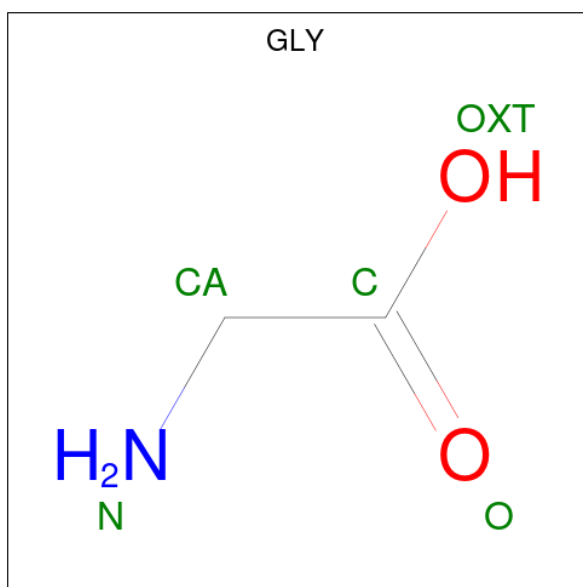
Chain	Residue	Modelled	Actual	Comment	Reference
E	-37	GLY	-	expression tag	UNP Q6DC22
E	-36	SER	-	expression tag	UNP Q6DC22
E	-35	GLY	-	expression tag	UNP Q6DC22
E	-34	GLY	-	expression tag	UNP Q6DC22
E	-33	GLY	-	expression tag	UNP Q6DC22
E	-32	SER	-	expression tag	UNP Q6DC22
E	-31	TRP	-	expression tag	UNP Q6DC22
E	-30	SER	-	expression tag	UNP Q6DC22
E	-29	HIS	-	expression tag	UNP Q6DC22
E	-28	PRO	-	expression tag	UNP Q6DC22
E	-27	GLN	-	expression tag	UNP Q6DC22
E	-26	PHE	-	expression tag	UNP Q6DC22
E	-25	GLU	-	expression tag	UNP Q6DC22
E	-24	LYS	-	expression tag	UNP Q6DC22
E	-23	GLY	-	expression tag	UNP Q6DC22
E	-22	GLY	-	expression tag	UNP Q6DC22
E	-21	GLY	-	expression tag	UNP Q6DC22
E	-20	SER	-	expression tag	UNP Q6DC22
E	-19	GLY	-	expression tag	UNP Q6DC22
E	-18	GLY	-	expression tag	UNP Q6DC22
E	-17	GLY	-	expression tag	UNP Q6DC22
E	-16	SER	-	expression tag	UNP Q6DC22
E	-15	GLY	-	expression tag	UNP Q6DC22
E	-14	GLY	-	expression tag	UNP Q6DC22
E	-13	GLY	-	expression tag	UNP Q6DC22
E	-12	SER	-	expression tag	UNP Q6DC22
E	-11	TRP	-	expression tag	UNP Q6DC22
E	-10	SER	-	expression tag	UNP Q6DC22
E	-9	HIS	-	expression tag	UNP Q6DC22
E	-8	PRO	-	expression tag	UNP Q6DC22
E	-7	GLN	-	expression tag	UNP Q6DC22
E	-6	PHE	-	expression tag	UNP Q6DC22
E	-5	GLU	-	expression tag	UNP Q6DC22
E	-4	LYS	-	expression tag	UNP Q6DC22
E	-3	GLY	-	expression tag	UNP Q6DC22
E	-2	GLY	-	expression tag	UNP Q6DC22
E	-1	GLY	-	expression tag	UNP Q6DC22
E	0	SER	-	expression tag	UNP Q6DC22
E	1	GLY	-	expression tag	UNP Q6DC22
E	2	GLY	-	expression tag	UNP Q6DC22
E	3	GLY	-	expression tag	UNP Q6DC22
E	4	SER	-	expression tag	UNP Q6DC22

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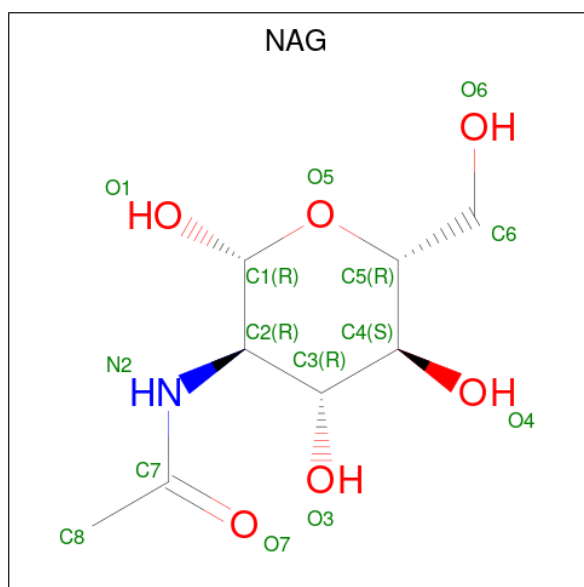
Chain	Residue	Modelled	Actual	Comment	Reference
E	5	GLY	-	expression tag	UNP Q6DC22
E	6	GLY	-	expression tag	UNP Q6DC22
E	7	GLY	-	expression tag	UNP Q6DC22
E	8	SER	-	expression tag	UNP Q6DC22
E	9	TRP	-	expression tag	UNP Q6DC22
E	10	SER	-	expression tag	UNP Q6DC22
E	11	HIS	-	expression tag	UNP Q6DC22
E	12	PRO	-	expression tag	UNP Q6DC22
E	13	GLN	-	expression tag	UNP Q6DC22
E	14	PHE	-	expression tag	UNP Q6DC22
E	15	GLU	-	expression tag	UNP Q6DC22
E	16	LYS	-	expression tag	UNP Q6DC22
E	17	GLU	-	expression tag	UNP Q6DC22
E	18	ASN	-	expression tag	UNP Q6DC22
E	19	LEU	-	expression tag	UNP Q6DC22
E	20	TYR	-	expression tag	UNP Q6DC22
E	21	PHE	-	expression tag	UNP Q6DC22
E	22	GLN	-	expression tag	UNP Q6DC22
E	23	GLY	-	expression tag	UNP Q6DC22
E	495	GLU	-	expression tag	UNP Q6DC22
E	496	ASN	-	expression tag	UNP Q6DC22
E	497	LEU	-	expression tag	UNP Q6DC22
E	498	TYR	-	expression tag	UNP Q6DC22
E	499	PHE	-	expression tag	UNP Q6DC22
E	500	GLN	-	expression tag	UNP Q6DC22
E	501	GLY	-	expression tag	UNP Q6DC22
E	502	THR	-	expression tag	UNP Q6DC22
E	503	GLU	-	expression tag	UNP Q6DC22
E	504	THR	-	expression tag	UNP Q6DC22
E	505	SER	-	expression tag	UNP Q6DC22
E	506	GLN	-	expression tag	UNP Q6DC22
E	507	VAL	-	expression tag	UNP Q6DC22
E	508	ALA	-	expression tag	UNP Q6DC22
E	509	PRO	-	expression tag	UNP Q6DC22
E	510	ALA	-	expression tag	UNP Q6DC22

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$) (labeled as "Ligand of Interest" by depositor).



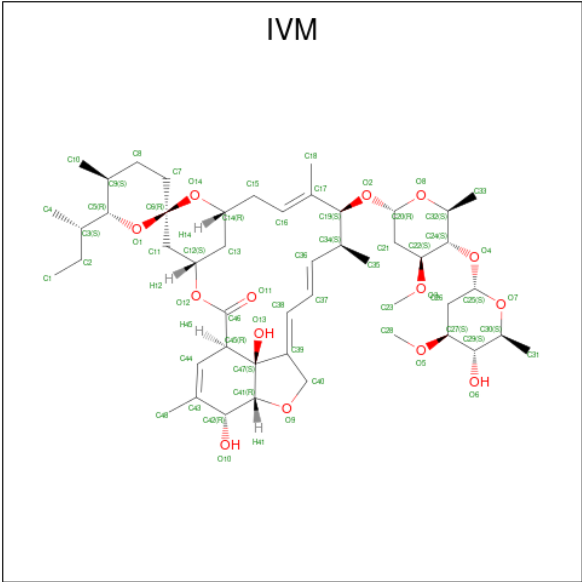
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			5	2	1	2	
3	A	1	Total	C	N	O	0
			5	2	1	2	
3	D	1	Total	C	N	O	0
			5	2	1	2	
3	C	1	Total	C	N	O	0
			5	2	1	2	
3	C	1	Total	C	N	O	0
			5	2	1	2	

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



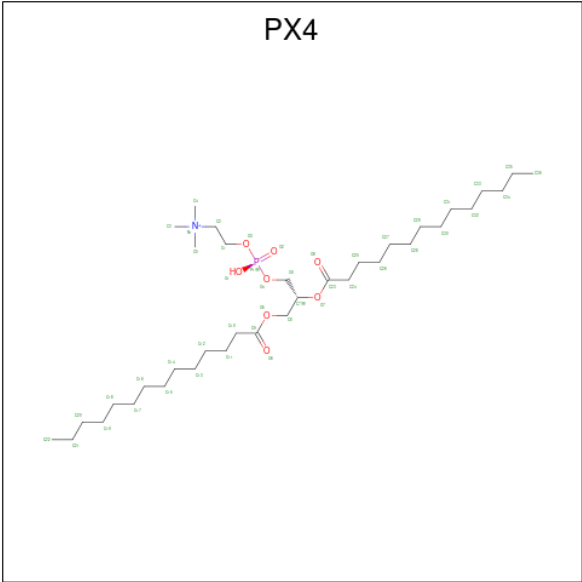
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is (2aE,4E,5'S,6S,6'R,7S,8E,11R,13R,15S,17aR,20R,20aR,20bS)-6'-[(2S)-butan-2-yl]-20,20b-dihydroxy-5',6,8,19-tetramethyl-17-oxo-3',4',5',6,6',10,11,14,15,17,17a,20,20a,20b-tetradecahydro-2H,7H-spiro[11,15-methanofuro[4,3,2-pq][2,6]benzodioxacyclooctadecine-13,2'-pyran]-7-yl 2,6-dideoxy-4-O-(2,6-dideoxy-3-O-methyl- α -L-arabino-hexopyranosyl)-3-O-methyl- α -L-arabino-hexopyranoside (three-letter code: IVM) (formula: C₄₈H₇₄O₁₄) (labeled as "Ligand of Interest" by depositor).



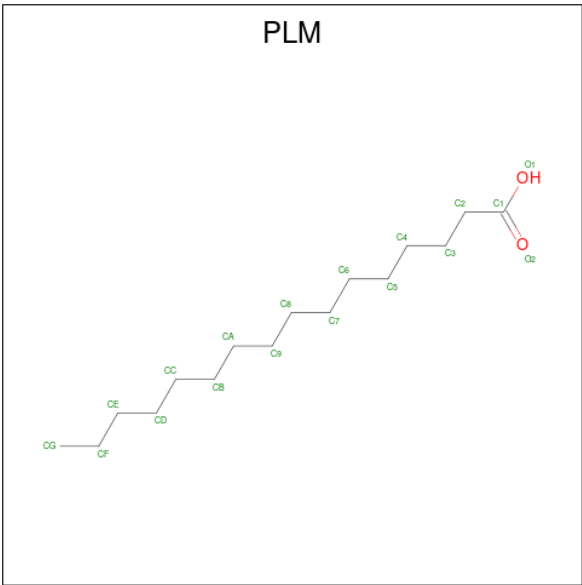
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			62	48	14	
5	A	1	Total	C	O	0
			62	48	14	
5	D	1	Total	C	O	0
			62	48	14	
5	C	1	Total	C	O	0
			62	48	14	
5	B	1	Total	C	O	0
			62	48	14	

- Molecule 6 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C₃₆H₇₃NO₈P).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			31	27	4	
6	D	1	Total	C	O	0
			34	30	4	
6	D	1	Total	C	O	0
			28	24	4	
6	C	1	Total	C	O	0
			31	27	4	
6	C	1	Total	C	O	0
			34	30	4	
6	B	1	Total	C	O	0
			33	29	4	
6	B	1	Total	C	O	0
			31	27	4	
6	E	1	Total	C	O	0
			31	27	4	

- Molecule 7 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



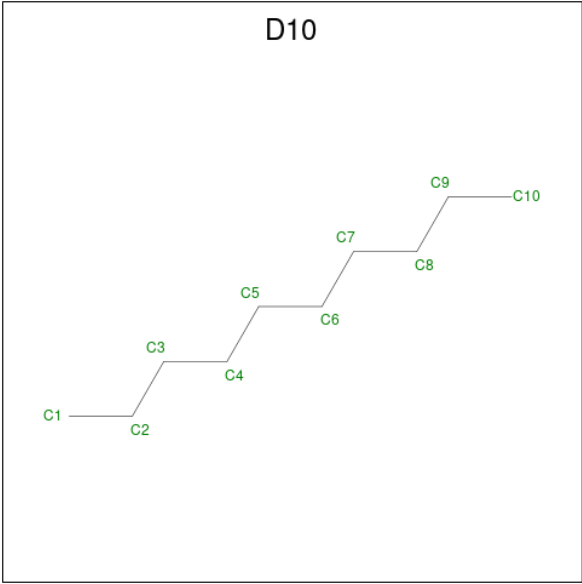
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			11	9	2	
7	A	1	Total	C	O	0
			12	10	2	
7	A	1	Total	C	O	0
			18	16	2	
7	A	1	Total	C	O	0
			17	15	2	
7	A	1	Total	C	O	0
			18	16	2	
7	D	1	Total	C	O	0
			13	11	2	
7	D	1	Total	C	O	0
			16	14	2	
7	D	1	Total	C	O	0
			15	13	2	
7	D	1	Total	C	O	0
			11	9	2	
7	D	1	Total	C	O	0
			13	11	2	
7	D	1	Total	C	O	0
			18	16	2	
7	C	1	Total	C	O	0
			13	11	2	
7	C	1	Total	C	O	0
			15	13	2	
7	C	1	Total	C	O	0
			14	12	2	

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Mol	Chain	Residues	Atoms			AltConf
7	C	1	Total	C	O	0
			17	15	2	
7	C	1	Total	C	O	0
			18	16	2	
7	C	1	Total	C	O	0
			14	12	2	
7	B	1	Total	C	O	0
			14	12	2	
7	B	1	Total	C	O	0
			11	9	2	
7	B	1	Total	C	O	0
			18	16	2	
7	B	1	Total	C	O	0
			11	9	2	
7	B	1	Total	C	O	0
			14	12	2	
7	B	1	Total	C	O	0
			18	16	2	
7	E	1	Total	C	O	0
			12	10	2	
7	E	1	Total	C	O	0
			15	13	2	
7	E	1	Total	C	O	0
			14	12	2	
7	E	1	Total	C	O	0
			14	12	2	
7	E	1	Total	C	O	0
			14	12	2	

- Molecule 8 is DECANE (three-letter code: D10) (formula: C₁₀H₂₂).

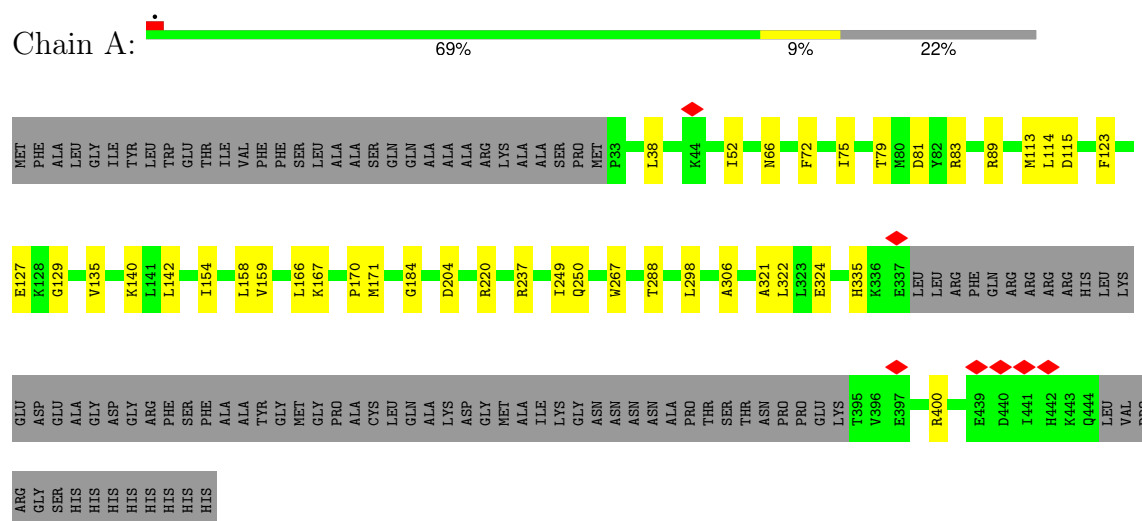


Mol	Chain	Residues	Atoms		AltConf
8	C	1	Total	C	0
			10	10	

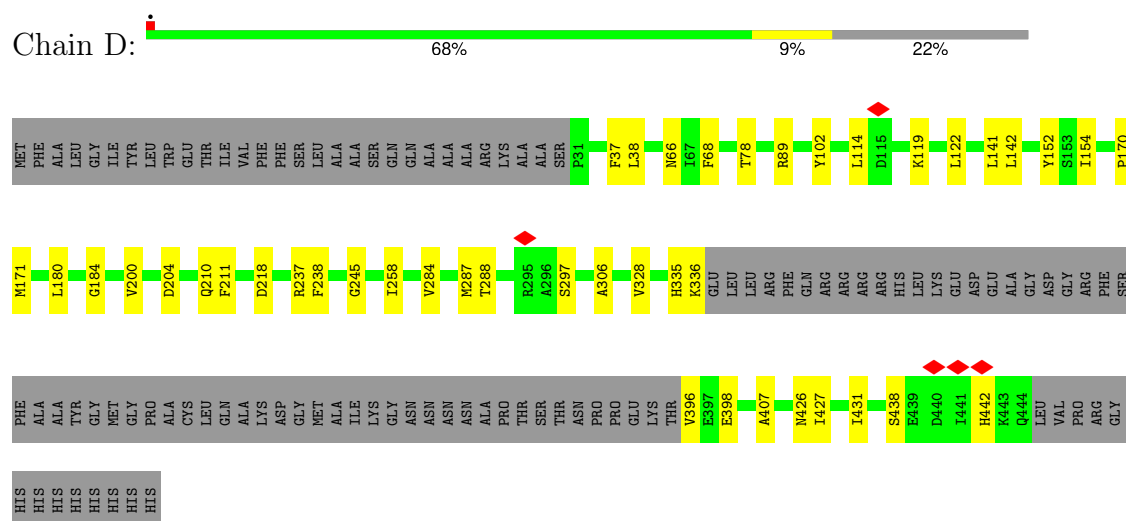
3 Residue-property plots

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: Glycine receptor subunit alphaZ1

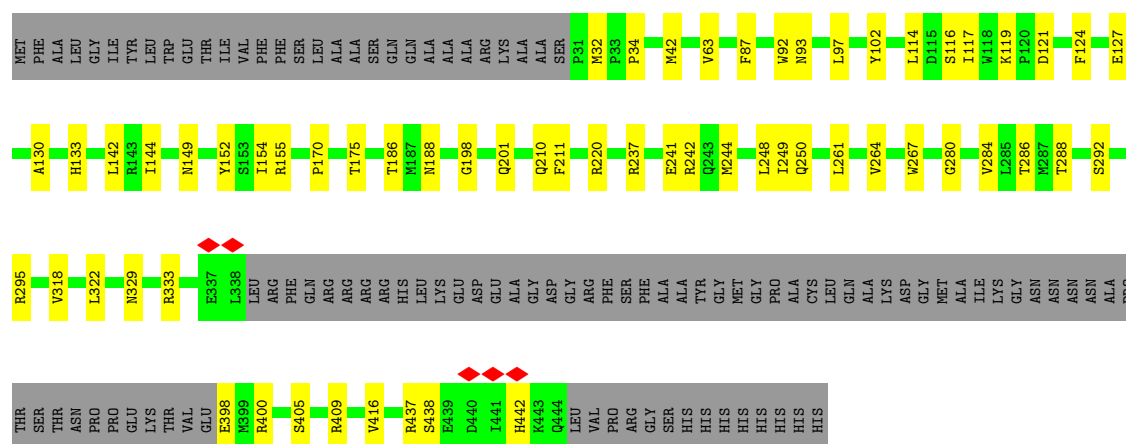


• Molecule 1: Glycine receptor subunit alphaZ1

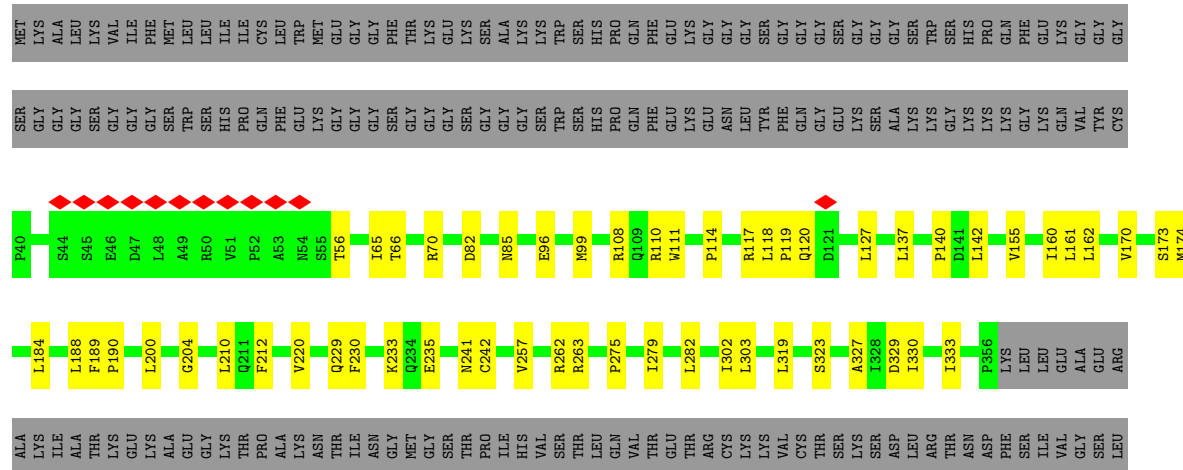


• Molecule 1: Glycine receptor subunit alphaZ1





- Molecule 2: Glycine receptor beta subunit 2



PRO	ARG	ASP	PHE	GLU	LEU	SER	ASN	PHE	ASP	CYS	TYR	GLY	LYS	PRO	ILE	GLU	VAL	GLY	SER	ALA	PHE	SER	LYS	SER	GLN	ALA	LYS	ASN	ASN	LYS	LYS	PRO	PRO	PRO	PRO	LYS	PRO	VAL	ILE	PRO	SER	A466	L494	GLU	ASN	LEU	TYR	PHE	GLN	GLY	THR	GLU	THR	SER	GLN	VAL	ALA	PRO
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ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	204512	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)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.739	Depositor
Minimum map value	-0.384	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	251.99998, 251.99998, 251.99998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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: PLM, NAG, D10, IVM, PX4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/2958	0.51	0/4009
1	B	0.29	0/2959	0.52	0/4010
1	C	0.24	0/2967	0.48	0/4021
1	D	0.25	0/2958	0.51	0/4009
2	E	0.27	0/2872	0.55	0/3906
All	All	0.27	0/14714	0.51	0/19955

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2887	0	2898	30	0
1	B	2887	0	2903	44	0
1	C	2895	0	2907	28	0
1	D	2886	0	2901	26	0
2	E	2800	0	2786	35	0
3	A	10	0	4	0	0
3	C	10	0	4	0	0
3	D	5	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
4	E	28	0	26	0	0
5	A	124	0	147	5	0
5	B	62	0	74	1	0
5	C	62	0	74	1	0
5	D	62	0	74	0	0
6	A	31	0	47	0	0
6	B	64	0	95	2	0
6	C	65	0	103	0	0
6	D	62	0	94	2	0
6	E	31	0	47	0	0
7	A	76	0	118	0	0
7	B	86	0	130	1	0
7	C	91	0	137	1	0
7	D	86	0	127	0	0
7	E	69	0	98	1	0
8	C	10	0	22	0	0
All	All	15445	0	15870	152	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 5.

All (152) 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:C:406:ARG:HH21	7:C:513:PLM:H22	1.57	0.70
1:B:198:GLY:O	1:B:201:GLN:NE2	2.28	0.66
1:A:166:LEU:HD13	1:A:298:LEU:HD12	1.78	0.64
2:E:161:LEU:HB3	2:E:173:SER:HB3	1.79	0.63
1:D:184:GLY:HA2	1:C:141:LEU:HD12	1.80	0.63
1:C:72:PHE:HD2	1:C:208:LEU:HD21	1.63	0.62
1:D:141:LEU:HD12	2:E:204:GLY:HA2	1.81	0.62
6:B:504:PX4:H23	6:B:504:PX4:H52	1.83	0.61
1:C:170:PRO:HD2	1:C:306:ALA:HB3	1.82	0.60
2:E:114:PRO:O	2:E:117:ARG:NH1	2.35	0.60
2:E:142:LEU:HD21	2:E:200:LEU:HD22	1.83	0.60
1:C:333:ARG:NH2	1:B:267:TRP:O	2.33	0.59
2:E:118:LEU:HD21	2:E:127:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:PHE:H	1:C:206:LEU:HD11	1.67	0.58
1:B:405:SER:OG	1:B:409:ARG:NH1	2.36	0.58
1:C:114:LEU:HD21	1:C:142:LEU:HB2	1.84	0.58
1:B:280:GLY:HA3	1:B:322:LEU:HD13	1.85	0.58
2:E:137:LEU:HD12	2:E:162:LEU:HD11	1.85	0.57
1:D:426:ASN:HD22	6:D:503:PX4:H69	1.70	0.57
1:D:218:ASP:HB2	1:D:237:ARG:HB2	1.85	0.56
1:D:328:VAL:HG13	1:D:407:ALA:HB1	1.88	0.56
1:B:249:ILE:HG13	1:B:250:GLN:HG2	1.88	0.56
1:A:140:LYS:HG2	1:A:154:ILE:HG22	1.88	0.56
1:A:267:TRP:O	1:B:333:ARG:NH1	2.39	0.55
2:E:140:PRO:HB3	2:E:210:LEU:HD11	1.89	0.55
1:D:38:LEU:HD13	2:E:70:ARG:HE	1.72	0.55
1:D:114:LEU:HD21	1:D:142:LEU:HB2	1.89	0.54
1:B:186:THR:HG23	1:B:188:ASN:H	1.73	0.54
1:C:122:LEU:HD11	1:C:180:LEU:HD23	1.91	0.53
1:A:321:ALA:O	1:A:324:GLU:HG3	2.09	0.53
1:B:114:LEU:HD21	1:B:142:LEU:HB2	1.90	0.52
1:B:97:LEU:HD23	1:B:144:ILE:HD13	1.90	0.52
2:E:220:VAL:HG21	2:E:257:VAL:HG21	1.92	0.52
1:A:322:LEU:HD23	2:E:282:LEU:HD22	1.91	0.51
1:A:115:ASP:N	1:A:115:ASP:OD1	2.44	0.51
1:A:127:GLU:OE2	1:A:129:GLY:N	2.44	0.51
1:B:42:MET:HE3	1:B:116:SER:HB2	1.93	0.51
1:B:329:ASN:HB3	1:B:333:ARG:HH22	1.73	0.51
5:A:504:IVM:H48	1:B:288:THR:HG23	1.92	0.51
1:A:220:ARG:HH12	1:A:237:ARG:CZ	2.24	0.51
1:D:37:PHE:CG	1:D:102:TYR:HE2	2.28	0.51
1:A:220:ARG:HH22	1:A:237:ARG:HD3	1.75	0.50
1:A:184:GLY:HA2	2:E:161:LEU:HD12	1.92	0.50
1:A:249:ILE:HD11	5:A:504:IVM:H31A	1.93	0.50
1:B:244:MET:HG3	1:B:248:LEU:HG	1.93	0.50
1:B:261:LEU:O	1:B:264:VAL:HG22	2.12	0.49
1:D:122:LEU:HD11	1:D:180:LEU:HD23	1.94	0.49
1:D:78:THR:OG1	1:D:297:SER:O	2.28	0.49
1:C:266:PHE:O	1:C:415:ARG:NH2	2.45	0.49
1:A:66:ASN:HB2	1:A:89:ARG:HB2	1.94	0.48
2:E:330:ILE:HG23	7:E:604:PLM:H92	1.95	0.48
1:D:170:PRO:HB2	1:D:171:MET:SD	2.53	0.48
1:A:250:GLN:HB3	1:B:295:ARG:HH11	1.79	0.48
1:C:186:THR:OG1	1:C:188:ASN:OD1	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:82:ASP:HB2	2:E:212:PHE:HD1	1.79	0.48
1:B:119:LYS:HD2	1:B:152:TYR:CZ	2.48	0.48
1:A:38:LEU:HB3	1:A:113:MET:HE1	1.95	0.47
1:A:83:ARG:HG2	1:A:159:VAL:HG22	1.97	0.47
1:A:114:LEU:HD21	1:A:142:LEU:HB2	1.96	0.47
1:B:175:THR:HG21	1:B:237:ARG:HH11	1.78	0.47
1:B:329:ASN:HB3	1:B:333:ARG:NH2	2.30	0.47
1:D:245:GLY:HA3	2:E:323:SER:HB2	1.97	0.47
1:D:119:LYS:HD2	1:D:152:TYR:CE2	2.50	0.47
2:E:210:LEU:HD21	2:E:212:PHE:CZ	2.50	0.46
1:B:438:SER:O	1:B:442:HIS:ND1	2.47	0.46
1:A:79:THR:OG1	1:A:81:ASP:OD1	2.22	0.46
1:A:123:PHE:HA	2:E:155:VAL:HG11	1.96	0.46
2:E:188:LEU:HA	2:E:327:ALA:HB2	1.95	0.46
6:D:503:PX4:H17	6:D:503:PX4:H19	1.65	0.46
2:E:329:ASP:O	2:E:333:ILE:HG13	2.14	0.46
1:B:152:TYR:CZ	1:B:154:ILE:HD11	2.51	0.46
2:E:229:GLN:HG3	2:E:230:PHE:CD2	2.51	0.46
1:D:427:ILE:O	1:D:431:ILE:HG12	2.17	0.45
2:E:190:PRO:HD2	2:E:327:ALA:HB3	1.99	0.45
1:B:170:PRO:HA	1:B:242:ARG:HD2	1.99	0.45
1:D:204:ASP:OD1	1:D:204:ASP:N	2.50	0.45
2:E:189:PHE:CE1	2:E:319:LEU:HD11	2.52	0.45
2:E:302:ILE:HG23	2:E:303:LEU:HD22	1.99	0.45
1:D:152:TYR:CE2	1:D:154:ILE:HD11	2.52	0.44
1:A:52:ILE:HD11	2:E:56:THR:HG23	2.00	0.44
1:B:124:PHE:HB2	1:B:127:GLU:HB2	1.99	0.44
1:B:152:TYR:CE2	1:B:154:ILE:HD11	2.53	0.44
1:C:204:ASP:OD1	1:C:205:GLY:N	2.47	0.44
1:B:241:GLU:OE2	1:B:437:ARG:NH2	2.50	0.44
1:A:250:GLN:HB3	1:B:295:ARG:NH1	2.32	0.44
1:D:335:HIS:CD2	1:D:336:LYS:HG3	2.52	0.44
5:A:504:IVM:H36	5:A:504:IVM:C16	2.47	0.44
1:C:152:TYR:CZ	1:C:154:ILE:HD11	2.52	0.44
1:A:167:LYS:HB3	1:A:167:LYS:HE3	1.77	0.44
1:D:170:PRO:HD2	1:D:306:ALA:HB3	2.00	0.44
1:C:285:LEU:HD13	1:B:286:THR:HG21	1.99	0.44
1:B:220:ARG:HD2	1:B:237:ARG:HH21	1.82	0.44
1:C:152:TYR:CE2	1:C:154:ILE:HD11	2.52	0.43
1:B:63:VAL:HG22	1:B:92:TRP:HB3	2.00	0.43
1:B:93:ASN:ND2	1:B:149:ASN:OD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ARG:HH11	1:B:250:GLN:HB3	1.83	0.43
2:E:65:ILE:HG23	2:E:66:THR:HG23	2.00	0.43
1:A:170:PRO:HB2	1:A:171:MET:SD	2.58	0.43
1:A:335:HIS:HB2	1:A:400:ARG:HA	2.00	0.43
1:C:180:LEU:HB2	1:C:234:ILE:HG13	2.00	0.43
1:C:127:GLU:OE2	1:B:133:HIS:ND1	2.51	0.43
1:C:119:LYS:HD2	1:C:152:TYR:CZ	2.53	0.43
2:E:85:ASN:HB2	2:E:108:ARG:HB2	2.00	0.43
1:B:210:GLN:HG3	1:B:211:PHE:CD1	2.53	0.43
1:A:72:PHE:HE1	1:A:75:ILE:HD11	1.83	0.43
1:A:204:ASP:N	1:A:204:ASP:OD1	2.52	0.43
1:A:220:ARG:NH2	1:A:237:ARG:HD3	2.34	0.42
2:E:119:PRO:O	2:E:120:GLN:HG3	2.19	0.42
1:A:135:VAL:HG23	1:B:130:ALA:CB	2.50	0.42
1:A:170:PRO:HD2	1:A:306:ALA:HB3	2.01	0.42
1:D:210:GLN:HG3	1:D:211:PHE:CD1	2.55	0.42
1:C:124:PHE:HA	1:C:179:GLN:O	2.18	0.42
1:B:284:VAL:HG22	1:B:318:VAL:HG23	2.00	0.42
1:B:292:SER:O	1:B:295:ARG:HG2	2.20	0.42
2:E:160:ILE:HG12	2:E:174:MET:HG2	2.00	0.42
1:D:66:ASN:HB2	1:D:89:ARG:HB2	2.02	0.42
1:D:200:VAL:HG11	1:D:238:PHE:HE1	1.84	0.42
1:B:97:LEU:HD21	1:B:117:ILE:HD12	2.01	0.42
2:E:233:LYS:HE3	2:E:235:GLU:HB2	2.01	0.42
1:B:220:ARG:HE	1:B:237:ARG:HE	1.68	0.42
2:E:110:ARG:HA	2:E:170:VAL:O	2.19	0.42
1:D:396:VAL:HG23	1:D:398:GLU:HG2	2.02	0.41
2:E:233:LYS:HE2	2:E:262:ARG:HH12	1.85	0.41
1:C:187:MET:HG2	1:C:232:THR:HB	2.02	0.41
2:E:96:GLU:OE2	2:E:263:ARG:NH1	2.49	0.41
1:A:127:GLU:HG3	1:A:158:LEU:HD22	2.02	0.41
1:D:258:ILE:HG21	1:D:287:MET:HB2	2.02	0.41
1:D:68:PHE:HB2	1:D:89:ARG:HH22	1.86	0.41
1:C:63:VAL:HG22	1:C:92:TRP:HB3	2.02	0.41
1:C:200:VAL:HG11	1:C:238:PHE:HE1	1.86	0.41
2:E:241:ASN:O	2:E:242:CYS:HB3	2.20	0.41
1:B:87:PHE:CE1	1:B:155:ARG:HG3	2.56	0.41
1:A:288:THR:HG23	5:A:503:IVM:H48	2.01	0.41
5:A:503:IVM:H25	5:A:503:IVM:H32	1.61	0.41
1:B:121:ASP:OD1	1:B:121:ASP:N	2.53	0.41
1:D:438:SER:O	1:D:442:HIS:ND1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ARG:HG2	1:C:159:VAL:HG22	2.02	0.41
1:C:420:LEU:O	1:C:424:ILE:HG12	2.21	0.41
5:B:503:IVM:H23	6:B:504:PX4:H65	2.03	0.41
1:C:136:THR:HG22	1:C:137:THR:HG23	2.03	0.40
1:B:32:MET:HB3	1:B:102:TYR:HE1	1.85	0.40
1:B:87:PHE:HE1	1:B:155:ARG:HG3	1.85	0.40
1:B:398:GLU:HG2	1:B:400:ARG:H	1.86	0.40
1:B:416:VAL:HG12	7:B:505:PLM:H51	2.04	0.40
1:C:52:ILE:HG12	1:B:34:PRO:HB2	2.03	0.40
1:C:71:SER:HB3	1:C:85:ASN:HB3	2.03	0.40
5:C:505:IVM:H36	5:C:505:IVM:H13A	2.04	0.40
2:E:275:PRO:O	2:E:279:ILE:HG12	2.21	0.40
1:D:284:VAL:O	1:D:288:THR:HG23	2.22	0.40
1:C:79:THR:OG1	1:C:81:ASP:OD1	2.23	0.40
2:E:82:ASP:OD1	2:E:111:TRP:HB3	2.21	0.40
2:E:99:MET:HE2	2:E:184:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	351/458 (77%)	348 (99%)	3 (1%)	0	100	100
1	B	351/458 (77%)	348 (99%)	3 (1%)	0	100	100
1	C	352/458 (77%)	348 (99%)	4 (1%)	0	100	100
1	D	351/458 (77%)	346 (99%)	5 (1%)	0	100	100
2	E	342/591 (58%)	333 (97%)	9 (3%)	0	100	100
All	All	1747/2423 (72%)	1723 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	320/400 (80%)	320 (100%)	0	100	100
1	B	320/400 (80%)	320 (100%)	0	100	100
1	C	321/400 (80%)	321 (100%)	0	100	100
1	D	320/400 (80%)	320 (100%)	0	100	100
2	E	315/509 (62%)	315 (100%)	0	100	100
All	All	1596/2109 (76%)	1596 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

53 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$
8	D10	C	506	-	9,9,9	0.11	0	8,8,8	0.17	0
7	PLM	A	508	-	11,11,17	1.13	1 (9%)	11,11,17	1.08	2 (18%)
5	IVM	C	505	-	67,68,68	3.68	44 (65%)	87,102,102	1.77	19 (21%)
6	PX4	D	503	-	33,33,45	2.19	7 (21%)	34,34,53	1.11	2 (5%)
7	PLM	B	509	-	13,13,17	1.04	1 (7%)	13,13,17	0.99	2 (15%)
6	PX4	C	502	-	30,30,45	2.21	7 (23%)	31,31,53	1.11	2 (6%)
7	PLM	E	605	-	14,14,17	1.02	1 (7%)	14,14,17	0.81	2 (14%)
7	PLM	D	510	-	12,12,17	1.08	1 (8%)	12,12,17	1.04	2 (16%)
7	PLM	E	604	-	11,11,17	1.12	1 (9%)	11,11,17	1.08	2 (18%)
7	PLM	B	506	-	10,10,17	1.17	1 (10%)	10,10,17	0.95	2 (20%)
7	PLM	A	510	-	16,16,17	0.96	1 (6%)	16,16,17	0.75	2 (12%)
4	NAG	E	601	2	14,14,15	0.37	0	17,19,21	1.15	1 (5%)
6	PX4	E	602	-	30,30,45	2.21	7 (23%)	31,31,53	1.07	2 (6%)
3	GLY	C	501	-	4,4,4	1.15	1 (25%)	3,4,4	1.66	1 (33%)
7	PLM	C	508	-	12,12,17	1.08	1 (8%)	12,12,17	0.86	2 (16%)
7	PLM	B	510	-	17,17,17	0.83	1 (5%)	17,17,17	0.77	2 (11%)
7	PLM	D	507	-	15,15,17	0.98	1 (6%)	15,15,17	0.93	2 (13%)
6	PX4	D	505	-	27,27,45	2.25	7 (25%)	28,28,53	1.17	2 (7%)
5	IVM	B	503	-	67,68,68	3.66	43 (64%)	87,102,102	1.85	20 (22%)
7	PLM	B	507	-	17,17,17	0.98	1 (5%)	17,17,17	0.72	1 (5%)
7	PLM	A	511	-	17,17,17	0.90	1 (5%)	17,17,17	0.73	2 (11%)
7	PLM	C	509	-	14,14,17	1.02	1 (7%)	14,14,17	0.81	2 (14%)
3	GLY	A	501	-	4,4,4	1.16	1 (25%)	3,4,4	1.65	1 (33%)
5	IVM	A	504	-	67,68,68	3.64	44 (65%)	87,102,102	1.79	18 (20%)
3	GLY	C	503	-	4,4,4	1.16	1 (25%)	3,4,4	1.64	1 (33%)
4	NAG	C	504	1	14,14,15	0.67	1 (7%)	17,19,21	0.73	1 (5%)
7	PLM	A	507	-	10,10,17	1.17	1 (10%)	10,10,17	0.96	2 (20%)
7	PLM	C	511	-	16,16,17	0.96	1 (6%)	16,16,17	0.75	2 (12%)
7	PLM	E	606	-	13,13,17	1.04	1 (7%)	13,13,17	1.00	2 (15%)
4	NAG	A	502	1	14,14,15	0.52	0	17,19,21	0.54	0
4	NAG	D	501	1	14,14,15	0.27	0	17,19,21	0.38	0
3	GLY	A	506	-	4,4,4	1.16	1 (25%)	3,4,4	1.64	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	IVM	A	503	-	67,68,68	3.68	43 (64%)	87,102,102	2.00	25 (28%)
4	NAG	B	502	1	14,14,15	0.61	0	17,19,21	0.82	1 (5%)
7	PLM	C	510	-	13,13,17	1.04	1 (7%)	13,13,17	0.99	2 (15%)
7	PLM	D	508	-	14,14,17	1.06	1 (7%)	14,14,17	0.98	2 (14%)
4	NAG	E	603	2	14,14,15	0.27	0	17,19,21	0.54	0
6	PX4	B	501	-	32,32,45	2.19	7 (21%)	33,33,53	1.15	2 (6%)
7	PLM	D	509	-	10,10,17	1.17	1 (10%)	10,10,17	0.95	2 (20%)
7	PLM	D	504	-	12,12,17	1.04	1 (8%)	12,12,17	1.04	2 (16%)
7	PLM	C	512	-	17,17,17	0.87	1 (5%)	17,17,17	0.76	2 (11%)
7	PLM	D	511	-	17,17,17	0.91	1 (5%)	17,17,17	0.74	2 (11%)
7	PLM	A	509	-	17,17,17	0.94	1 (5%)	17,17,17	0.73	2 (11%)
7	PLM	B	505	-	13,13,17	1.04	1 (7%)	13,13,17	0.85	2 (15%)
6	PX4	A	505	-	30,30,45	2.21	7 (23%)	31,31,53	1.15	2 (6%)
7	PLM	B	508	-	10,10,17	1.16	1 (10%)	10,10,17	1.13	2 (20%)
6	PX4	B	504	-	30,30,45	2.21	7 (23%)	31,31,53	1.13	2 (6%)
3	GLY	D	506	-	4,4,4	1.16	1 (25%)	3,4,4	1.65	1 (33%)
6	PX4	C	507	-	33,33,45	2.18	7 (21%)	34,34,53	1.12	2 (5%)
7	PLM	E	607	-	13,13,17	1.05	1 (7%)	13,13,17	1.00	2 (15%)
5	IVM	D	502	-	67,68,68	3.67	43 (64%)	87,102,102	1.76	22 (25%)
7	PLM	C	513	-	13,13,17	1.02	1 (7%)	13,13,17	0.85	2 (15%)
7	PLM	E	608	-	13,13,17	1.03	1 (7%)	13,13,17	1.00	2 (15%)

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
8	D10	C	506	-	-	0/7/7/7	-
7	PLM	A	508	-	-	0/9/9/15	-
5	IVM	C	505	-	-	7/45/141/141	2/7/7/7
6	PX4	D	503	-	-	9/33/33/49	-
7	PLM	B	509	-	-	2/11/11/15	-
6	PX4	C	502	-	-	6/30/30/49	-
7	PLM	E	605	-	-	3/12/12/15	-
7	PLM	D	510	-	-	2/10/10/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PLM	E	604	-	-	2/9/9/15	-
7	PLM	B	506	-	-	2/8/8/15	-
7	PLM	A	510	-	-	4/14/14/15	-
4	NAG	E	601	2	-	4/6/23/26	0/1/1/1
6	PX4	E	602	-	-	4/30/30/49	-
3	GLY	C	501	-	-	0/2/2/2	-
7	PLM	C	508	-	-	2/10/10/15	-
7	PLM	B	510	-	-	2/15/15/15	-
7	PLM	D	507	-	-	3/13/13/15	-
6	PX4	D	505	-	-	5/27/27/49	-
5	IVM	B	503	-	-	9/45/141/141	2/7/7/7
7	PLM	B	507	-	-	2/15/15/15	-
7	PLM	A	511	-	-	3/15/15/15	-
7	PLM	C	509	-	-	2/12/12/15	-
3	GLY	A	501	-	-	2/2/2/2	-
5	IVM	A	504	-	-	6/45/141/141	2/7/7/7
3	GLY	C	503	-	-	1/2/2/2	-
4	NAG	C	504	1	-	2/6/23/26	0/1/1/1
7	PLM	A	507	-	-	2/8/8/15	-
7	PLM	C	511	-	-	3/14/14/15	-
7	PLM	E	606	-	-	2/11/11/15	-
4	NAG	A	502	1	-	2/6/23/26	0/1/1/1
4	NAG	D	501	1	-	2/6/23/26	0/1/1/1
3	GLY	A	506	-	-	0/2/2/2	-
5	IVM	A	503	-	-	11/45/141/141	1/7/7/7
4	NAG	B	502	1	-	2/6/23/26	0/1/1/1
7	PLM	C	510	-	-	3/11/11/15	-
7	PLM	D	508	-	-	4/12/12/15	-
4	NAG	E	603	2	-	4/6/23/26	0/1/1/1
6	PX4	B	501	-	-	6/32/32/49	-
7	PLM	D	509	-	-	2/8/8/15	-
7	PLM	D	504	-	-	5/10/10/15	-
7	PLM	C	512	-	-	2/15/15/15	-
7	PLM	D	511	-	-	4/15/15/15	-
7	PLM	A	509	-	-	2/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PLM	B	505	-	-	2/11/11/15	-
6	PX4	A	505	-	-	5/30/30/49	-
7	PLM	B	508	-	-	2/8/8/15	-
6	PX4	B	504	-	-	5/30/30/49	-
3	GLY	D	506	-	-	0/2/2/2	-
6	PX4	C	507	-	-	9/33/33/49	-
7	PLM	E	607	-	-	5/11/11/15	-
5	IVM	D	502	-	-	4/45/141/141	1/7/7/7
7	PLM	C	513	-	-	3/11/11/15	-
7	PLM	E	608	-	-	2/11/11/15	-

All (307) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	IVM	C48-C43	8.38	1.66	1.50
5	C	505	IVM	C48-C43	8.33	1.65	1.50
5	A	503	IVM	C48-C43	8.32	1.65	1.50
5	D	502	IVM	C48-C43	8.26	1.65	1.50
5	A	504	IVM	C48-C43	8.12	1.65	1.50
5	D	502	IVM	C3-C5	8.07	1.67	1.53
5	A	503	IVM	C3-C5	8.01	1.67	1.53
5	C	505	IVM	C3-C5	7.99	1.67	1.53
5	A	504	IVM	C3-C5	7.87	1.67	1.53
5	B	503	IVM	C3-C5	7.76	1.66	1.53
5	D	502	IVM	C34-C36	7.51	1.68	1.51
5	B	503	IVM	C40-C39	7.44	1.62	1.50
5	D	502	IVM	C40-C39	7.42	1.62	1.50
5	A	503	IVM	C40-C39	7.39	1.62	1.50
5	C	505	IVM	C40-C39	7.37	1.62	1.50
5	B	503	IVM	C34-C36	7.37	1.68	1.51
5	A	504	IVM	C40-C39	7.36	1.62	1.50
5	A	503	IVM	C34-C36	7.36	1.68	1.51
5	A	504	IVM	C18-C17	7.35	1.64	1.50
5	A	503	IVM	C18-C17	7.33	1.64	1.50
5	C	505	IVM	C18-C17	7.31	1.64	1.50
5	B	503	IVM	C18-C17	7.29	1.64	1.50
5	A	503	IVM	C47-C41	7.27	1.61	1.54
5	C	505	IVM	C34-C36	7.25	1.68	1.51
5	C	505	IVM	C47-C41	7.24	1.61	1.54
5	A	504	IVM	C34-C36	7.23	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	IVM	C18-C17	7.19	1.63	1.50
5	A	504	IVM	C47-C41	7.02	1.61	1.54
5	B	503	IVM	C47-C41	6.75	1.60	1.54
5	D	502	IVM	C47-C41	6.73	1.60	1.54
5	C	505	IVM	C47-C45	-6.06	1.50	1.56
5	D	502	IVM	C47-C45	-5.93	1.50	1.56
5	B	503	IVM	C26-C27	-5.69	1.41	1.52
5	C	505	IVM	C26-C27	-5.61	1.41	1.52
5	A	504	IVM	C26-C27	-5.58	1.41	1.52
5	A	503	IVM	C26-C27	-5.53	1.41	1.52
5	A	504	IVM	C47-C45	-5.51	1.50	1.56
5	A	503	IVM	C11-C6	5.49	1.60	1.52
5	C	505	IVM	C11-C6	5.44	1.60	1.52
5	D	502	IVM	C26-C27	-5.39	1.41	1.52
5	B	503	IVM	C37-C38	5.36	1.59	1.43
5	B	503	IVM	C11-C6	5.33	1.59	1.52
5	A	503	IVM	C37-C38	5.32	1.59	1.43
5	A	504	IVM	C11-C6	5.31	1.59	1.52
5	D	502	IVM	C37-C38	5.31	1.59	1.43
5	D	502	IVM	C11-C6	5.29	1.59	1.52
5	C	505	IVM	C37-C38	5.28	1.59	1.43
5	B	503	IVM	C47-C45	-5.27	1.50	1.56
5	A	504	IVM	C37-C38	5.26	1.59	1.43
5	A	503	IVM	C47-C45	-5.18	1.51	1.56
6	E	602	PX4	O7-C23	4.86	1.47	1.33
6	D	505	PX4	O7-C23	4.85	1.47	1.33
6	B	501	PX4	O7-C23	4.84	1.47	1.33
6	C	502	PX4	O7-C23	4.83	1.47	1.33
6	D	503	PX4	O7-C23	4.83	1.47	1.33
6	C	507	PX4	O7-C23	4.82	1.47	1.33
6	B	504	PX4	O7-C23	4.81	1.47	1.33
6	A	505	PX4	O7-C23	4.80	1.47	1.33
6	D	503	PX4	O5-C9	4.78	1.47	1.33
6	A	505	PX4	O5-C9	4.75	1.47	1.33
6	D	505	PX4	O5-C9	4.74	1.47	1.33
6	B	504	PX4	O5-C9	4.74	1.47	1.33
6	C	502	PX4	O5-C9	4.74	1.47	1.33
6	E	602	PX4	O5-C9	4.73	1.47	1.33
5	A	503	IVM	O1-C6	4.72	1.50	1.42
6	B	501	PX4	O5-C9	4.72	1.47	1.33
6	C	507	PX4	O5-C9	4.70	1.47	1.33
5	C	505	IVM	O1-C6	4.66	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	IVM	C7-C6	4.64	1.60	1.51
5	D	502	IVM	O1-C6	4.60	1.50	1.42
5	B	503	IVM	O1-C6	4.59	1.50	1.42
5	A	504	IVM	O1-C6	4.54	1.50	1.42
5	C	505	IVM	O12-C46	4.50	1.44	1.34
5	C	505	IVM	C7-C6	4.49	1.60	1.51
5	A	504	IVM	O2-C20	-4.49	1.29	1.41
5	C	505	IVM	O2-C20	-4.46	1.29	1.41
5	B	503	IVM	C7-C6	4.46	1.60	1.51
5	A	504	IVM	C7-C6	4.46	1.60	1.51
5	D	502	IVM	O2-C20	-4.44	1.29	1.41
5	A	503	IVM	C13-C14	4.44	1.62	1.52
5	D	502	IVM	C45-C46	-4.44	1.45	1.52
5	B	503	IVM	O12-C46	4.43	1.44	1.34
5	A	503	IVM	C7-C6	4.43	1.60	1.51
5	B	503	IVM	O2-C20	-4.41	1.29	1.41
5	A	503	IVM	O12-C46	4.41	1.44	1.34
5	A	503	IVM	O8-C20	4.38	1.53	1.42
5	A	503	IVM	O1-C5	4.35	1.50	1.44
5	A	504	IVM	C13-C14	4.33	1.62	1.52
5	A	504	IVM	O12-C46	4.32	1.44	1.34
5	A	503	IVM	C10-C9	4.28	1.63	1.53
5	D	502	IVM	C13-C14	4.28	1.62	1.52
5	C	505	IVM	C13-C14	4.27	1.62	1.52
5	C	505	IVM	O1-C5	4.27	1.50	1.44
5	B	503	IVM	C13-C14	4.27	1.62	1.52
5	B	503	IVM	C10-C9	4.26	1.63	1.53
5	B	503	IVM	O1-C5	4.25	1.50	1.44
5	B	503	IVM	C45-C46	-4.25	1.46	1.52
5	A	503	IVM	O2-C20	-4.25	1.30	1.41
5	D	502	IVM	O12-C46	4.22	1.43	1.34
5	A	504	IVM	O8-C20	4.21	1.53	1.42
5	A	504	IVM	C10-C9	4.20	1.63	1.53
5	C	505	IVM	C10-C9	4.20	1.63	1.53
5	A	503	IVM	C45-C46	-4.19	1.46	1.52
5	A	504	IVM	O1-C5	4.19	1.50	1.44
5	D	502	IVM	C10-C9	4.17	1.63	1.53
5	C	505	IVM	O8-C20	4.14	1.53	1.42
5	B	503	IVM	C45-C44	4.13	1.55	1.50
5	A	503	IVM	C4-C3	4.08	1.63	1.53
5	B	503	IVM	C4-C3	4.07	1.63	1.53
5	B	503	IVM	O8-C20	4.05	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	IVM	C45-C44	4.04	1.55	1.50
5	D	502	IVM	O8-C20	4.04	1.52	1.42
5	D	502	IVM	C35-C34	4.03	1.63	1.53
5	D	502	IVM	C4-C3	4.00	1.63	1.53
5	D	502	IVM	O14-C6	3.98	1.49	1.42
5	D	502	IVM	O1-C5	3.97	1.49	1.44
5	A	504	IVM	C4-C3	3.96	1.63	1.53
5	C	505	IVM	C45-C46	-3.96	1.46	1.52
5	C	505	IVM	C4-C3	3.91	1.63	1.53
5	A	504	IVM	C45-C46	-3.91	1.46	1.52
5	D	502	IVM	C34-C19	3.87	1.60	1.54
5	C	505	IVM	C45-C44	3.85	1.55	1.50
5	A	504	IVM	C35-C34	3.85	1.63	1.53
5	A	503	IVM	C45-C44	3.83	1.55	1.50
5	B	503	IVM	C35-C34	3.82	1.63	1.53
5	A	503	IVM	O14-C6	3.82	1.49	1.42
5	B	503	IVM	O14-C6	3.81	1.49	1.42
5	C	505	IVM	O14-C6	3.76	1.49	1.42
5	A	503	IVM	C35-C34	3.73	1.63	1.53
5	C	505	IVM	C35-C34	3.68	1.63	1.53
5	B	503	IVM	C34-C19	3.68	1.60	1.54
5	D	502	IVM	C45-C44	3.67	1.54	1.50
5	A	504	IVM	O14-C6	3.67	1.49	1.42
6	E	602	PX4	C24-C23	3.62	1.61	1.50
5	A	503	IVM	C9-C5	3.62	1.60	1.53
6	C	507	PX4	C24-C23	3.60	1.61	1.50
5	C	505	IVM	C34-C19	3.60	1.60	1.54
5	C	505	IVM	C9-C5	3.58	1.60	1.53
5	A	504	IVM	C34-C19	3.56	1.60	1.54
6	A	505	PX4	C24-C23	3.56	1.61	1.50
6	D	505	PX4	C24-C23	3.54	1.61	1.50
5	A	503	IVM	C34-C19	3.54	1.60	1.54
6	D	503	PX4	C24-C23	3.53	1.61	1.50
6	B	504	PX4	C24-C23	3.53	1.61	1.50
6	B	501	PX4	C24-C23	3.52	1.60	1.50
5	A	503	IVM	O2-C19	3.51	1.52	1.42
6	C	502	PX4	C24-C23	3.51	1.60	1.50
5	A	504	IVM	C9-C5	3.50	1.60	1.53
5	D	502	IVM	O2-C19	3.50	1.52	1.42
6	B	504	PX4	C10-C9	3.48	1.60	1.50
5	C	505	IVM	O2-C19	3.48	1.52	1.42
6	A	505	PX4	C10-C9	3.47	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	501	PX4	C10-C9	3.47	1.60	1.50
6	D	505	PX4	C10-C9	3.47	1.60	1.50
5	B	503	IVM	O2-C19	3.46	1.52	1.42
6	C	507	PX4	C10-C9	3.46	1.60	1.50
6	D	503	PX4	C10-C9	3.46	1.60	1.50
6	C	502	PX4	C10-C9	3.45	1.60	1.50
5	D	502	IVM	O14-C14	3.45	1.52	1.44
6	E	602	PX4	C10-C9	3.44	1.60	1.50
5	B	503	IVM	C9-C5	3.43	1.60	1.53
5	B	503	IVM	O14-C14	3.42	1.51	1.44
5	A	504	IVM	O14-C14	3.41	1.51	1.44
5	A	504	IVM	O2-C19	3.41	1.52	1.42
5	D	502	IVM	C9-C5	3.39	1.60	1.53
5	A	503	IVM	O14-C14	3.35	1.51	1.44
5	D	502	IVM	C7-C8	3.31	1.60	1.53
5	C	505	IVM	O14-C14	3.30	1.51	1.44
5	A	504	IVM	C7-C8	3.20	1.59	1.53
5	C	505	IVM	C7-C8	3.20	1.59	1.53
7	D	508	PLM	C2-C1	3.19	1.58	1.50
5	C	505	IVM	O4-C24	3.15	1.51	1.43
5	A	503	IVM	O4-C24	3.14	1.51	1.43
5	B	503	IVM	O4-C24	3.14	1.51	1.43
5	D	502	IVM	O9-C41	3.13	1.49	1.44
5	B	503	IVM	C7-C8	3.13	1.59	1.53
5	C	505	IVM	C38-C39	3.12	1.38	1.33
5	D	502	IVM	O4-C24	3.12	1.51	1.43
5	B	503	IVM	C38-C39	3.12	1.38	1.33
5	A	504	IVM	C41-C42	-3.11	1.46	1.52
5	A	503	IVM	C7-C8	3.10	1.59	1.53
7	B	507	PLM	C2-C1	3.09	1.57	1.50
5	A	504	IVM	O4-C24	3.09	1.51	1.43
5	D	502	IVM	C38-C39	3.08	1.38	1.33
5	A	503	IVM	O9-C41	3.06	1.49	1.44
5	A	503	IVM	C38-C39	3.04	1.38	1.33
5	B	503	IVM	O9-C41	3.03	1.49	1.44
7	E	607	PLM	C2-C1	3.01	1.57	1.50
5	A	503	IVM	C2-C3	2.99	1.63	1.53
5	C	505	IVM	O9-C41	2.98	1.49	1.44
7	A	508	PLM	C2-C1	2.98	1.57	1.50
7	D	507	PLM	C2-C1	2.97	1.57	1.50
7	C	509	PLM	C2-C1	2.97	1.57	1.50
7	D	510	PLM	C2-C1	2.97	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	509	PLM	C2-C1	2.97	1.57	1.50
7	D	509	PLM	C2-C1	2.96	1.57	1.50
5	D	502	IVM	C2-C3	2.96	1.63	1.53
7	E	606	PLM	C2-C1	2.96	1.57	1.50
7	B	509	PLM	C2-C1	2.96	1.57	1.50
7	C	510	PLM	C2-C1	2.96	1.57	1.50
7	E	605	PLM	C2-C1	2.96	1.57	1.50
7	E	604	PLM	C2-C1	2.95	1.57	1.50
7	B	505	PLM	C2-C1	2.95	1.57	1.50
7	C	508	PLM	C2-C1	2.95	1.57	1.50
7	B	506	PLM	C2-C1	2.95	1.57	1.50
7	B	508	PLM	C2-C1	2.95	1.57	1.50
7	C	511	PLM	C2-C1	2.95	1.57	1.50
7	E	608	PLM	C2-C1	2.93	1.57	1.50
5	A	504	IVM	C38-C39	2.93	1.38	1.33
7	A	507	PLM	C2-C1	2.92	1.57	1.50
5	B	503	IVM	C2-C3	2.91	1.63	1.53
7	A	510	PLM	C2-C1	2.91	1.57	1.50
5	A	504	IVM	O9-C41	2.91	1.49	1.44
7	A	511	PLM	C2-C1	2.91	1.57	1.50
5	A	504	IVM	C2-C3	2.90	1.62	1.53
5	C	505	IVM	C2-C3	2.89	1.62	1.53
7	D	511	PLM	C2-C1	2.88	1.57	1.50
7	C	513	PLM	C2-C1	2.86	1.57	1.50
5	D	502	IVM	C19-C17	2.85	1.56	1.51
5	D	502	IVM	C41-C42	-2.81	1.47	1.52
7	D	504	PLM	C2-C1	2.80	1.57	1.50
5	A	504	IVM	C21-C22	-2.78	1.46	1.52
5	B	503	IVM	C19-C17	2.77	1.56	1.51
5	A	503	IVM	C41-C42	-2.77	1.47	1.52
5	A	504	IVM	O3-C23	2.76	1.51	1.42
5	A	503	IVM	C21-C22	-2.76	1.46	1.52
5	A	504	IVM	C19-C17	2.76	1.56	1.51
5	C	505	IVM	O3-C23	2.75	1.51	1.42
5	D	502	IVM	C37-C36	2.74	1.43	1.33
5	A	503	IVM	O10-C42	-2.74	1.36	1.42
7	C	512	PLM	C2-C1	2.73	1.56	1.50
5	B	503	IVM	O3-C23	2.73	1.51	1.42
5	A	503	IVM	C19-C17	2.72	1.56	1.51
5	A	503	IVM	O13-C47	2.72	1.47	1.42
5	A	503	IVM	O3-C23	2.70	1.51	1.42
5	C	505	IVM	C41-C42	-2.70	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	IVM	C41-C42	-2.70	1.47	1.52
5	D	502	IVM	O10-C42	-2.70	1.36	1.42
5	B	503	IVM	C21-C22	-2.68	1.46	1.52
5	D	502	IVM	O3-C23	2.68	1.51	1.42
5	C	505	IVM	C21-C22	-2.67	1.46	1.52
5	B	503	IVM	C37-C36	2.66	1.43	1.33
5	C	505	IVM	C37-C36	2.64	1.43	1.33
7	B	510	PLM	C2-C1	2.64	1.56	1.50
5	B	503	IVM	O13-C47	2.62	1.47	1.42
5	C	505	IVM	C19-C17	2.62	1.56	1.51
5	A	503	IVM	C37-C36	2.62	1.43	1.33
5	A	504	IVM	O10-C42	-2.60	1.37	1.42
5	C	505	IVM	O10-C42	-2.58	1.37	1.42
5	D	502	IVM	O13-C47	2.57	1.47	1.42
5	B	503	IVM	O10-C42	-2.52	1.37	1.42
5	D	502	IVM	O6-C29	2.49	1.49	1.43
5	C	505	IVM	O13-C47	2.49	1.46	1.42
5	A	504	IVM	C37-C36	2.48	1.42	1.33
5	C	505	IVM	C29-C27	-2.48	1.47	1.53
6	E	602	PX4	C25-C24	2.47	1.61	1.52
5	D	502	IVM	C21-C22	-2.47	1.47	1.52
5	A	504	IVM	C29-C27	-2.45	1.47	1.53
5	A	504	IVM	O13-C47	2.44	1.46	1.42
6	C	502	PX4	C25-C24	2.41	1.61	1.52
5	B	503	IVM	C29-C27	-2.40	1.47	1.53
5	D	502	IVM	O5-C28	2.39	1.50	1.42
4	C	504	NAG	O5-C1	-2.39	1.39	1.43
5	A	503	IVM	C29-C27	-2.39	1.47	1.53
6	B	501	PX4	C25-C24	2.39	1.60	1.52
6	D	505	PX4	C25-C24	2.39	1.60	1.52
5	A	504	IVM	O6-C29	2.38	1.48	1.43
6	A	505	PX4	C25-C24	2.38	1.60	1.52
5	B	503	IVM	O6-C29	2.37	1.48	1.43
6	C	507	PX4	C25-C24	2.37	1.60	1.52
5	A	504	IVM	O5-C28	2.37	1.50	1.42
6	B	504	PX4	C25-C24	2.37	1.60	1.52
5	A	503	IVM	O5-C28	2.37	1.50	1.42
5	A	503	IVM	O6-C29	2.36	1.48	1.43
6	D	503	PX4	C25-C24	2.36	1.60	1.52
5	B	503	IVM	O5-C28	2.36	1.50	1.42
5	C	505	IVM	O5-C28	2.35	1.50	1.42
6	D	503	PX4	C8-C7	2.35	1.60	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	IVM	C29-C27	-2.34	1.48	1.53
6	E	602	PX4	C8-C7	2.34	1.60	1.49
6	D	505	PX4	C8-C7	2.33	1.60	1.49
6	A	505	PX4	C8-C7	2.33	1.60	1.49
6	C	502	PX4	C8-C7	2.32	1.60	1.49
6	C	502	PX4	C11-C10	2.32	1.60	1.52
6	B	504	PX4	C8-C7	2.32	1.60	1.49
5	C	505	IVM	O6-C29	2.32	1.48	1.43
6	B	501	PX4	C8-C7	2.32	1.60	1.49
6	C	507	PX4	C8-C7	2.32	1.60	1.49
6	D	505	PX4	C11-C10	2.30	1.60	1.52
6	B	501	PX4	C11-C10	2.29	1.60	1.52
6	B	504	PX4	C11-C10	2.29	1.60	1.52
6	A	505	PX4	C11-C10	2.28	1.60	1.52
6	D	503	PX4	C11-C10	2.27	1.60	1.52
6	E	602	PX4	C11-C10	2.27	1.60	1.52
6	C	507	PX4	C11-C10	2.24	1.60	1.52
3	D	506	GLY	OXT-C	-2.22	1.23	1.30
3	C	503	GLY	OXT-C	-2.21	1.23	1.30
3	A	501	GLY	OXT-C	-2.21	1.23	1.30
3	A	506	GLY	OXT-C	-2.20	1.23	1.30
3	C	501	GLY	OXT-C	-2.18	1.23	1.30
5	A	503	IVM	C8-C9	2.18	1.58	1.53
5	A	504	IVM	C8-C9	2.18	1.58	1.53
5	C	505	IVM	C8-C9	2.17	1.58	1.53
5	A	504	IVM	C24-C32	-2.13	1.48	1.52
5	D	502	IVM	C8-C9	2.13	1.58	1.53
5	C	505	IVM	C24-C32	-2.12	1.48	1.52
5	B	503	IVM	C8-C9	2.09	1.58	1.53

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	503	IVM	C35-C34-C19	6.78	120.13	110.78
5	A	504	IVM	C35-C34-C19	6.40	119.60	110.78
5	C	505	IVM	C35-C34-C19	6.07	119.14	110.78
5	A	503	IVM	C34-C19-C17	-5.91	102.41	113.19
5	A	503	IVM	O2-C19-C17	-5.78	101.03	111.69
5	A	503	IVM	C35-C34-C19	5.55	118.42	110.78
5	D	502	IVM	C35-C34-C19	5.45	118.29	110.78
5	D	502	IVM	O12-C46-C45	5.45	119.18	110.91
5	C	505	IVM	O12-C46-C45	5.30	118.95	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	IVM	O12-C46-C45	5.29	118.94	110.91
5	B	503	IVM	O12-C46-C45	4.78	118.17	110.91
5	C	505	IVM	C34-C19-C17	-4.78	104.48	113.19
5	A	504	IVM	C34-C19-C17	-4.65	104.72	113.19
5	A	504	IVM	O12-C46-C45	4.53	117.79	110.91
5	B	503	IVM	C34-C19-C17	-4.24	105.47	113.19
5	A	504	IVM	O2-C19-C17	-4.10	104.13	111.69
5	A	504	IVM	C15-C16-C17	-4.08	118.89	127.71
5	C	505	IVM	O2-C19-C17	-4.05	104.23	111.69
4	E	601	NAG	C1-O5-C5	3.89	117.40	112.19
5	B	503	IVM	C15-C16-C17	-3.89	119.31	127.71
5	D	502	IVM	C6-O1-C5	-3.89	108.90	114.21
5	A	504	IVM	C37-C38-C39	-3.69	120.03	125.87
5	A	503	IVM	O11-C46-C45	-3.64	119.54	125.06
5	A	503	IVM	O4-C24-C32	3.58	115.90	106.77
5	A	503	IVM	C13-C14-C15	-3.58	108.81	113.05
5	D	502	IVM	C47-C45-C44	-3.55	108.61	112.74
5	C	505	IVM	O11-C46-C45	-3.54	119.70	125.06
5	B	503	IVM	O2-C19-C17	-3.51	105.21	111.69
5	C	505	IVM	C15-C16-C17	-3.42	120.32	127.71
5	B	503	IVM	O11-C46-C45	-3.41	119.89	125.06
5	D	502	IVM	C15-C16-C17	-3.33	120.51	127.71
5	D	502	IVM	C34-C19-C17	-3.31	107.16	113.19
5	D	502	IVM	O11-C46-C45	-3.29	120.07	125.06
5	B	503	IVM	C37-C38-C39	-3.29	120.66	125.87
5	D	502	IVM	O2-C19-C17	-3.29	105.62	111.69
5	B	503	IVM	C10-C9-C5	-3.09	107.41	112.32
5	A	504	IVM	C47-C45-C44	-3.05	109.18	112.74
5	B	503	IVM	C7-C6-C11	-3.03	107.19	112.22
5	C	505	IVM	C47-C45-C44	-2.99	109.26	112.74
5	B	503	IVM	C13-C14-C15	-2.99	109.51	113.05
4	B	502	NAG	C1-O5-C5	2.98	116.18	112.19
5	A	503	IVM	C31-C30-C29	-2.97	107.65	113.08
5	A	504	IVM	C10-C9-C5	-2.96	107.61	112.32
5	A	503	IVM	O14-C14-C13	2.96	114.22	109.02
5	B	503	IVM	C38-C37-C36	-2.89	117.73	124.43
6	C	507	PX4	O7-C23-C24	2.85	120.51	111.83
5	A	504	IVM	O11-C46-C45	-2.84	120.76	125.06
5	A	503	IVM	C2-C3-C5	-2.84	107.91	112.02
5	A	503	IVM	C47-C45-C44	-2.83	109.44	112.74
5	A	503	IVM	C10-C9-C5	-2.82	107.84	112.32
6	D	505	PX4	O7-C23-C24	2.82	120.42	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	503	PX4	O5-C9-C10	2.81	120.39	111.83
6	B	501	PX4	O5-C9-C10	2.78	120.30	111.83
5	A	504	IVM	C6-O1-C5	-2.77	110.42	114.21
5	B	503	IVM	C31-C30-C29	-2.76	108.03	113.08
6	B	501	PX4	O7-C23-C24	2.75	120.21	111.83
7	D	508	PLM	O2-C1-C2	-2.74	114.41	123.09
6	A	505	PX4	O5-C9-C10	2.73	120.15	111.83
7	D	504	PLM	O2-C1-C2	-2.72	114.47	123.09
5	A	503	IVM	C33-C32-C24	-2.72	109.35	113.39
5	A	503	IVM	O2-C20-C21	-2.71	103.06	108.28
5	B	503	IVM	C8-C9-C5	2.71	112.09	108.33
6	C	502	PX4	O7-C23-C24	2.71	120.10	111.83
6	A	505	PX4	O7-C23-C24	2.71	120.10	111.83
7	D	510	PLM	O2-C1-C2	-2.70	114.53	123.09
7	A	508	PLM	O2-C1-C2	-2.70	114.53	123.09
7	E	607	PLM	O2-C1-C2	-2.70	114.53	123.09
7	E	608	PLM	O2-C1-C2	-2.70	114.54	123.09
7	E	606	PLM	O2-C1-C2	-2.69	114.55	123.09
7	B	509	PLM	O2-C1-C2	-2.69	114.55	123.09
7	E	604	PLM	O2-C1-C2	-2.69	114.55	123.09
7	C	510	PLM	O2-C1-C2	-2.69	114.57	123.09
7	B	508	PLM	O2-C1-C2	-2.69	114.57	123.09
5	C	505	IVM	C10-C9-C5	-2.69	108.05	112.32
7	D	507	PLM	O2-C1-C2	-2.68	114.58	123.09
5	A	503	IVM	C38-C37-C36	-2.68	118.23	124.43
6	B	504	PX4	O7-C23-C24	2.66	119.96	111.83
6	D	505	PX4	O5-C9-C10	2.66	119.94	111.83
6	C	507	PX4	O5-C9-C10	2.64	119.89	111.83
6	C	502	PX4	O5-C9-C10	2.62	119.81	111.83
5	D	502	IVM	C10-C9-C5	-2.61	108.17	112.32
5	D	502	IVM	C7-C6-C11	-2.60	107.90	112.22
6	B	504	PX4	O5-C9-C10	2.60	119.77	111.83
5	A	504	IVM	C2-C3-C5	-2.59	108.27	112.02
5	C	505	IVM	C31-C30-C29	-2.59	108.35	113.08
6	D	503	PX4	O7-C23-C24	2.56	119.63	111.83
5	A	504	IVM	O14-C14-C13	2.55	113.50	109.02
5	A	504	IVM	O4-C24-C32	2.54	113.25	106.77
5	A	503	IVM	C35-C34-C36	-2.52	104.21	109.91
5	C	505	IVM	C13-C14-C15	-2.52	110.07	113.05
5	A	503	IVM	C8-C9-C5	2.49	111.79	108.33
5	D	502	IVM	C48-C43-C44	-2.49	117.46	123.36
5	C	505	IVM	C37-C38-C39	-2.48	121.94	125.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	505	IVM	C2-C3-C5	-2.48	108.42	112.02
5	B	503	IVM	C2-C3-C5	-2.46	108.45	112.02
5	C	505	IVM	C6-O1-C5	-2.46	110.85	114.21
5	C	505	IVM	C35-C34-C36	-2.44	104.38	109.91
5	D	502	IVM	C38-C37-C36	-2.43	118.79	124.43
4	C	504	NAG	C1-O5-C5	2.43	115.45	112.19
5	C	505	IVM	O4-C24-C32	2.43	112.96	106.77
5	A	503	IVM	C14-C15-C16	-2.43	106.45	111.59
5	A	503	IVM	C18-C17-C19	2.41	120.72	115.96
5	C	505	IVM	C38-C37-C36	-2.40	118.86	124.43
6	E	602	PX4	O7-C23-C24	2.40	119.16	111.83
5	D	502	IVM	C2-C3-C5	-2.39	108.55	112.02
5	A	503	IVM	C15-C16-C17	-2.38	122.56	127.71
5	D	502	IVM	O14-C14-C15	2.37	109.29	106.53
5	B	503	IVM	C7-C8-C9	2.36	116.64	112.26
5	D	502	IVM	C47-C45-C46	-2.34	106.64	109.05
5	B	503	IVM	O14-C14-C13	2.32	113.11	109.02
6	E	602	PX4	O5-C9-C10	2.32	118.90	111.83
5	D	502	IVM	C31-C30-C29	-2.30	108.87	113.08
5	D	502	IVM	C7-C8-C9	2.30	116.53	112.26
5	A	503	IVM	C37-C38-C39	-2.30	122.23	125.87
5	A	504	IVM	C35-C34-C36	-2.30	104.71	109.91
5	D	502	IVM	C13-C14-C15	-2.29	110.33	113.05
5	D	502	IVM	O14-C14-C13	2.29	113.04	109.02
5	B	503	IVM	C47-C45-C44	-2.28	110.08	112.74
5	B	503	IVM	C48-C43-C44	-2.27	117.98	123.36
5	D	502	IVM	O7-C30-C29	2.26	113.62	109.55
5	A	504	IVM	C13-C14-C15	-2.25	110.38	113.05
5	A	503	IVM	O1-C5-C9	2.22	114.18	110.55
5	B	503	IVM	O14-C14-C15	2.21	109.10	106.53
5	A	503	IVM	C7-C6-C11	-2.21	108.56	112.22
5	A	504	IVM	C48-C43-C44	-2.21	118.14	123.36
5	A	504	IVM	C31-C30-C29	-2.20	109.06	113.08
5	A	504	IVM	C38-C37-C36	-2.19	119.36	124.43
7	C	512	PLM	O1-C1-O2	2.18	128.94	123.33
7	B	510	PLM	O1-C1-O2	2.17	128.92	123.33
7	C	509	PLM	O1-C1-O2	2.15	128.87	123.33
7	D	511	PLM	O1-C1-O2	2.15	128.86	123.33
5	D	502	IVM	O1-C6-C7	2.15	113.63	110.93
7	D	507	PLM	O1-C1-O2	2.15	128.85	123.33
7	A	508	PLM	O1-C1-O2	2.15	128.85	123.33
7	B	505	PLM	O1-C1-O2	2.15	128.85	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	504	PLM	O1-C1-O2	2.14	128.85	123.33
7	E	606	PLM	O1-C1-O2	2.14	128.84	123.33
7	E	608	PLM	O1-C1-O2	2.14	128.84	123.33
7	A	511	PLM	O1-C1-O2	2.14	128.84	123.33
5	D	502	IVM	C33-C32-C24	-2.14	110.21	113.39
7	B	506	PLM	O1-C1-O2	2.14	128.83	123.33
7	C	510	PLM	O1-C1-O2	2.14	128.82	123.33
7	B	510	PLM	O2-C1-C2	-2.13	116.33	123.09
7	D	510	PLM	O1-C1-O2	2.13	128.82	123.33
7	E	607	PLM	O1-C1-O2	2.13	128.82	123.33
7	A	507	PLM	O1-C1-O2	2.13	128.81	123.33
7	C	513	PLM	O1-C1-O2	2.13	128.81	123.33
7	E	605	PLM	O1-C1-O2	2.13	128.81	123.33
7	C	511	PLM	O1-C1-O2	2.13	128.81	123.33
7	B	509	PLM	O1-C1-O2	2.13	128.80	123.33
7	A	509	PLM	O1-C1-O2	2.12	128.80	123.33
7	D	509	PLM	O1-C1-O2	2.12	128.80	123.33
7	B	508	PLM	O1-C1-O2	2.12	128.79	123.33
5	C	505	IVM	O14-C14-C13	2.12	112.75	109.02
7	E	604	PLM	O1-C1-O2	2.12	128.79	123.33
5	C	505	IVM	C48-C43-C44	-2.12	118.34	123.36
7	C	508	PLM	O1-C1-O2	2.11	128.77	123.33
7	A	510	PLM	O1-C1-O2	2.11	128.77	123.33
5	A	503	IVM	C21-C22-C24	-2.11	106.43	110.53
3	C	501	GLY	OXT-C-O	-2.09	117.94	123.33
3	A	501	GLY	OXT-C-O	-2.09	117.97	123.33
3	A	506	GLY	OXT-C-O	-2.08	117.97	123.33
3	D	506	GLY	OXT-C-O	-2.07	118.00	123.33
5	C	505	IVM	C18-C17-C19	2.07	120.04	115.96
7	C	513	PLM	O2-C1-C2	-2.06	116.55	123.09
7	D	508	PLM	O1-C1-O2	2.06	128.63	123.33
3	C	503	GLY	OXT-C-O	-2.06	118.03	123.33
7	B	505	PLM	O2-C1-C2	-2.06	116.56	123.09
7	B	507	PLM	O1-C1-O2	2.06	128.63	123.33
7	A	507	PLM	O2-C1-C2	-2.06	116.57	123.09
7	C	509	PLM	O2-C1-C2	-2.05	116.60	123.09
7	D	511	PLM	O2-C1-C2	-2.04	116.62	123.09
7	B	506	PLM	O2-C1-C2	-2.04	116.63	123.09
7	E	605	PLM	O2-C1-C2	-2.04	116.63	123.09
7	C	511	PLM	O2-C1-C2	-2.04	116.63	123.09
7	A	511	PLM	O2-C1-C2	-2.03	116.64	123.09
5	B	503	IVM	O1-C5-C9	2.03	113.88	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	510	PLM	O2-C1-C2	-2.03	116.64	123.09
7	A	509	PLM	O2-C1-C2	-2.03	116.65	123.09
5	A	503	IVM	C6-O1-C5	-2.03	111.44	114.21
7	D	509	PLM	O2-C1-C2	-2.03	116.67	123.09
7	C	508	PLM	O2-C1-C2	-2.03	116.67	123.09
7	C	512	PLM	O2-C1-C2	-2.03	116.67	123.09

There are no chirality outliers.

All (177) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GLY	O-C-CA-N
3	A	501	GLY	OXT-C-CA-N
4	E	601	NAG	C8-C7-N2-C2
4	E	601	NAG	O7-C7-N2-C2
5	A	503	IVM	C1-C2-C3-C5
5	A	503	IVM	O2-C19-C34-C36
5	A	503	IVM	C36-C37-C38-C39
5	A	504	IVM	C36-C37-C38-C39
5	D	502	IVM	C1-C2-C3-C5
5	C	505	IVM	C26-C25-O4-C24
5	B	503	IVM	O7-C25-O4-C24
5	B	503	IVM	C36-C37-C38-C39
6	A	505	PX4	O8-C23-O7-C7
6	A	505	PX4	C24-C23-O7-C7
6	D	503	PX4	O6-C9-O5-C8
6	D	503	PX4	C10-C9-O5-C8
6	D	505	PX4	O8-C23-O7-C7
6	D	505	PX4	C24-C23-O7-C7
6	C	507	PX4	O8-C23-O7-C7
6	C	507	PX4	C24-C23-O7-C7
6	B	501	PX4	O8-C23-O7-C7
6	B	501	PX4	C24-C23-O7-C7
5	B	503	IVM	C32-C24-O4-C25
5	A	504	IVM	C32-C24-O4-C25
5	C	505	IVM	C32-C24-O4-C25
6	D	505	PX4	O6-C9-O5-C8
6	C	502	PX4	O6-C9-O5-C8
5	A	503	IVM	C32-C24-O4-C25
6	D	505	PX4	C10-C9-O5-C8
6	C	502	PX4	C10-C9-O5-C8
4	E	601	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	B	504	PX4	C24-C23-O7-C7
6	B	504	PX4	O8-C23-O7-C7
4	C	504	NAG	O5-C5-C6-O6
4	B	502	NAG	O5-C5-C6-O6
4	E	601	NAG	C4-C5-C6-O6
6	A	505	PX4	O7-C7-C8-O5
5	B	503	IVM	C21-C22-O3-C23
5	B	503	IVM	C26-C25-O4-C24
5	C	505	IVM	C36-C37-C38-C39
5	A	503	IVM	O8-C20-O2-C19
5	C	505	IVM	O7-C25-O4-C24
4	E	603	NAG	O5-C5-C6-O6
6	E	602	PX4	O7-C7-C8-O5
4	C	504	NAG	C4-C5-C6-O6
6	C	502	PX4	O7-C7-C8-O5
6	B	501	PX4	O7-C7-C8-O5
4	A	502	NAG	C8-C7-N2-C2
4	A	502	NAG	O7-C7-N2-C2
4	E	603	NAG	C8-C7-N2-C2
4	E	603	NAG	O7-C7-N2-C2
4	B	502	NAG	C4-C5-C6-O6
6	D	503	PX4	C28-C29-C30-C31
5	A	503	IVM	C21-C22-O3-C23
7	A	510	PLM	C1-C2-C3-C4
7	D	504	PLM	C2-C3-C4-C5
7	C	510	PLM	C3-C4-C5-C6
6	C	507	PX4	C10-C9-O5-C8
7	D	504	PLM	C1-C2-C3-C4
5	A	503	IVM	C1-C2-C3-C4
5	D	502	IVM	C1-C2-C3-C4
6	E	602	PX4	C28-C29-C30-C31
6	C	507	PX4	O6-C9-O5-C8
4	E	603	NAG	C4-C5-C6-O6
5	A	504	IVM	C26-C25-O4-C24
5	B	503	IVM	C1-C2-C3-C5
7	D	507	PLM	C3-C4-C5-C6
4	D	501	NAG	O5-C5-C6-O6
7	A	511	PLM	C6-C7-C8-C9
6	C	507	PX4	C7-C8-O5-C9
6	D	503	PX4	C24-C23-O7-C7
4	D	501	NAG	C4-C5-C6-O6
6	B	501	PX4	C11-C10-C9-O5

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Mol	Chain	Res	Type	Atoms
6	B	504	PX4	O7-C7-C8-O5
5	C	505	IVM	C35-C34-C36-C37
5	A	503	IVM	C26-C25-O4-C24
6	C	502	PX4	C10-C11-C12-C13
6	C	507	PX4	O7-C7-C8-O5
6	A	505	PX4	C11-C10-C9-O5
5	A	504	IVM	O7-C25-O4-C24
6	D	503	PX4	O8-C23-O7-C7
6	D	503	PX4	C10-C11-C12-C13
7	D	508	PLM	C4-C5-C6-C7
6	E	602	PX4	C26-C27-C28-C29
5	C	505	IVM	C19-C34-C36-C37
6	D	503	PX4	O7-C7-C8-O5
7	C	511	PLM	C8-C9-CA-CB
7	E	607	PLM	C8-C9-CA-CB
5	A	503	IVM	O7-C25-O4-C24
7	E	608	PLM	C5-C6-C7-C8
5	A	503	IVM	C17-C19-O2-C20
5	A	504	IVM	C17-C19-O2-C20
5	C	505	IVM	C17-C19-O2-C20
5	B	503	IVM	C17-C19-O2-C20
5	A	503	IVM	C35-C34-C36-C37
5	A	504	IVM	C35-C34-C36-C37
6	C	502	PX4	C11-C12-C13-C14
6	D	505	PX4	C12-C13-C14-C15
7	E	607	PLM	C7-C8-C9-CA
7	D	511	PLM	C6-C7-C8-C9
6	B	501	PX4	C30-C31-C32-C33
5	B	503	IVM	C35-C34-C36-C37
6	B	504	PX4	C16-C17-C18-C19
7	E	608	PLM	C3-C4-C5-C6
6	B	501	PX4	C11-C10-C9-O6
7	A	510	PLM	C2-C3-C4-C5
7	B	505	PLM	O2-C1-C2-C3
7	A	511	PLM	O2-C1-C2-C3
7	D	508	PLM	O1-C1-C2-C3
7	D	504	PLM	C7-C8-C9-CA
3	C	503	GLY	O-C-CA-N
7	A	510	PLM	O2-C1-C2-C3
7	D	504	PLM	O2-C1-C2-C3
7	E	607	PLM	C6-C7-C8-C9
7	A	507	PLM	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	C	508	PLM	O2-C1-C2-C3
7	D	508	PLM	O2-C1-C2-C3
6	E	602	PX4	C27-C28-C29-C30
7	E	605	PLM	O1-C1-C2-C3
7	C	513	PLM	C3-C4-C5-C6
7	C	511	PLM	O1-C1-C2-C3
7	B	505	PLM	O1-C1-C2-C3
7	A	507	PLM	O1-C1-C2-C3
7	B	506	PLM	O1-C1-C2-C3
7	B	507	PLM	O1-C1-C2-C3
7	A	510	PLM	O1-C1-C2-C3
7	A	511	PLM	O1-C1-C2-C3
7	D	504	PLM	O1-C1-C2-C3
7	C	508	PLM	O1-C1-C2-C3
7	B	510	PLM	O1-C1-C2-C3
7	E	605	PLM	C9-CA-CB-CC
7	E	607	PLM	O1-C1-C2-C3
7	B	508	PLM	O1-C1-C2-C3
7	A	509	PLM	O1-C1-C2-C3
7	C	511	PLM	O2-C1-C2-C3
7	C	513	PLM	O1-C1-C2-C3
7	E	605	PLM	O2-C1-C2-C3
7	E	606	PLM	O1-C1-C2-C3
7	D	507	PLM	O1-C1-C2-C3
7	D	509	PLM	O1-C1-C2-C3
7	D	511	PLM	O1-C1-C2-C3
7	C	512	PLM	O1-C1-C2-C3
7	E	604	PLM	O1-C1-C2-C3
7	D	510	PLM	O1-C1-C2-C3
7	B	507	PLM	O2-C1-C2-C3
7	B	509	PLM	O1-C1-C2-C3
7	D	508	PLM	C5-C6-C7-C8
7	C	509	PLM	O1-C1-C2-C3
7	B	506	PLM	O2-C1-C2-C3
7	C	510	PLM	O1-C1-C2-C3
7	E	607	PLM	O2-C1-C2-C3
7	D	507	PLM	O2-C1-C2-C3
7	D	510	PLM	O2-C1-C2-C3
7	B	509	PLM	O2-C1-C2-C3
7	C	512	PLM	O2-C1-C2-C3
7	E	604	PLM	O2-C1-C2-C3
7	A	509	PLM	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	E	606	PLM	O2-C1-C2-C3
7	D	509	PLM	O2-C1-C2-C3
7	D	511	PLM	O2-C1-C2-C3
7	C	509	PLM	O2-C1-C2-C3
7	C	510	PLM	O2-C1-C2-C3
7	B	508	PLM	O2-C1-C2-C3
7	B	510	PLM	O2-C1-C2-C3
5	D	502	IVM	C14-C15-C16-C17
7	C	513	PLM	O2-C1-C2-C3
6	A	505	PX4	C11-C10-C9-O6
6	C	507	PX4	C11-C12-C13-C14
5	D	502	IVM	C26-C27-O5-C28
6	D	503	PX4	C32-C33-C34-C35
6	C	507	PX4	C24-C25-C26-C27
6	D	503	PX4	C30-C31-C32-C33
6	C	502	PX4	C12-C13-C14-C15
7	D	511	PLM	C5-C6-C7-C8
6	C	507	PX4	C23-C24-C25-C26
5	B	503	IVM	C1-C2-C3-C4
6	B	504	PX4	C11-C10-C9-O5

All (8) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	IVM	C20-C21-C22-C24-C32-O8
5	B	503	IVM	C20-C21-C22-C24-C32-O8
5	B	503	IVM	C25-C26-C27-C29-C30-O7
5	C	505	IVM	C20-C21-C22-C24-C32-O8
5	A	503	IVM	C25-C26-C27-C29-C30-O7
5	A	504	IVM	C25-C26-C27-C29-C30-O7
5	D	502	IVM	C20-C21-C22-C24-C32-O8
5	C	505	IVM	C25-C26-C27-C29-C30-O7

9 monomers are involved in 13 short contacts:

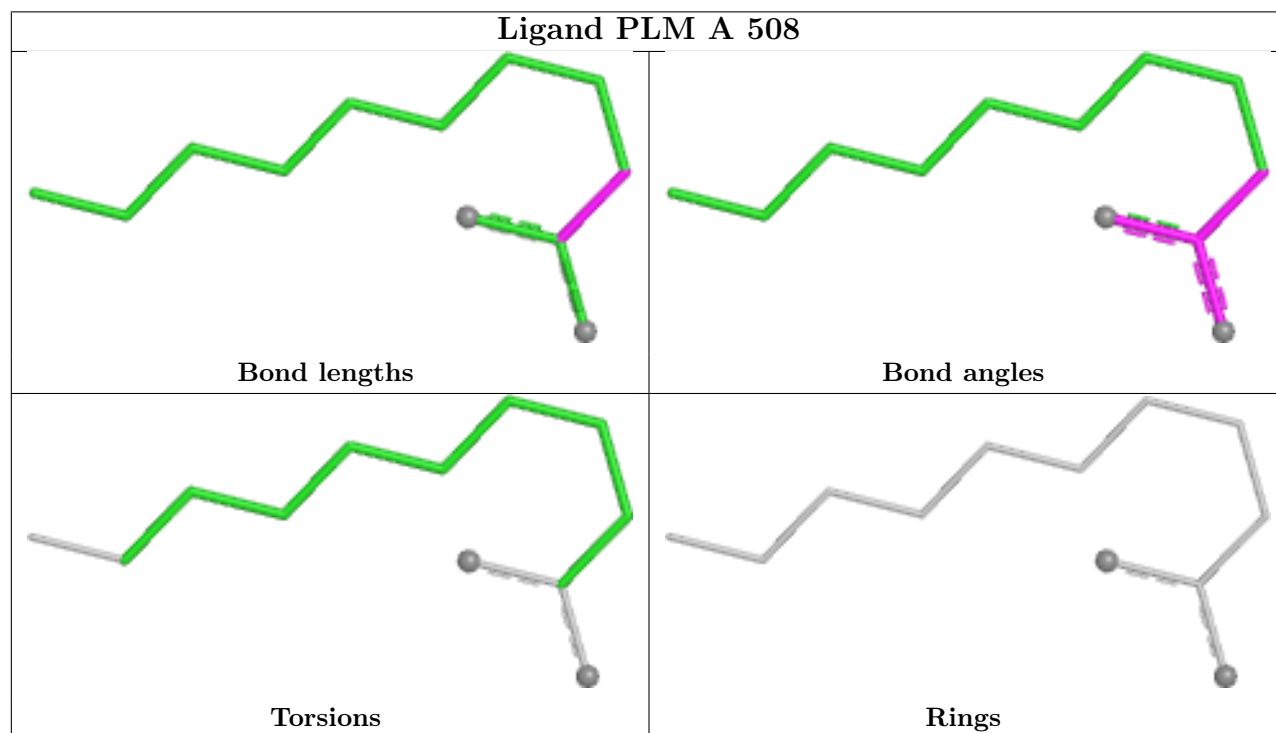
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	505	IVM	1	0
6	D	503	PX4	2	0
7	E	604	PLM	1	0
5	B	503	IVM	1	0
5	A	504	IVM	3	0
5	A	503	IVM	2	0

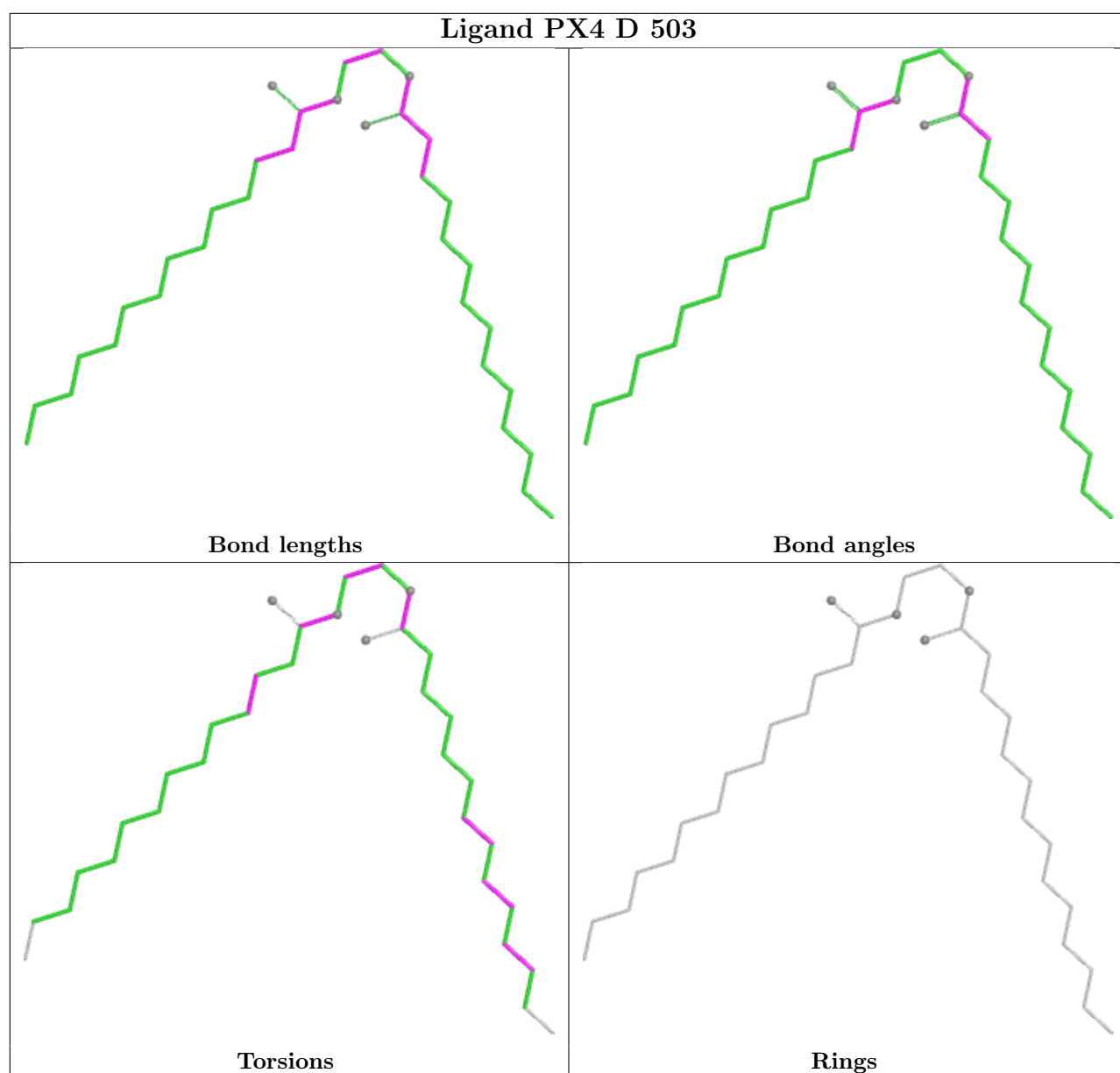
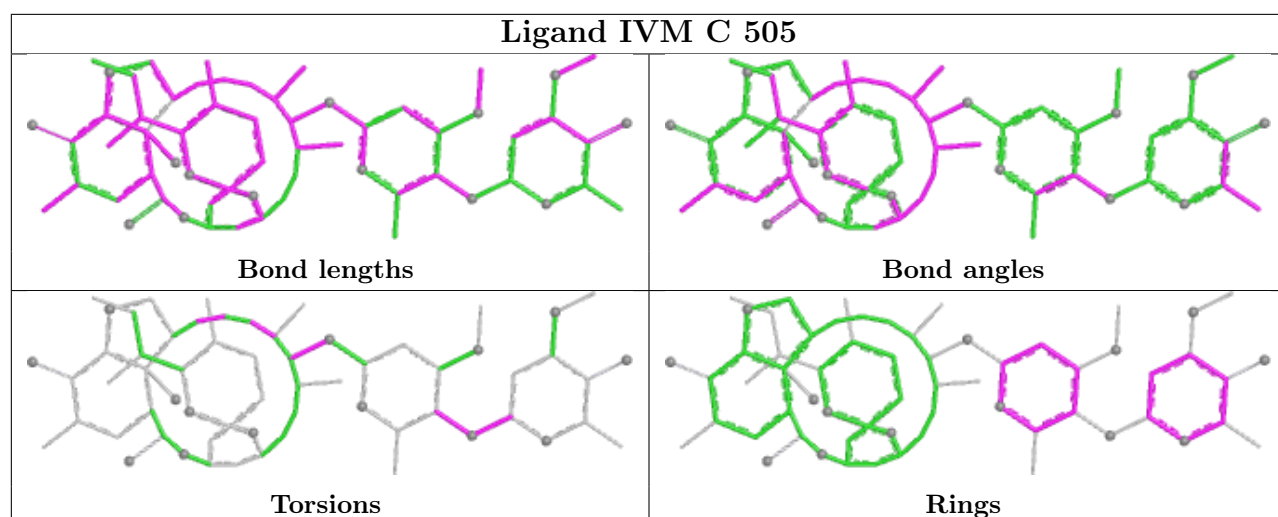
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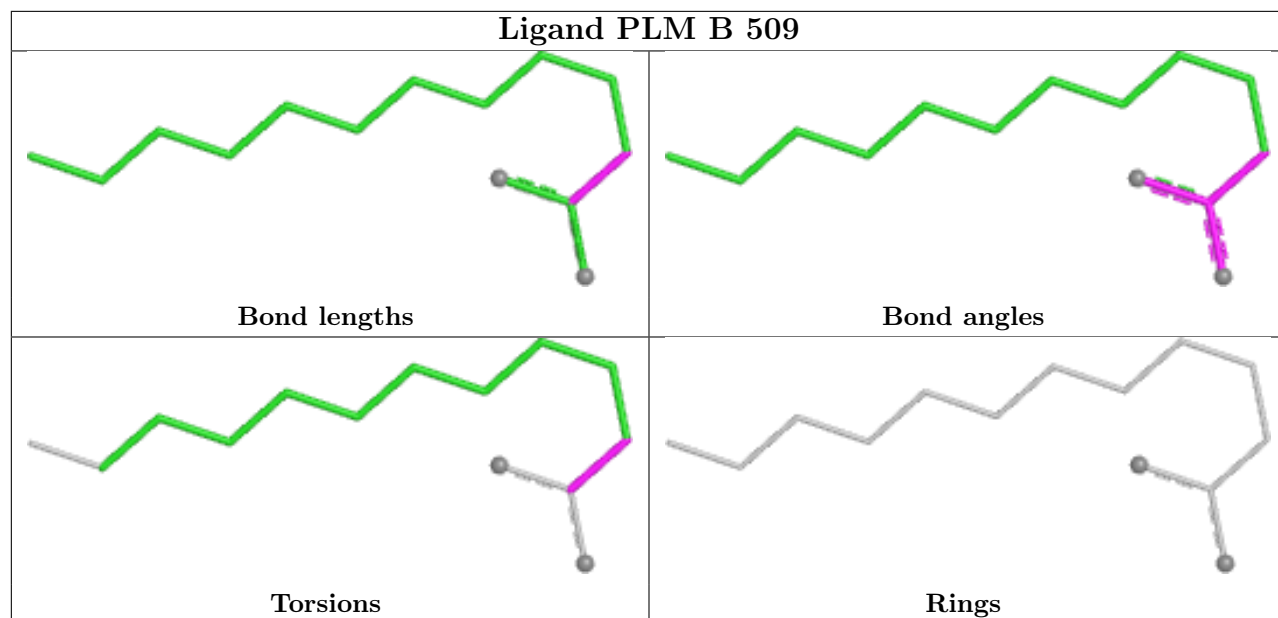
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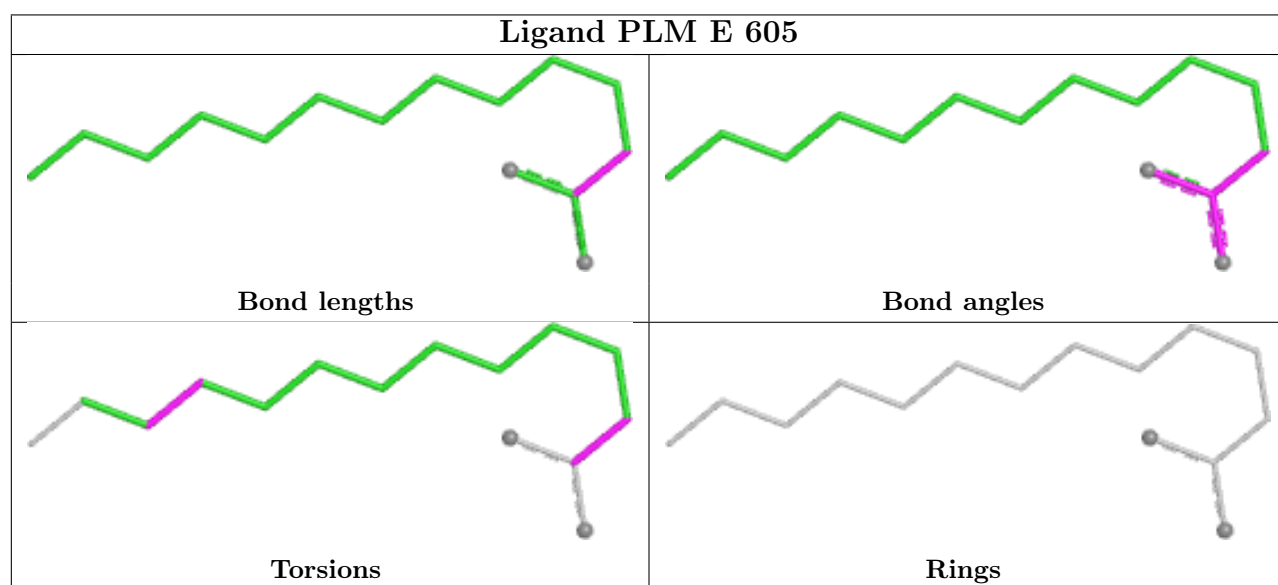
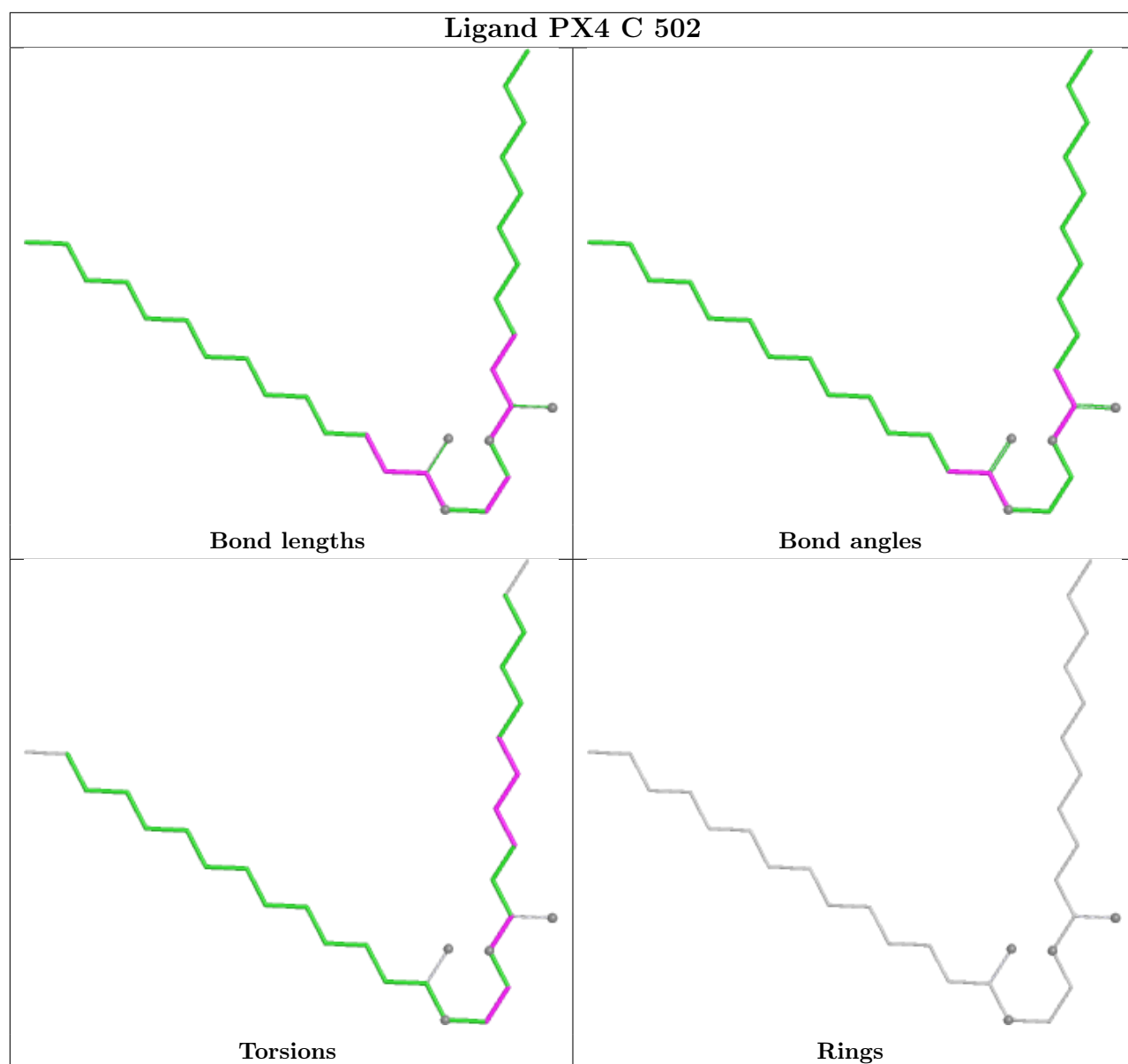
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	505	PLM	1	0
6	B	504	PX4	2	0
7	C	513	PLM	1	0

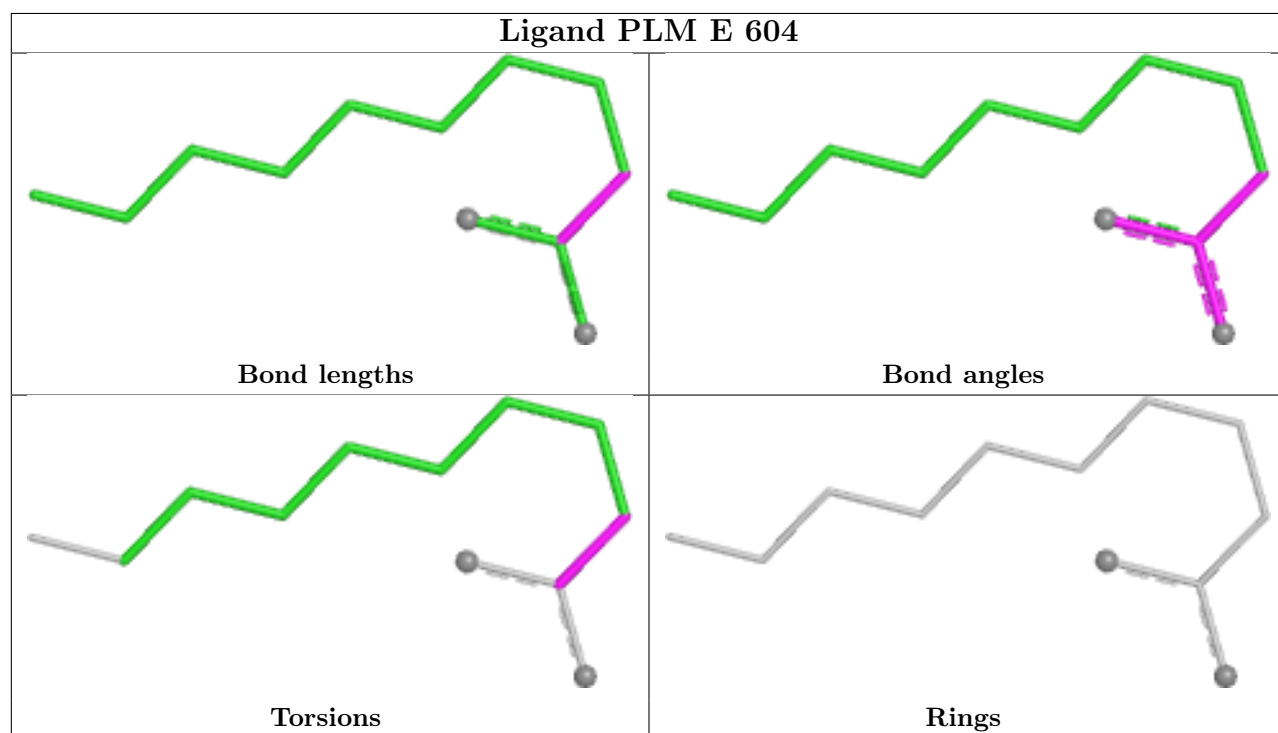
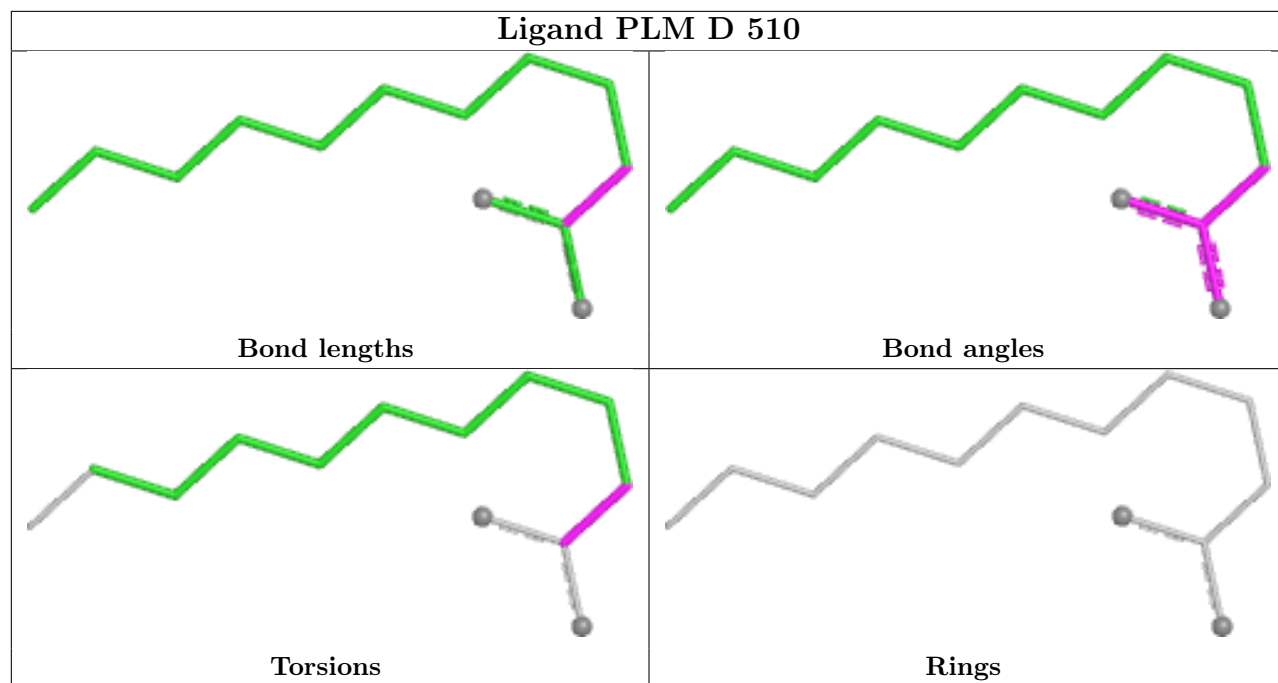
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

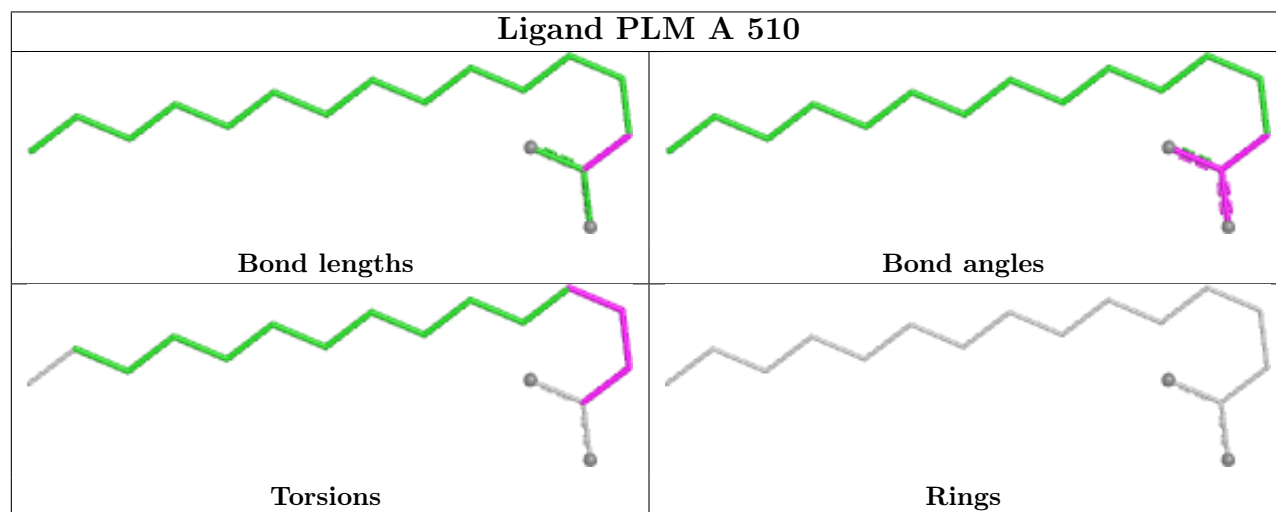
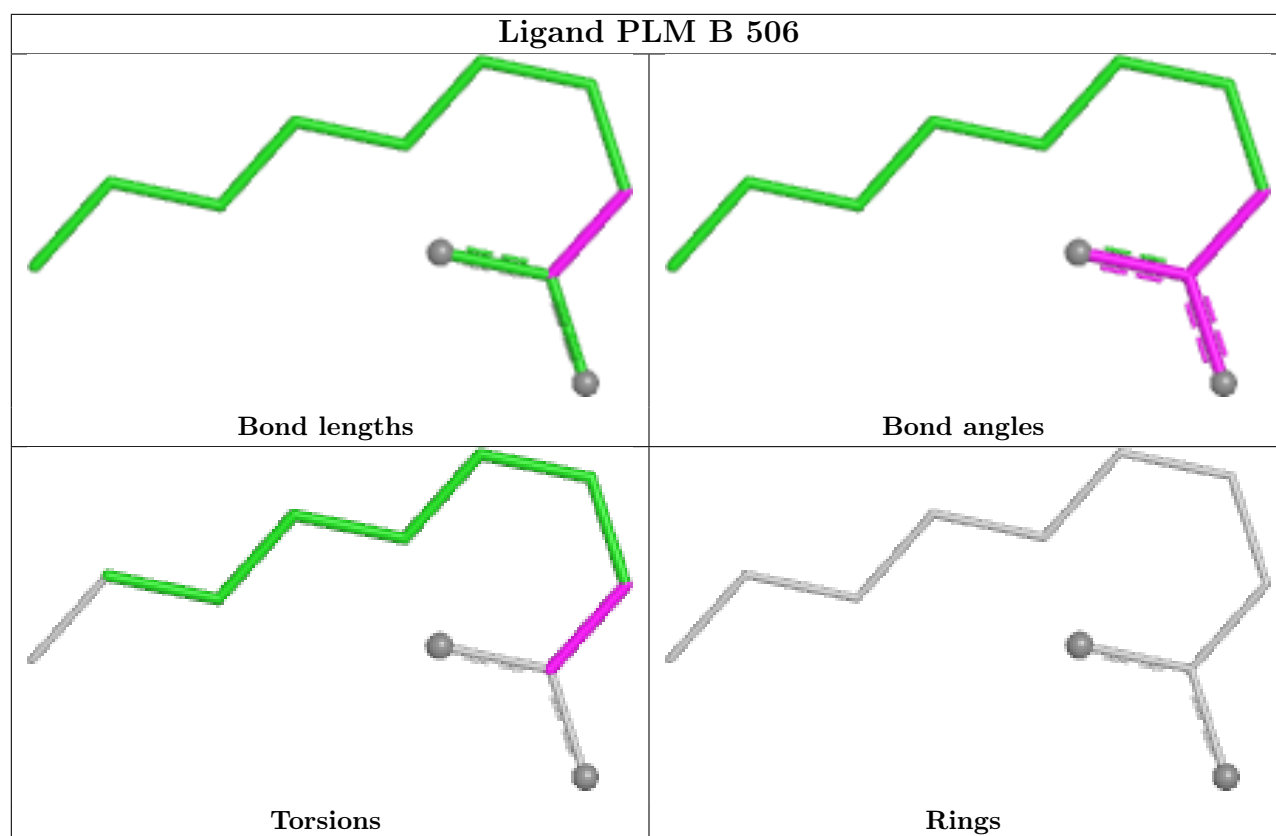


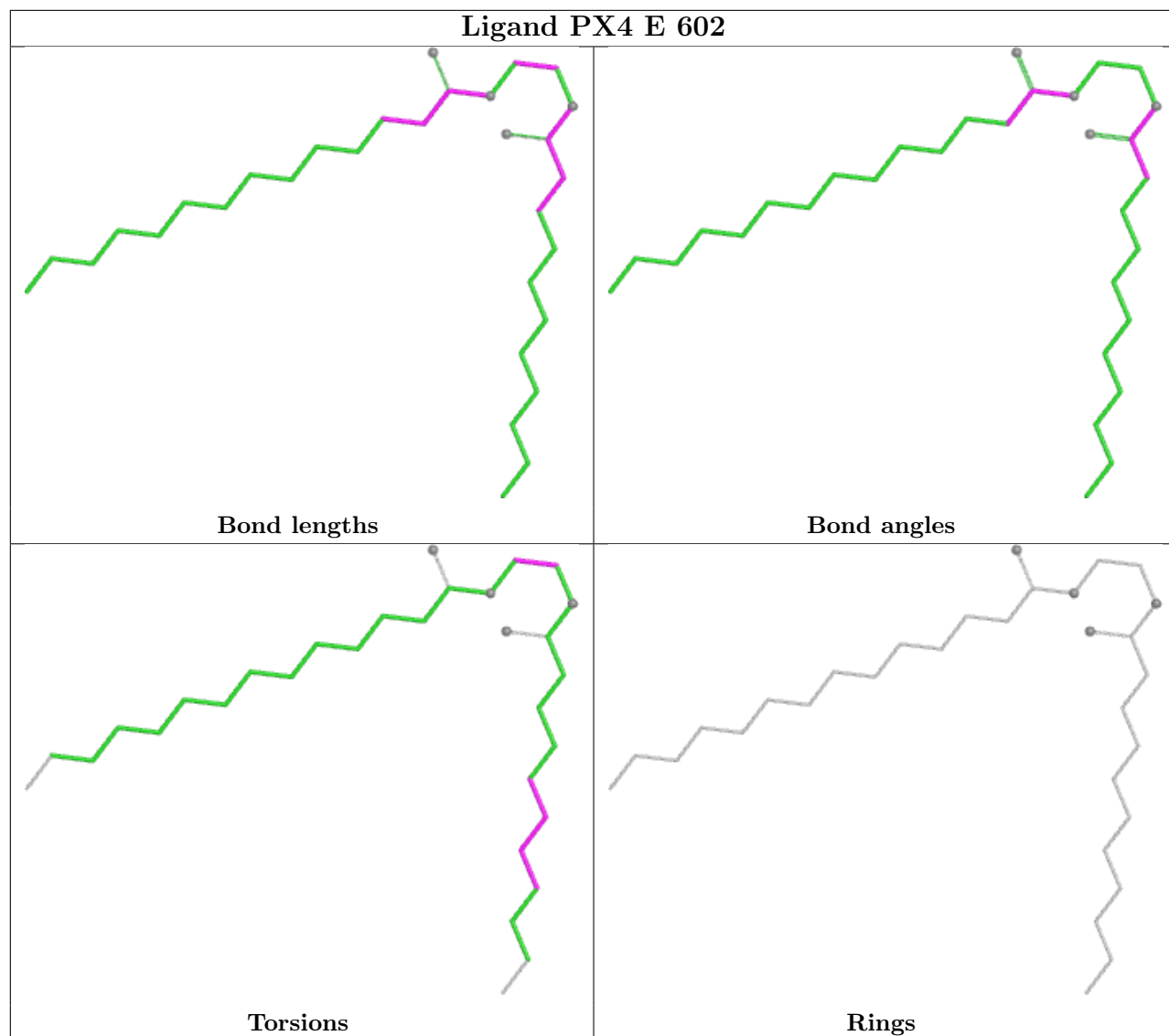


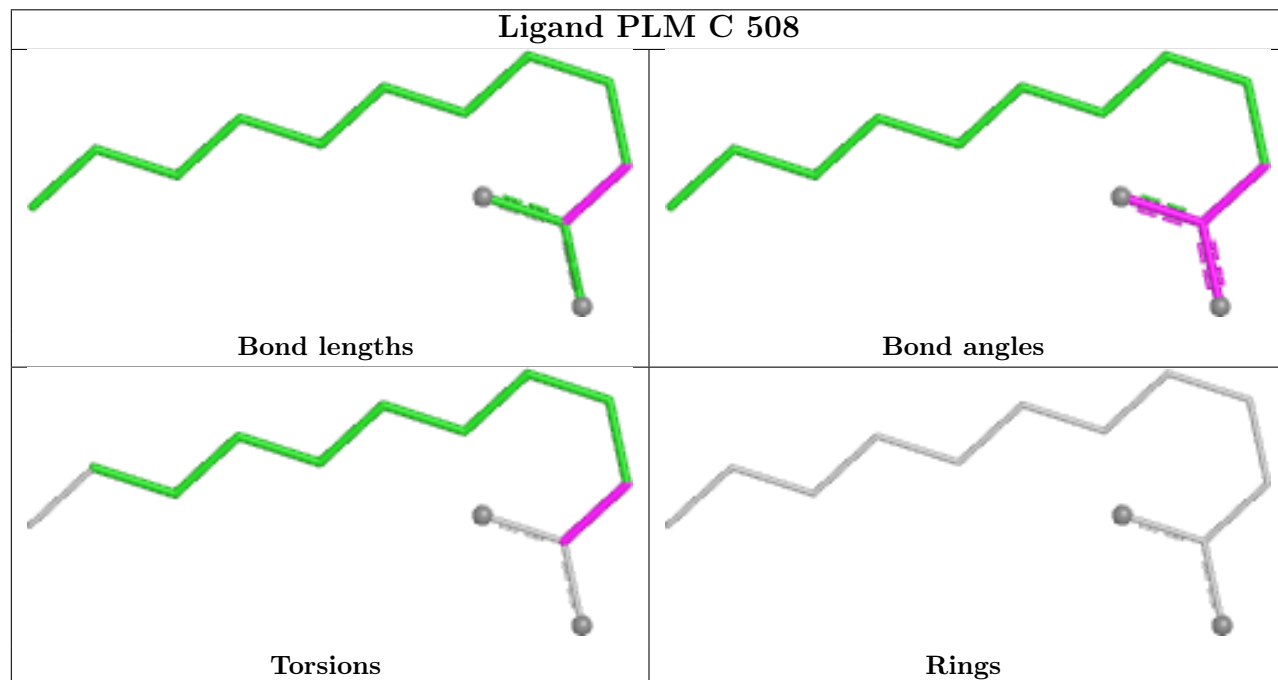
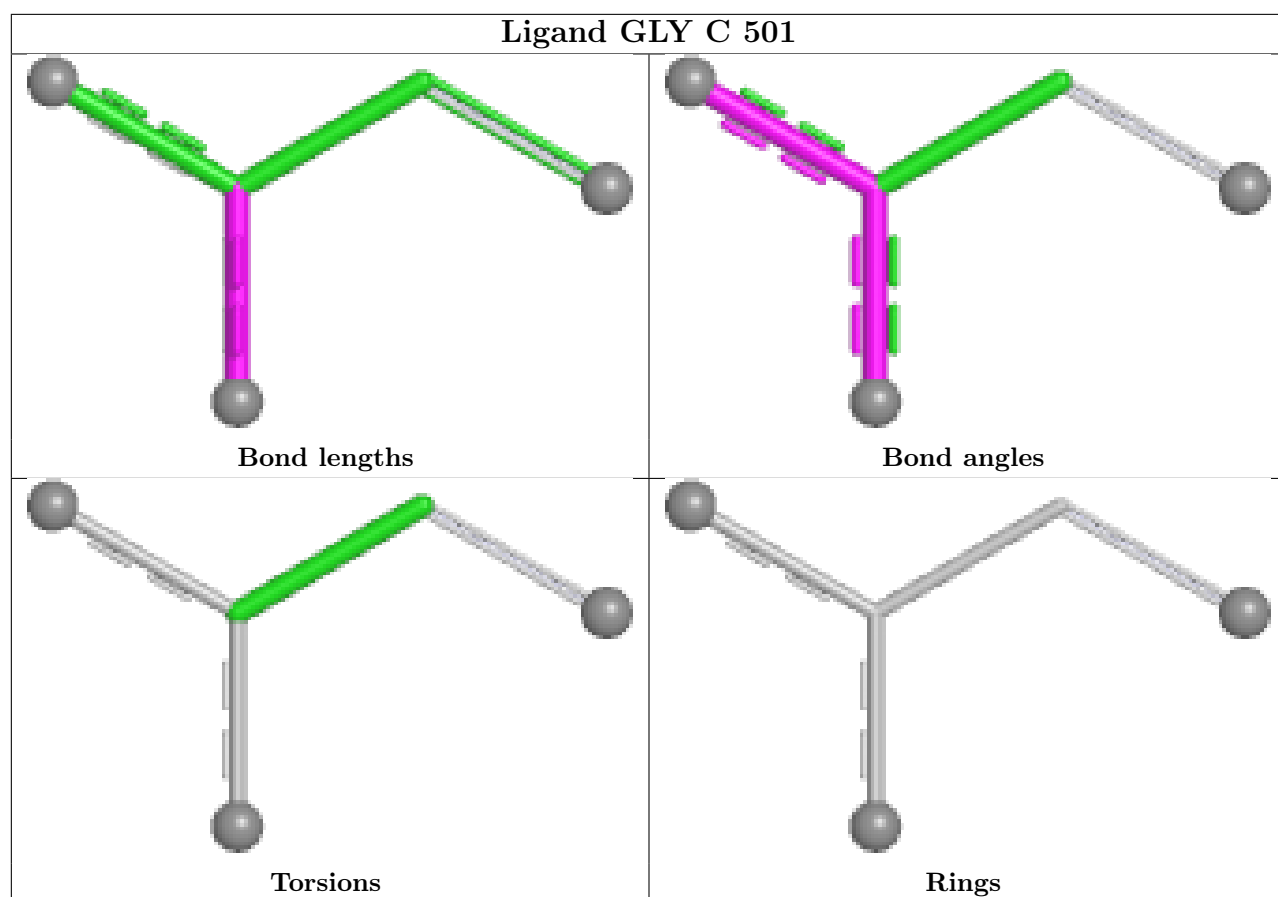


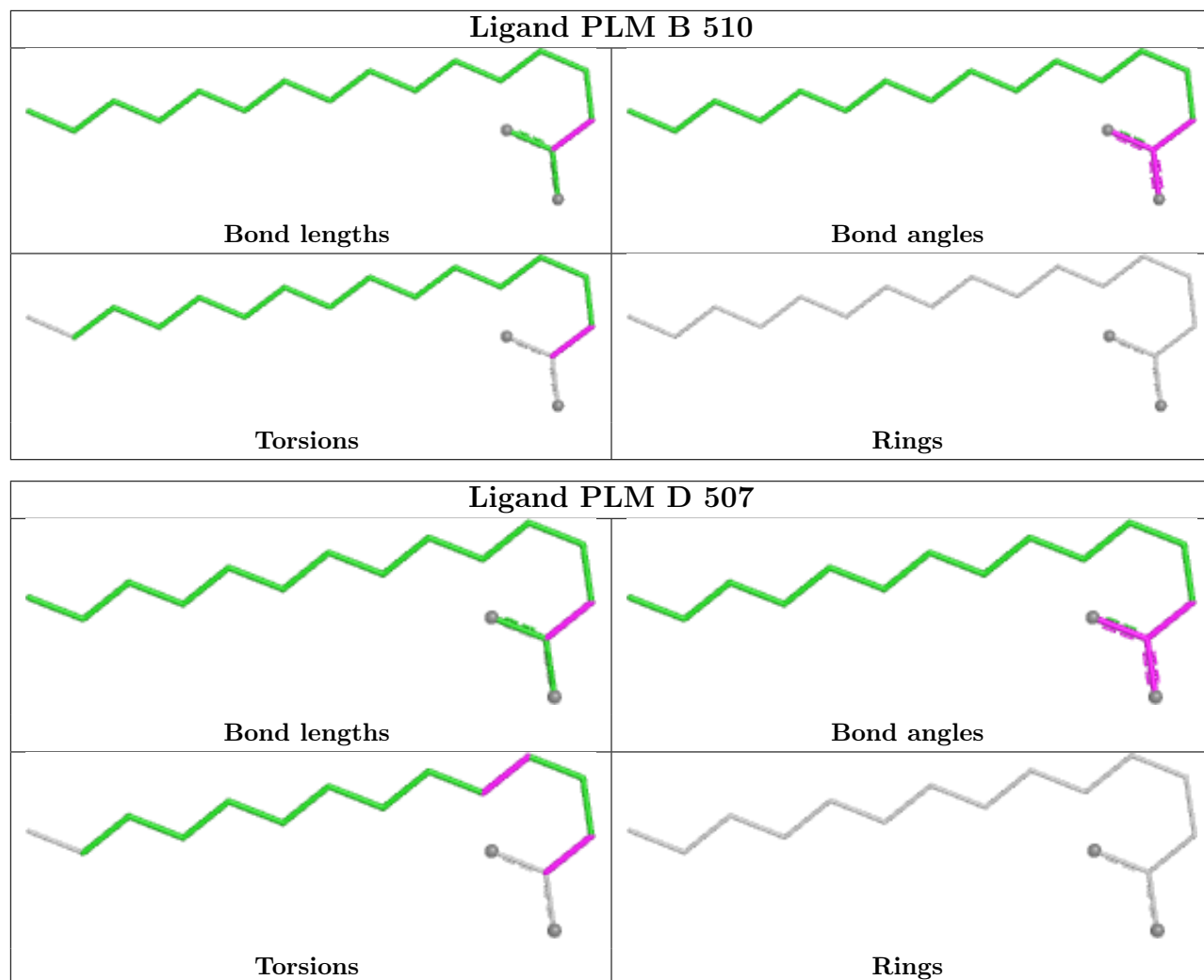


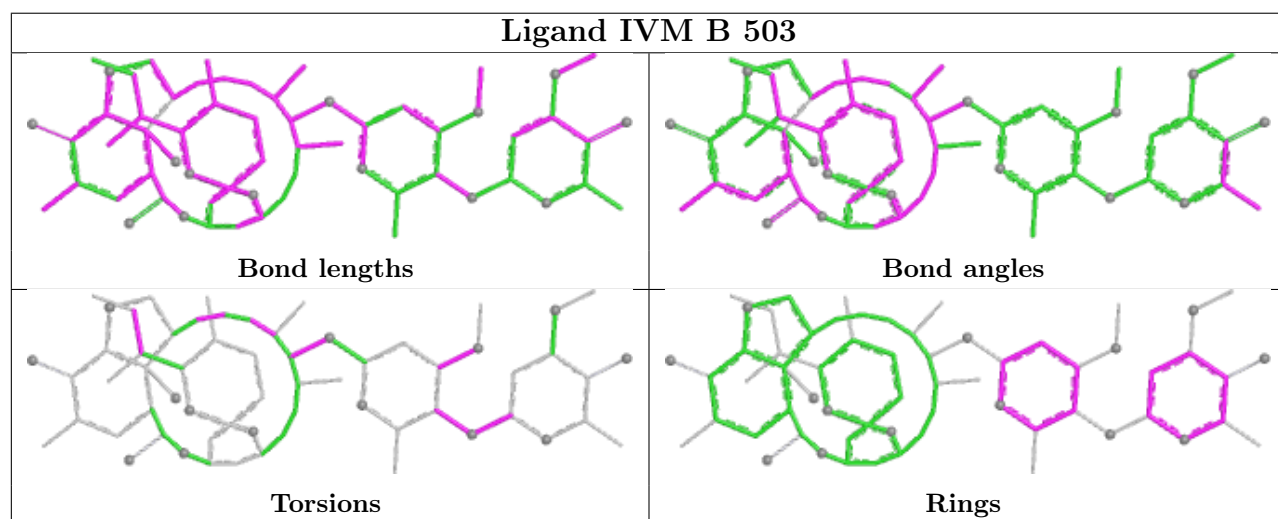
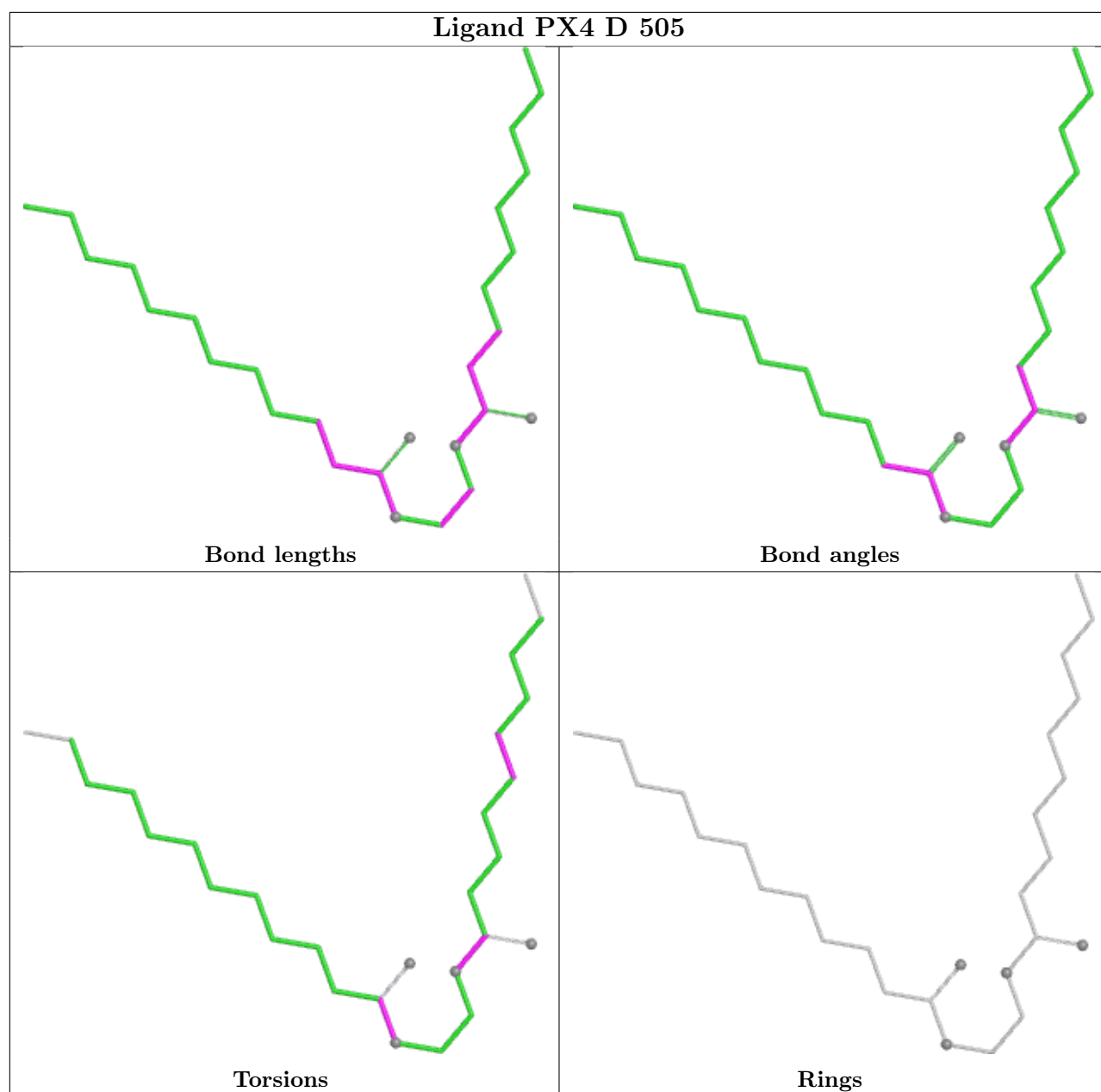


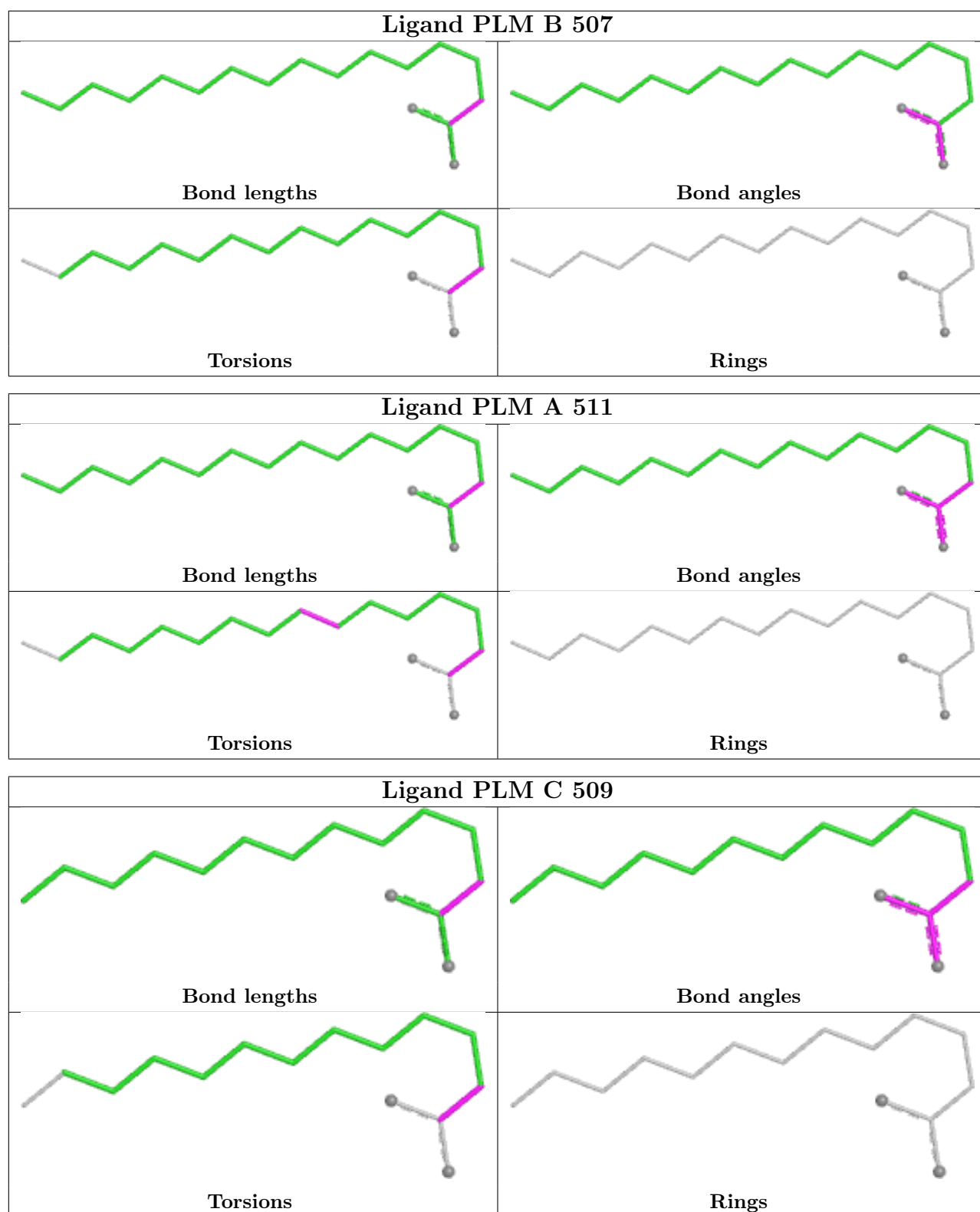


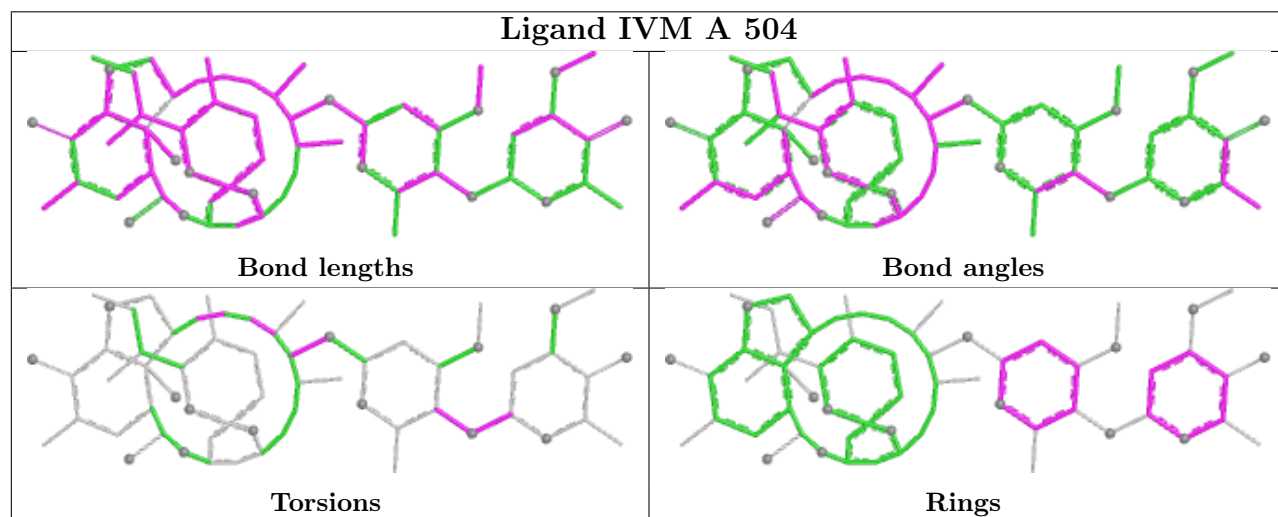
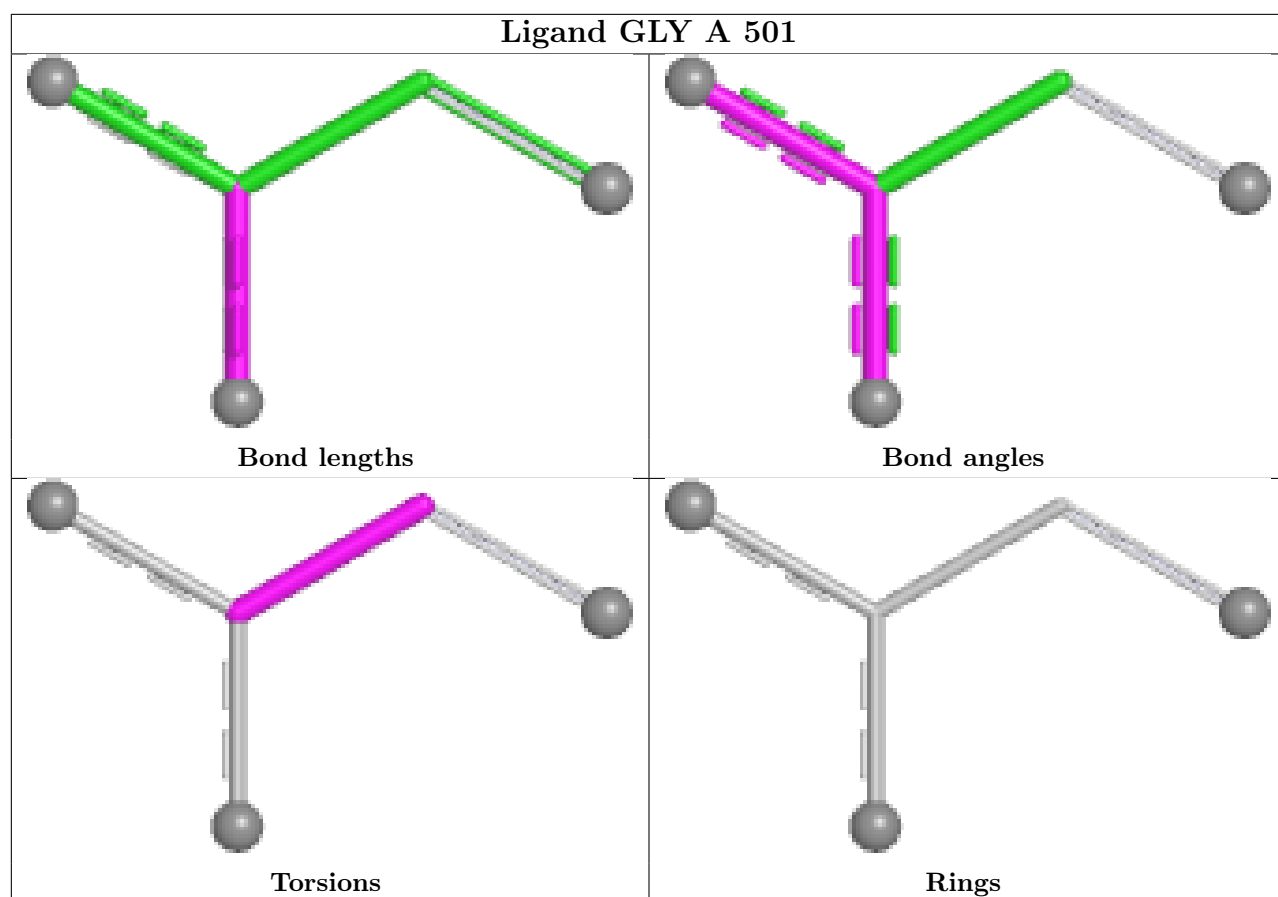


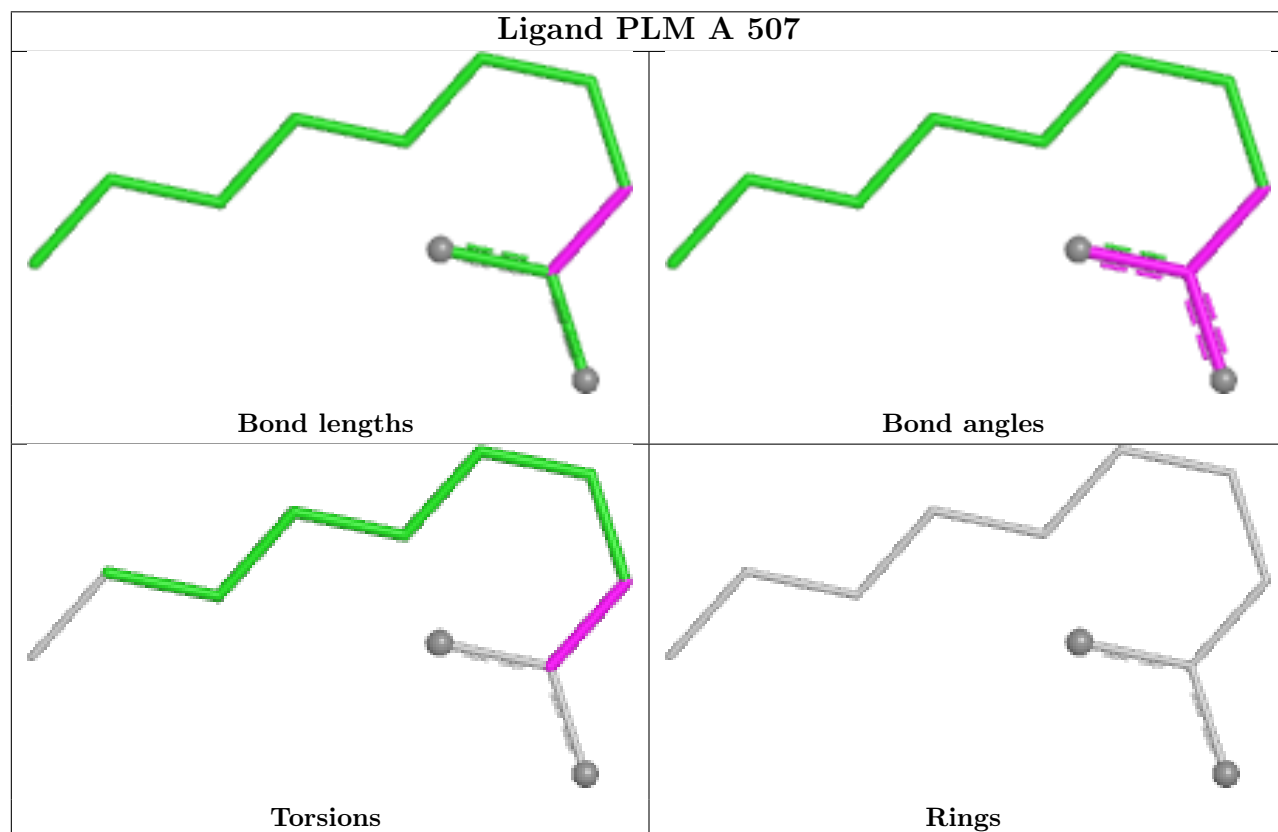
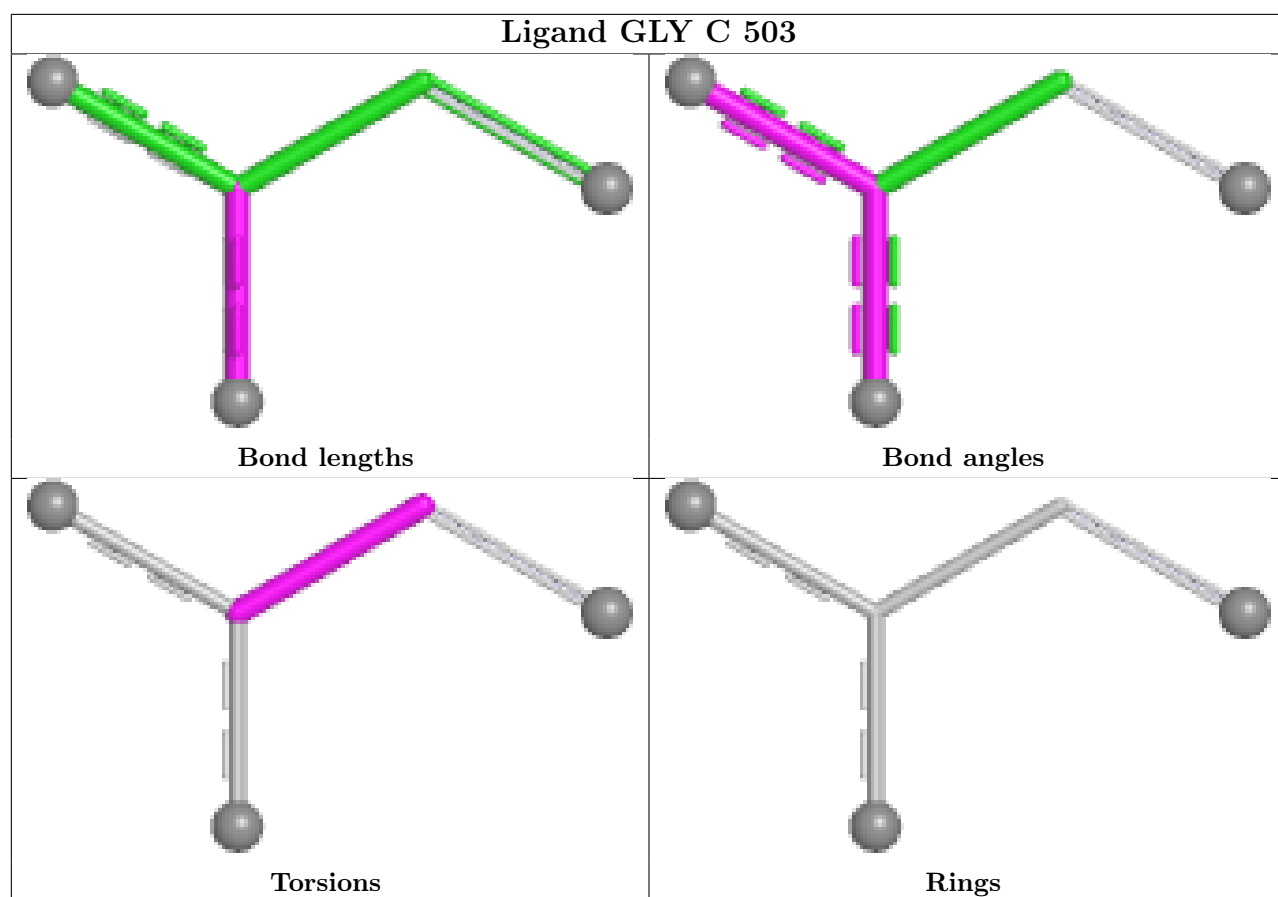


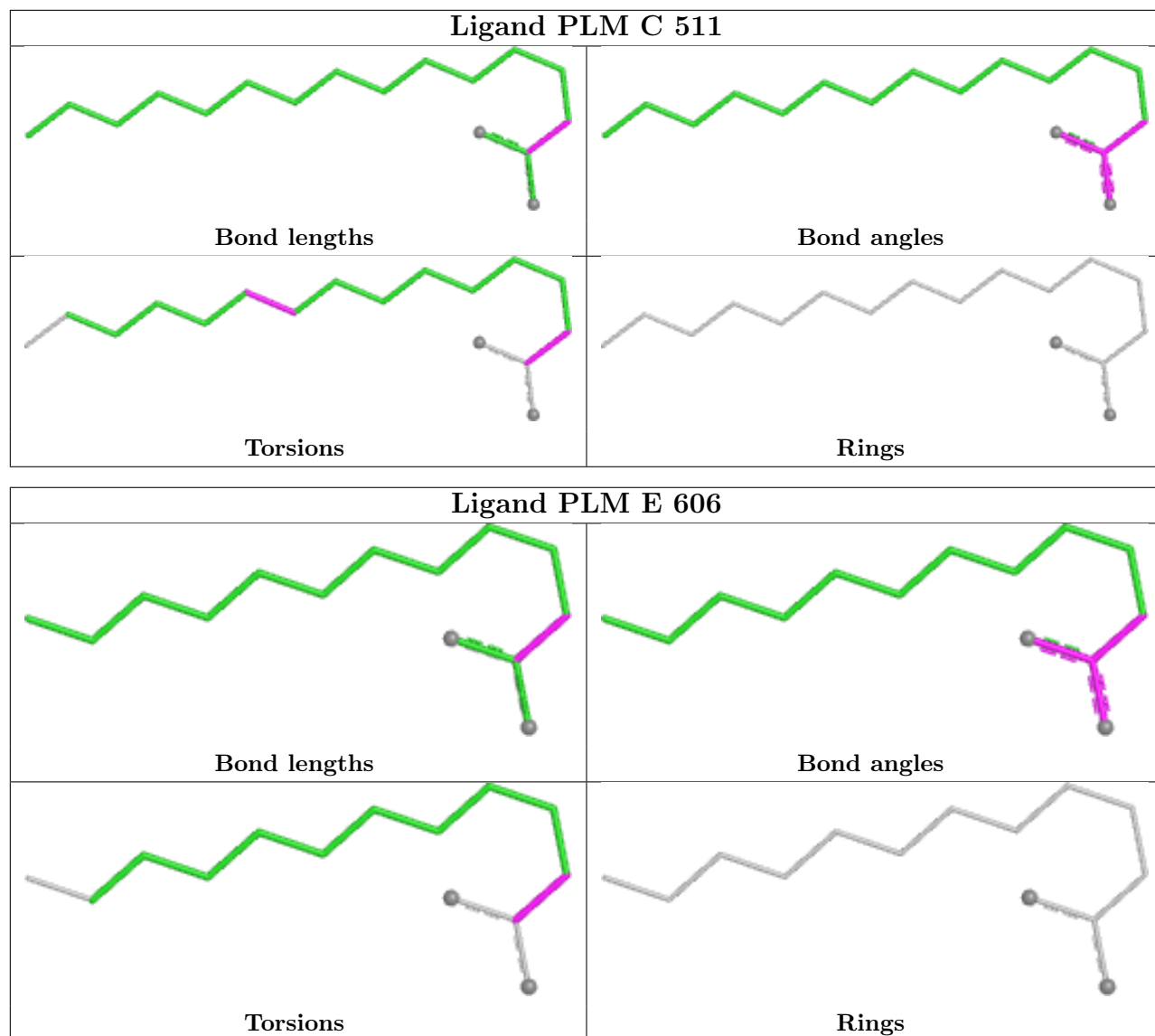


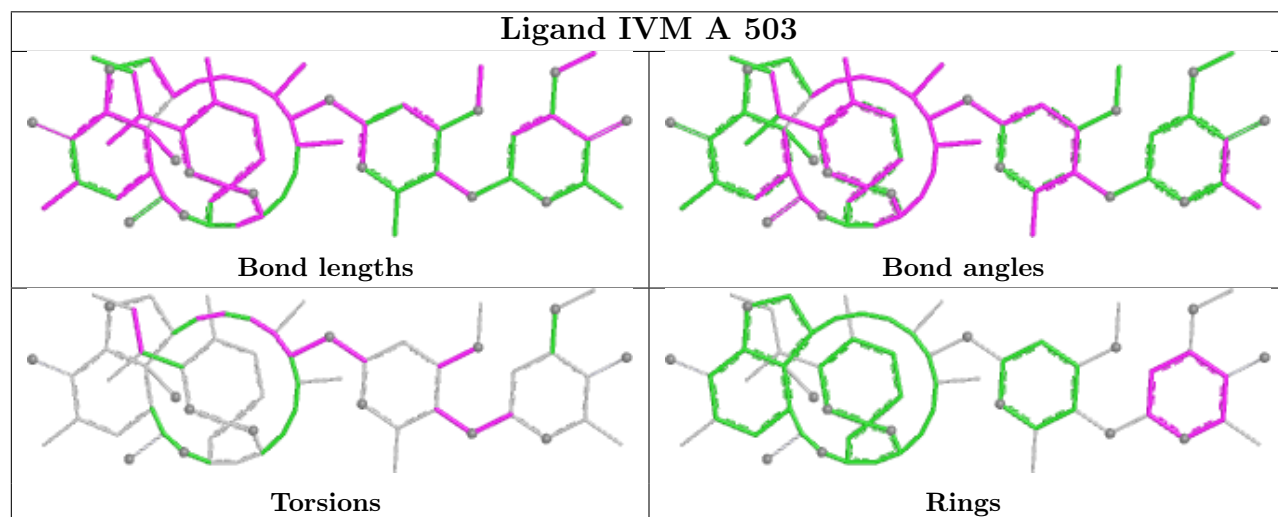
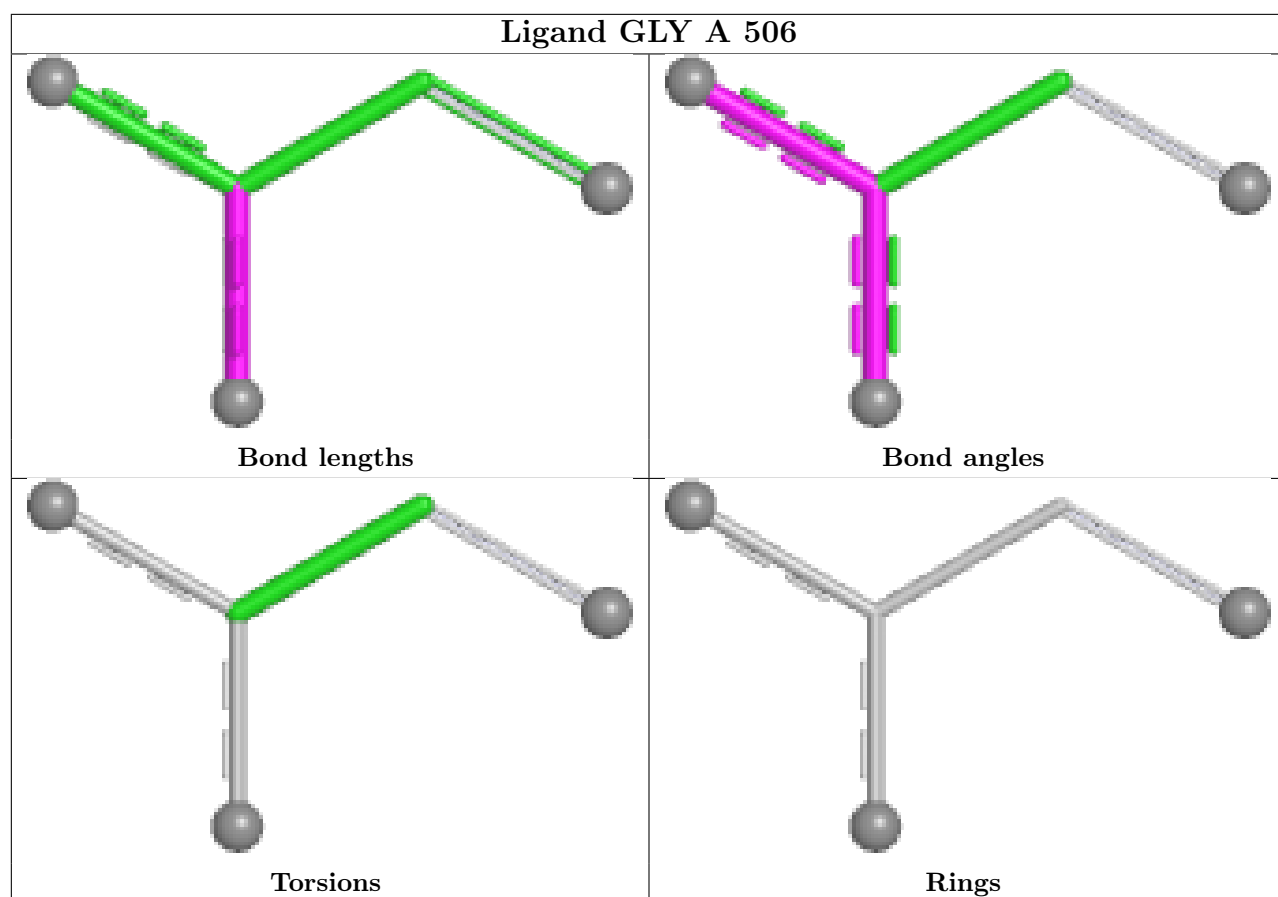


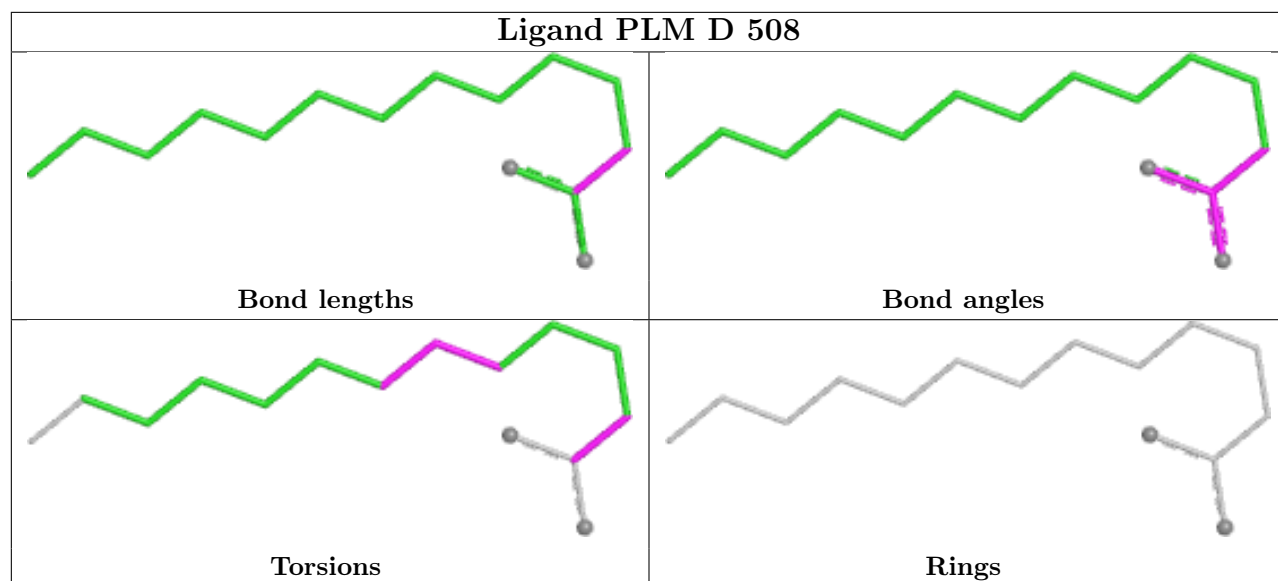
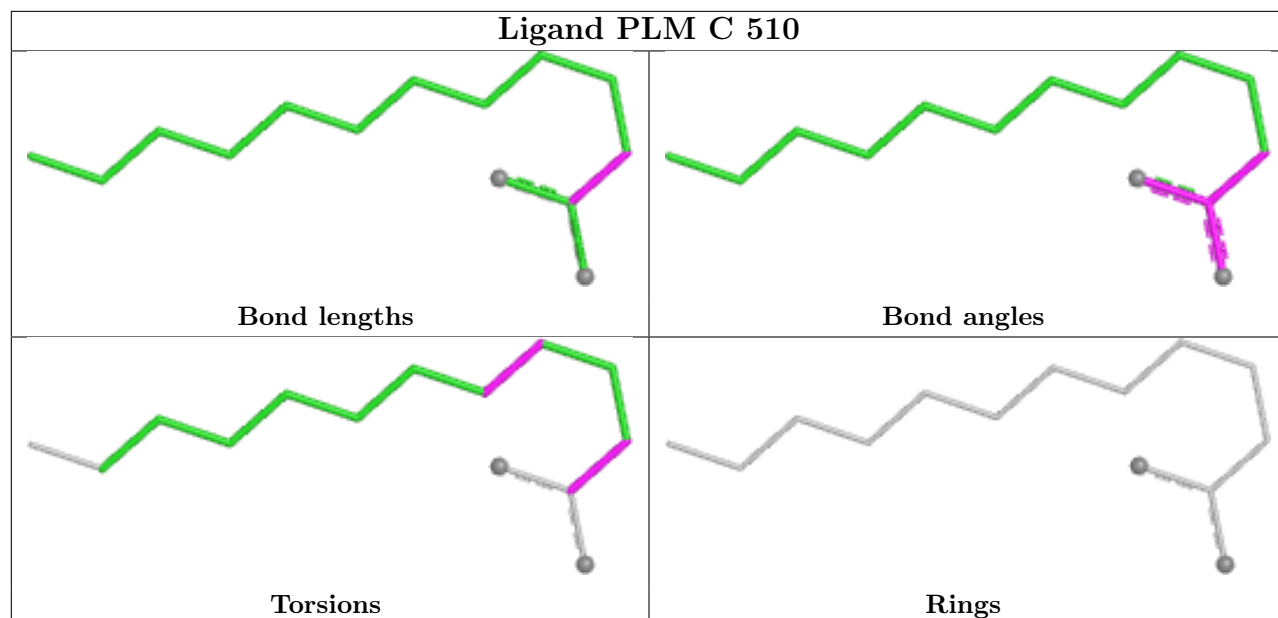


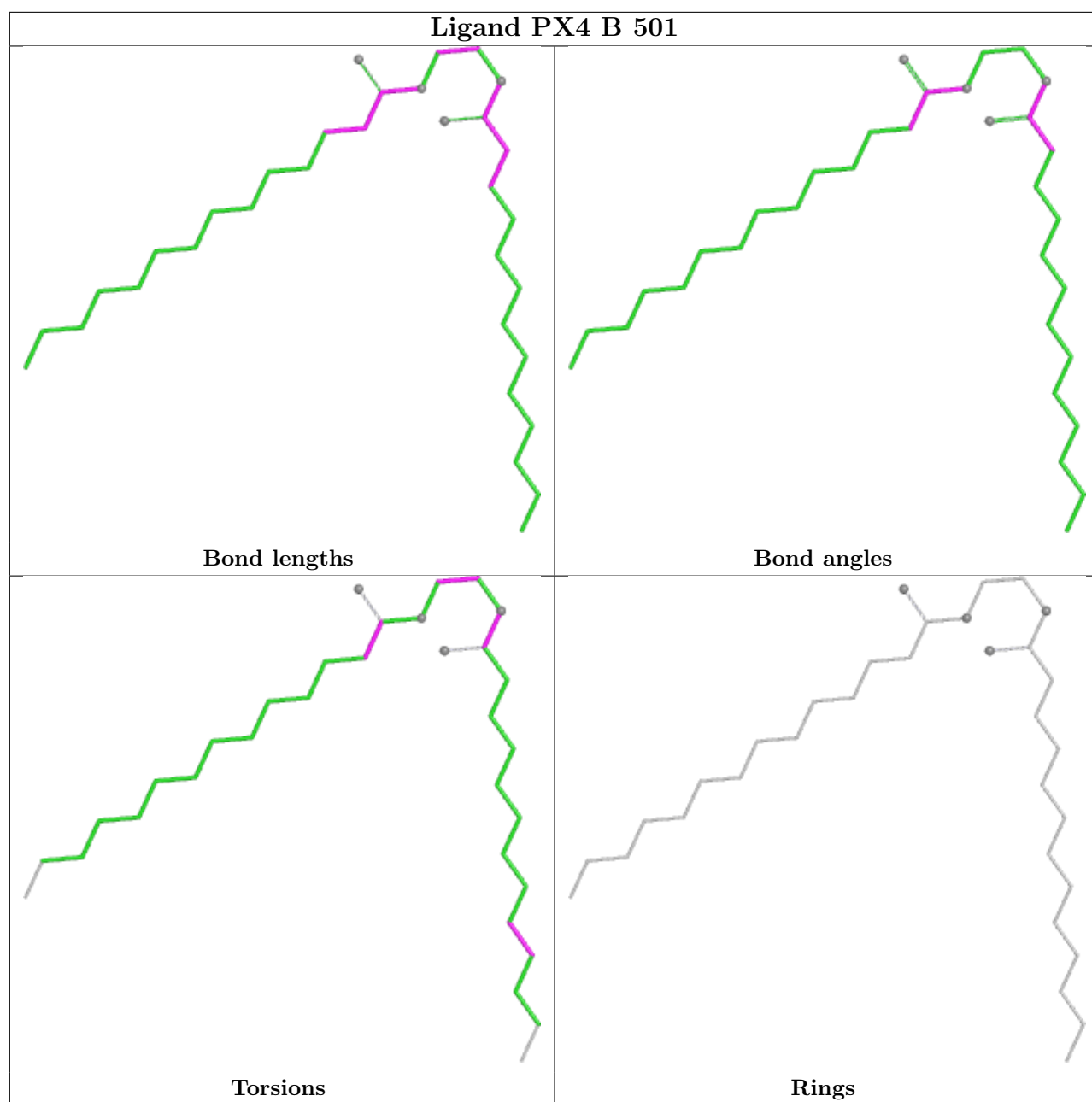


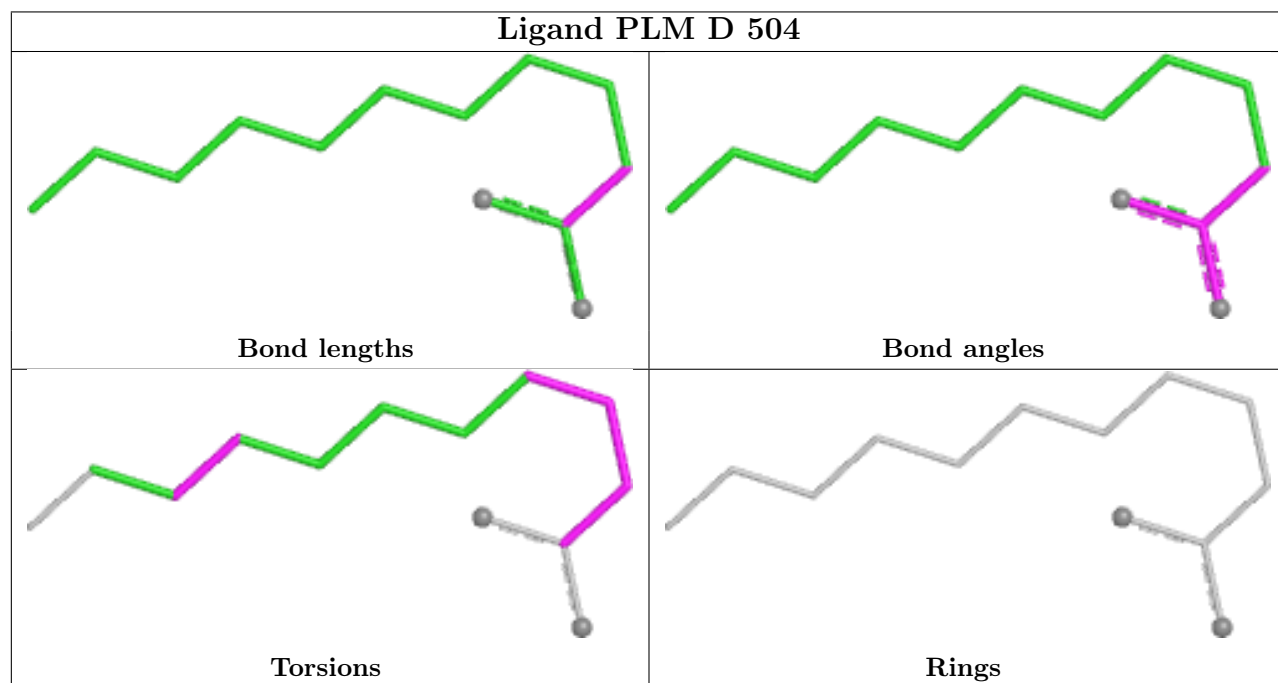
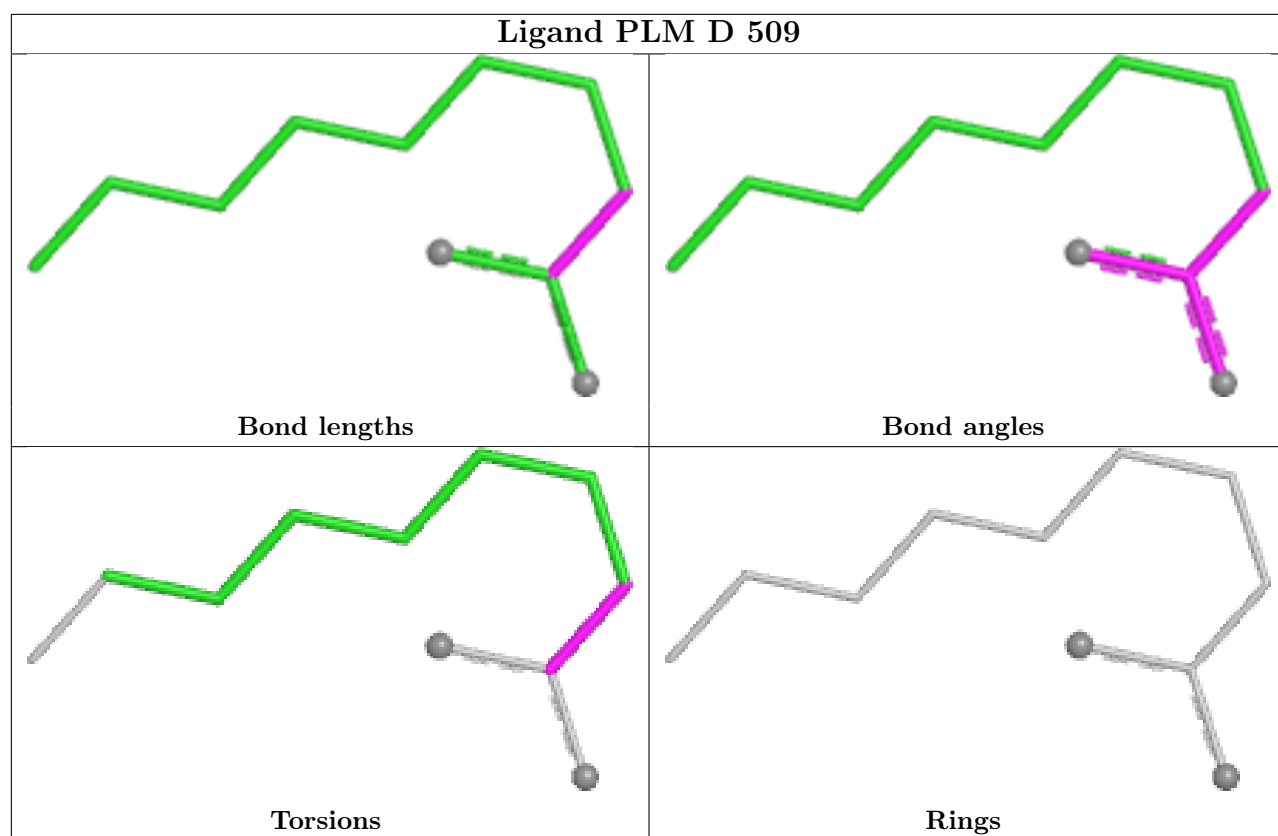


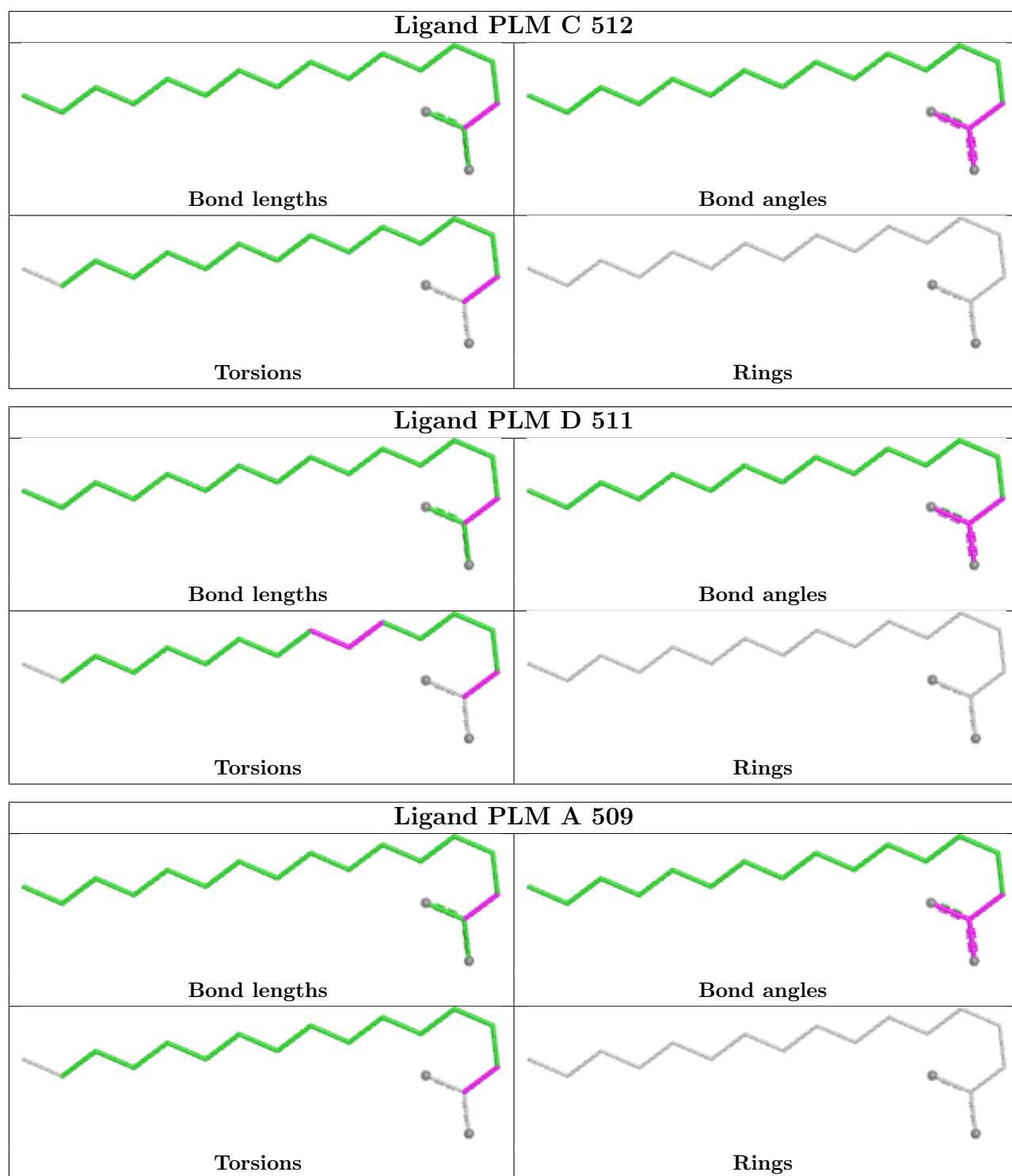


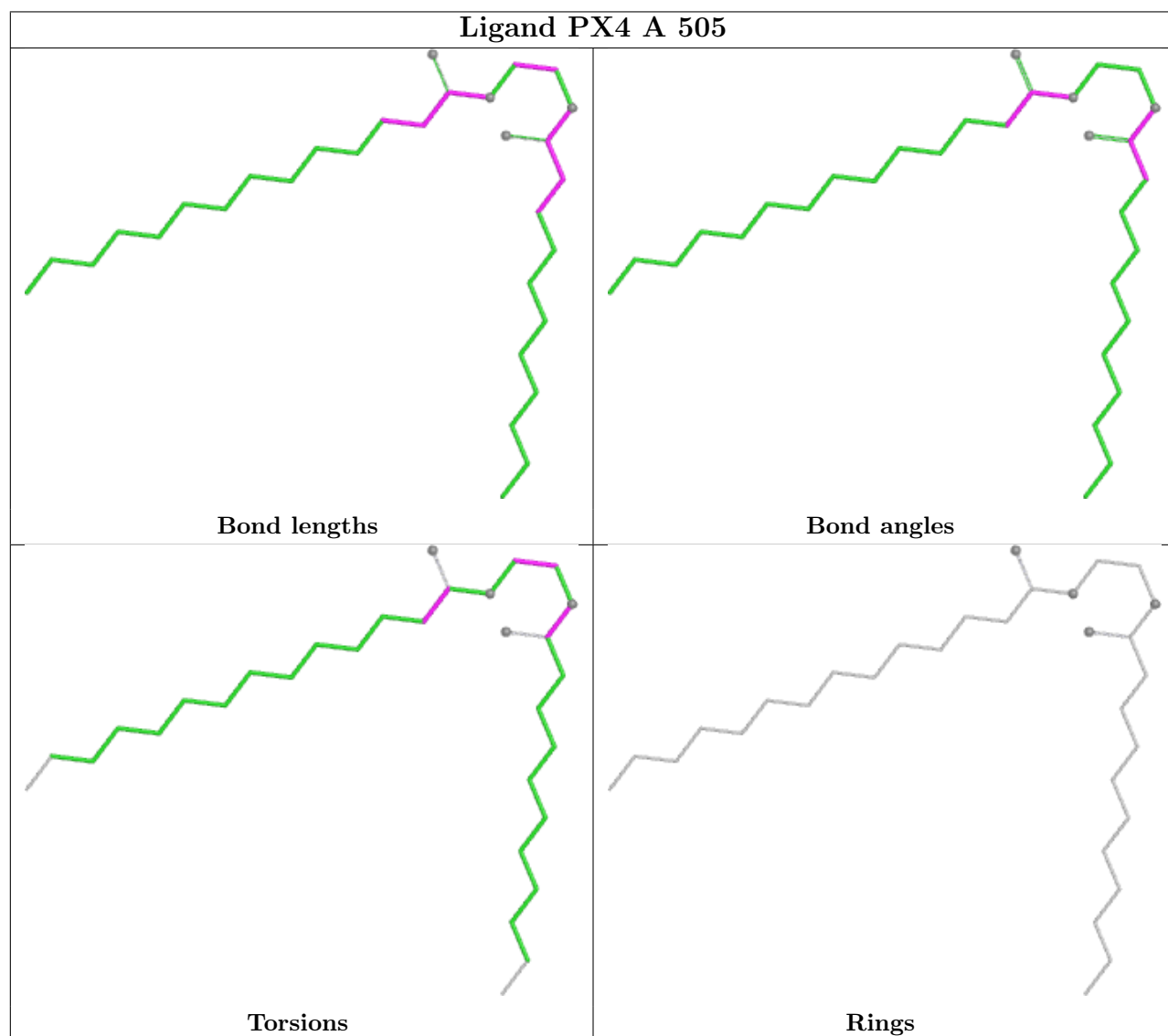
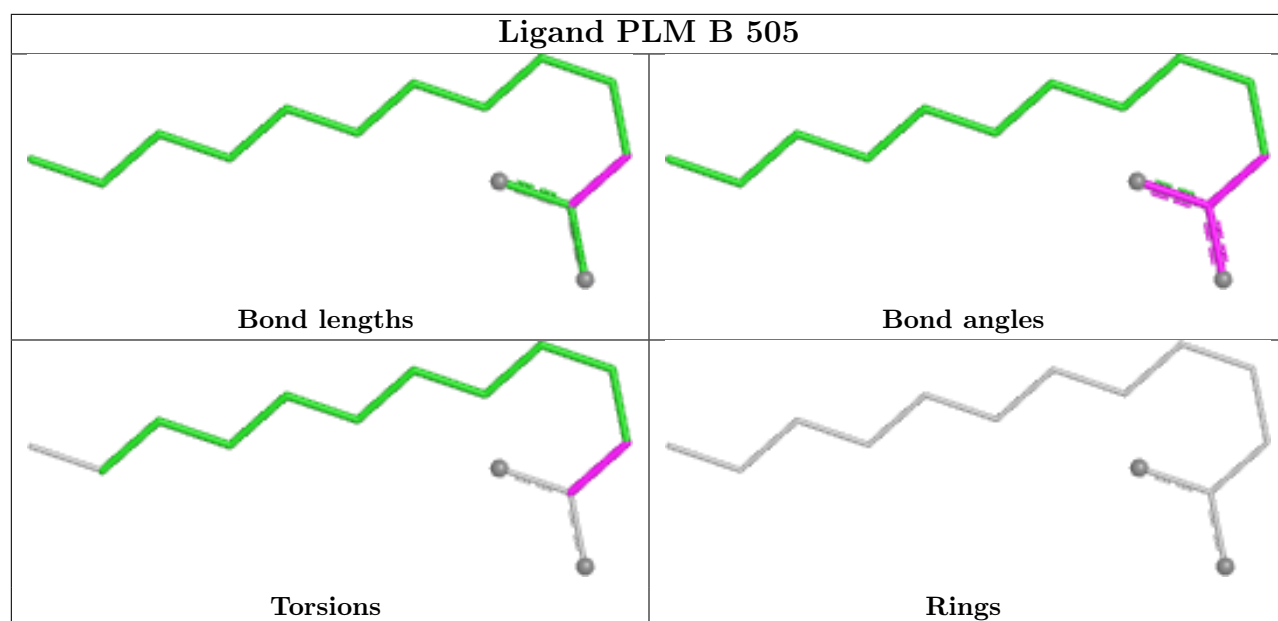


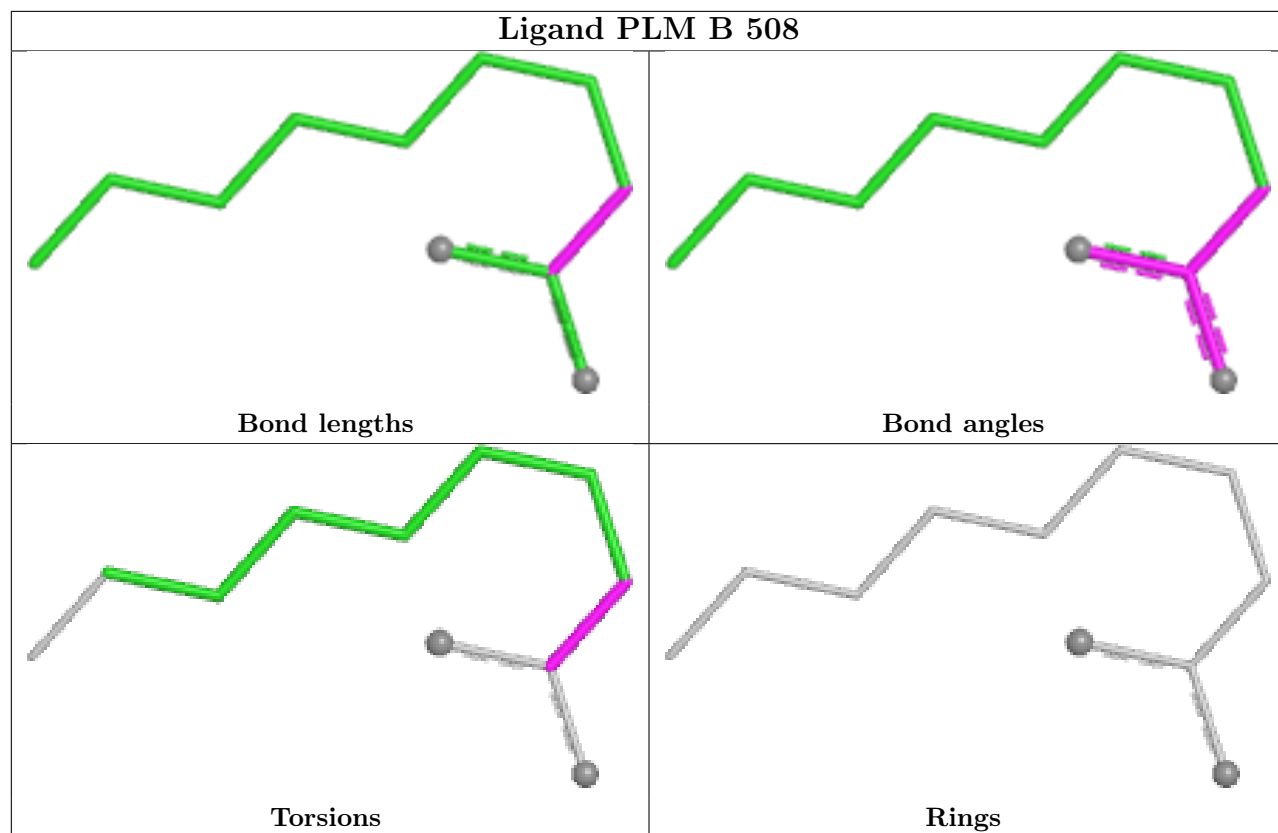


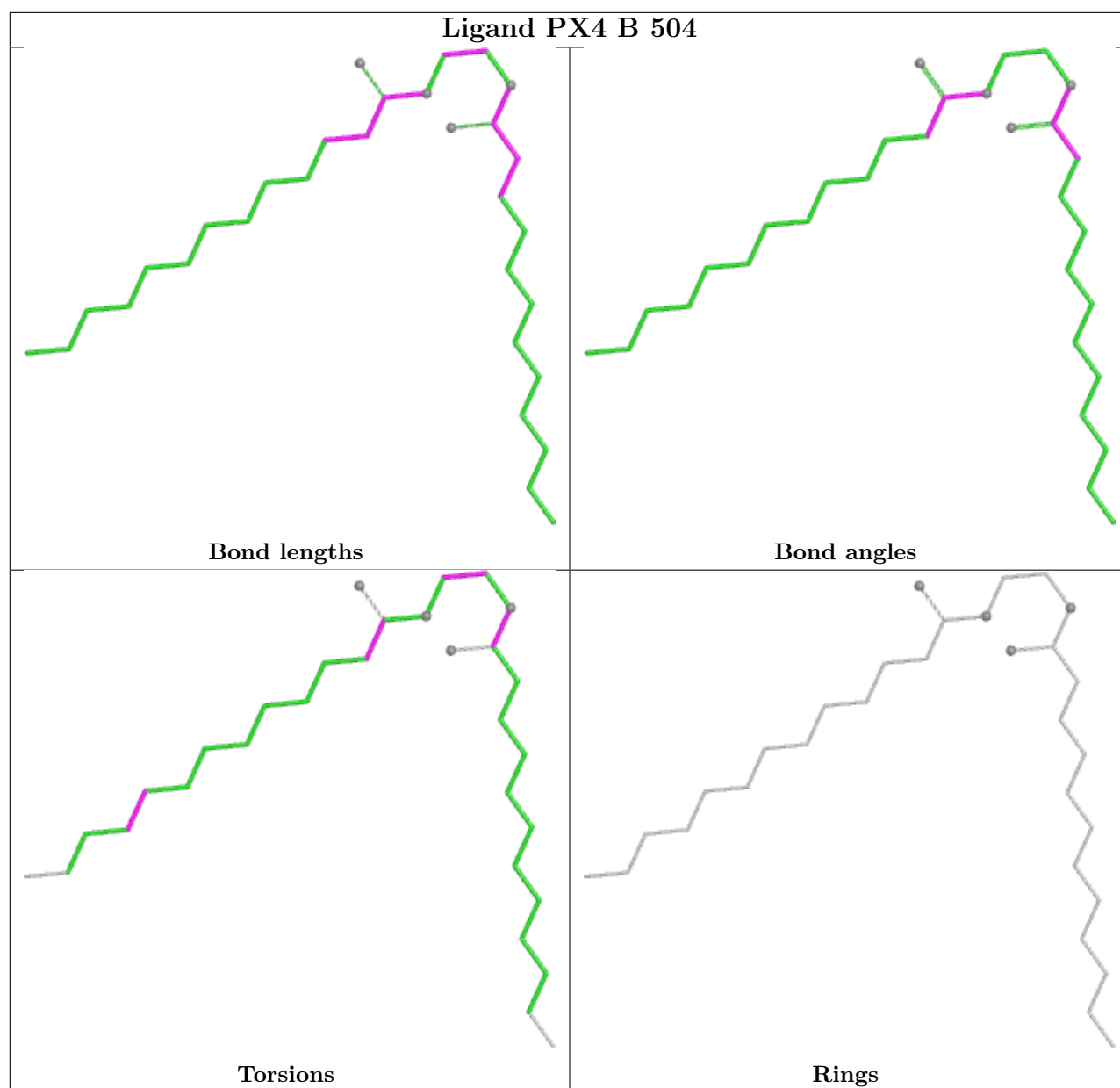


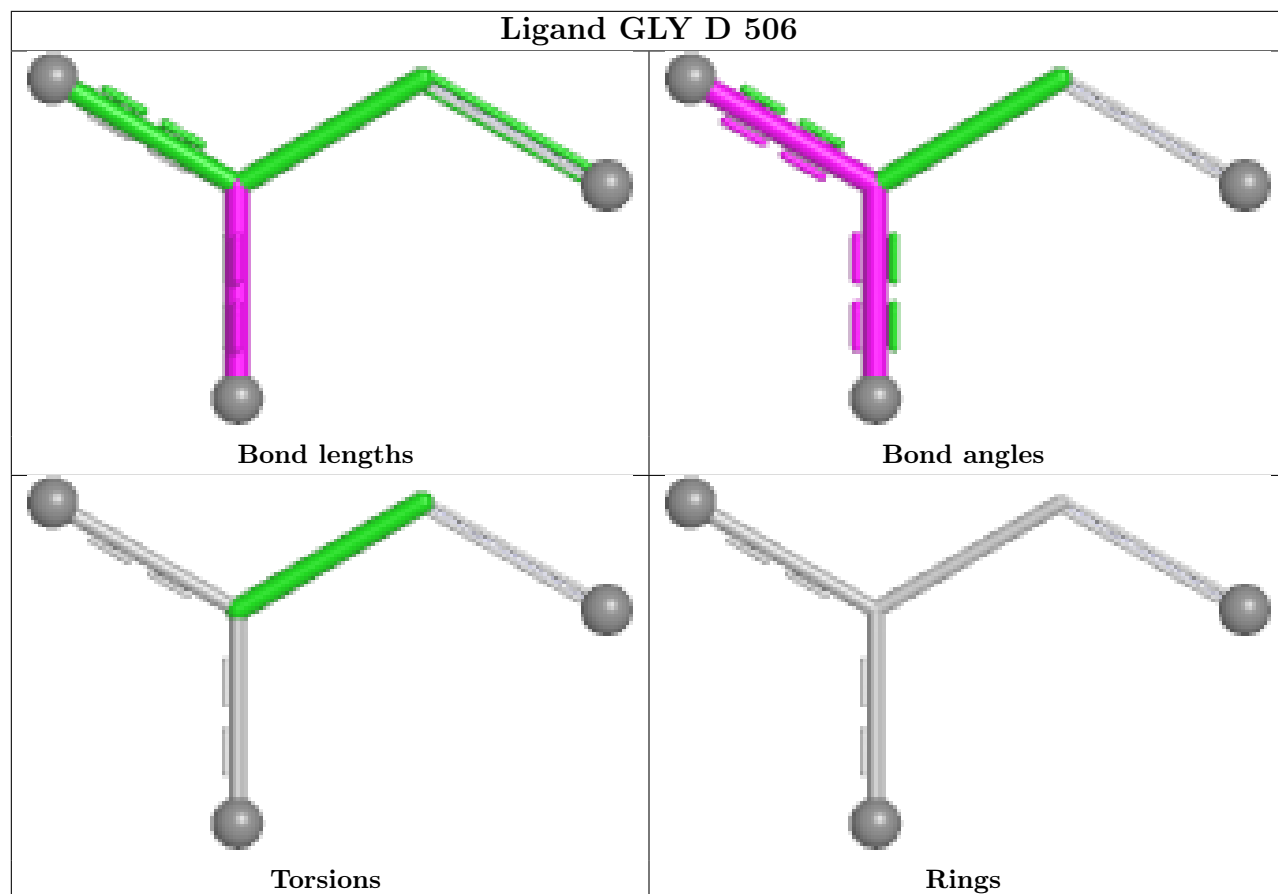


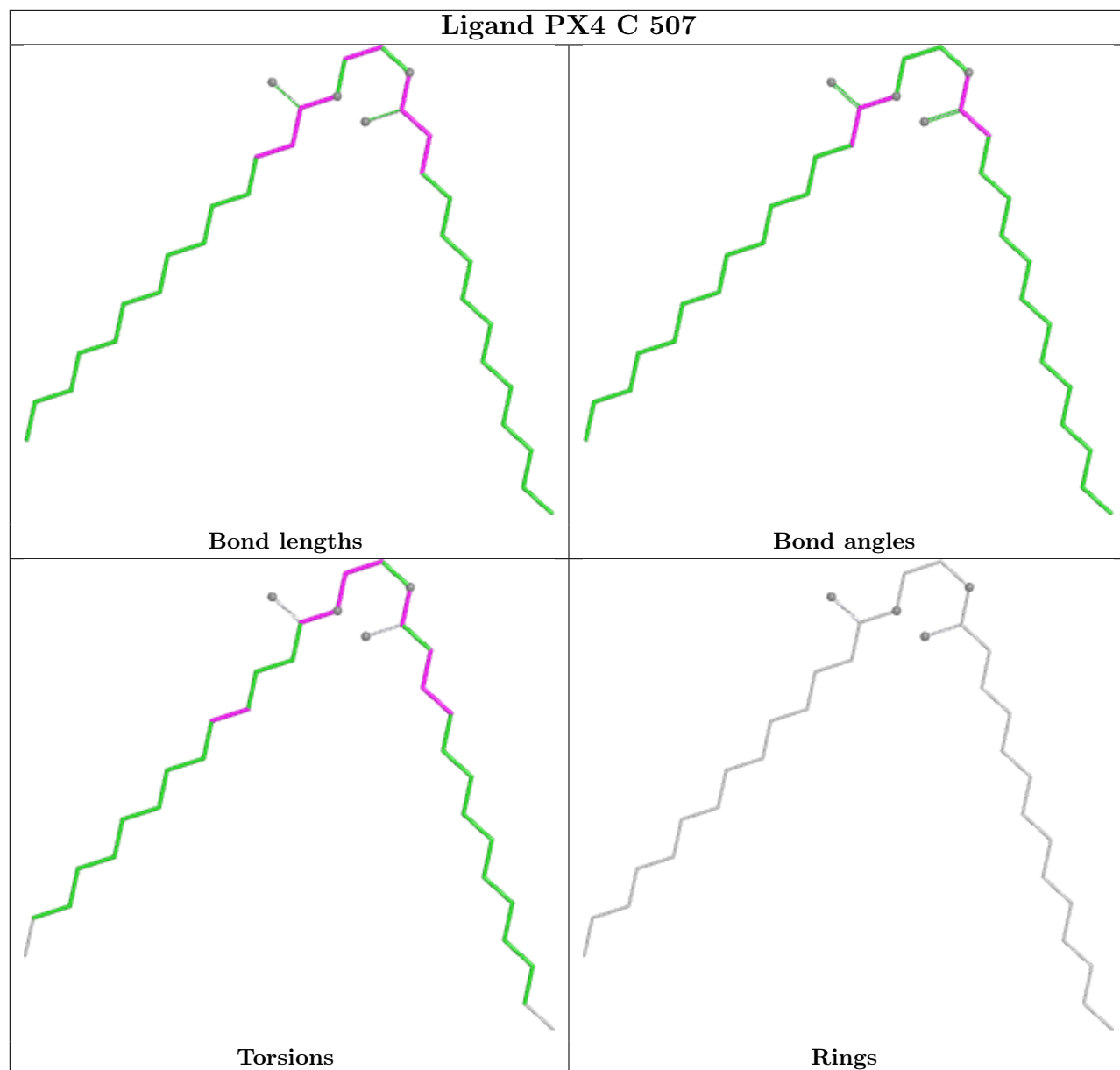


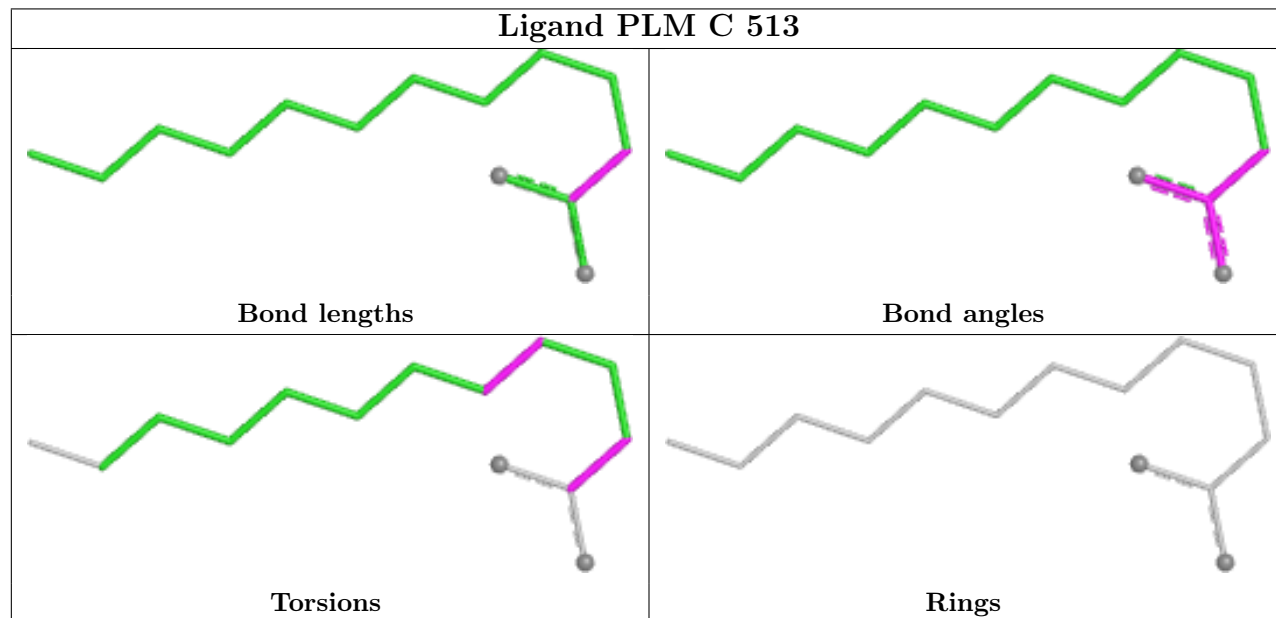
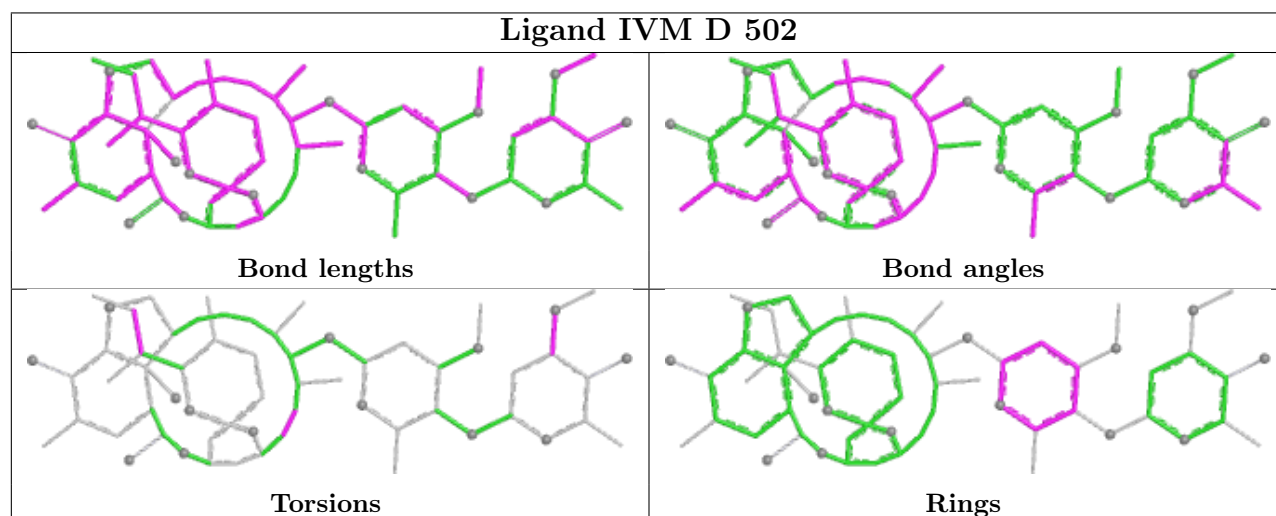
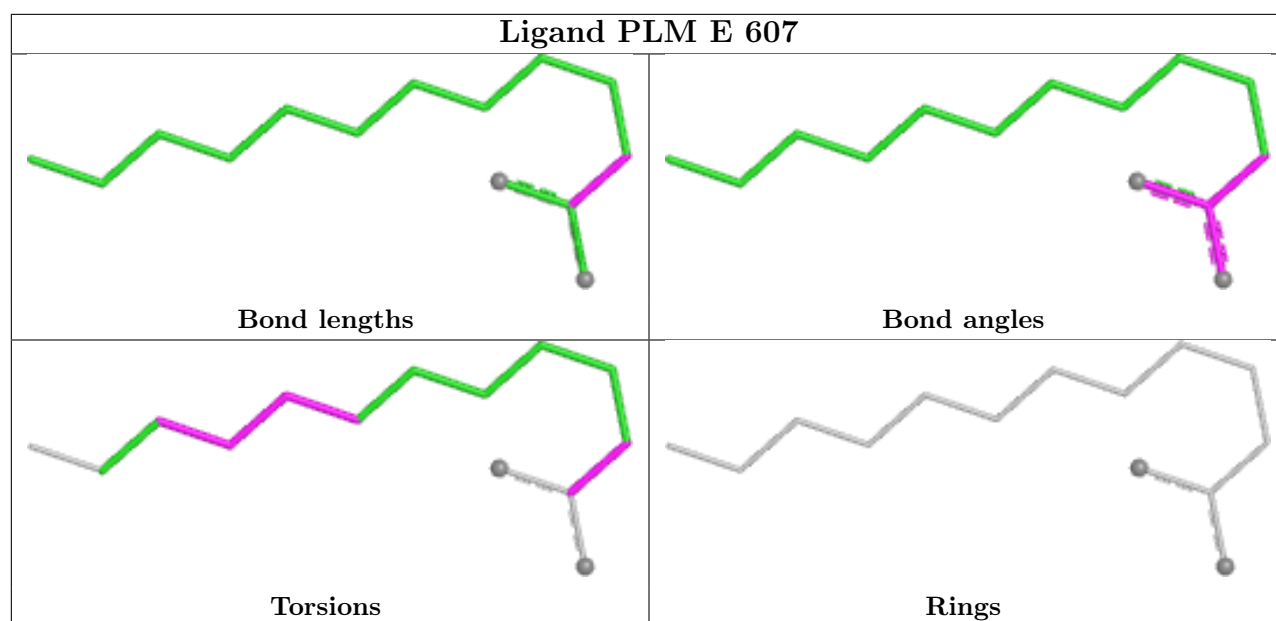


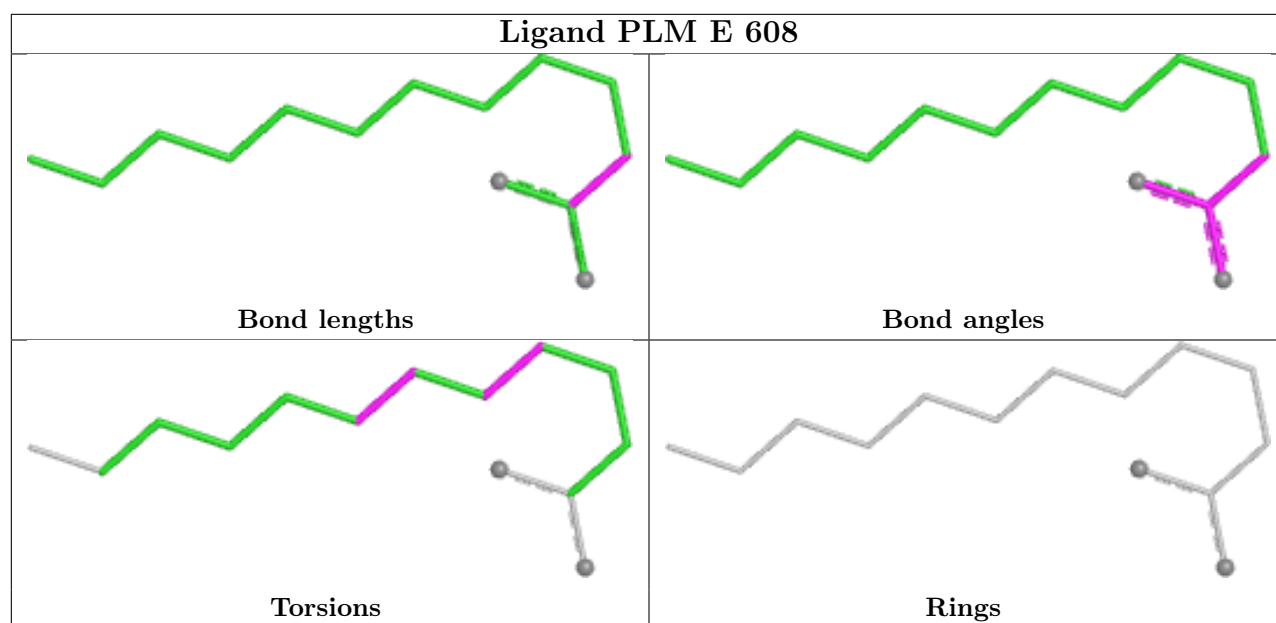












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

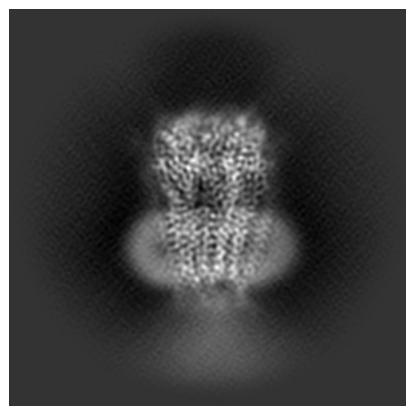
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29019. These allow visual inspection of the internal detail of the map and identification of artifacts.

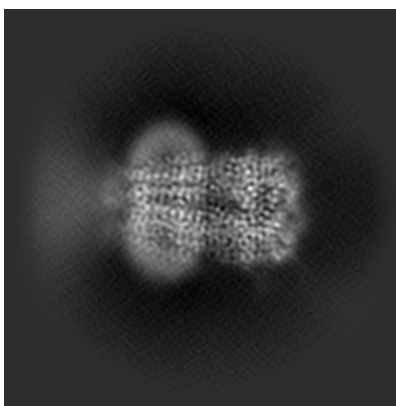
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

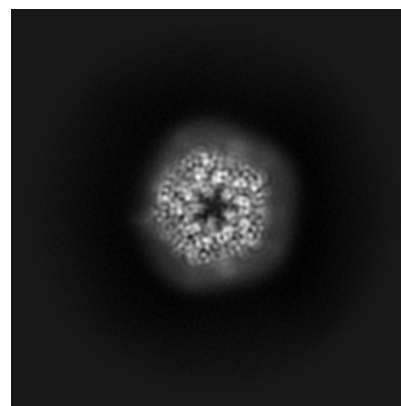
6.1.1 Primary map



X

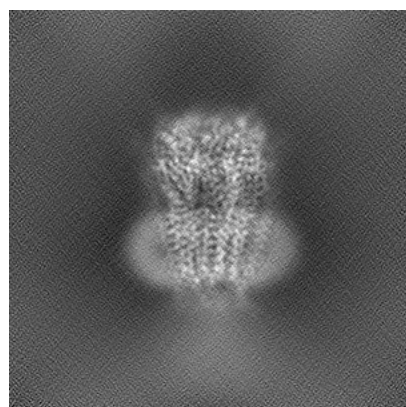


Y

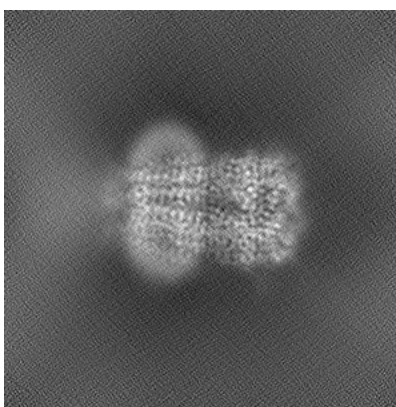


Z

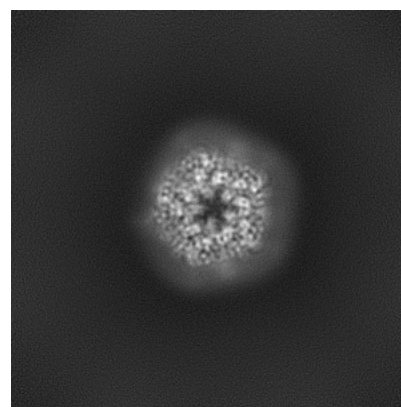
6.1.2 Raw map



X



Y

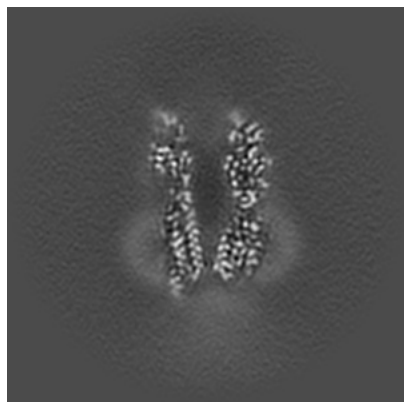


Z

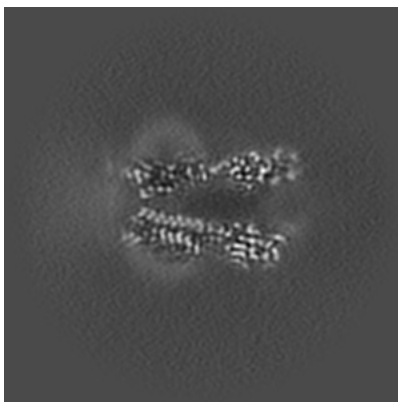
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

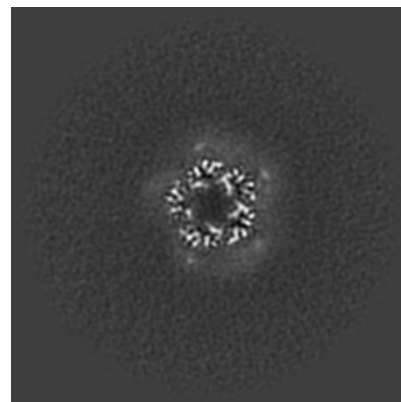
6.2.1 Primary map



X Index: 150

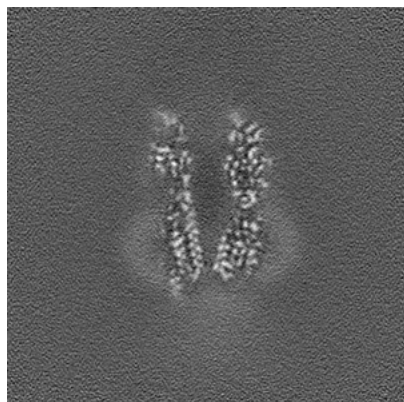


Y Index: 150

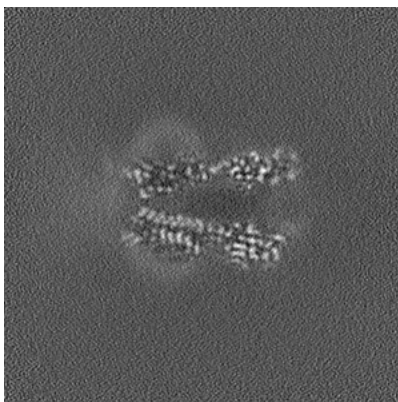


Z Index: 150

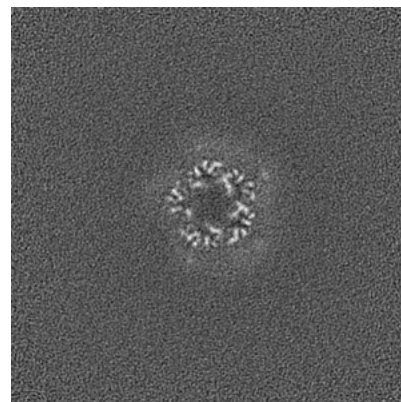
6.2.2 Raw map



X Index: 150



Y Index: 150

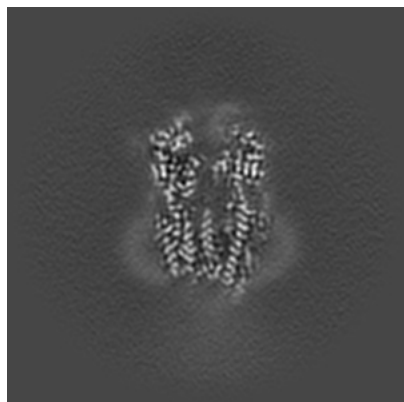


Z Index: 150

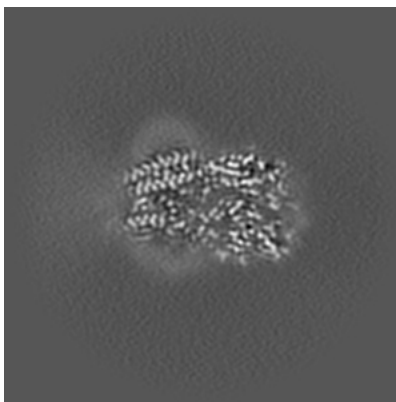
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

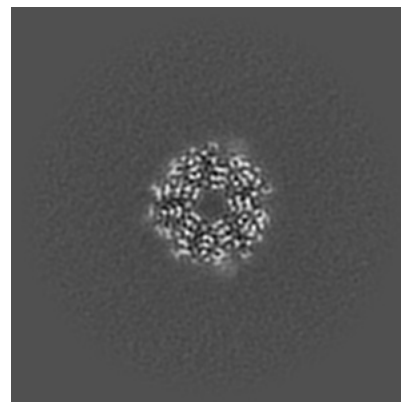
6.3.1 Primary map



X Index: 139

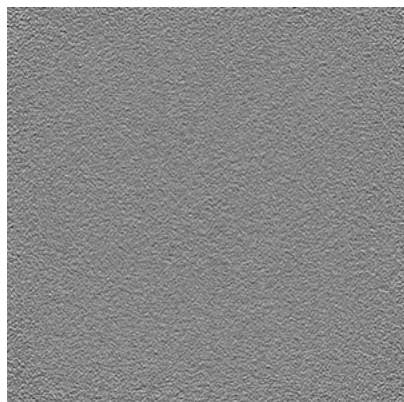


Y Index: 168

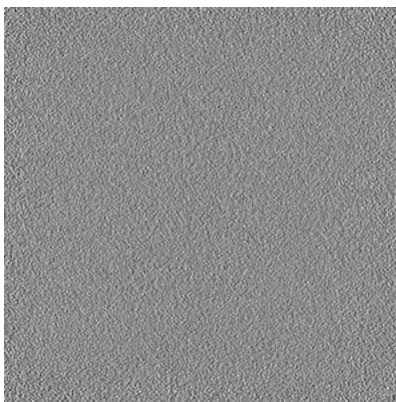


Z Index: 182

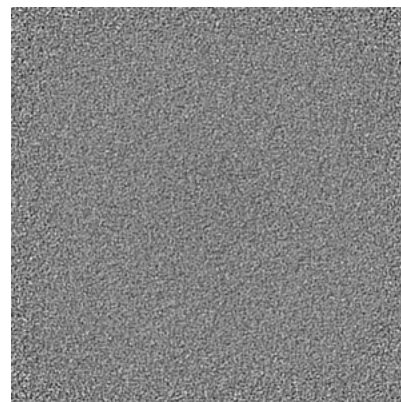
6.3.2 Raw map



X Index: 0



Y Index: 0

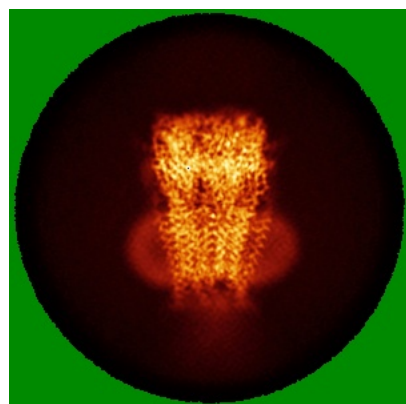


Z Index: 0

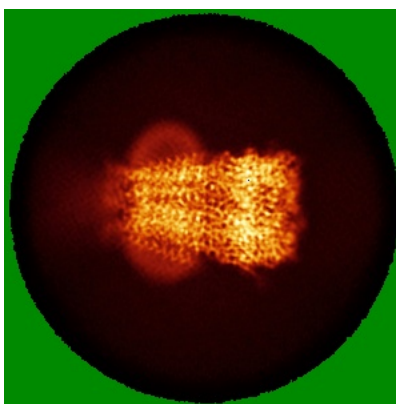
The images above show the largest variance slices of the map in three orthogonal directions.

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

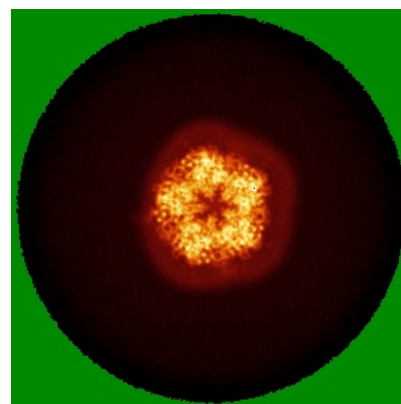
6.4.1 Primary map



X

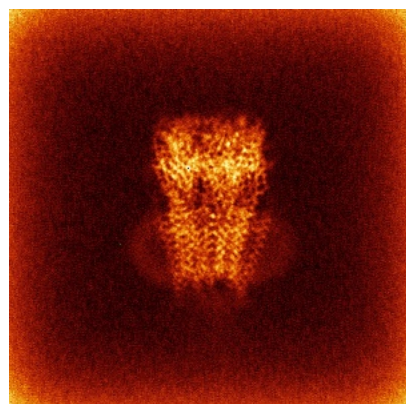


Y

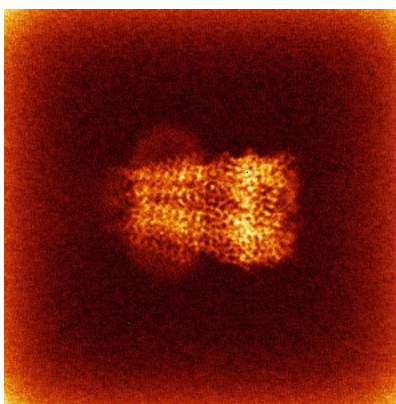


Z

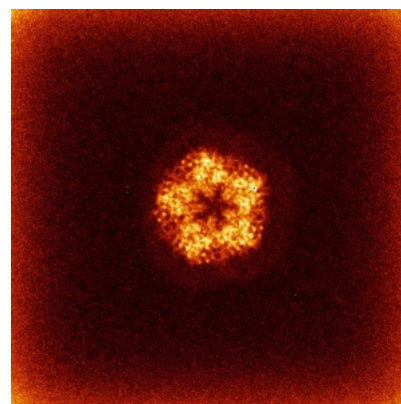
6.4.2 Raw map



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.

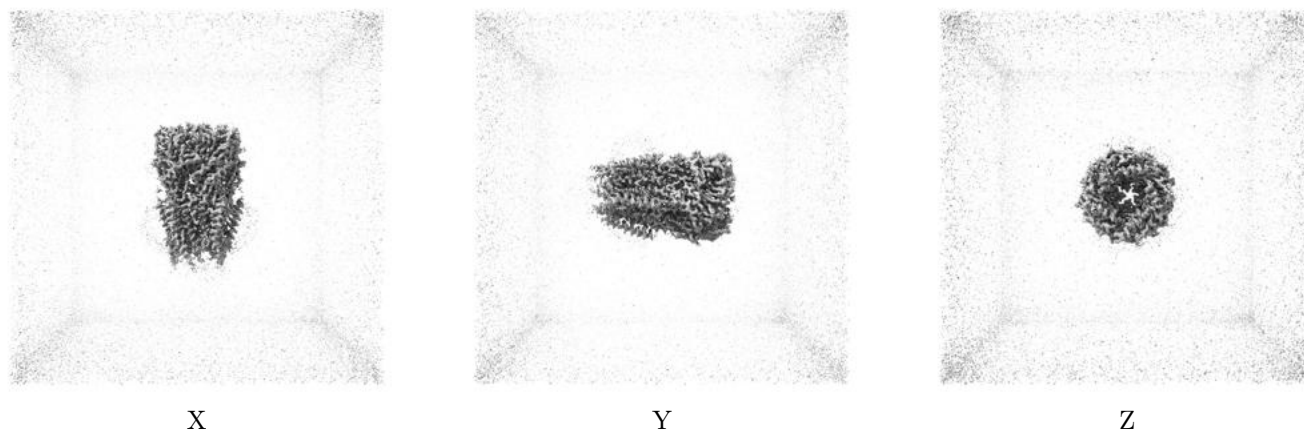
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. 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.

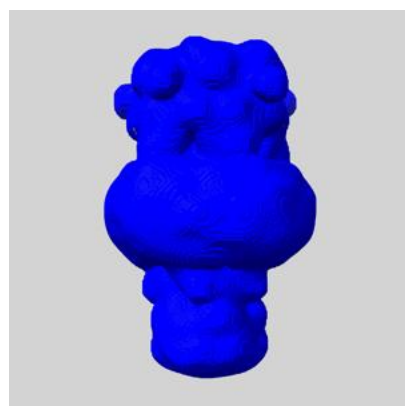
6.6 Mask visualisation [i](#)

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

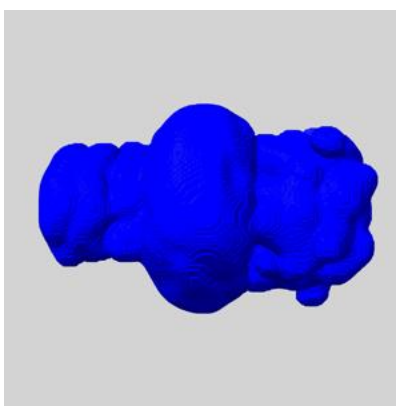
A mask typically either:

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

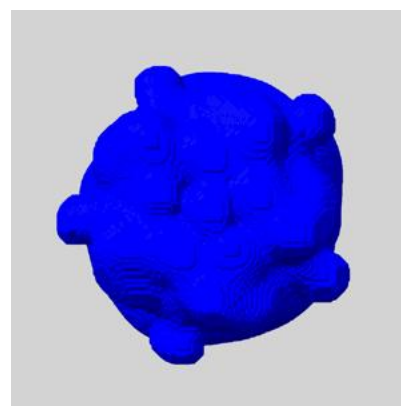
6.6.1 emd_29019_msk_1.map [i](#)



X



Y

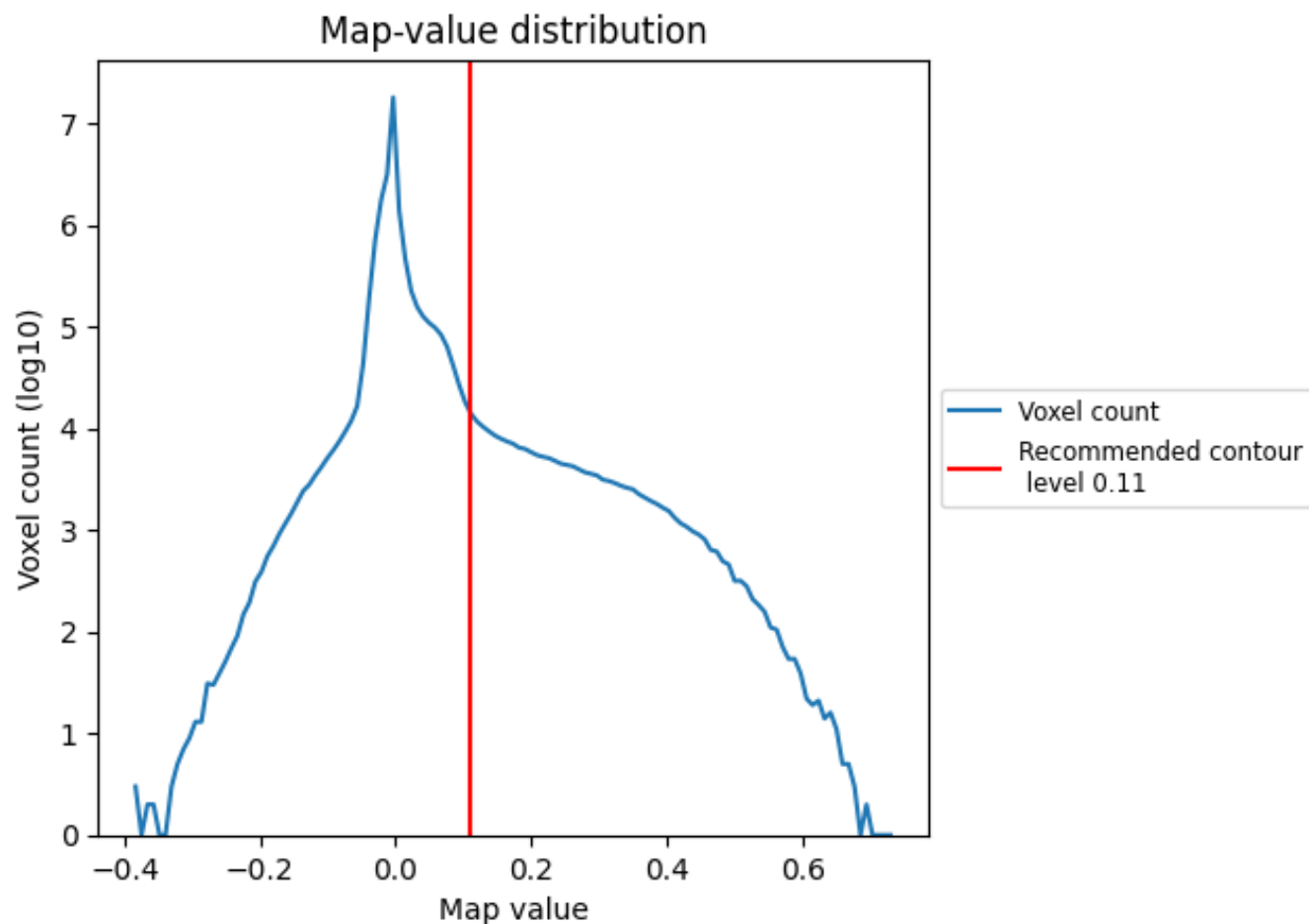


Z

7 Map analysis [i](#)

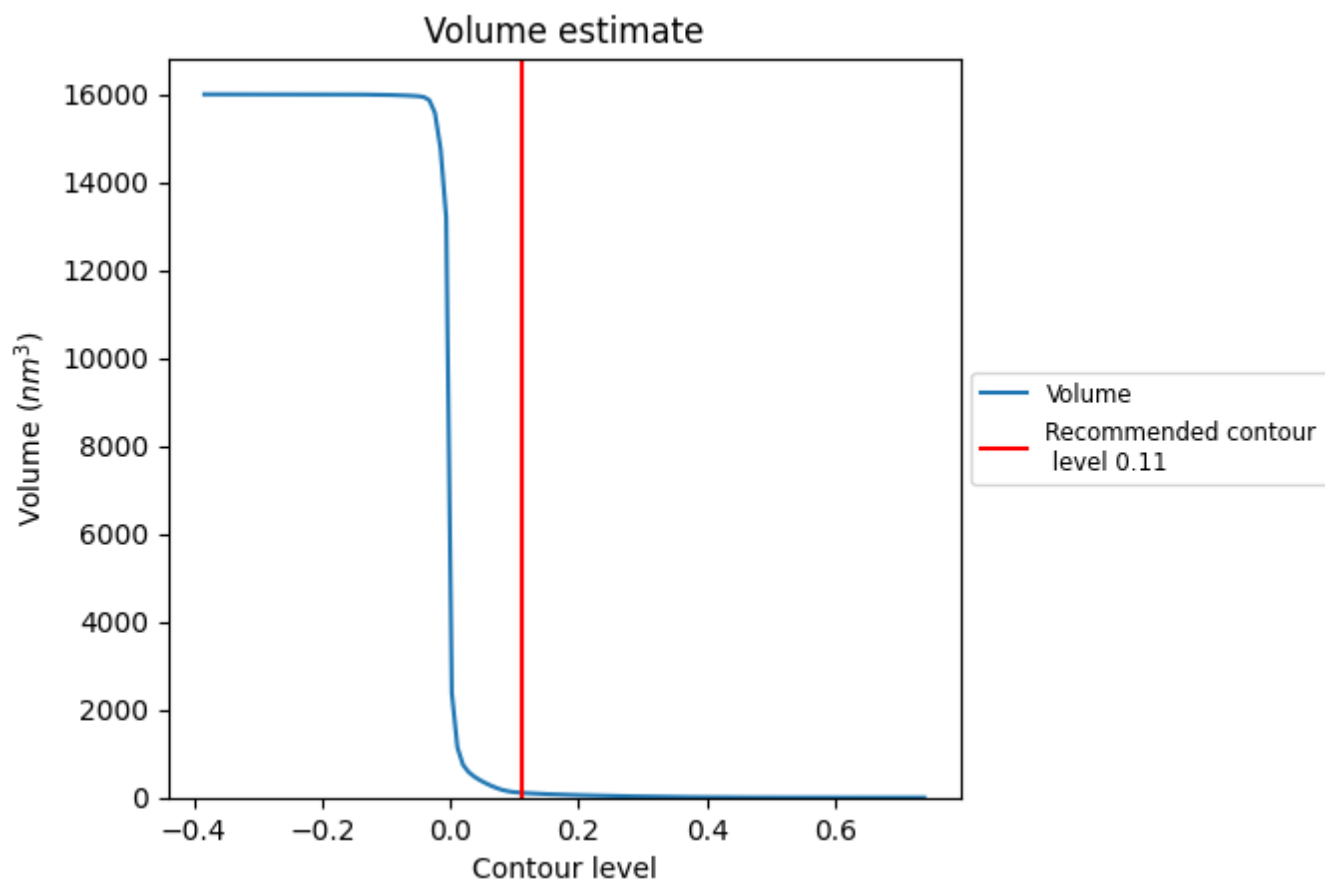
This section contains the results of statistical analysis of the map.

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.

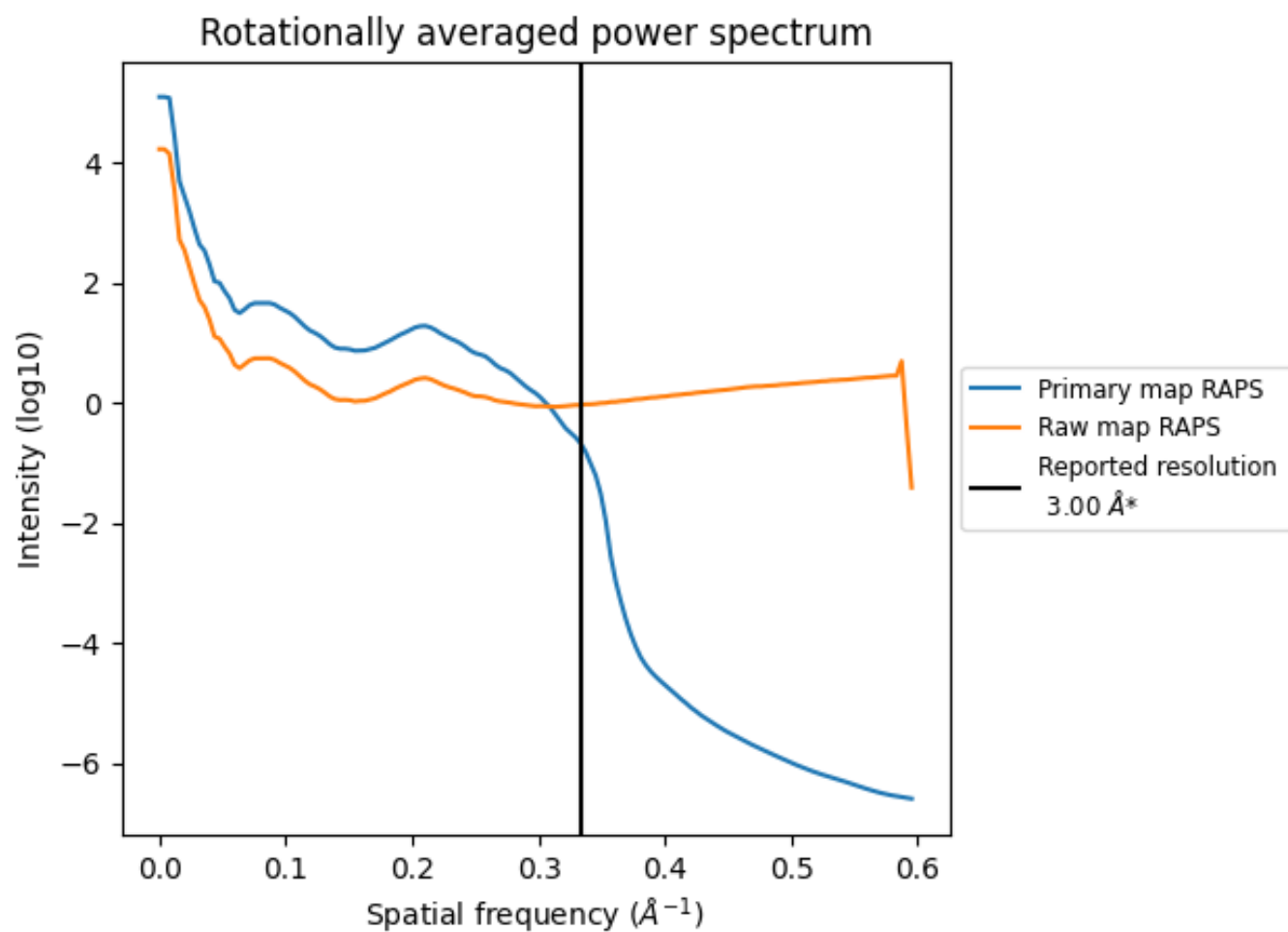
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm³; this corresponds to an approximate mass of 99 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 ⓘ

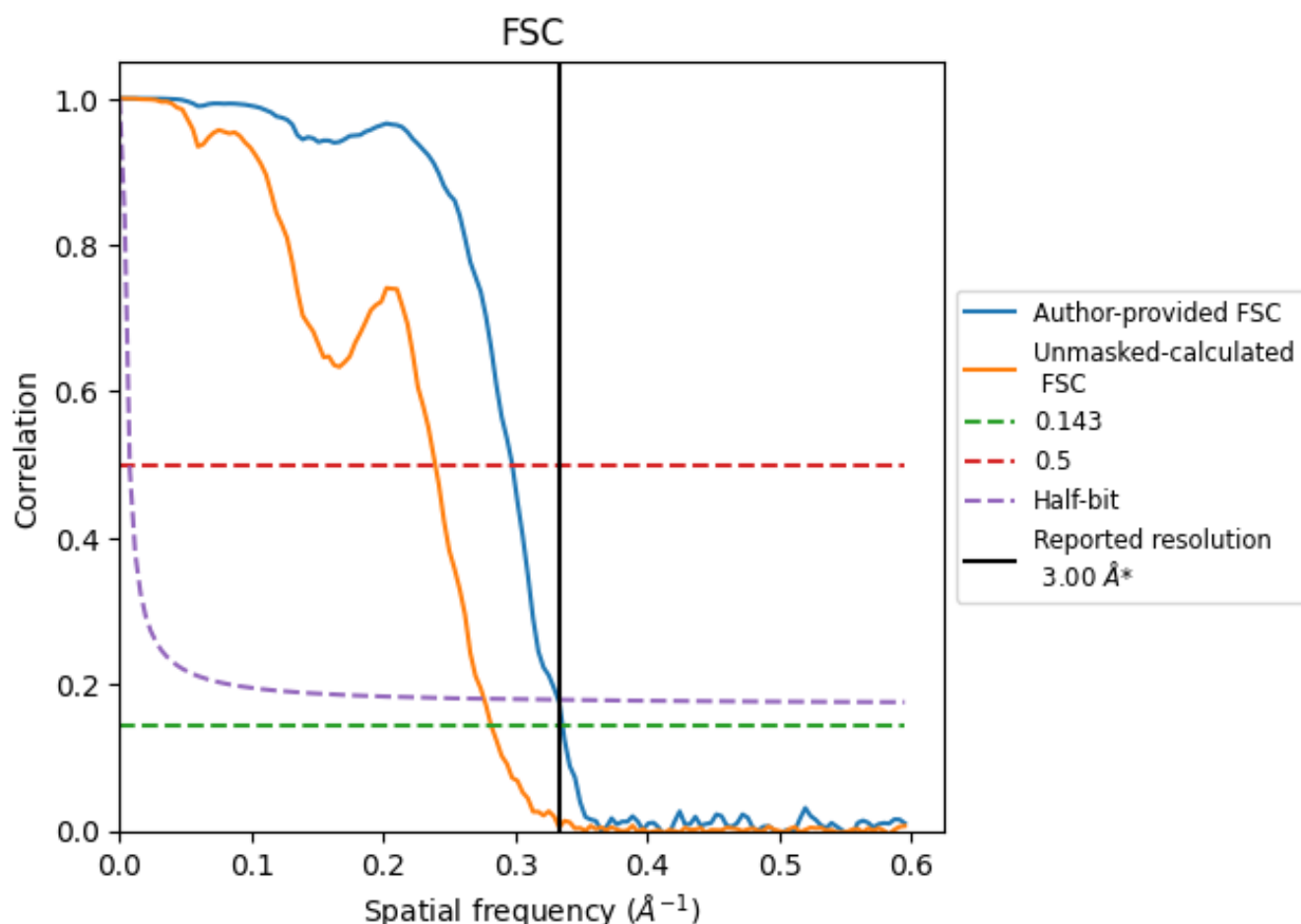


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

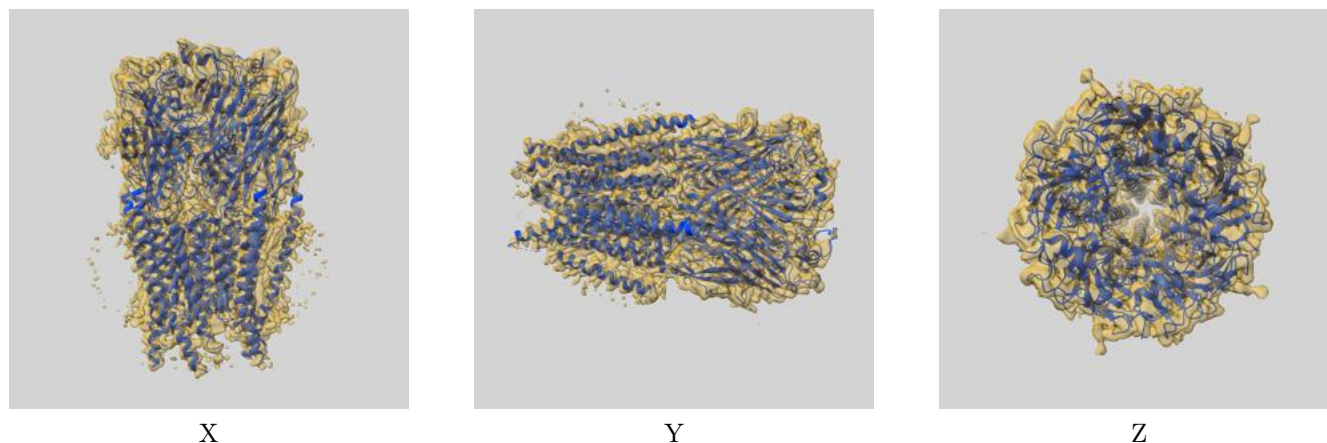
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.36	3.01
Unmasked-calculated*	3.55	4.18	3.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.55 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

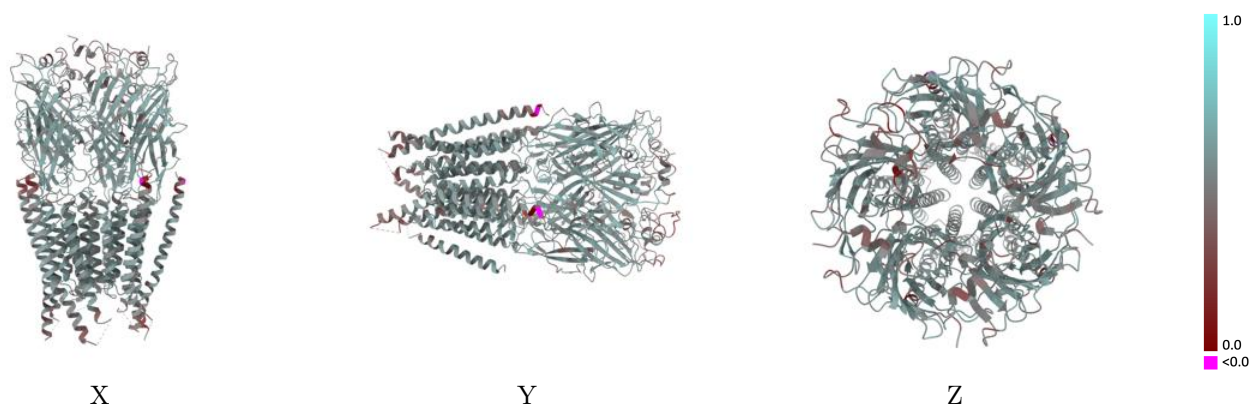
This section contains information regarding the fit between EMDB map EMD-29019 and PDB model 8FE1. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



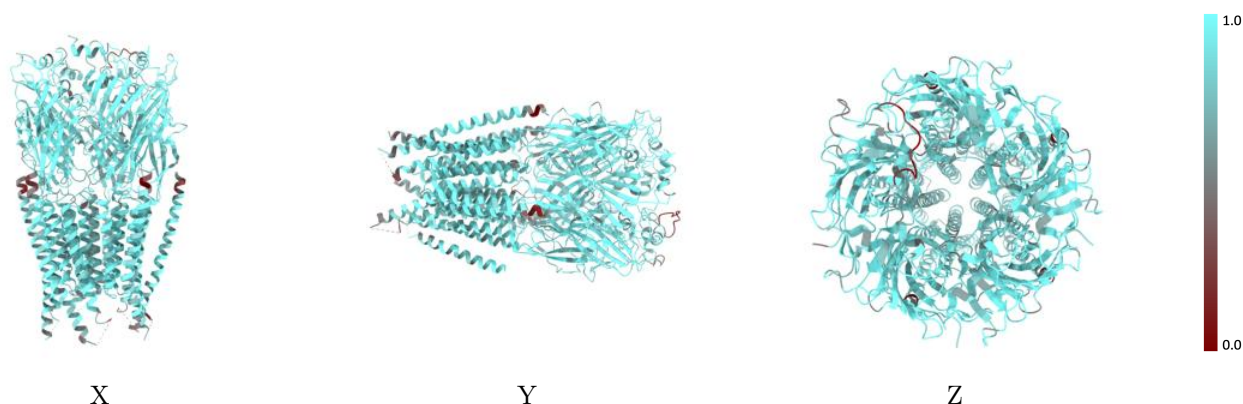
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



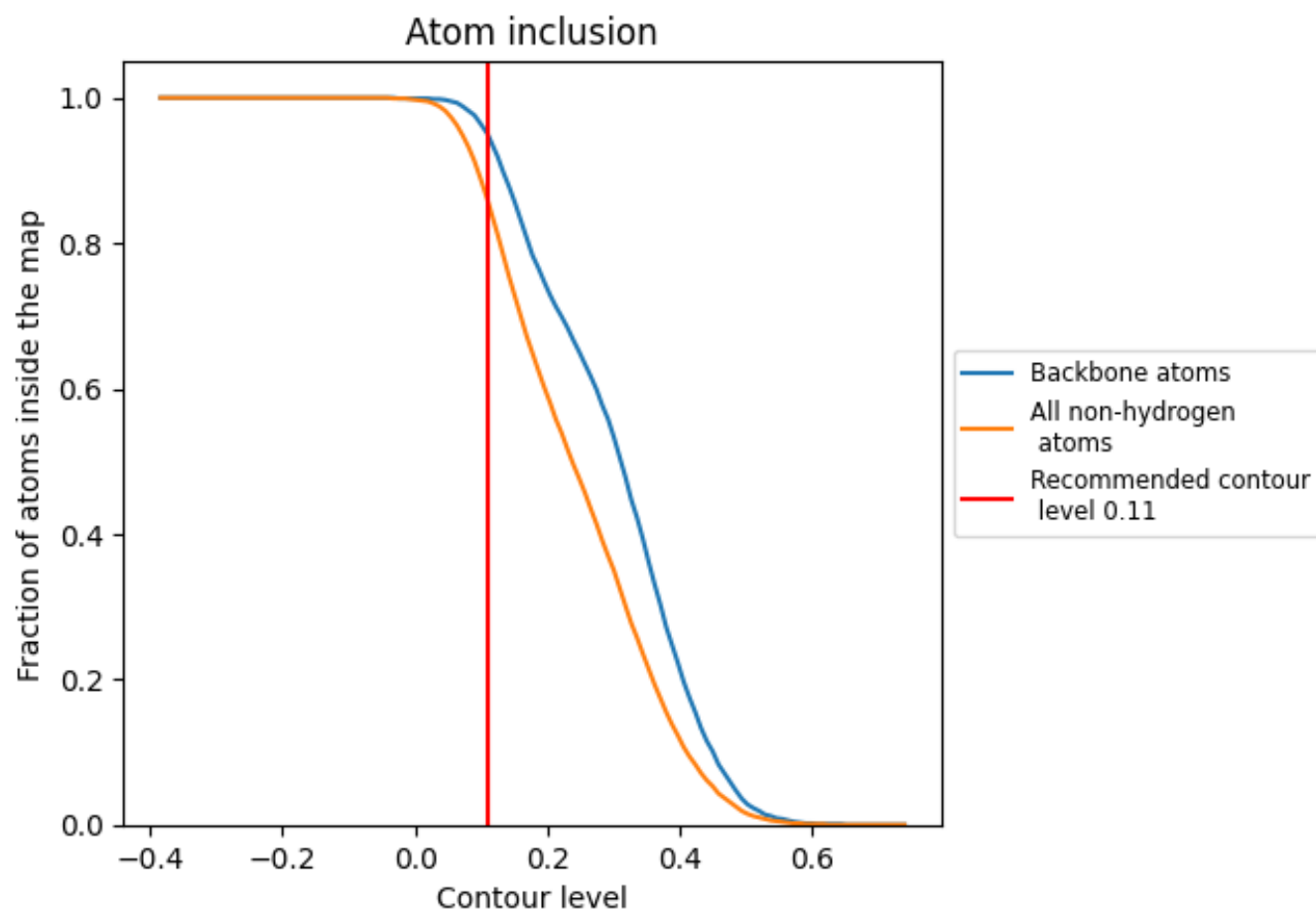
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 86% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8590	<div></div> 0.5270
A	<div></div> 0.8690	<div></div> 0.5290
B	<div></div> 0.8680	<div></div> 0.5310
C	<div></div> 0.8620	<div></div> 0.5290
D	<div></div> 0.8630	<div></div> 0.5320
E	<div></div> 0.8300	<div></div> 0.5130

