



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:13 PM UTC

PDB ID : 7AP5 / pdb_00007ap5
Title : Crystal structure of phycoerythrin from cyanobacterium Nostoc sp. WR13 contains multiple stacks of hexameric assemblies which resemble the rods of phycobilisome.
Authors : Patel, H.M.; Roszak, A.W.; Cogdell, R.J.; Madamwar, D.; Liu, H.; Gross, M.L.; Blankenship, R.E.
Deposited on : 2020-10-15
Resolution : 2.13 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

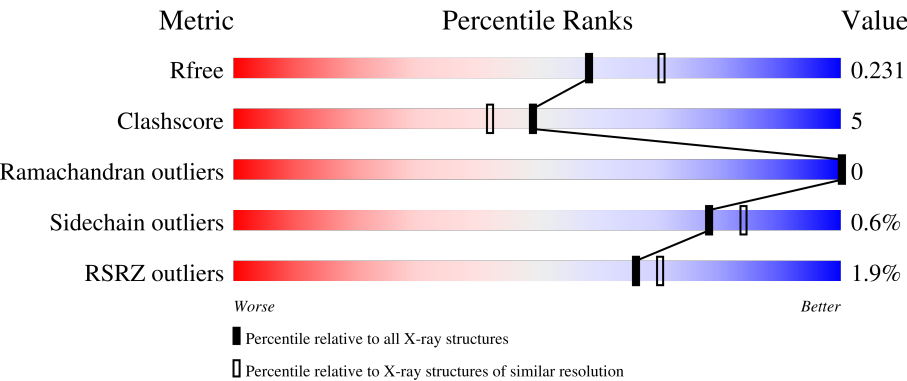
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 Å.

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



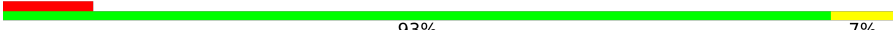
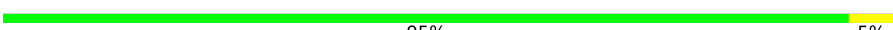
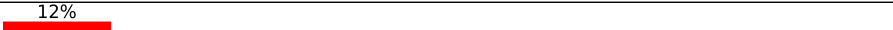
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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

Mol	Chain	Length	Quality of chain
1	AAA	164	94%6%
1	CCC	164	95%. .
1	EEE	164	98%. .
1	GGG	164	%93%7%
1	III	164	95%5%

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Mol	Chain	Length	Quality of chain
1	KKK	164	 91% 9%
1	MMM	164	 94% 6% 2%
1	OOO	164	 93% 7% 10%
2	BBB	184	 95% 5%
2	DDD	184	 92% 8%
2	FFF	184	 92% 8% 2%
2	HHH	184	 92% 8%
2	JJJ	184	 92% 8%
2	LLL	184	 90% 10% 2%
2	NNN	184	 93% 7% 2%
2	PPP	184	 91% 9% 12%

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
14	EDO	FFF	203	-	-	-	X
4	PG4	AAA	203	-	-	X	-
4	PG4	AAA	204	-	-	X	-
4	PG4	MMM	203	-	-	X	-
6	PEG	CCC	210	-	-	X	-
7	PO4	KKK	215	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 26483 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha subunit of cyanobacterial protein phycoerythrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	164	Total	C	N	O	S	0	4	0
			1257	785	220	245	7			
1	CCC	164	Total	C	N	O	S	0	4	0
			1256	785	219	245	7			
1	EEE	164	Total	C	N	O	S	0	4	0
			1254	784	219	244	7			
1	GGG	164	Total	C	N	O	S	0	2	0
			1244	777	218	242	7			
1	III	164	Total	C	N	O	S	0	2	0
			1244	777	218	242	7			
1	KKK	164	Total	C	N	O	S	0	3	0
			1245	780	217	241	7			
1	MMM	164	Total	C	N	O	S	0	3	0
			1247	780	217	243	7			
1	OOO	164	Total	C	N	O	S	0	1	0
			1238	774	217	240	7			

- Molecule 2 is a protein called Beta subunit of cyanobacterial protein phycoerythrin.

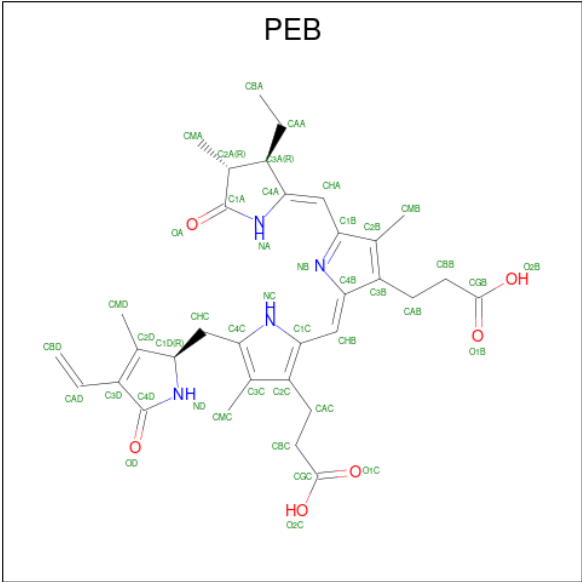
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	184	Total	C	N	O	S	0	6	0
			1378	845	253	268	12			
2	DDD	184	Total	C	N	O	S	0	9	0
			1382	849	251	270	12			
2	FFF	184	Total	C	N	O	S	0	6	0
			1370	840	250	268	12			
2	HHH	184	Total	C	N	O	S	0	7	0
			1368	839	247	270	12			
2	JJJ	184	Total	C	N	O	S	0	8	0
			1376	844	250	270	12			
2	LLL	184	Total	C	N	O	S	0	7	0
			1381	847	253	269	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	NNN	184	Total	C	N	O	S	0	3	0
			1355	830	247	266	12			
2	PPP	184	Total	C	N	O	S	0	4	0
			1363	835	250	266	12			

- Molecule 3 is PHYCOERYTHROBILIN (CCD ID: PEB) (formula: C₃₃H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	N	O		0	0
			43	33	4	6			
3	AAA	1	Total	C	N	O		0	0
			43	33	4	6			
3	BBB	1	Total	C	N	O		0	0
			43	33	4	6			
3	BBB	1	Total	C	N	O		0	0
			43	33	4	6			
3	BBB	1	Total	C	N	O		0	0
			43	33	4	6			
3	CCC	1	Total	C	N	O		0	0
			43	33	4	6			
3	CCC	1	Total	C	N	O		0	0
			43	33	4	6			
3	DDD	1	Total	C	N	O		0	0
			43	33	4	6			
3	DDD	1	Total	C	N	O		0	0
			43	33	4	6			

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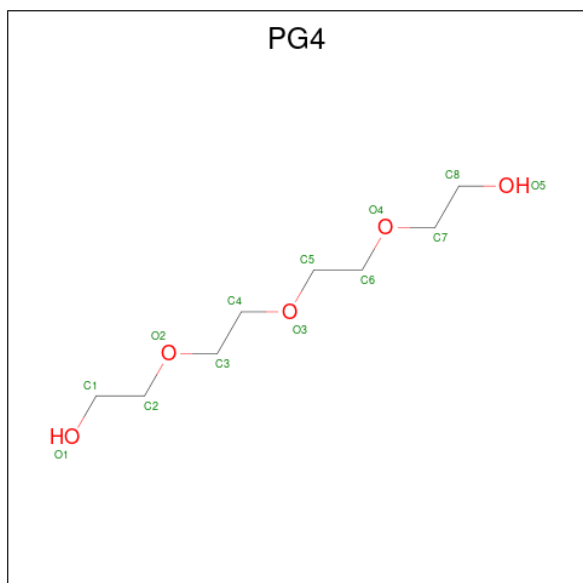
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	DDD	1	Total	C	N	O	0	0
			43	33	4	6		
3	EEE	1	Total	C	N	O	0	0
			43	33	4	6		
3	EEE	1	Total	C	N	O	0	0
			43	33	4	6		
3	FFF	1	Total	C	N	O	0	0
			43	33	4	6		
3	FFF	1	Total	C	N	O	0	0
			43	33	4	6		
3	FFF	1	Total	C	N	O	0	0
			43	33	4	6		
3	GGG	1	Total	C	N	O	0	0
			43	33	4	6		
3	GGG	1	Total	C	N	O	0	0
			43	33	4	6		
3	HHH	1	Total	C	N	O	0	0
			43	33	4	6		
3	HHH	1	Total	C	N	O	0	0
			43	33	4	6		
3	HHH	1	Total	C	N	O	0	0
			43	33	4	6		
3	III	1	Total	C	N	O	0	0
			43	33	4	6		
3	III	1	Total	C	N	O	0	0
			43	33	4	6		
3	JJJ	1	Total	C	N	O	0	0
			43	33	4	6		
3	JJJ	1	Total	C	N	O	0	0
			43	33	4	6		
3	JJJ	1	Total	C	N	O	0	0
			43	33	4	6		
3	KKK	1	Total	C	N	O	0	0
			43	33	4	6		
3	KKK	1	Total	C	N	O	0	0
			43	33	4	6		
3	LLL	1	Total	C	N	O	0	0
			43	33	4	6		
3	LLL	1	Total	C	N	O	0	0
			43	33	4	6		
3	LLL	1	Total	C	N	O	0	0
			43	33	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	MMM	1	Total	C	N	O	0	0
			43	33	4	6		
3	MMM	1	Total	C	N	O	0	0
			43	33	4	6		
3	NNN	1	Total	C	N	O	0	0
			43	33	4	6		
3	NNN	1	Total	C	N	O	0	0
			43	33	4	6		
3	NNN	1	Total	C	N	O	0	0
			43	33	4	6		
3	OOO	1	Total	C	N	O	0	0
			43	33	4	6		
3	OOO	1	Total	C	N	O	0	0
			43	33	4	6		
3	PPP	1	Total	C	N	O	0	0
			43	33	4	6		
3	PPP	1	Total	C	N	O	0	0
			43	33	4	6		
3	PPP	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			13	8	5		

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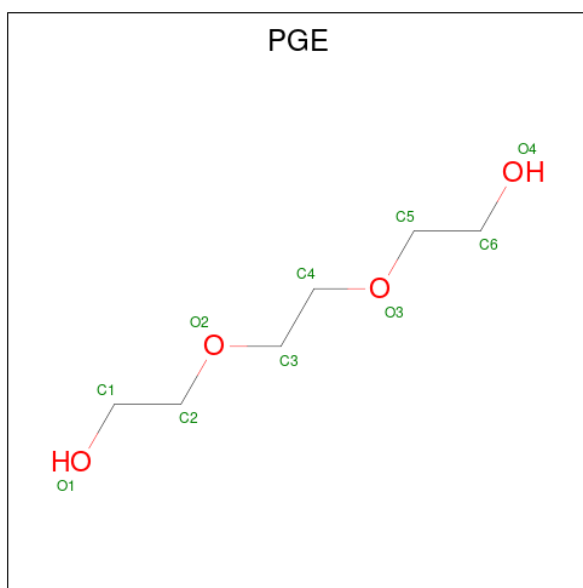
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			13	8	5		
4	AAA	1	Total	C	O	0	0
			13	8	5		
4	CCC	1	Total	C	O	0	0
			13	8	5		
4	DDD	1	Total	C	O	0	0
			13	8	5		
4	DDD	1	Total	C	O	0	0
			13	8	5		
4	FFF	1	Total	C	O	0	0
			13	8	5		
4	FFF	1	Total	C	O	0	0
			13	8	5		
4	FFF	1	Total	C	O	0	0
			13	8	5		
4	FFF	1	Total	C	O	0	0
			13	8	5		
4	GGG	1	Total	C	O	0	0
			13	8	5		
4	GGG	1	Total	C	O	0	0
			13	8	5		
4	GGG	1	Total	C	O	0	0
			13	8	5		
4	HHH	1	Total	C	O	0	0
			13	8	5		
4	HHH	1	Total	C	O	0	0
			13	8	5		
4	JJJ	1	Total	C	O	0	0
			13	8	5		
4	KKK	1	Total	C	O	0	0
			13	8	5		
4	KKK	1	Total	C	O	0	0
			13	8	5		
4	KKK	1	Total	C	O	0	0
			13	8	5		
4	LLL	1	Total	C	O	0	0
			13	8	5		
4	LLL	1	Total	C	O	0	0
			13	8	5		
4	LLL	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	MMM	1	Total	C	O	0	0
			13	8	5		
4	MMM	1	Total	C	O	0	0
			13	8	5		
4	MMM	1	Total	C	O	0	0
			13	8	5		
4	MMM	1	Total	C	O	0	0
			13	8	5		
4	NNN	1	Total	C	O	0	0
			13	8	5		
4	NNN	1	Total	C	O	0	0
			13	8	5		
4	NNN	1	Total	C	O	0	0
			13	8	5		
4	NNN	1	Total	C	O	0	0
			13	8	5		
4	NNN	1	Total	C	O	0	0
			13	8	5		
4	OOO	1	Total	C	O	0	0
			13	8	5		
4	PPP	1	Total	C	O	0	0
			13	8	5		
4	PPP	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			10	6	4		
5	AAA	1	Total	C	O	0	0
			10	6	4		
5	AAA	1	Total	C	O	0	0
			10	6	4		
5	AAA	1	Total	C	O	0	0
			10	6	4		
5	AAA	1	Total	C	O	0	0
			10	6	4		
5	BBB	1	Total	C	O	0	0
			10	6	4		
5	BBB	1	Total	C	O	0	0
			10	6	4		
5	BBB	1	Total	C	O	0	0
			10	6	4		
5	CCC	1	Total	C	O	0	0
			10	6	4		
5	CCC	1	Total	C	O	0	0
			10	6	4		
5	CCC	1	Total	C	O	0	0
			10	6	4		
5	CCC	1	Total	C	O	0	0
			10	6	4		
5	DDD	1	Total	C	O	0	0
			10	6	4		
5	DDD	1	Total	C	O	0	0
			10	6	4		
5	DDD	1	Total	C	O	0	0
			10	6	4		
5	EEE	1	Total	C	O	0	0
			10	6	4		
5	EEE	1	Total	C	O	0	0
			10	6	4		
5	EEE	1	Total	C	O	0	0
			10	6	4		
5	FFF	1	Total	C	O	0	0
			10	6	4		

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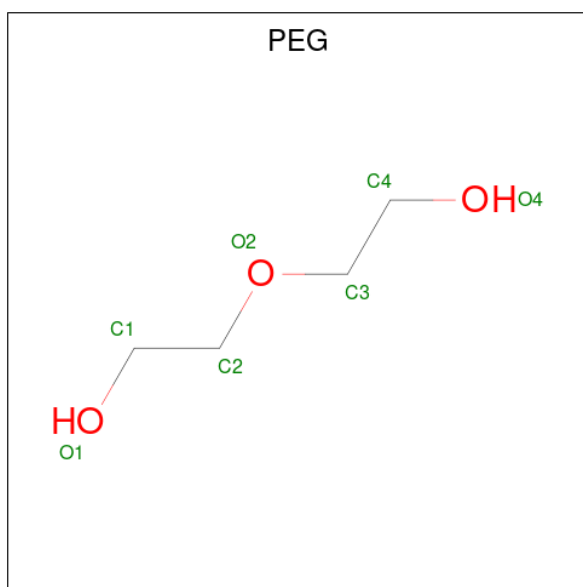
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	FFF	1	Total	C	O	0	0
			10	6	4		
5	FFF	1	Total	C	O	0	0
			10	6	4		
5	GGG	1	Total	C	O	0	0
			10	6	4		
5	GGG	1	Total	C	O	0	0
			10	6	4		
5	GGG	1	Total	C	O	0	0
			10	6	4		
5	GGG	1	Total	C	O	0	0
			10	6	4		
5	HHH	1	Total	C	O	0	0
			10	6	4		
5	HHH	1	Total	C	O	0	0
			10	6	4		
5	HHH	1	Total	C	O	0	0
			10	6	4		
5	HHH	1	Total	C	O	0	0
			10	6	4		
5	HHH	1	Total	C	O	0	0
			10	6	4		
5	HHH	1	Total	C	O	0	0
			10	6	4		
5	III	1	Total	C	O	0	0
			10	6	4		
5	III	1	Total	C	O	0	0
			10	6	4		
5	III	1	Total	C	O	0	0
			10	6	4		
5	III	1	Total	C	O	0	0
			10	6	4		
5	JJJ	1	Total	C	O	0	0
			10	6	4		
5	JJJ	1	Total	C	O	0	0
			10	6	4		
5	JJJ	1	Total	C	O	0	0
			10	6	4		
5	KKK	1	Total	C	O	0	0
			10	6	4		
5	KKK	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	LLL	1	Total	C	O	0	0
			10	6	4		
5	LLL	1	Total	C	O	0	0
			10	6	4		
5	LLL	1	Total	C	O	0	0
			10	6	4		
5	LLL	1	Total	C	O	0	0
			10	6	4		
5	MMM	1	Total	C	O	0	0
			10	6	4		
5	MMM	1	Total	C	O	0	0
			10	6	4		
5	NNN	1	Total	C	O	0	0
			10	6	4		
5	NNN	1	Total	C	O	0	0
			10	6	4		
5	NNN	1	Total	C	O	0	0
			10	6	4		
5	NNN	1	Total	C	O	0	0
			10	6	4		
5	OOO	1	Total	C	O	0	0
			10	6	4		
5	OOO	1	Total	C	O	0	0
			10	6	4		
5	OOO	1	Total	C	O	0	0
			10	6	4		
5	PPP	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	C	O	0	0
			7	4	3		
6	AAA	1	Total	C	O	0	0
			7	4	3		
6	BBB	1	Total	C	O	0	0
			7	4	3		
6	BBB	1	Total	C	O	0	0
			7	4	3		
6	BBB	1	Total	C	O	0	0
			7	4	3		
6	BBB	1	Total	C	O	0	0
			7	4	3		
6	BBB	1	Total	C	O	0	0
			7	4	3		
6	BBB	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	CCC	1	Total	C	O	0	0
			7	4	3		
6	DDD	1	Total	C	O	0	0
			7	4	3		
6	DDD	1	Total	C	O	0	0
			7	4	3		
6	DDD	1	Total	C	O	0	0
			7	4	3		
6	DDD	1	Total	C	O	0	0
			7	4	3		
6	DDD	1	Total	C	O	0	0
			7	4	3		
6	EEE	1	Total	C	O	0	0
			7	4	3		
6	EEE	1	Total	C	O	0	0
			7	4	3		
6	FFF	1	Total	C	O	0	0
			7	4	3		
6	FFF	1	Total	C	O	0	0
			7	4	3		
6	FFF	1	Total	C	O	0	0
			7	4	3		
6	FFF	1	Total	C	O	0	0
			7	4	3		
6	FFF	1	Total	C	O	0	0
			7	4	3		
6	GGG	1	Total	C	O	0	0
			7	4	3		
6	GGG	1	Total	C	O	0	0
			7	4	3		
6	GGG	1	Total	C	O	0	0
			7	4	3		
6	GGG	1	Total	C	O	0	0
			7	4	3		
6	GGG	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	HHH	1	Total	C	O	0	0
			7	4	3		
6	HHH	1	Total	C	O	0	0
			7	4	3		
6	HHH	1	Total	C	O	0	0
			7	4	3		
6	HHH	1	Total	C	O	0	0
			7	4	3		
6	HHH	1	Total	C	O	0	0
			7	4	3		
6	III	1	Total	C	O	0	0
			7	4	3		
6	III	1	Total	C	O	0	0
			7	4	3		
6	III	1	Total	C	O	0	0
			7	4	3		
6	III	1	Total	C	O	0	0
			7	4	3		
6	III	1	Total	C	O	0	0
			7	4	3		
6	III	1	Total	C	O	0	0
			7	4	3		
6	JJJ	1	Total	C	O	0	0
			7	4	3		
6	JJJ	1	Total	C	O	0	0
			7	4	3		
6	JJJ	1	Total	C	O	0	0
			7	4	3		
6	KKK	1	Total	C	O	0	0
			7	4	3		
6	KKK	1	Total	C	O	0	0
			7	4	3		
6	KKK	1	Total	C	O	0	0
			7	4	3		
6	KKK	1	Total	C	O	0	0
			7	4	3		
6	KKK	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		

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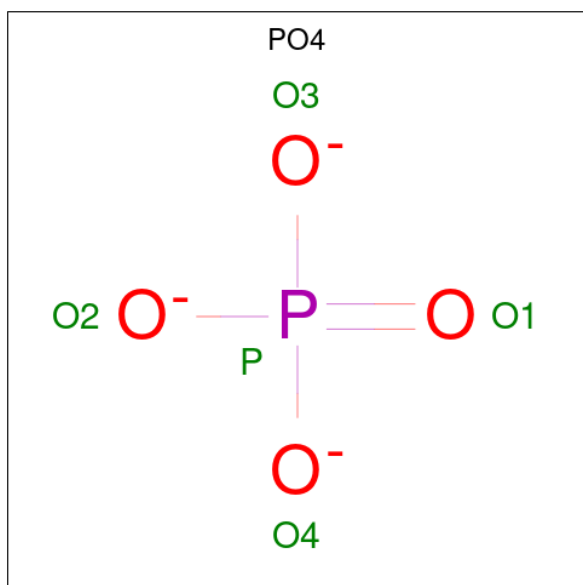
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	1
			14	8	6		
6	MMM	1	Total	C	O	0	0
			7	4	3		
6	MMM	1	Total	C	O	0	0
			7	4	3		
6	MMM	1	Total	C	O	0	0
			7	4	3		
6	NNN	1	Total	C	O	0	0
			7	4	3		
6	NNN	1	Total	C	O	0	0
			7	4	3		
6	NNN	1	Total	C	O	0	0
			7	4	3		
6	OOO	1	Total	C	O	0	0
			7	4	3		
6	OOO	1	Total	C	O	0	0
			7	4	3		
6	OOO	1	Total	C	O	0	0
			7	4	3		
6	OOO	1	Total	C	O	0	0
			7	4	3		
6	PPP	1	Total	C	O	0	0
			7	4	3		
6	PPP	1	Total	C	O	0	0
			7	4	3		
6	PPP	1	Total	C	O	0	0
			7	4	3		
6	PPP	1	Total	C	O	0	0
			7	4	3		
6	PPP	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	PPP	1	Total	C	O	0	0
			7	4	3		
6	PPP	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	O	P	0	0
			5	4	1		
7	AAA	1	Total	O	P	0	0
			5	4	1		
7	BBB	1	Total	O	P	0	0
			5	4	1		
7	BBB	1	Total	O	P	0	0
			5	4	1		
7	BBB	1	Total	O	P	0	0
			5	4	1		
7	BBB	1	Total	O	P	0	0
			5	4	1		
7	CCC	1	Total	O	P	0	0
			5	4	1		
7	CCC	1	Total	O	P	0	0
			5	4	1		
7	CCC	1	Total	O	P	0	0
			5	4	1		

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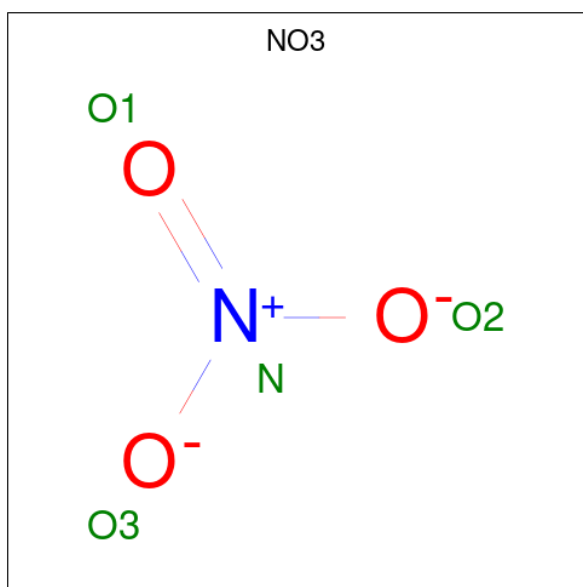
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	FFF	1	Total	O	P	0	0
			5	4	1		
7	FFF	1	Total	O	P	0	0
			5	4	1		
7	FFF	1	Total	O	P	0	0
			5	4	1		
7	FFF	1	Total	O	P	0	0
			5	4	1		
7	GGG	1	Total	O	P	0	0
			5	4	1		
7	GGG	1	Total	O	P	0	0
			5	4	1		
7	HHH	1	Total	O	P	0	0
			5	4	1		
7	HHH	1	Total	O	P	0	0
			5	4	1		
7	HHH	1	Total	O	P	0	0
			5	4	1		
7	HHH	1	Total	O	P	0	0
			5	4	1		
7	III	1	Total	O	P	0	0
			5	4	1		
7	III	1	Total	O	P	0	0
			5	4	1		
7	III	1	Total	O	P	0	0
			5	4	1		
7	JJJ	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	JJJ	1	Total	O	P	0	0
			5	4	1		
7	JJJ	1	Total	O	P	0	0
			5	4	1		
7	JJJ	1	Total	O	P	0	0
			5	4	1		
7	JJJ	1	Total	O	P	0	0
			5	4	1		
7	JJJ	1	Total	O	P	0	0
			5	4	1		
7	KKK	1	Total	O	P	0	0
			5	4	1		
7	KKK	1	Total	O	P	0	0
			5	4	1		
7	KKK	1	Total	O	P	0	0
			5	4	1		
7	LLL	1	Total	O	P	0	0
			5	4	1		
7	LLL	1	Total	O	P	0	0
			5	4	1		
7	NNN	1	Total	O	P	0	0
			5	4	1		
7	NNN	1	Total	O	P	0	0
			5	4	1		
7	NNN	1	Total	O	P	0	0
			5	4	1		
7	NNN	1	Total	O	P	0	0
			5	4	1		
7	NNN	1	Total	O	P	0	0
			5	4	1		
7	OOO	1	Total	O	P	0	0
			5	4	1		
7	PPP	1	Total	O	P	0	0
			5	4	1		
7	PPP	1	Total	O	P	0	0
			5	4	1		
7	PPP	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



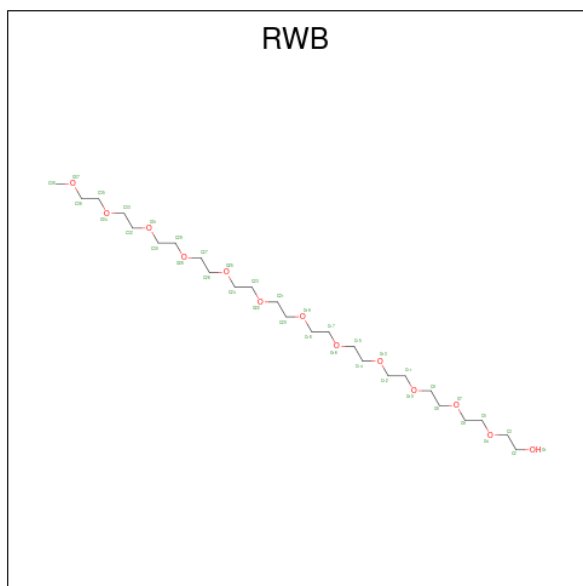
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	AAA	1	Total	N	O	0	0
			4	1	3		
8	AAA	1	Total	N	O	0	0
			4	1	3		
8	BBB	1	Total	N	O	0	0
			4	1	3		
8	CCC	1	Total	N	O	0	0
			4	1	3		
8	DDD	1	Total	N	O	0	0
			4	1	3		
8	DDD	1	Total	N	O	0	0
			4	1	3		
8	EEE	1	Total	N	O	0	0
			4	1	3		
8	EEE	1	Total	N	O	0	0
			4	1	3		
8	FFF	1	Total	N	O	0	0
			4	1	3		
8	GGG	1	Total	N	O	0	0
			4	1	3		
8	HHH	1	Total	N	O	0	0
			4	1	3		
8	HHH	1	Total	N	O	0	0
			4	1	3		
8	III	1	Total	N	O	0	0
			4	1	3		
8	JJJ	1	Total	N	O	0	0
			4	1	3		

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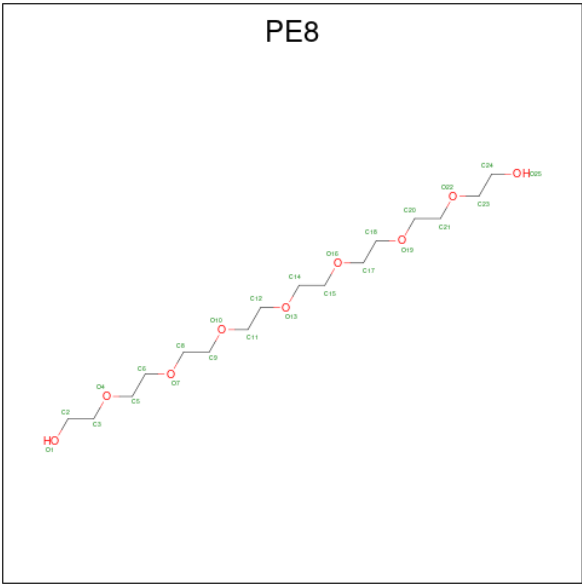
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	JJJ	1	Total	N	O	0	0
			4	1	3		
8	KKK	1	Total	N	O	0	0
			4	1	3		
8	KKK	1	Total	N	O	0	0
			4	1	3		
8	LLL	1	Total	N	O	0	0
			4	1	3		
8	LLL	1	Total	N	O	0	0
			4	1	3		
8	LLL	1	Total	N	O	0	0
			4	1	3		
8	MMM	1	Total	N	O	0	0
			4	1	3		
8	OOO	1	Total	N	O	0	0
			4	1	3		
8	PPP	1	Total	N	O	0	0
			4	1	3		

- Molecule 9 is dodecaethylene glycol monomethyl ether (CCD ID: RWB) (formula: $C_{25}H_{52}O_{13}$).



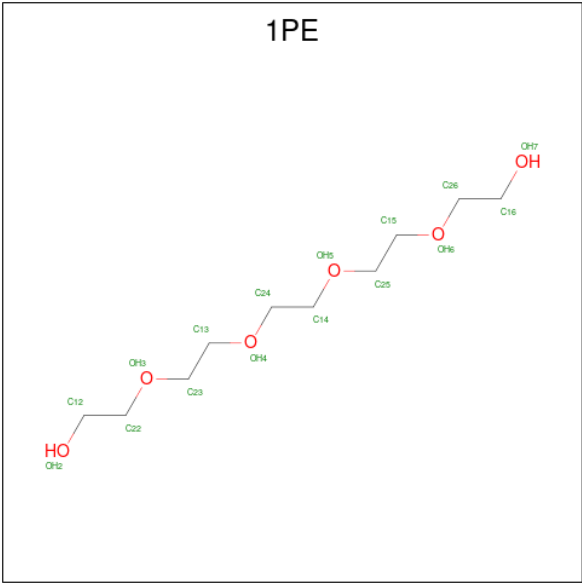
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	BBB	1	Total	C	O	0	0
			38	25	13		
9	LLL	1	Total	C	O	0	0
			38	25	13		

- Molecule 10 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: C₁₆H₃₄O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	BBB	1	Total	C	O	0	0
			25	16	9		

- Molecule 11 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



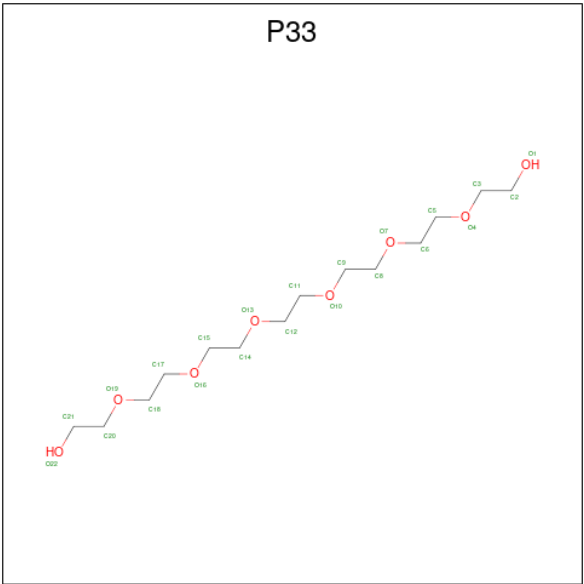
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	BBB	1	Total	C	O	0	0
			16	10	6		

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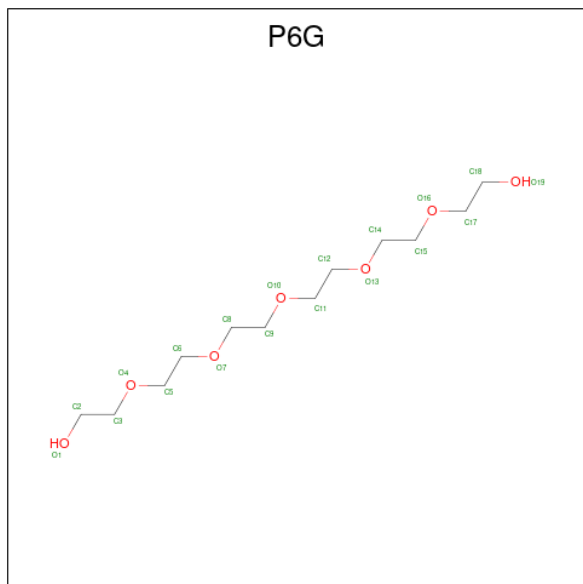
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	BBB	1	Total	C	O	0	0
			16	10	6		
11	BBB	1	Total	C	O	0	0
			16	10	6		
11	DDD	1	Total	C	O	0	0
			16	10	6		
11	EEE	1	Total	C	O	0	0
			16	10	6		
11	FFF	1	Total	C	O	0	0
			16	10	6		
11	HHH	1	Total	C	O	0	0
			16	10	6		
11	JJJ	1	Total	C	O	0	0
			16	10	6		
11	JJJ	1	Total	C	O	0	0
			16	10	6		
11	JJJ	1	Total	C	O	0	0
			16	10	6		
11	LLL	1	Total	C	O	0	0
			16	10	6		
11	PPP	1	Total	C	O	0	0
			16	10	6		

- Molecule 12 is 3,6,9,12,15,18-HEXAIOXAICOSANE-1,20-DIOL (CCD ID: P33) (formula: C₁₄H₃₀O₈).



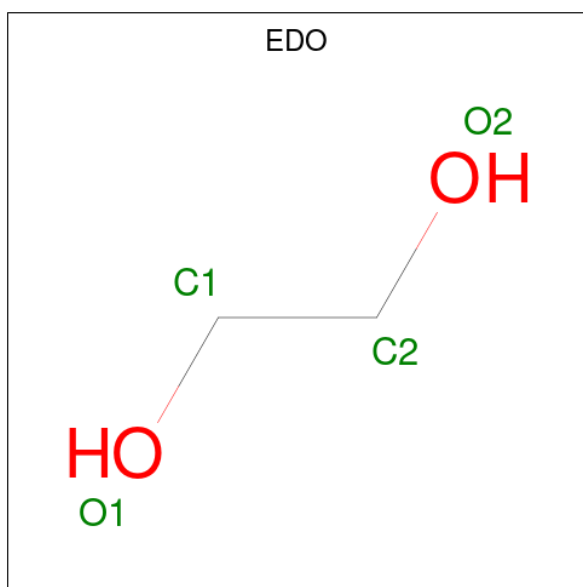
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	DDD	1	Total	C	O	0	0
			22	14	8		
12	DDD	1	Total	C	O	0	0
			22	14	8		
12	FFF	1	Total	C	O	0	0
			22	14	8		
12	HHH	1	Total	C	O	0	0
			22	14	8		
12	HHH	1	Total	C	O	0	0
			22	14	8		
12	JJJ	1	Total	C	O	0	0
			22	14	8		

- Molecule 13 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	DDD	1	Total	C	O	0	0
			19	12	7		

- Molecule 14 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



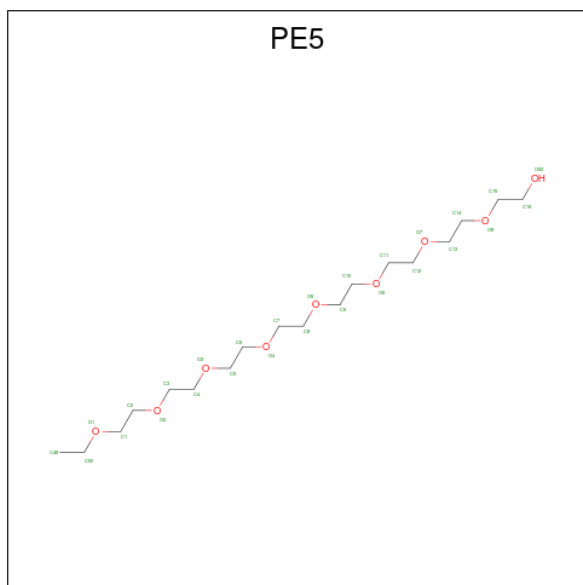
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	DDD	1	Total	C	O	0	0
			4	2	2		
14	DDD	1	Total	C	O	0	0
			4	2	2		
14	EEE	1	Total	C	O	0	0
			4	2	2		
14	EEE	1	Total	C	O	0	0
			4	2	2		
14	FFF	1	Total	C	O	0	0
			4	2	2		
14	FFF	1	Total	C	O	0	0
			4	2	2		
14	HHH	1	Total	C	O	0	0
			4	2	2		
14	HHH	1	Total	C	O	0	0
			4	2	2		
14	III	1	Total	C	O	0	0
			4	2	2		
14	III	1	Total	C	O	0	0
			4	2	2		
14	LLL	1	Total	C	O	0	0
			4	2	2		
14	NNN	1	Total	C	O	0	0
			4	2	2		
14	NNN	1	Total	C	O	0	0
			4	2	2		
14	NNN	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	PPP	1	Total	C	O	0	0
			4	2	2		

- Molecule 15 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (CCD ID: PE5) (formula: C₁₈H₃₈O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	NNN	1	Total	C	O	0	0
			27	18	9		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	AAA	93	Total	O	0	0
			93	93		
16	BBB	90	Total	O	0	0
			90	90		
16	CCC	90	Total	O	0	0
			90	90		
16	DDD	97	Total	O	0	0
			97	97		
16	EEE	82	Total	O	0	0
			82	82		
16	FFF	110	Total	O	0	0
			110	110		
16	GGG	77	Total	O	0	0
			77	77		

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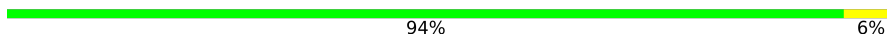
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	HHH	92	Total 92	O 92	0	0
16	III	79	Total 79	O 79	0	0
16	JJJ	106	Total 106	O 106	0	0
16	KKK	86	Total 86	O 86	0	0
16	LLL	97	Total 97	O 97	0	0
16	MMM	76	Total 76	O 76	0	0
16	NNN	76	Total 76	O 76	0	0
16	OOO	57	Total 57	O 57	0	0
16	PPP	57	Total 57	O 57	0	0

3 Residue-property plots [i](#)

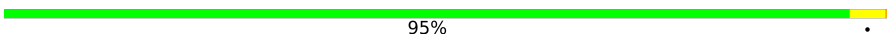
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

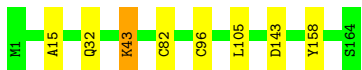
- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain AAA:  94% 6%

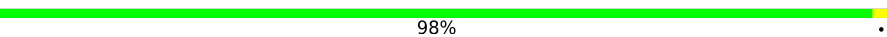


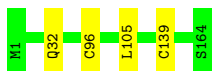
- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain CCC:  95% ..

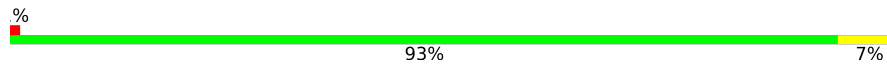


- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain EEE:  98% .



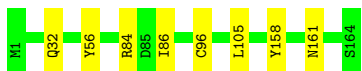
- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain GGG:  93% 7%

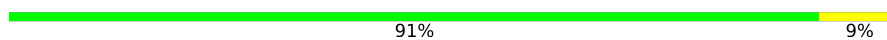


- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain III:  95% 5%

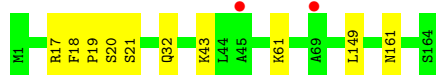


- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

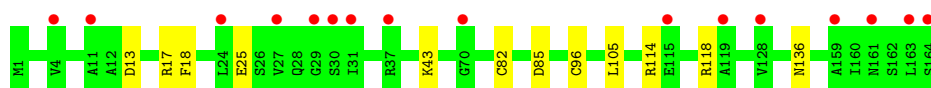
Chain KKK:  91% 9%



- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin



- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin



- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin



- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin



- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin

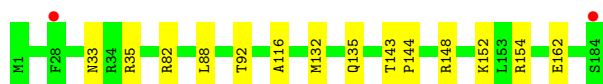


- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin

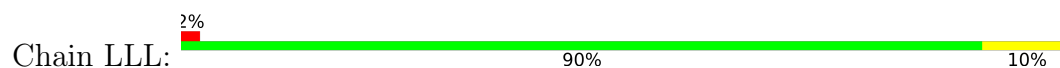


- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin





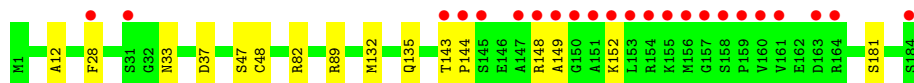
- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin



- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin



- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	192.76Å 192.76Å 524.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.01 – 2.13 49.01 – 2.13	Depositor EDS
% Data completeness (in resolution range)	75.0 (49.01-2.13) 75.0 (49.01-2.13)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.177 , 0.225 0.188 , 0.231	Depositor DCC
R_{free} test set	7767 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26483	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, MEN, RWB, NO3, PEB, PEG, P6G, EDO, PE5, PE8, PG4, P33, 1PE, PO4

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	AAA	1.03	0/1283	1.32	0/1739
1	CCC	0.98	0/1285	1.32	0/1741
1	EEE	0.99	0/1283	1.31	0/1739
1	GGG	1.00	0/1267	1.31	0/1717
1	III	0.99	0/1267	1.33	0/1717
1	KKK	0.99	0/1274	1.32	0/1727
1	MMM	0.98	0/1276	1.33	0/1729
1	OOO	1.05	0/1261	1.33	0/1709
2	BBB	1.02	0/1401	1.33	0/1892
2	DDD	1.02	0/1411	1.32	0/1905
2	FFF	1.03	0/1390	1.31	0/1878
2	HHH	1.01	0/1391	1.31	0/1880
2	JJJ	1.02	0/1402	1.34	0/1894
2	LLL	1.02	0/1407	1.32	1/1900 (0.1%)
2	NNN	1.01	0/1366	1.34	0/1846
2	PPP	1.02	0/1377	1.34	0/1860
All	All	1.01	0/21341	1.32	1/28873 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	LLL	154	ARG	CG-CD-NE	-5.17	100.64	112.00

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	AAA	1257	0	1252	20	0
1	CCC	1256	0	1252	11	0
1	EEE	1254	0	1253	5	0
1	GGG	1244	0	1238	11	0
1	III	1244	0	1238	10	0
1	KKK	1245	0	1248	17	0
1	MMM	1247	0	1245	24	0
1	OOO	1238	0	1234	6	0
2	BBB	1378	0	1410	9	0
2	DDD	1382	0	1420	11	0
2	FFF	1370	0	1397	14	0
2	HHH	1368	0	1394	21	0
2	JJJ	1376	0	1407	13	0
2	LLL	1381	0	1415	19	0
2	NNN	1355	0	1372	11	0
2	PPP	1363	0	1385	18	0
3	AAA	86	0	74	2	0
3	BBB	129	0	110	7	0
3	CCC	86	0	74	3	0
3	DDD	129	0	110	7	0
3	EEE	86	0	74	3	0
3	FFF	129	0	110	5	0
3	GGG	86	0	74	1	0
3	HHH	129	0	110	5	0
3	III	86	0	74	0	0
3	JJJ	129	0	110	3	0
3	KKK	86	0	74	2	0
3	LLL	129	0	110	7	0
3	MMM	86	0	74	5	0
3	NNN	129	0	110	7	0
3	OOO	86	0	74	3	0
3	PPP	129	0	110	13	0
4	AAA	39	0	54	18	0
4	CCC	13	0	18	0	0
4	DDD	26	0	36	0	0
4	FFF	52	0	72	5	0
4	GGG	39	0	54	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	HHH	26	0	36	2	0
4	JJJ	13	0	18	3	0
4	KKK	39	0	54	2	0
4	LLL	39	0	54	2	0
4	MMM	52	0	72	24	0
4	NNN	65	0	90	2	0
4	OOO	13	0	18	0	0
4	PPP	26	0	36	3	0
5	AAA	60	0	84	1	0
5	BBB	30	0	42	0	0
5	CCC	50	0	70	3	0
5	DDD	30	0	42	0	0
5	EEE	40	0	56	0	0
5	FFF	30	0	42	6	0
5	GGG	40	0	56	4	0
5	HHH	60	0	84	6	0
5	III	40	0	56	5	0
5	JJJ	30	0	42	0	0
5	KKK	20	0	28	1	0
5	LLL	40	0	56	7	0
5	MMM	20	0	28	0	0
5	NNN	40	0	56	2	0
5	OOO	30	0	42	0	0
5	PPP	10	0	14	0	0
6	AAA	14	0	20	0	0
6	BBB	49	0	70	0	0
6	CCC	63	0	90	7	0
6	DDD	35	0	50	1	0
6	EEE	14	0	20	0	0
6	FFF	35	0	50	0	0
6	GGG	35	0	50	0	0
6	HHH	35	0	50	1	0
6	III	42	0	60	1	0
6	JJJ	21	0	30	1	0
6	KKK	35	0	50	6	0
6	LLL	63	0	90	0	0
6	MMM	21	0	30	3	0
6	NNN	21	0	30	3	0
6	OOO	28	0	40	0	0
6	PPP	49	0	70	2	0
7	AAA	10	0	0	0	0
7	BBB	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	CCC	15	0	0	0	0
7	DDD	30	0	0	0	0
7	FFF	25	0	0	0	0
7	GGG	10	0	0	1	0
7	HHH	20	0	0	0	0
7	III	15	0	0	0	0
7	JJJ	30	0	0	0	0
7	KKK	15	0	0	2	0
7	LLL	10	0	0	0	0
7	NNN	25	0	0	0	0
7	OOO	5	0	0	1	0
7	PPP	15	0	0	0	0
8	AAA	8	0	0	0	0
8	BBB	4	0	0	0	0
8	CCC	4	0	0	0	0
8	DDD	8	0	0	0	0
8	EEE	8	0	0	0	0
8	FFF	4	0	0	0	0
8	GGG	4	0	0	0	0
8	HHH	8	0	0	0	0
8	III	4	0	0	0	0
8	JJJ	8	0	0	0	0
8	KKK	8	0	0	0	0
8	LLL	12	0	0	0	0
8	MMM	4	0	0	0	0
8	OOO	4	0	0	0	0
8	PPP	4	0	0	0	0
9	BBB	38	0	0	1	0
9	LLL	38	0	0	2	0
10	BBB	25	0	34	0	0
11	BBB	48	0	66	1	0
11	DDD	16	0	22	1	0
11	EEE	16	0	22	0	0
11	FFF	16	0	22	1	0
11	HHH	16	0	22	3	0
11	JJJ	48	0	66	2	0
11	LLL	16	0	22	0	0
11	PPP	16	0	22	0	0
12	DDD	44	0	60	2	0
12	FFF	22	0	30	2	0
12	HHH	44	0	60	3	0
12	JJJ	22	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	DDD	19	0	26	2	0
14	DDD	8	0	12	0	0
14	EEE	8	0	12	0	0
14	FFF	8	0	12	0	0
14	HHH	8	0	12	0	0
14	III	8	0	12	0	0
14	LLL	4	0	6	0	0
14	NNN	12	0	18	0	0
14	PPP	4	0	6	0	0
15	NNN	27	0	38	6	0
16	AAA	93	0	0	0	0
16	BBB	90	0	0	2	0
16	CCC	90	0	0	0	0
16	DDD	97	0	0	1	0
16	EEE	82	0	0	0	0
16	FFF	110	0	0	2	0
16	GGG	77	0	0	0	0
16	HHH	92	0	0	1	0
16	III	79	0	0	0	0
16	JJJ	106	0	0	1	0
16	KKK	86	0	0	3	0
16	LLL	97	0	0	1	0
16	MMM	76	0	0	0	0
16	NNN	76	0	0	3	0
16	OOO	57	0	0	0	0
16	PPP	57	0	0	1	0
All	All	26483	0	25474	273	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.

The worst 5 of 273 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:AAA:47:ASN:HA	4:AAA:203:PG4:H52	1.34	1.08
1:GGG:49:ASP:HB2	5:GGG:208:PGE:H1	1.28	1.08
1:AAA:49:ASP:HB2	4:AAA:203:PG4:H61	1.47	0.93
1:CCC:32[A]:GLN:HG3	1:EEE:32[A]:GLN:HG3	1.50	0.91
1:GGG:32:GLN:HG3	1:III:32:GLN:HG3	1.55	0.88

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	165/164 (101%)	162 (98%)	3 (2%)	0	100	100
1	CCC	165/164 (101%)	162 (98%)	3 (2%)	0	100	100
1	EEE	165/164 (101%)	162 (98%)	3 (2%)	0	100	100
1	GGG	163/164 (99%)	160 (98%)	3 (2%)	0	100	100
1	III	163/164 (99%)	160 (98%)	3 (2%)	0	100	100
1	KKK	164/164 (100%)	161 (98%)	3 (2%)	0	100	100
1	MMM	164/164 (100%)	161 (98%)	3 (2%)	0	100	100
1	OOO	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
2	BBB	188/184 (102%)	184 (98%)	4 (2%)	0	100	100
2	DDD	190/184 (103%)	186 (98%)	4 (2%)	0	100	100
2	FFF	187/184 (102%)	183 (98%)	4 (2%)	0	100	100
2	HHH	188/184 (102%)	183 (97%)	5 (3%)	0	100	100
2	JJJ	189/184 (103%)	184 (97%)	5 (3%)	0	100	100
2	LLL	189/184 (103%)	185 (98%)	4 (2%)	0	100	100
2	NNN	184/184 (100%)	180 (98%)	4 (2%)	0	100	100
2	PPP	185/184 (100%)	181 (98%)	4 (2%)	0	100	100
All	All	2811/2784 (101%)	2753 (98%)	58 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	128/124 (103%)	128 (100%)	0	100	100
1	CCC	128/124 (103%)	127 (99%)	1 (1%)	73	79
1	EEE	128/124 (103%)	128 (100%)	0	100	100
1	GGG	126/124 (102%)	124 (98%)	2 (2%)	55	61
1	III	126/124 (102%)	126 (100%)	0	100	100
1	KKK	127/124 (102%)	126 (99%)	1 (1%)	73	79
1	MMM	127/124 (102%)	127 (100%)	0	100	100
1	OOO	125/124 (101%)	121 (97%)	4 (3%)	34	35
2	BBB	145/138 (105%)	145 (100%)	0	100	100
2	DDD	147/138 (106%)	145 (99%)	2 (1%)	59	65
2	FFF	144/138 (104%)	144 (100%)	0	100	100
2	HHH	145/138 (105%)	145 (100%)	0	100	100
2	JJJ	146/138 (106%)	143 (98%)	3 (2%)	47	51
2	LLL	146/138 (106%)	146 (100%)	0	100	100
2	NNN	141/138 (102%)	140 (99%)	1 (1%)	76	81
2	PPP	142/138 (103%)	140 (99%)	2 (1%)	59	65
All	All	2171/2096 (104%)	2155 (99%)	16 (1%)	78	81

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	PPP	47	SER
1	OOO	118	ARG
1	KKK	43	LYS
1	OOO	114	ARG
2	JJJ	162	GLU

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MEN	HHH	70	2	7,8,9	0.59	0	4,9,11	0.78	0
2	MEN	NNN	70	2	7,8,9	0.71	0	4,9,11	0.41	0
2	MEN	FFF	70	2	7,8,9	0.61	0	4,9,11	0.73	0
2	MEN	DDD	70	2	7,8,9	0.72	0	4,9,11	0.80	0
2	MEN	PPP	70	2	7,8,9	0.74	0	4,9,11	0.29	0
2	MEN	BBB	70	2	7,8,9	0.68	0	4,9,11	0.84	0
2	MEN	LLL	70	2	7,8,9	0.65	0	4,9,11	0.37	0
2	MEN	JJJ	70	2	7,8,9	0.59	0	4,9,11	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	HHH	70	2	-	2/7/8/10	-
2	MEN	NNN	70	2	-	2/7/8/10	-
2	MEN	FFF	70	2	-	2/7/8/10	-
2	MEN	DDD	70	2	-	2/7/8/10	-
2	MEN	PPP	70	2	-	2/7/8/10	-
2	MEN	BBB	70	2	-	2/7/8/10	-
2	MEN	LLL	70	2	-	2/7/8/10	-
2	MEN	JJJ	70	2	-	2/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	DDD	70	MEN	CA-CB-CG-ND2
2	FFF	70	MEN	CA-CB-CG-ND2
2	HHH	70	MEN	CA-CB-CG-ND2
2	JJJ	70	MEN	CA-CB-CG-ND2
2	LLL	70	MEN	CA-CB-CG-ND2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	NNN	70	MEN	1	0
2	DDD	70	MEN	1	0
2	LLL	70	MEN	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

321 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	$\# Z > 2$
5	PGE	JJJ	301	-	9,9,9	0.29	0	8,8,8	0.15	0
5	PGE	III	205	-	9,9,9	0.28	0	8,8,8	0.08	0
5	PGE	AAA	206	-	9,9,9	0.49	0	8,8,8	0.35	0
6	PEG	BBB	212	-	6,6,6	0.25	0	5,5,5	0.24	0
7	PO4	KKK	213	-	4,4,4	0.88	0	6,6,6	0.62	0
6	PEG	HHH	314	-	6,6,6	0.16	0	5,5,5	0.08	0
4	PG4	MMM	212	-	12,12,12	0.26	0	11,11,11	0.19	0
6	PEG	HHH	316	-	6,6,6	0.69	0	5,5,5	0.57	0
6	PEG	OOO	209	-	6,6,6	0.30	0	5,5,5	0.18	0
3	PEB	JJJ	305	2	46,46,46	0.98	1 (2%)	56,67,67	0.89	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEB	BBB	202	2	46,46,46	0.97	3 (6%)	56,67,67	1.02	3 (5%)
7	PO4	BBB	218	-	4,4,4	0.75	0	6,6,6	0.35	0
6	PEG	HHH	315	-	6,6,6	0.29	0	5,5,5	0.20	0
7	PO4	PPP	217	-	4,4,4	0.92	0	6,6,6	0.78	0
6	PEG	OOO	208	-	6,6,6	0.27	0	5,5,5	0.14	0
8	NO3	GGG	216	-	1,3,3	0.88	0	0,3,3	-	-
5	PGE	EEE	207	-	9,9,9	0.49	0	8,8,8	0.27	0
8	NO3	BBB	221	-	1,3,3	0.98	0	0,3,3	-	-
3	PEB	III	202	1	46,46,46	1.18	3 (6%)	56,67,67	1.57	6 (10%)
4	PG4	PPP	206	-	12,12,12	0.29	0	11,11,11	0.12	0
5	PGE	KKK	206	-	9,9,9	0.51	0	8,8,8	0.27	0
7	PO4	AAA	215	-	4,4,4	0.69	0	6,6,6	0.37	0
5	PGE	EEE	204	-	9,9,9	0.22	0	8,8,8	0.11	0
6	PEG	BBB	213	-	6,6,6	0.25	0	5,5,5	0.07	0
4	PG4	LLL	207	-	12,12,12	0.36	0	11,11,11	0.20	0
3	PEB	AAA	201	1	46,46,46	1.08	4 (8%)	56,67,67	1.47	10 (17%)
3	PEB	OOO	202	1	46,46,46	0.74	1 (2%)	56,67,67	0.89	2 (3%)
5	PGE	JJJ	310	-	9,9,9	0.20	0	8,8,8	0.10	0
8	NO3	HHH	326	-	1,3,3	0.23	0	0,3,3	-	-
14	EDO	NNN	217	-	3,3,3	0.15	0	2,2,2	0.17	0
7	PO4	FFF	220	-	4,4,4	0.94	0	6,6,6	0.40	0
7	PO4	CCC	216	-	4,4,4	0.61	0	6,6,6	0.65	0
11	1PE	HHH	301	-	15,15,15	0.71	0	14,14,14	0.57	0
7	PO4	DDD	220	-	4,4,4	0.87	0	6,6,6	0.59	0
8	NO3	HHH	325	-	1,3,3	1.20	0	0,3,3	-	-
6	PEG	EEE	212	-	6,6,6	0.18	0	5,5,5	0.11	0
7	PO4	BBB	219	-	4,4,4	0.80	0	6,6,6	0.51	0
5	PGE	HHH	309	-	9,9,9	0.35	0	8,8,8	0.42	0
5	PGE	CCC	208	-	9,9,9	0.48	0	8,8,8	0.34	0
6	PEG	CCC	209	-	6,6,6	0.44	0	5,5,5	0.26	0
8	NO3	CCC	218	-	1,3,3	1.16	0	0,3,3	-	-
6	PEG	CCC	213	-	6,6,6	0.23	0	5,5,5	0.09	0
7	PO4	BBB	220	-	4,4,4	0.65	0	6,6,6	0.51	0
7	PO4	NNN	224	-	4,4,4	0.87	0	6,6,6	0.49	0
5	PGE	CCC	206	-	9,9,9	0.28	0	8,8,8	0.25	0
6	PEG	PPP	210	-	6,6,6	0.30	0	5,5,5	0.20	0
8	NO3	PPP	219	-	1,3,3	0.42	0	0,3,3	-	-
5	PGE	III	206	-	9,9,9	0.21	0	8,8,8	0.09	0
5	PGE	LLL	226	-	9,9,9	0.43	0	8,8,8	0.26	0
3	PEB	OOO	201	1	46,46,46	1.22	4 (8%)	56,67,67	1.21	4 (7%)
8	NO3	LLL	223	-	1,3,3	0.07	0	0,3,3	-	-
5	PGE	OOO	205	-	9,9,9	0.25	0	8,8,8	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	HHH	318	-	6,6,6	0.24	0	5,5,5	0.13	0
14	EDO	HHH	320	-	3,3,3	0.17	0	2,2,2	0.27	0
5	PGE	HHH	327	-	9,9,9	0.33	0	8,8,8	0.26	0
7	PO4	DDD	223	-	4,4,4	0.92	0	6,6,6	0.60	0
4	PG4	PPP	207	-	12,12,12	0.23	0	11,11,11	0.22	0
5	PGE	NNN	210	-	9,9,9	0.55	0	8,8,8	0.38	0
14	EDO	NNN	219	-	3,3,3	0.25	0	2,2,2	0.19	0
6	PEG	GGG	213	-	6,6,6	0.17	0	5,5,5	0.19	0
6	PEG	GGG	210	-	6,6,6	0.21	0	5,5,5	0.15	0
6	PEG	OOO	210	-	6,6,6	0.34	0	5,5,5	0.27	0
3	PEB	MMM	201	1	46,46,46	1.14	4 (8%)	56,67,67	1.36	9 (16%)
6	PEG	CCC	212	-	6,6,6	0.30	0	5,5,5	0.16	0
6	PEG	OOO	207	-	6,6,6	0.22	0	5,5,5	0.11	0
4	PG4	GGG	205	-	12,12,12	0.22	0	11,11,11	0.13	0
14	EDO	NNN	218	-	3,3,3	0.10	0	2,2,2	0.01	0
4	PG4	AAA	205	-	12,12,12	0.31	0	11,11,11	0.19	0
6	PEG	PPP	212	-	6,6,6	0.22	0	5,5,5	0.13	0
8	NO3	FFF	225	-	1,3,3	1.15	0	0,3,3	-	-
6	PEG	KKK	209	-	6,6,6	0.24	0	5,5,5	0.27	0
5	PGE	AAA	210	-	9,9,9	0.25	0	8,8,8	0.10	0
6	PEG	BBB	211	-	6,6,6	0.16	0	5,5,5	0.11	0
3	PEB	FFF	206	2	46,46,46	0.74	1 (2%)	56,67,67	1.02	4 (7%)
7	PO4	III	214	-	4,4,4	1.52	1 (25%)	6,6,6	0.69	0
4	PG4	LLL	206	-	12,12,12	0.24	0	11,11,11	0.26	0
11	1PE	BBB	207	-	15,15,15	0.67	0	14,14,14	0.78	0
5	PGE	FFF	213	-	9,9,9	0.40	0	8,8,8	0.41	0
12	P33	FFF	207	-	21,21,21	0.73	0	20,20,20	0.80	0
8	NO3	KKK	216	-	1,3,3	0.41	0	0,3,3	-	-
7	PO4	HHH	323	-	4,4,4	0.51	0	6,6,6	0.57	0
6	PEG	PPP	214	-	6,6,6	0.33	0	5,5,5	0.29	0
7	PO4	JJJ	319	-	4,4,4	0.84	0	6,6,6	0.48	0
5	PGE	BBB	210	-	9,9,9	0.36	0	8,8,8	0.22	0
7	PO4	JJJ	317	-	4,4,4	0.82	0	6,6,6	0.51	0
5	PGE	LLL	225	-	9,9,9	0.31	0	8,8,8	0.20	0
6	PEG	KKK	212	-	6,6,6	0.40	0	5,5,5	0.19	0
14	EDO	PPP	215	-	3,3,3	0.07	0	2,2,2	0.08	0
6	PEG	LLL	212	-	6,6,6	0.22	0	5,5,5	0.10	0
7	PO4	FFF	224	-	4,4,4	0.96	0	6,6,6	0.52	0
6	PEG	LLL	218[B]	-	6,6,6	0.37	0	5,5,5	0.18	0
5	PGE	GGG	217	-	9,9,9	0.30	0	8,8,8	0.20	0
4	PG4	NNN	207	-	12,12,12	0.35	0	11,11,11	0.22	0
7	PO4	NNN	220	-	4,4,4	0.72	0	6,6,6	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PGE	FFF	212	-	9,9,9	0.34	0	8,8,8	0.31	0
5	PGE	HHH	313	-	9,9,9	0.34	0	8,8,8	0.15	0
7	PO4	BBB	217	-	4,4,4	0.93	0	6,6,6	0.48	0
5	PGE	AAA	207	-	9,9,9	0.25	0	8,8,8	0.21	0
3	PEB	BBB	203	2	46,46,46	0.85	1 (2%)	56,67,67	1.04	4 (7%)
6	PEG	HHH	317	-	6,6,6	0.40	0	5,5,5	0.21	0
4	PG4	AAA	204	-	12,12,12	0.30	0	11,11,11	0.22	0
7	PO4	LLL	220	-	4,4,4	1.00	0	6,6,6	0.44	0
4	PG4	FFF	210	-	12,12,12	0.40	0	11,11,11	0.23	0
3	PEB	GGG	202	1	46,46,46	0.80	1 (2%)	56,67,67	1.01	4 (7%)
4	PG4	KKK	204	-	12,12,12	0.17	0	11,11,11	0.21	0
8	NO3	DDD	226	-	1,3,3	0.38	0	0,3,3	-	-
14	EDO	DDD	217	-	3,3,3	0.37	0	2,2,2	0.34	0
6	PEG	JJJ	313	-	6,6,6	0.35	0	5,5,5	0.19	0
14	EDO	III	217	-	3,3,3	0.20	0	2,2,2	0.19	0
6	PEG	LLL	213	-	6,6,6	0.36	0	5,5,5	0.30	0
6	PEG	KKK	211	-	6,6,6	0.20	0	5,5,5	0.14	0
6	PEG	FFF	217	-	6,6,6	0.17	0	5,5,5	0.11	0
7	PO4	NNN	223	-	4,4,4	0.90	0	6,6,6	0.54	0
8	NO3	JJJ	320	-	1,3,3	0.74	0	0,3,3	-	-
7	PO4	OOO	211	-	4,4,4	0.51	0	6,6,6	0.53	0
6	PEG	JJJ	312	-	6,6,6	0.24	0	5,5,5	0.09	0
6	PEG	MMM	208	-	6,6,6	0.11	0	5,5,5	0.27	0
7	PO4	DDD	224	-	4,4,4	0.84	0	6,6,6	0.52	0
7	PO4	CCC	220	-	4,4,4	1.32	1 (25%)	6,6,6	0.27	0
4	PG4	DDD	209	-	12,12,12	0.30	0	11,11,11	0.21	0
5	PGE	III	207	-	9,9,9	0.43	0	8,8,8	0.25	0
14	EDO	EEE	208	-	3,3,3	0.20	0	2,2,2	0.38	0
3	PEB	DDD	202	2	46,46,46	0.81	1 (2%)	56,67,67	0.94	1 (1%)
9	RWB	LLL	204	-	37,37,37	0.96	0	36,36,36	0.82	0
7	PO4	PPP	218	-	4,4,4	0.59	0	6,6,6	0.60	0
3	PEB	HHH	303	2	46,46,46	0.98	3 (6%)	56,67,67	1.08	3 (5%)
7	PO4	III	216	-	4,4,4	1.01	0	6,6,6	0.46	0
5	PGE	CCC	205	-	9,9,9	0.23	0	8,8,8	0.14	0
6	PEG	MMM	209	-	6,6,6	0.56	0	5,5,5	0.33	0
5	PGE	MMM	207	-	9,9,9	0.25	0	8,8,8	0.12	0
6	PEG	EEE	213	-	6,6,6	0.22	0	5,5,5	0.13	0
6	PEG	III	208	-	6,6,6	0.22	0	5,5,5	0.16	0
7	PO4	PPP	216	-	4,4,4	0.35	0	6,6,6	0.66	0
6	PEG	MMM	210	-	6,6,6	0.29	0	5,5,5	0.21	0
6	PEG	LLL	214	-	6,6,6	0.16	0	5,5,5	0.13	0
8	NO3	AAA	216	-	1,3,3	1.16	0	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEB	PPP	203	2	46,46,46	0.89	2 (4%)	56,67,67	1.05	4 (7%)
7	PO4	NNN	222	-	4,4,4	0.59	0	6,6,6	0.69	0
12	P33	JJJ	306	-	21,21,21	0.71	0	20,20,20	0.66	0
4	PG4	AAA	203	-	12,12,12	0.39	0	11,11,11	0.21	0
5	PGE	NNN	213	-	9,9,9	0.46	0	8,8,8	0.27	0
7	PO4	HHH	321	-	4,4,4	0.87	0	6,6,6	0.76	0
3	PEB	PPP	202	2	46,46,46	1.13	3 (6%)	56,67,67	1.32	6 (10%)
3	PEB	NNN	204	2	46,46,46	0.89	1 (2%)	56,67,67	1.13	3 (5%)
6	PEG	LLL	211	-	6,6,6	0.44	0	5,5,5	0.39	0
6	PEG	LLL	216	-	6,6,6	0.30	0	5,5,5	0.28	0
5	PGE	AAA	211	-	9,9,9	0.22	0	8,8,8	0.38	0
8	NO3	AAA	217	-	1,3,3	0.53	0	0,3,3	-	-
11	1PE	BBB	208	-	15,15,15	0.68	0	14,14,14	0.56	0
7	PO4	JJJ	318	-	4,4,4	0.62	0	6,6,6	0.59	0
5	PGE	CCC	207	-	9,9,9	0.32	0	8,8,8	0.25	0
14	EDO	III	213	-	3,3,3	0.21	0	2,2,2	0.18	0
4	PG4	KKK	203	-	12,12,12	0.27	0	11,11,11	0.09	0
6	PEG	FFF	218	-	6,6,6	0.44	0	5,5,5	0.31	0
4	PG4	FFF	208	-	12,12,12	0.30	0	11,11,11	0.20	0
5	PGE	CCC	204	-	9,9,9	0.30	0	8,8,8	0.32	0
5	PGE	AAA	209	-	9,9,9	0.40	0	8,8,8	0.24	0
7	PO4	FFF	221	-	4,4,4	0.89	0	6,6,6	0.72	0
3	PEB	III	203	1	46,46,46	0.77	1 (2%)	56,67,67	1.03	2 (3%)
6	PEG	BBB	214	-	6,6,6	0.26	0	5,5,5	0.14	0
7	PO4	FFF	222	-	4,4,4	0.94	0	6,6,6	0.54	0
6	PEG	NNN	215	-	6,6,6	0.24	0	5,5,5	0.12	0
3	PEB	FFF	204	2	46,46,46	0.94	4 (8%)	56,67,67	1.26	6 (10%)
7	PO4	DDD	222	-	4,4,4	0.77	0	6,6,6	0.56	0
6	PEG	CCC	219	-	6,6,6	0.25	0	5,5,5	0.15	0
4	PG4	CCC	203	-	12,12,12	0.38	0	11,11,11	0.19	0
6	PEG	BBB	216	-	6,6,6	0.31	0	5,5,5	0.15	0
3	PEB	HHH	304	2	46,46,46	0.73	1 (2%)	56,67,67	1.02	2 (3%)
5	PGE	LLL	209	-	9,9,9	0.30	0	8,8,8	0.13	0
14	EDO	FFF	219	-	3,3,3	0.22	0	2,2,2	0.32	0
6	PEG	GGG	209	-	6,6,6	0.23	0	5,5,5	0.15	0
5	PGE	PPP	208	-	9,9,9	0.17	0	8,8,8	0.17	0
14	EDO	HHH	319	-	3,3,3	0.40	0	2,2,2	0.41	0
11	1PE	DDD	207	-	15,15,15	0.78	0	14,14,14	0.51	0
6	PEG	LLL	215	-	6,6,6	0.32	0	5,5,5	0.21	0
3	PEB	EEE	202	1	46,46,46	0.82	0	56,67,67	1.08	4 (7%)
5	PGE	MMM	206	-	9,9,9	0.33	0	8,8,8	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	AAA	213	-	6,6,6	0.14	0	5,5,5	0.09	0
12	P33	DDD	204	-	21,21,21	0.72	0	20,20,20	0.98	1 (5%)
6	PEG	PPP	201	-	6,6,6	0.23	0	5,5,5	0.14	0
6	PEG	PPP	211	-	6,6,6	0.52	0	5,5,5	0.33	0
4	PG4	NNN	201	-	12,12,12	0.24	0	11,11,11	0.25	0
8	NO3	KKK	217	-	1,3,3	0.12	0	0,3,3	-	-
3	PEB	LLL	202	2	46,46,46	0.89	1 (2%)	56,67,67	0.93	1 (1%)
6	PEG	CCC	214	-	6,6,6	0.20	0	5,5,5	0.09	0
6	PEG	III	209	-	6,6,6	0.19	0	5,5,5	0.22	0
4	PG4	HHH	307	-	12,12,12	0.30	0	11,11,11	0.16	0
10	PE8	BBB	205	-	24,24,24	0.50	0	23,23,23	0.37	0
12	P33	DDD	205	-	21,21,21	0.83	0	20,20,20	1.04	0
6	PEG	CCC	211	-	6,6,6	0.19	0	5,5,5	0.13	0
5	PGE	EEE	206	-	9,9,9	0.26	0	8,8,8	0.07	0
7	PO4	GGG	214	-	4,4,4	0.52	0	6,6,6	0.61	0
8	NO3	EEE	211	-	1,3,3	0.02	0	0,3,3	-	-
4	PG4	NNN	208	-	12,12,12	0.37	0	11,11,11	0.21	0
8	NO3	EEE	210	-	1,3,3	0.83	0	0,3,3	-	-
5	PGE	HHH	311	-	9,9,9	0.29	0	8,8,8	0.18	0
4	PG4	OOO	203	-	12,12,12	0.31	0	11,11,11	0.19	0
5	PGE	DDD	212	-	9,9,9	0.46	0	8,8,8	0.29	0
11	1PE	JJJ	307	-	15,15,15	0.77	0	14,14,14	0.95	0
11	1PE	JJJ	308	-	15,15,15	0.73	0	14,14,14	0.59	0
3	PEB	DDD	203	2	46,46,46	0.80	0	56,67,67	1.09	5 (8%)
3	PEB	AAA	202	1	46,46,46	0.90	1 (2%)	56,67,67	1.11	6 (10%)
6	PEG	III	212	-	6,6,6	0.40	0	5,5,5	0.17	0
6	PEG	PPP	213	-	6,6,6	0.43	0	5,5,5	0.30	0
3	PEB	BBB	201	2	46,46,46	0.99	3 (6%)	56,67,67	1.29	8 (14%)
4	PG4	JJJ	309	-	12,12,12	0.16	0	11,11,11	0.27	0
5	PGE	OOO	206	-	9,9,9	0.27	0	8,8,8	0.13	0
6	PEG	DDD	215	-	6,6,6	0.22	0	5,5,5	0.12	0
7	PO4	NNN	221	-	4,4,4	0.67	0	6,6,6	0.61	0
3	PEB	NNN	205	2	46,46,46	0.81	1 (2%)	56,67,67	0.91	1 (1%)
8	NO3	LLL	224	-	1,3,3	0.10	0	0,3,3	-	-
6	PEG	LLL	218[A]	-	6,6,6	0.32	0	5,5,5	0.15	0
8	NO3	OOO	212	-	1,3,3	0.07	0	0,3,3	-	-
4	PG4	GGG	203	-	12,12,12	0.25	0	11,11,11	0.15	0
3	PEB	NNN	203	2	46,46,46	0.87	2 (4%)	56,67,67	1.33	6 (10%)
6	PEG	CCC	221	-	6,6,6	0.14	0	5,5,5	0.04	0
6	PEG	BBB	215	-	6,6,6	0.29	0	5,5,5	0.16	0
5	PGE	GGG	208	-	9,9,9	0.50	0	8,8,8	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	AAA	212	-	6,6,6	0.10	0	5,5,5	0.14	0
3	PEB	EEE	201	1	46,46,46	0.91	2 (4%)	56,67,67	1.33	7 (12%)
4	PG4	KKK	205	-	12,12,12	0.31	0	11,11,11	0.13	0
4	PG4	MMM	205	-	12,12,12	0.33	0	11,11,11	0.16	0
6	PEG	CCC	215	-	6,6,6	0.26	0	5,5,5	0.22	0
5	PGE	GGG	206	-	9,9,9	0.36	0	8,8,8	0.19	0
11	1PE	FFF	201	-	15,15,15	0.63	0	14,14,14	0.85	0
5	PGE	DDD	211	-	9,9,9	0.29	0	8,8,8	0.13	0
3	PEB	HHH	302	2	46,46,46	0.94	2 (4%)	56,67,67	1.21	8 (14%)
7	PO4	GGG	215	-	4,4,4	0.75	0	6,6,6	0.55	0
5	PGE	HHH	310	-	9,9,9	0.42	0	8,8,8	0.21	0
14	EDO	FFF	203	-	3,3,3	0.26	0	2,2,2	0.16	0
4	PG4	LLL	208	-	12,12,12	0.30	0	11,11,11	0.11	0
3	PEB	GGG	201	1	46,46,46	1.08	3 (6%)	56,67,67	1.30	7 (12%)
3	PEB	CCC	202	1	46,46,46	0.91	2 (4%)	56,67,67	1.19	5 (8%)
6	PEG	KKK	208	-	6,6,6	0.43	0	5,5,5	0.49	0
8	NO3	MMM	211	-	1,3,3	0.64	0	0,3,3	-	-
13	P6G	DDD	206	-	18,18,18	0.69	0	17,17,17	0.68	0
7	PO4	LLL	221	-	4,4,4	1.18	0	6,6,6	0.71	0
3	PEB	JJJ	303	2	46,46,46	1.07	4 (8%)	56,67,67	1.38	7 (12%)
7	PO4	FFF	223	-	4,4,4	0.71	0	6,6,6	0.62	0
15	PE5	NNN	206	-	26,26,26	0.25	0	25,25,25	0.34	0
6	PEG	DDD	227	-	6,6,6	0.16	0	5,5,5	0.16	0
4	PG4	DDD	208	-	12,12,12	0.40	0	11,11,11	0.24	0
11	1PE	BBB	206	-	15,15,15	0.61	0	14,14,14	0.51	0
8	NO3	JJJ	322	-	1,3,3	0.40	0	0,3,3	-	-
4	PG4	HHH	308	-	12,12,12	0.27	0	11,11,11	0.14	0
6	PEG	CCC	210	-	6,6,6	0.30	0	5,5,5	0.57	0
6	PEG	BBB	223	-	6,6,6	0.20	0	5,5,5	0.11	0
5	PGE	OOO	204	-	9,9,9	0.21	0	8,8,8	0.11	0
8	NO3	LLL	222	-	1,3,3	0.21	0	0,3,3	-	-
3	PEB	JJJ	304	2	46,46,46	0.90	1 (2%)	56,67,67	1.49	5 (8%)
14	EDO	LLL	219	-	3,3,3	0.35	0	2,2,2	0.26	0
5	PGE	HHH	312	-	9,9,9	0.36	0	8,8,8	0.26	0
5	PGE	NNN	212	-	9,9,9	0.34	0	8,8,8	0.43	0
4	PG4	MMM	204	-	12,12,12	0.20	0	11,11,11	0.14	0
6	PEG	GGG	212	-	6,6,6	0.14	0	5,5,5	0.11	0
6	PEG	III	201	-	6,6,6	0.56	0	5,5,5	0.36	0
12	P33	HHH	305	-	21,21,21	0.70	0	20,20,20	0.93	1 (5%)
3	PEB	PPP	204	2	46,46,46	0.88	3 (6%)	56,67,67	1.23	6 (10%)
5	PGE	BBB	222	-	9,9,9	0.32	0	8,8,8	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PO4	DDD	219	-	4,4,4	1.08	0	6,6,6	0.80	0
6	PEG	NNN	214	-	6,6,6	0.39	0	5,5,5	0.36	0
7	PO4	CCC	217	-	4,4,4	0.64	0	6,6,6	0.56	0
4	PG4	NNN	202	-	12,12,12	0.27	0	11,11,11	0.15	0
6	PEG	III	211	-	6,6,6	0.34	0	5,5,5	0.16	0
9	RWB	BBB	204	-	37,37,37	1.22	2 (5%)	36,36,36	1.35	6 (16%)
5	PGE	EEE	205	-	9,9,9	0.21	0	8,8,8	0.23	0
6	PEG	III	210	-	6,6,6	0.14	0	5,5,5	0.17	0
11	1PE	JJJ	302	-	15,15,15	0.93	0	14,14,14	1.12	0
7	PO4	KKK	214	-	4,4,4	0.69	0	6,6,6	0.55	0
4	PG4	FFF	202	-	12,12,12	0.30	0	11,11,11	0.21	0
6	PEG	PPP	209	-	6,6,6	0.17	0	5,5,5	0.20	0
3	PEB	LLL	201	2	46,46,46	0.84	0	56,67,67	1.17	7 (12%)
7	PO4	JJJ	315	-	4,4,4	0.59	0	6,6,6	0.52	0
4	PG4	NNN	209	-	12,12,12	0.33	0	11,11,11	0.16	0
5	PGE	KKK	207	-	9,9,9	0.26	0	8,8,8	0.10	0
5	PGE	LLL	210	-	9,9,9	0.31	0	8,8,8	0.19	0
6	PEG	KKK	210	-	6,6,6	0.50	0	5,5,5	0.39	0
5	PGE	NNN	211	-	9,9,9	0.17	0	8,8,8	0.14	0
6	PEG	NNN	216	-	6,6,6	0.18	0	5,5,5	0.12	0
6	PEG	DDD	214	-	6,6,6	0.18	0	5,5,5	0.10	0
6	PEG	FFF	214	-	6,6,6	0.34	0	5,5,5	0.27	0
6	PEG	LLL	217	-	6,6,6	0.29	0	5,5,5	0.12	0
11	1PE	LLL	205	-	15,15,15	0.72	0	14,14,14	0.35	0
8	NO3	III	218	-	1,3,3	0.34	0	0,3,3	-	-
3	PEB	KKK	202	1	46,46,46	1.01	3 (6%)	56,67,67	1.14	4 (7%)
6	PEG	DDD	216	-	6,6,6	0.41	0	5,5,5	0.30	0
8	NO3	DDD	225	-	1,3,3	1.37	0	0,3,3	-	-
5	PGE	DDD	210	-	9,9,9	0.29	0	8,8,8	0.20	0
5	PGE	JJJ	311	-	9,9,9	0.20	0	8,8,8	0.19	0
3	PEB	CCC	201	1	46,46,46	1.05	3 (6%)	56,67,67	1.10	6 (10%)
7	PO4	KKK	215	-	4,4,4	0.39	0	6,6,6	0.79	0
3	PEB	LLL	203	2	46,46,46	0.83	1 (2%)	56,67,67	0.90	2 (3%)
5	PGE	BBB	209	-	9,9,9	0.32	0	8,8,8	0.14	0
5	PGE	III	204	-	9,9,9	0.44	0	8,8,8	0.47	0
4	PG4	MMM	203	-	12,12,12	0.29	0	11,11,11	0.40	0
7	PO4	DDD	221	-	4,4,4	0.81	0	6,6,6	0.43	0
6	PEG	GGG	211	-	6,6,6	0.32	0	5,5,5	0.21	0
14	EDO	EEE	209	-	3,3,3	0.10	0	2,2,2	0.07	0
7	PO4	HHH	322	-	4,4,4	1.02	0	6,6,6	0.48	0
3	PEB	FFF	205	2	46,46,46	0.74	1 (2%)	56,67,67	0.81	2 (3%)
4	PG4	FFF	209	-	12,12,12	0.34	0	11,11,11	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PO4	JJJ	321	-	4,4,4	1.24	1 (25%)	6,6,6	0.39	0
7	PO4	III	215	-	4,4,4	0.91	0	6,6,6	0.54	0
4	PG4	GGG	204	-	12,12,12	0.50	0	11,11,11	0.35	0
3	PEB	DDD	201	2	46,46,46	1.04	4 (8%)	56,67,67	1.37	8 (14%)
7	PO4	JJJ	316	-	4,4,4	0.88	0	6,6,6	0.61	0
6	PEG	DDD	213	-	6,6,6	0.24	0	5,5,5	0.17	0
7	PO4	HHH	324	-	4,4,4	0.72	0	6,6,6	0.55	0
3	PEB	KKK	201	1	46,46,46	1.12	4 (8%)	56,67,67	1.18	6 (10%)
14	EDO	DDD	218	-	3,3,3	0.16	0	2,2,2	0.10	0
6	PEG	JJJ	314	-	6,6,6	0.43	0	5,5,5	0.29	0
11	1PE	PPP	205	-	15,15,15	0.66	0	14,14,14	0.45	0
5	PGE	GGG	207	-	9,9,9	0.13	0	8,8,8	0.12	0
7	PO4	AAA	214	-	4,4,4	0.72	0	6,6,6	0.47	0
6	PEG	FFF	215	-	6,6,6	0.33	0	5,5,5	0.18	0
12	P33	HHH	306	-	21,21,21	0.79	0	20,20,20	0.64	0
5	PGE	AAA	208	-	9,9,9	0.22	0	8,8,8	0.15	0
3	PEB	MMM	202	1	46,46,46	0.79	0	56,67,67	1.12	4 (7%)
11	1PE	EEE	203	-	15,15,15	1.06	0	14,14,14	1.44	3 (21%)
6	PEG	FFF	216	-	6,6,6	0.10	0	5,5,5	0.13	0
5	PGE	FFF	211	-	9,9,9	0.30	0	8,8,8	0.18	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
5	PGE	JJJ	301	-	-	4/7/7/7	-
3	PEB	HHH	304	2	-	5/26/74/74	0/4/4/4
5	PGE	III	205	-	-	3/7/7/7	-
6	PEG	LLL	212	-	-	3/4/4/4	-
5	PGE	LLL	209	-	-	4/7/7/7	-
14	EDO	FFF	219	-	-	0/1/1/1	-
6	PEG	GGG	209	-	-	2/4/4/4	-
5	PGE	AAA	206	-	-	2/7/7/7	-
4	PG4	DDD	208	-	-	7/10/10/10	-
5	PGE	PPP	208	-	-	3/7/7/7	-
6	PEG	BBB	212	-	-	3/4/4/4	-
6	PEG	DDD	227	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	1PE	BBB	206	-	-	4/13/13/13	-
6	PEG	LLL	218[B]	-	-	3/4/4/4	-
15	PE5	NNN	206	-	-	11/24/24/24	-
6	PEG	HHH	314	-	-	3/4/4/4	-
5	PGE	GGG	217	-	-	5/7/7/7	-
4	PG4	HHH	308	-	-	4/10/10/10	-
4	PG4	MMM	212	-	-	5/10/10/10	-
14	EDO	HHH	319	-	-	1/1/1/1	-
6	PEG	HHH	316	-	-	2/4/4/4	-
4	PG4	NNN	207	-	-	5/10/10/10	-
11	1PE	DDD	207	-	-	9/13/13/13	-
5	PGE	FFF	212	-	-	2/7/7/7	-
5	PGE	HHH	313	-	-	3/7/7/7	-
6	PEG	CCC	210	-	-	4/4/4/4	-
6	PEG	LLL	215	-	-	2/4/4/4	-
3	PEB	EEE	202	1	-	7/26/74/74	0/4/4/4
6	PEG	OOO	209	-	-	2/4/4/4	-
5	PGE	AAA	207	-	-	4/7/7/7	-
3	PEB	JJJ	305	2	-	4/26/74/74	0/4/4/4
6	PEG	BBB	223	-	-	1/4/4/4	-
5	PGE	MMM	206	-	-	4/7/7/7	-
5	PGE	OOO	204	-	-	5/7/7/7	-
3	PEB	BBB	202	2	-	6/26/74/74	0/4/4/4
3	PEB	BBB	203	2	-	6/26/74/74	0/4/4/4
6	PEG	HHH	317	-	-	3/4/4/4	-
4	PG4	AAA	204	-	-	4/10/10/10	-
6	PEG	HHH	315	-	-	4/4/4/4	-
6	PEG	AAA	213	-	-	1/4/4/4	-
3	PEB	JJJ	304	2	-	7/26/74/74	0/4/4/4
6	PEG	OOO	208	-	-	4/4/4/4	-
4	PG4	FFF	210	-	-	5/10/10/10	-
5	PGE	EEE	207	-	-	6/7/7/7	-
14	EDO	LLL	219	-	-	1/1/1/1	-
3	PEB	GGG	202	1	-	6/26/74/74	0/4/4/4
3	PEB	III	202	1	-	5/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	HHH	312	-	-	5/7/7/7	-
4	PG4	KKK	204	-	-	4/10/10/10	-
4	PG4	PPP	206	-	-	7/10/10/10	-
5	PGE	KKK	206	-	-	3/7/7/7	-
12	P33	DDD	204	-	-	9/19/19/19	-
5	PGE	NNN	212	-	-	4/7/7/7	-
14	EDO	DDD	217	-	-	1/1/1/1	-
5	PGE	EEE	204	-	-	4/7/7/7	-
6	PEG	PPP	201	-	-	2/4/4/4	-
6	PEG	PPP	211	-	-	2/4/4/4	-
4	PG4	MMM	204	-	-	6/10/10/10	-
6	PEG	BBB	213	-	-	3/4/4/4	-
4	PG4	LLL	207	-	-	5/10/10/10	-
4	PG4	NNN	201	-	-	3/10/10/10	-
3	PEB	LLL	202	2	-	7/26/74/74	0/4/4/4
3	PEB	AAA	201	1	-	6/26/74/74	0/4/4/4
6	PEG	CCC	214	-	-	1/4/4/4	-
3	PEB	OOO	202	1	-	6/26/74/74	0/4/4/4
6	PEG	GGG	212	-	-	2/4/4/4	-
6	PEG	III	201	-	-	1/4/4/4	-
6	PEG	III	209	-	-	1/4/4/4	-
6	PEG	JJJ	313	-	-	3/4/4/4	-
3	PEB	PPP	204	2	-	6/26/74/74	0/4/4/4
5	PGE	JJJ	310	-	-	4/7/7/7	-
12	P33	HHH	305	-	-	7/19/19/19	-
4	PG4	HHH	307	-	-	7/10/10/10	-
14	EDO	III	217	-	-	1/1/1/1	-
5	PGE	BBB	222	-	-	7/7/7/7	-
6	PEG	LLL	213	-	-	3/4/4/4	-
10	PE8	BBB	205	-	-	8/22/22/22	-
6	PEG	NNN	214	-	-	3/4/4/4	-
14	EDO	NNN	217	-	-	1/1/1/1	-
6	PEG	KKK	211	-	-	2/4/4/4	-
4	PG4	NNN	202	-	-	7/10/10/10	-
6	PEG	III	211	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	1PE	HHH	301	-	-	6/13/13/13	-
6	PEG	FFF	217	-	-	3/4/4/4	-
12	P33	DDD	205	-	-	14/19/19/19	-
6	PEG	CCC	211	-	-	2/4/4/4	-
9	RWB	BBB	204	-	-	18/35/35/35	-
5	PGE	EEE	205	-	-	4/7/7/7	-
6	PEG	III	210	-	-	2/4/4/4	-
11	1PE	JJJ	302	-	-	8/13/13/13	-
4	PG4	FFF	202	-	-	7/10/10/10	-
6	PEG	JJJ	312	-	-	3/4/4/4	-
6	PEG	MMM	208	-	-	3/4/4/4	-
6	PEG	PPP	209	-	-	3/4/4/4	-
6	PEG	EEE	212	-	-	1/4/4/4	-
3	PEB	LLL	201	2	-	10/26/74/74	0/4/4/4
4	PG4	NNN	209	-	-	5/10/10/10	-
5	PGE	HHH	309	-	-	4/7/7/7	-
5	PGE	CCC	208	-	-	4/7/7/7	-
4	PG4	DDD	209	-	-	5/10/10/10	-
5	PGE	EEE	206	-	-	3/7/7/7	-
5	PGE	KKK	207	-	-	5/7/7/7	-
6	PEG	CCC	209	-	-	1/4/4/4	-
5	PGE	LLL	210	-	-	4/7/7/7	-
6	PEG	KKK	210	-	-	2/4/4/4	-
5	PGE	III	207	-	-	6/7/7/7	-
5	PGE	NNN	211	-	-	5/7/7/7	-
6	PEG	NNN	216	-	-	1/4/4/4	-
4	PG4	NNN	208	-	-	7/10/10/10	-
14	EDO	EEE	208	-	-	1/1/1/1	-
6	PEG	DDD	214	-	-	4/4/4/4	-
6	PEG	CCC	213	-	-	3/4/4/4	-
3	PEB	DDD	202	2	-	6/26/74/74	0/4/4/4
6	PEG	FFF	214	-	-	3/4/4/4	-
9	RWB	LLL	204	-	-	16/35/35/35	-
5	PGE	HHH	311	-	-	6/7/7/7	-
6	PEG	LLL	217	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	CCC	206	-	-	4/7/7/7	-
6	PEG	PPP	210	-	-	2/4/4/4	-
3	PEB	HHH	303	2	-	7/26/74/74	0/4/4/4
11	1PE	LLL	205	-	-	4/13/13/13	-
4	PG4	OOO	203	-	-	5/10/10/10	-
5	PGE	DDD	212	-	-	4/7/7/7	-
5	PGE	III	206	-	-	6/7/7/7	-
11	1PE	JJJ	307	-	-	7/13/13/13	-
5	PGE	LLL	226	-	-	5/7/7/7	-
11	1PE	JJJ	308	-	-	8/13/13/13	-
5	PGE	CCC	205	-	-	0/7/7/7	-
3	PEB	OOO	201	1	-	8/26/74/74	0/4/4/4
3	PEB	DDD	203	2	-	2/26/74/74	0/4/4/4
3	PEB	KKK	202	1	-	7/26/74/74	0/4/4/4
3	PEB	AAA	202	1	-	6/26/74/74	0/4/4/4
6	PEG	III	212	-	-	4/4/4/4	-
6	PEG	PPP	213	-	-	2/4/4/4	-
3	PEB	BBB	201	2	-	8/26/74/74	0/4/4/4
5	PGE	MMM	207	-	-	5/7/7/7	-
6	PEG	DDD	216	-	-	1/4/4/4	-
6	PEG	EEE	213	-	-	4/4/4/4	-
6	PEG	MMM	209	-	-	3/4/4/4	-
4	PG4	JJJ	309	-	-	3/10/10/10	-
5	PGE	OOO	205	-	-	3/7/7/7	-
6	PEG	III	208	-	-	3/4/4/4	-
6	PEG	MMM	210	-	-	2/4/4/4	-
6	PEG	HHH	318	-	-	3/4/4/4	-
14	EDO	HHH	320	-	-	0/1/1/1	-
5	PGE	OOO	206	-	-	6/7/7/7	-
6	PEG	LLL	214	-	-	2/4/4/4	-
6	PEG	DDD	215	-	-	3/4/4/4	-
5	PGE	HHH	327	-	-	4/7/7/7	-
3	PEB	NNN	205	2	-	8/26/74/74	0/4/4/4
3	PEB	PPP	203	2	-	5/26/74/74	0/4/4/4
5	PGE	DDD	210	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	P33	JJJ	306	-	-	8/19/19/19	-
4	PG4	AAA	203	-	-	5/10/10/10	-
5	PGE	JJJ	311	-	-	5/7/7/7	-
5	PGE	NNN	213	-	-	5/7/7/7	-
3	PEB	CCC	201	1	-	6/26/74/74	0/4/4/4
4	PG4	PPP	207	-	-	6/10/10/10	-
5	PGE	NNN	210	-	-	5/7/7/7	-
6	PEG	LLL	218[A]	-	-	4/4/4/4	-
3	PEB	LLL	203	2	-	6/26/74/74	0/4/4/4
14	EDO	NNN	219	-	-	0/1/1/1	-
3	PEB	PPP	202	2	-	8/26/74/74	0/4/4/4
6	PEG	GGG	213	-	-	2/4/4/4	-
3	PEB	NNN	204	2	-	8/26/74/74	0/4/4/4
6	PEG	GGG	210	-	-	0/4/4/4	-
6	PEG	OOO	210	-	-	2/4/4/4	-
4	PG4	GGG	203	-	-	7/10/10/10	-
5	PGE	BBB	209	-	-	5/7/7/7	-
3	PEB	NNN	203	2	-	9/26/74/74	0/4/4/4
5	PGE	III	204	-	-	6/7/7/7	-
6	PEG	CCC	221	-	-	4/4/4/4	-
6	PEG	LLL	211	-	-	1/4/4/4	-
6	PEG	BBB	215	-	-	3/4/4/4	-
3	PEB	MMM	201	1	-	6/26/74/74	0/4/4/4
5	PGE	GGG	208	-	-	2/7/7/7	-
4	PG4	MMM	203	-	-	7/10/10/10	-
6	PEG	CCC	212	-	-	3/4/4/4	-
6	PEG	OOO	207	-	-	2/4/4/4	-
4	PG4	GGG	205	-	-	8/10/10/10	-
6	PEG	GGG	211	-	-	1/4/4/4	-
6	PEG	AAA	212	-	-	1/4/4/4	-
3	PEB	EEE	201	1	-	8/26/74/74	0/4/4/4
4	PG4	KKK	205	-	-	7/10/10/10	-
4	PG4	MMM	205	-	-	7/10/10/10	-
14	EDO	NNN	218	-	-	1/1/1/1	-
6	PEG	CCC	215	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	GGG	206	-	-	6/7/7/7	-
5	PGE	AAA	211	-	-	3/7/7/7	-
6	PEG	LLL	216	-	-	2/4/4/4	-
11	1PE	BBB	208	-	-	12/13/13/13	-
5	PGE	CCC	207	-	-	5/7/7/7	-
11	1PE	FFF	201	-	-	2/13/13/13	-
4	PG4	KKK	203	-	-	7/10/10/10	-
6	PEG	FFF	218	-	-	4/4/4/4	-
14	EDO	EEE	209	-	-	1/1/1/1	-
14	EDO	III	213	-	-	1/1/1/1	-
4	PG4	FFF	208	-	-	4/10/10/10	-
4	PG4	AAA	205	-	-	7/10/10/10	-
6	PEG	PPP	212	-	-	2/4/4/4	-
6	PEG	KKK	209	-	-	3/4/4/4	-
3	PEB	FFF	205	2	-	6/26/74/74	0/4/4/4
5	PGE	CCC	204	-	-	4/7/7/7	-
5	PGE	AAA	210	-	-	5/7/7/7	-
4	PG4	FFF	209	-	-	7/10/10/10	-
5	PGE	DDD	211	-	-	5/7/7/7	-
6	PEG	BBB	211	-	-	2/4/4/4	-
3	PEB	HHH	302	2	-	7/26/74/74	0/4/4/4
3	PEB	FFF	206	2	-	6/26/74/74	0/4/4/4
5	PGE	AAA	209	-	-	6/7/7/7	-
4	PG4	GGG	204	-	-	3/10/10/10	-
3	PEB	DDD	201	2	-	7/26/74/74	0/4/4/4
4	PG4	LLL	206	-	-	5/10/10/10	-
11	1PE	BBB	207	-	-	11/13/13/13	-
5	PGE	FFF	213	-	-	5/7/7/7	-
6	PEG	DDD	213	-	-	1/4/4/4	-
3	PEB	III	203	1	-	6/26/74/74	0/4/4/4
12	P33	FFF	207	-	-	8/19/19/19	-
5	PGE	HHH	310	-	-	5/7/7/7	-
14	EDO	FFF	203	-	-	0/1/1/1	-
4	PG4	LLL	208	-	-	6/10/10/10	-
6	PEG	BBB	214	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	NNN	215	-	-	3/4/4/4	-
3	PEB	KKK	201	1	-	6/26/74/74	0/4/4/4
14	EDO	DDD	218	-	-	0/1/1/1	-
3	PEB	GGG	201	1	-	6/26/74/74	0/4/4/4
6	PEG	JJJ	314	-	-	3/4/4/4	-
11	1PE	PPP	205	-	-	10/13/13/13	-
3	PEB	CCC	202	1	-	8/26/74/74	0/4/4/4
6	PEG	PPP	214	-	-	1/4/4/4	-
3	PEB	FFF	204	2	-	6/26/74/74	0/4/4/4
5	PGE	GGG	207	-	-	1/7/7/7	-
5	PGE	BBB	210	-	-	4/7/7/7	-
6	PEG	KKK	208	-	-	2/4/4/4	-
13	P6G	DDD	206	-	-	12/16/16/16	-
5	PGE	LLL	225	-	-	4/7/7/7	-
3	PEB	JJJ	303	2	-	10/26/74/74	0/4/4/4
6	PEG	KKK	212	-	-	2/4/4/4	-
6	PEG	FFF	215	-	-	2/4/4/4	-
6	PEG	CCC	219	-	-	3/4/4/4	-
12	P33	HHH	306	-	-	11/19/19/19	-
5	PGE	AAA	208	-	-	4/7/7/7	-
3	PEB	MMM	202	1	-	6/26/74/74	0/4/4/4
4	PG4	CCC	203	-	-	8/10/10/10	-
11	1PE	EEE	203	-	-	8/13/13/13	-
14	EDO	PPP	215	-	-	1/1/1/1	-
6	PEG	BBB	216	-	-	3/4/4/4	-
6	PEG	FFF	216	-	-	3/4/4/4	-
5	PGE	FFF	211	-	-	3/7/7/7	-

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	III	202	PEB	CHA-C4A	5.29	1.45	1.36
3	OOO	201	PEB	CHA-C4A	5.29	1.45	1.36
3	PPP	202	PEB	CHA-C4A	4.98	1.44	1.36
3	GGG	201	PEB	CHA-C4A	4.48	1.43	1.36
3	MMM	201	PEB	CHA-C4A	4.47	1.43	1.36

The worst 5 of 202 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	III	202	PEB	CHA-C4A-NA	6.79	134.10	125.63
3	PPP	202	PEB	CHC-C1D-ND	-5.48	107.01	113.73
3	NNN	203	PEB	CHC-C1D-ND	-5.35	107.17	113.73
3	AAA	201	PEB	CHA-C4A-NA	5.24	132.18	125.63
3	JJJ	304	PEB	CHA-C4A-NA	5.07	131.96	125.63

There are no chirality outliers.

5 of 1112 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	201	PEB	NA-C4A-CHA-C1B
3	AAA	201	PEB	C3A-C4A-CHA-C1B
3	AAA	202	PEB	NB-C1B-CHA-C4A
3	AAA	202	PEB	C2B-C1B-CHA-C4A
3	BBB	201	PEB	NB-C1B-CHA-C4A

There are no ring outliers.

91 monomers are involved in 222 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	HHH	316	PEG	1	0
3	BBB	202	PEB	4	0
5	KKK	206	PGE	1	0
4	LLL	207	PG4	1	0
3	AAA	201	PEB	1	0
11	HHH	301	1PE	3	0
5	HHH	309	PGE	2	0
5	CCC	208	PGE	1	0
5	LLL	226	PGE	3	0
3	OOO	201	PEB	3	0
4	PPP	207	PG4	3	0
3	MMM	201	PEB	1	0
6	KKK	209	PEG	1	0
3	FFF	206	PEB	1	0
4	LLL	206	PG4	1	0
5	FFF	213	PGE	5	0
12	FFF	207	P33	2	0
6	PPP	214	PEG	2	0
5	LLL	225	PGE	4	0
6	KKK	212	PEG	2	0
5	FFF	212	PGE	1	0

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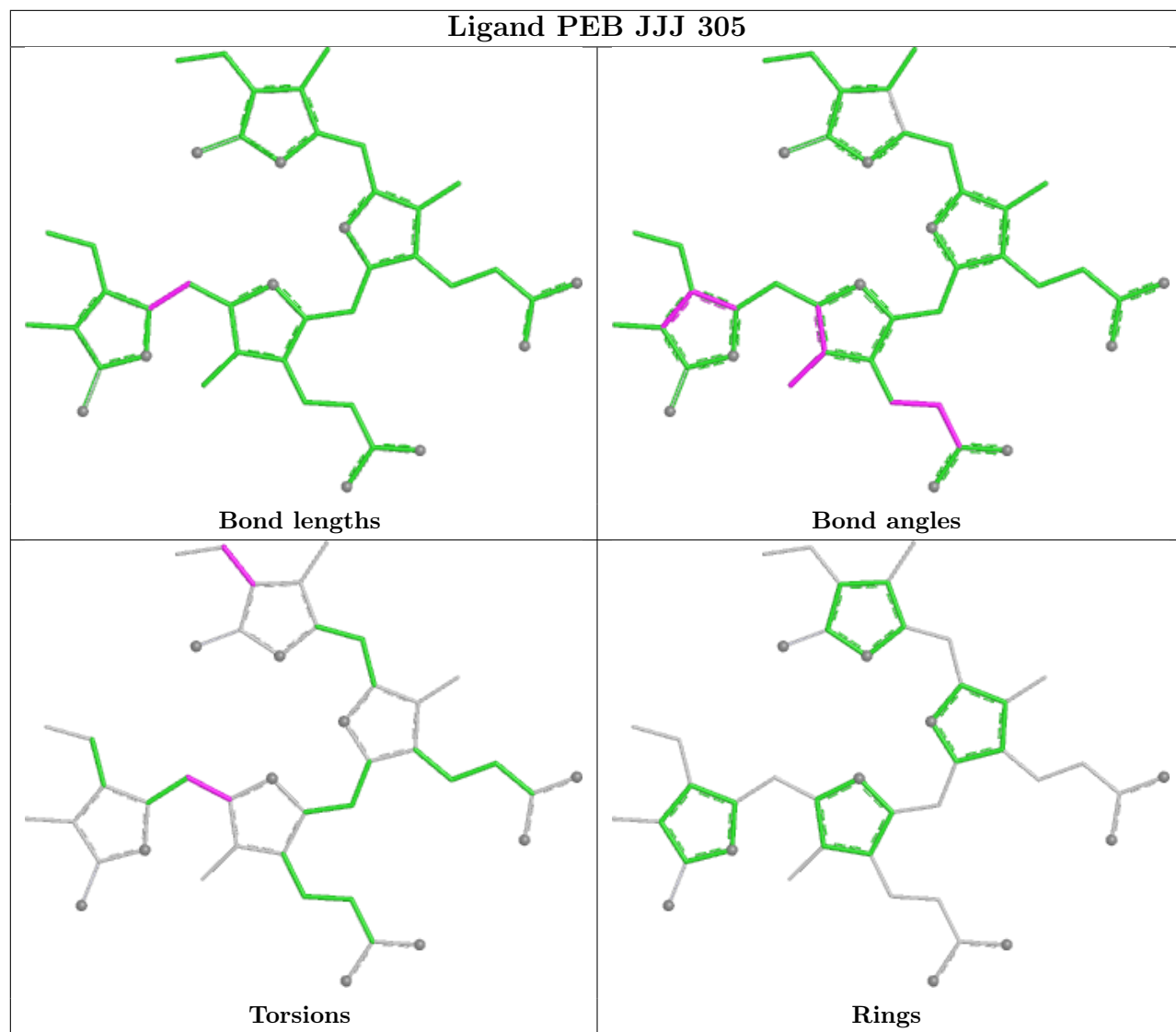
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	207	PGE	1	0
4	AAA	204	PG4	10	0
4	KKK	204	PG4	2	0
7	OOO	211	PO4	1	0
6	JJJ	312	PEG	1	0
3	DDD	202	PEB	4	0
9	LLL	204	RWB	2	0
5	CCC	205	PGE	1	0
6	MMM	209	PEG	2	0
6	MMM	210	PEG	1	0
3	PPP	203	PEB	2	0
12	JJJ	306	P33	4	0
4	AAA	203	PG4	8	0
3	PPP	202	PEB	3	0
3	NNN	204	PEB	3	0
5	CCC	204	PGE	1	0
3	FFF	204	PEB	4	0
3	HHH	304	PEB	2	0
11	DDD	207	1PE	1	0
3	EEE	202	PEB	2	0
12	DDD	204	P33	1	0
4	NNN	201	PG4	1	0
3	LLL	202	PEB	1	0
4	HHH	307	PG4	2	0
12	DDD	205	P33	1	0
7	GGG	214	PO4	1	0
4	NNN	208	PG4	1	0
5	HHH	311	PGE	2	0
11	JJJ	307	1PE	1	0
3	AAA	202	PEB	1	0
3	BBB	201	PEB	3	0
4	JJJ	309	PG4	3	0
3	NNN	205	PEB	2	0
3	NNN	203	PEB	2	0
5	GGG	208	PGE	3	0
3	EEE	201	PEB	1	0
4	MMM	205	PG4	1	0
11	FFF	201	1PE	1	0
3	HHH	302	PEB	3	0
3	GGG	201	PEB	1	0
3	CCC	202	PEB	1	0
6	KKK	208	PEG	3	0

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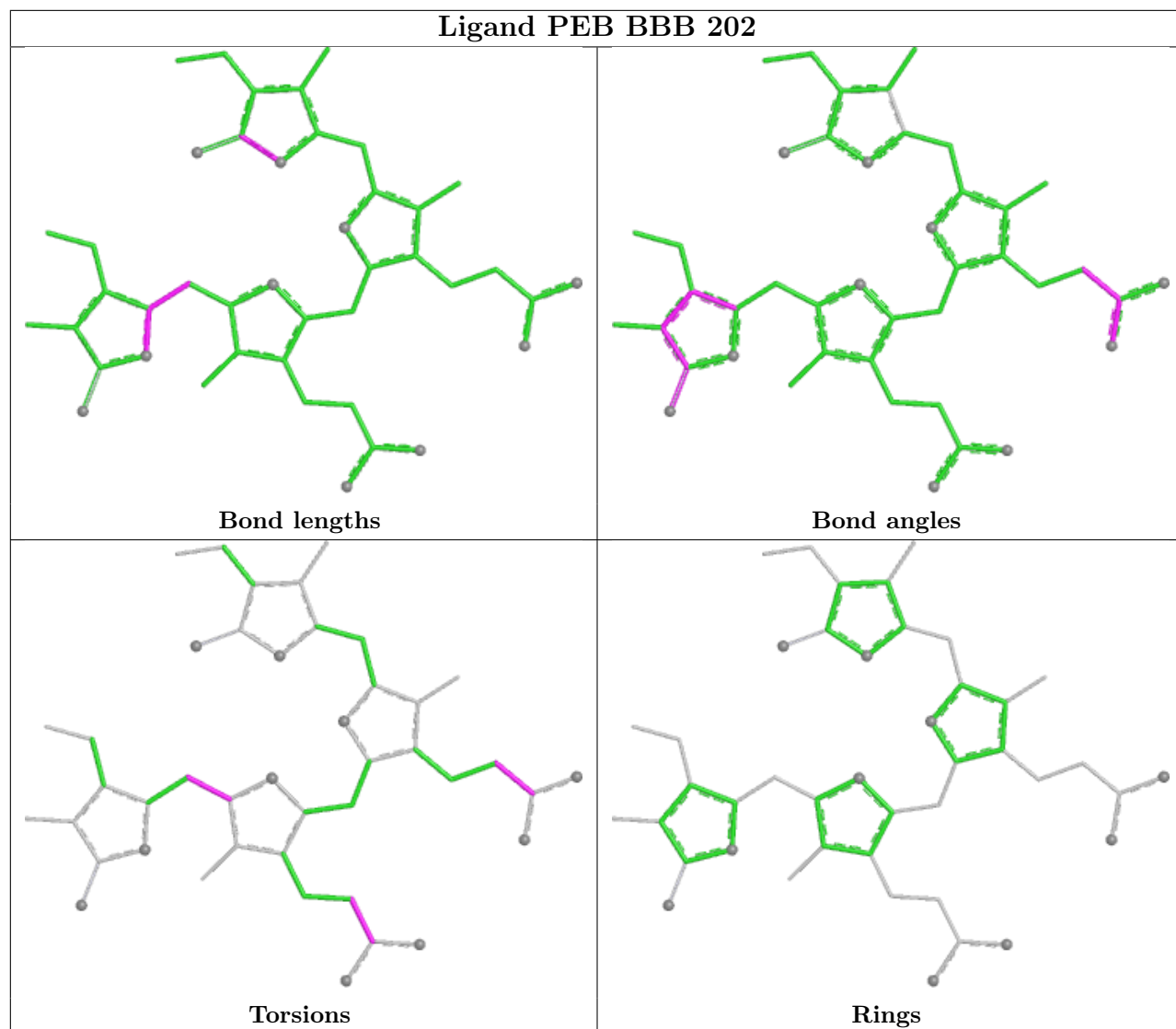
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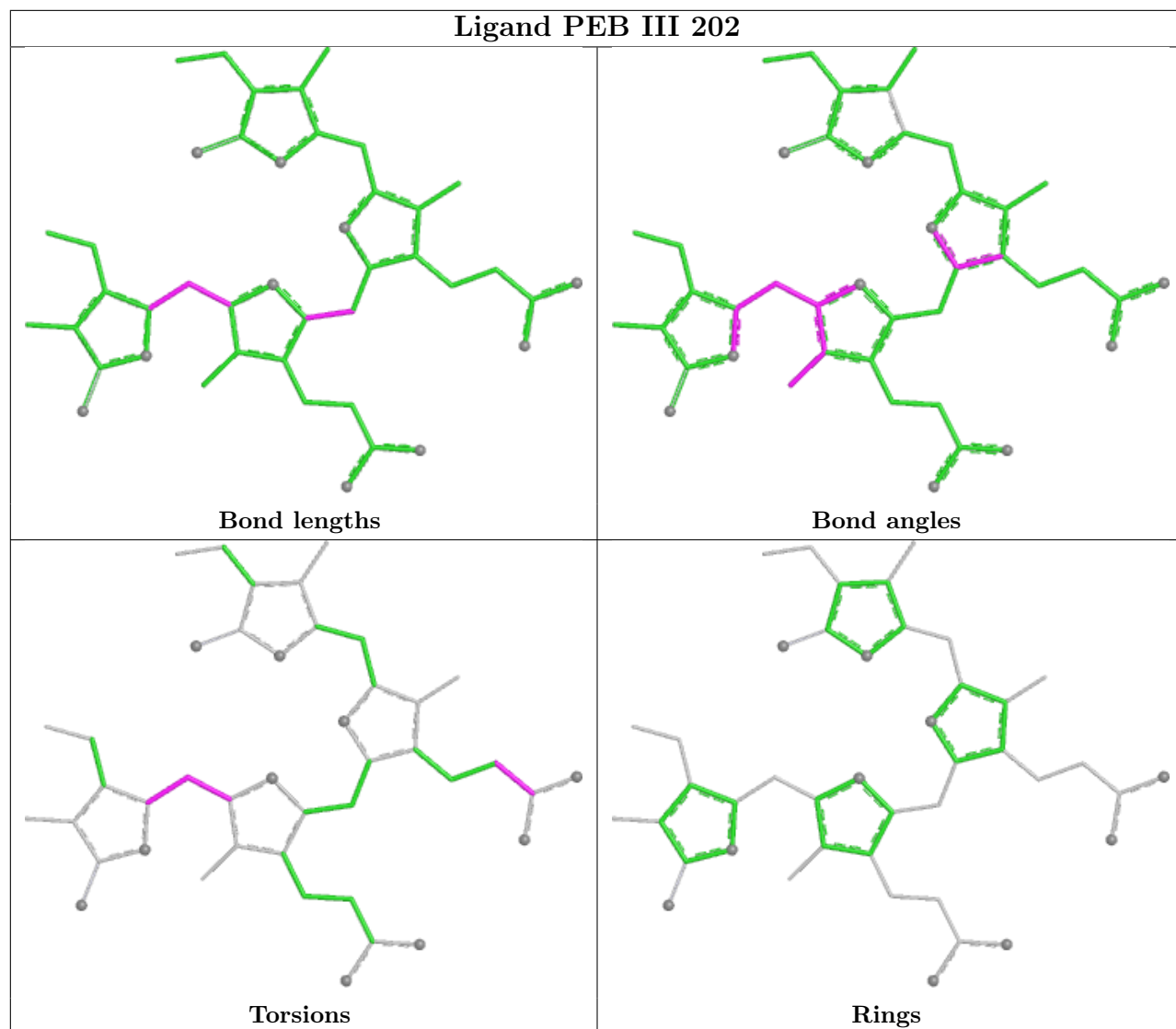
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	DDD	206	P6G	2	0
3	JJJ	303	PEB	2	0
15	NNN	206	PE5	6	0
11	BBB	206	1PE	1	0
6	CCC	210	PEG	7	0
3	JJJ	304	PEB	1	0
5	HHH	312	PGE	2	0
5	NNN	212	PGE	2	0
6	III	201	PEG	1	0
12	HHH	305	P33	3	0
3	PPP	204	PEB	8	0
6	NNN	214	PEG	3	0
9	BBB	204	RWB	1	0
11	JJJ	302	1PE	1	0
4	FFF	202	PG4	1	0
3	LLL	201	PEB	4	0
3	KKK	202	PEB	1	0
3	CCC	201	PEB	2	0
7	KKK	215	PO4	2	0
3	LLL	203	PEB	2	0
5	III	204	PGE	5	0
4	MMM	203	PG4	23	0
4	FFF	209	PG4	4	0
3	DDD	201	PEB	3	0
6	DDD	213	PEG	1	0
3	KKK	201	PEB	1	0
5	GGG	207	PGE	1	0
3	MMM	202	PEB	4	0

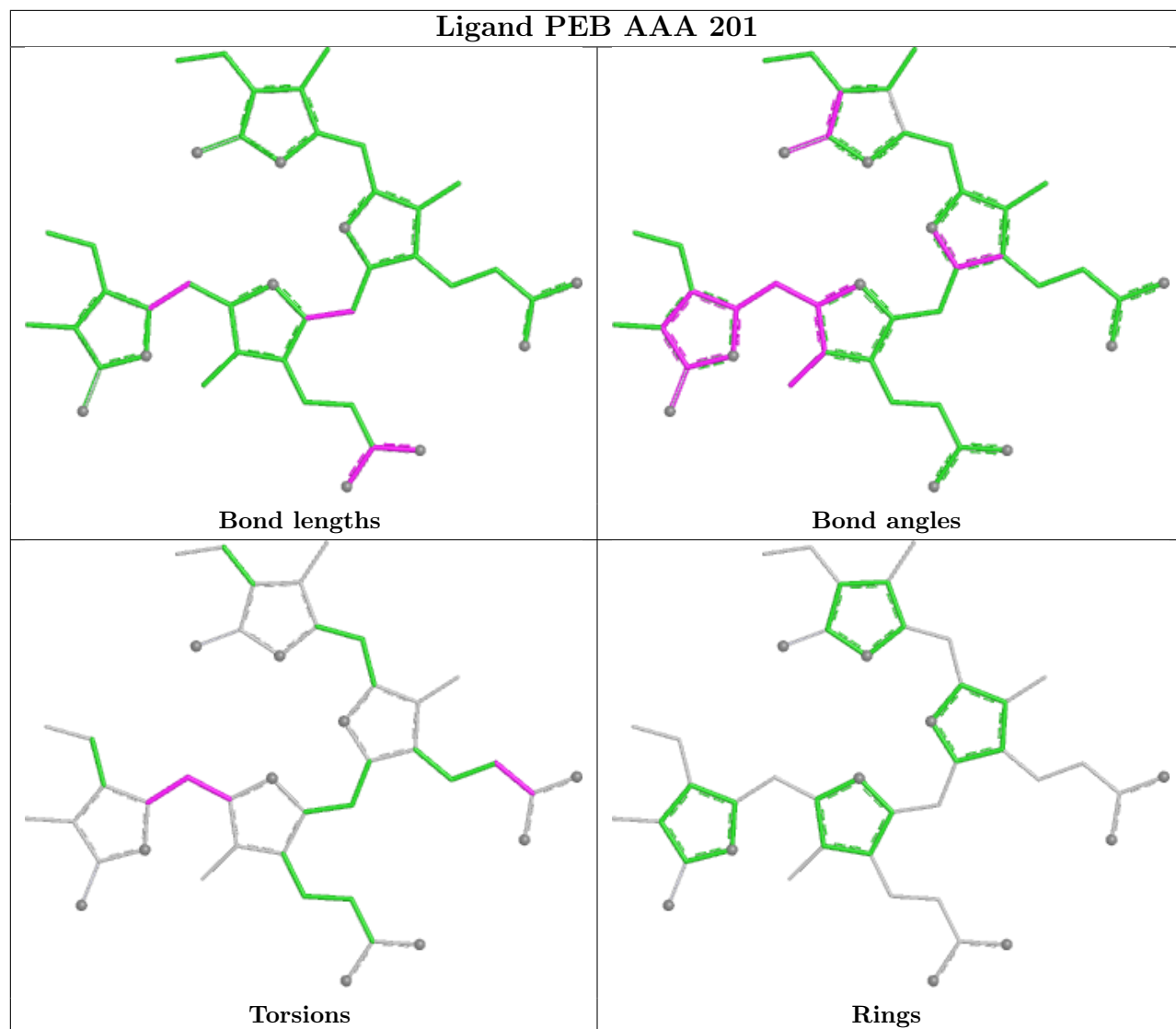
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

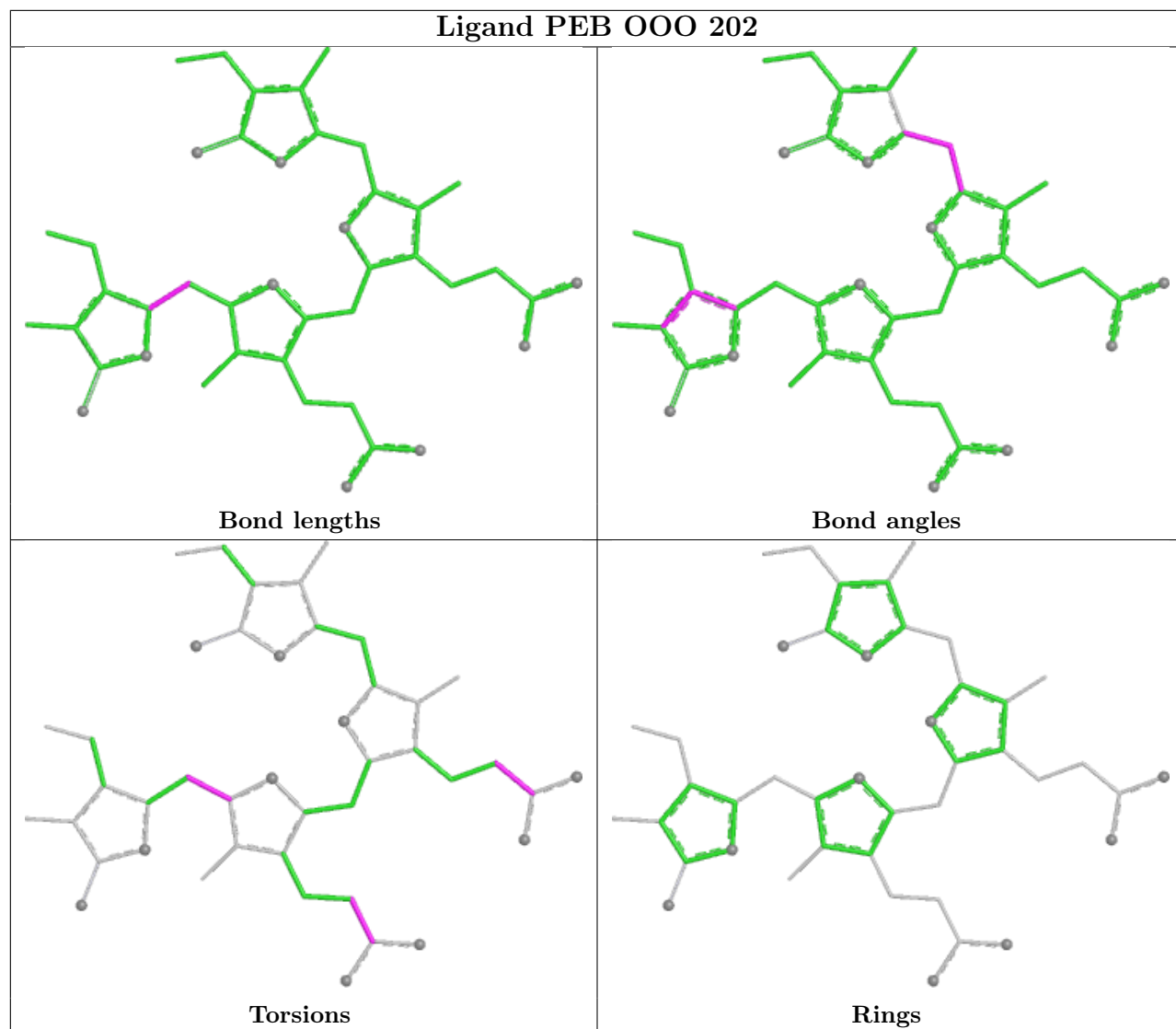


Ligand PEB BBB 202

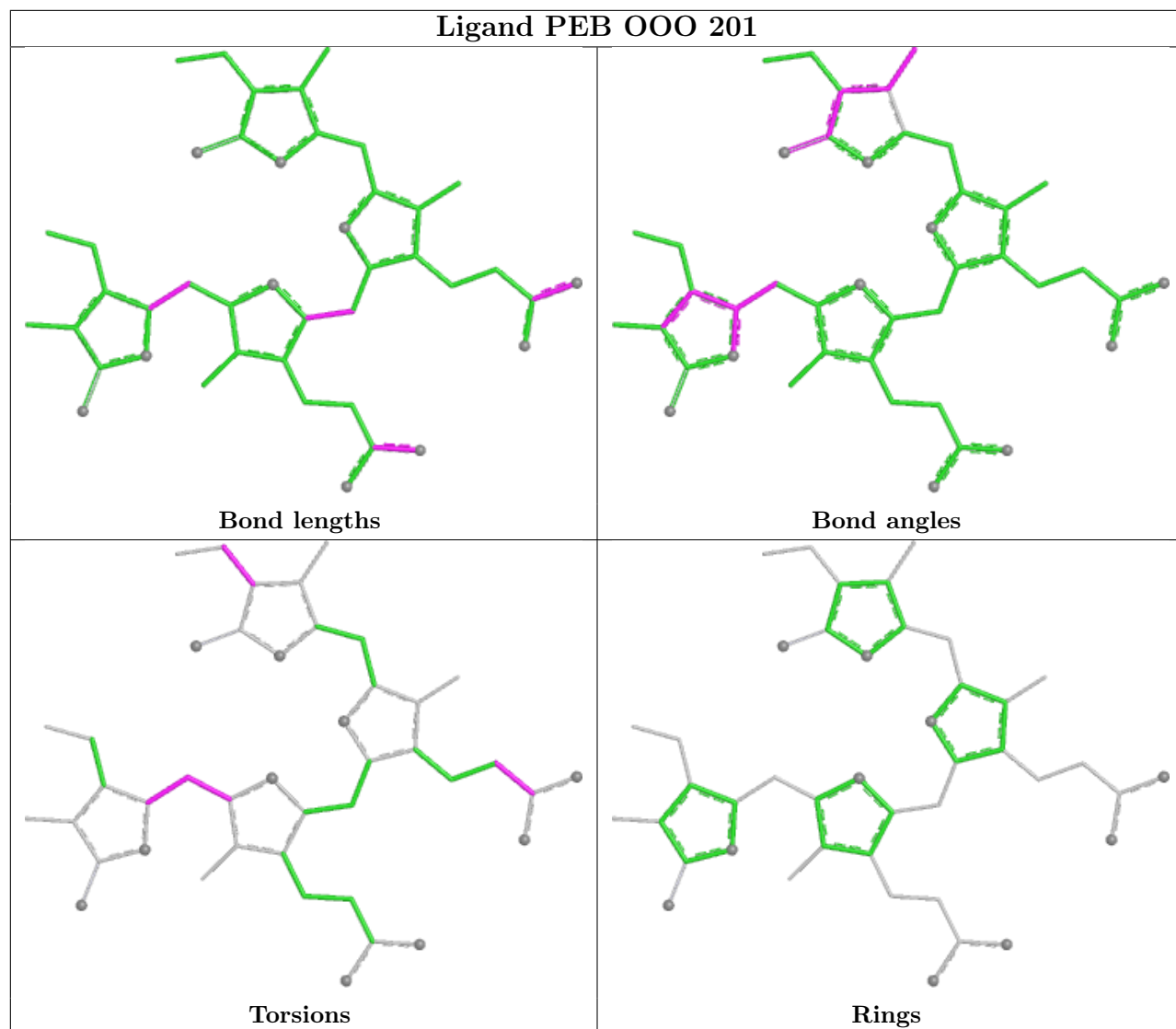




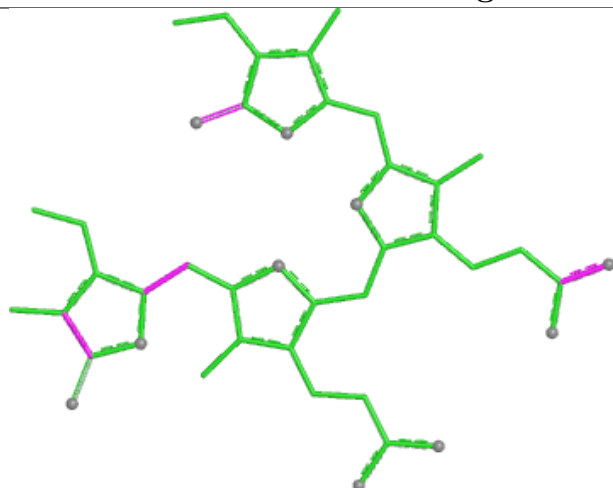




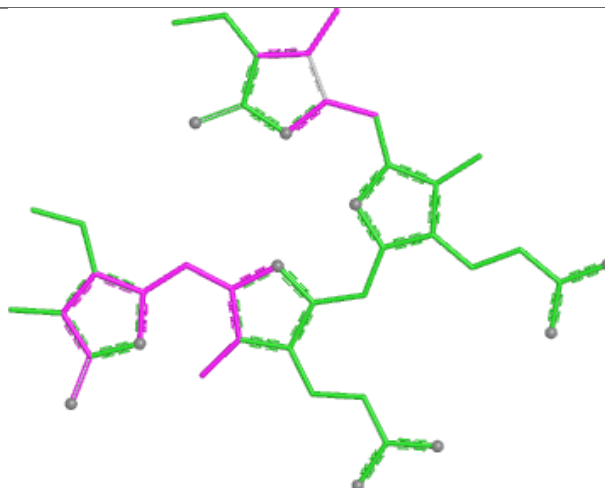
Ligand PEB_OOO_201



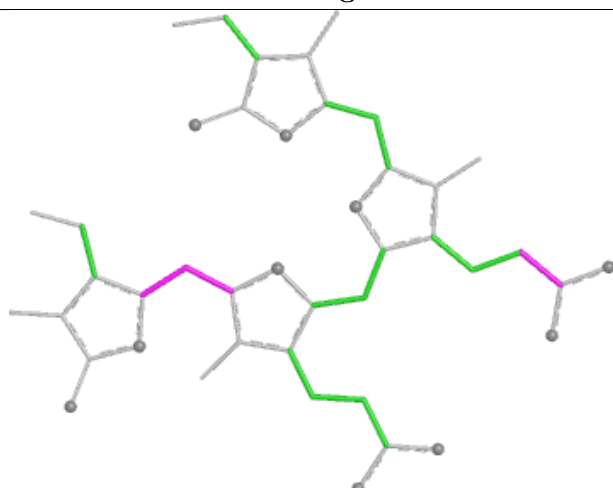
Ligand PEB MMM 201



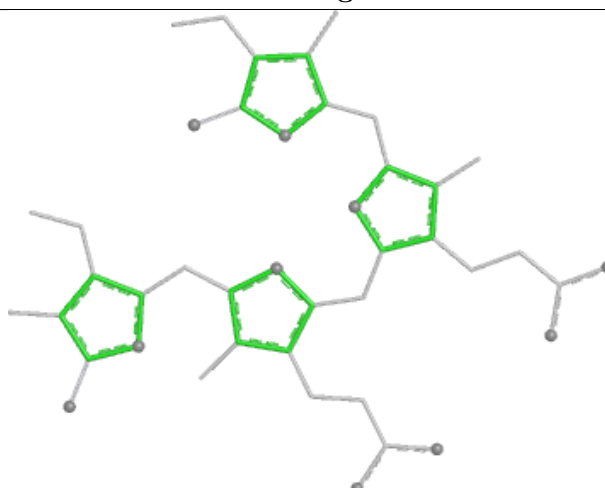
Bond lengths



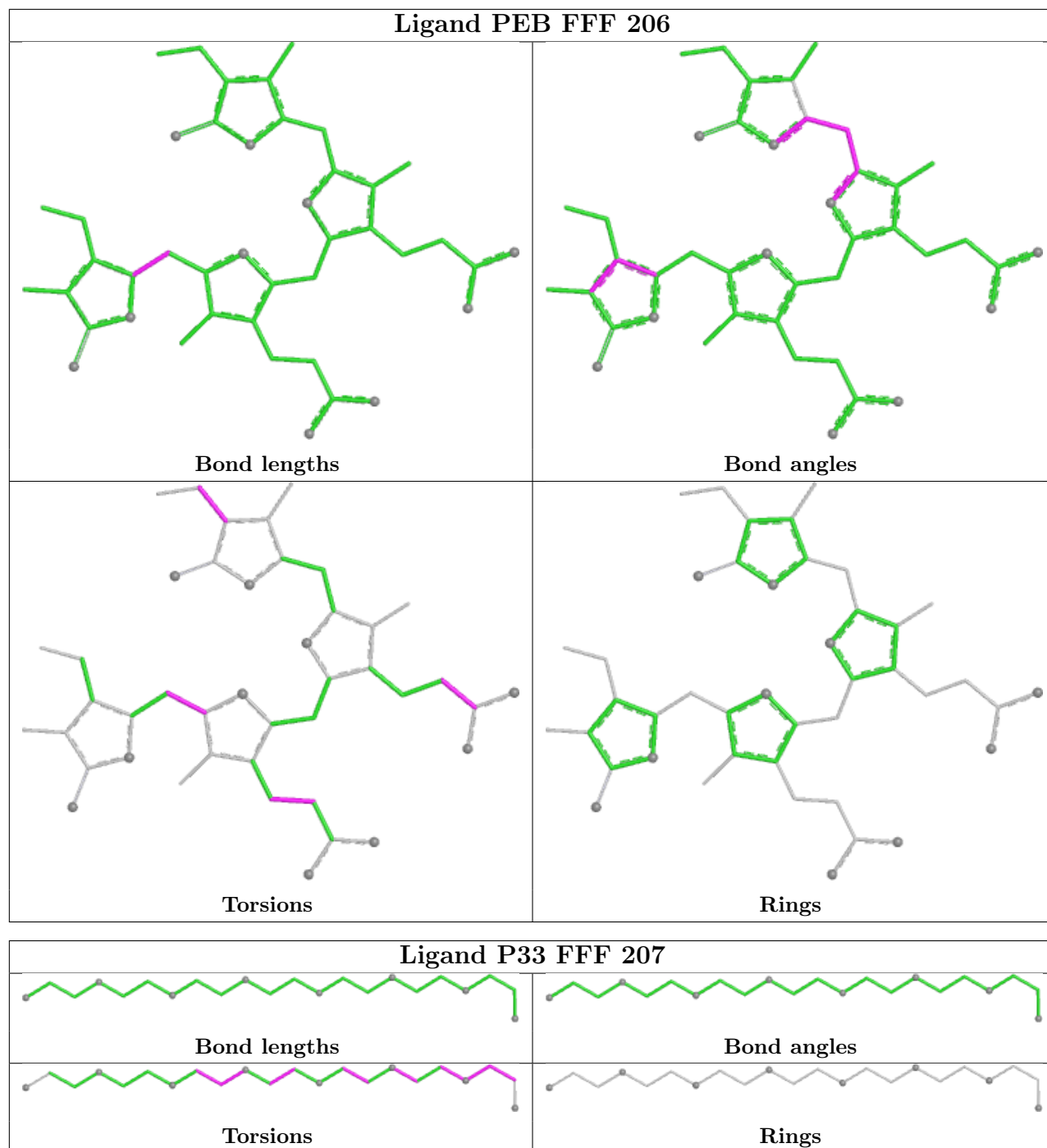
Bond angles

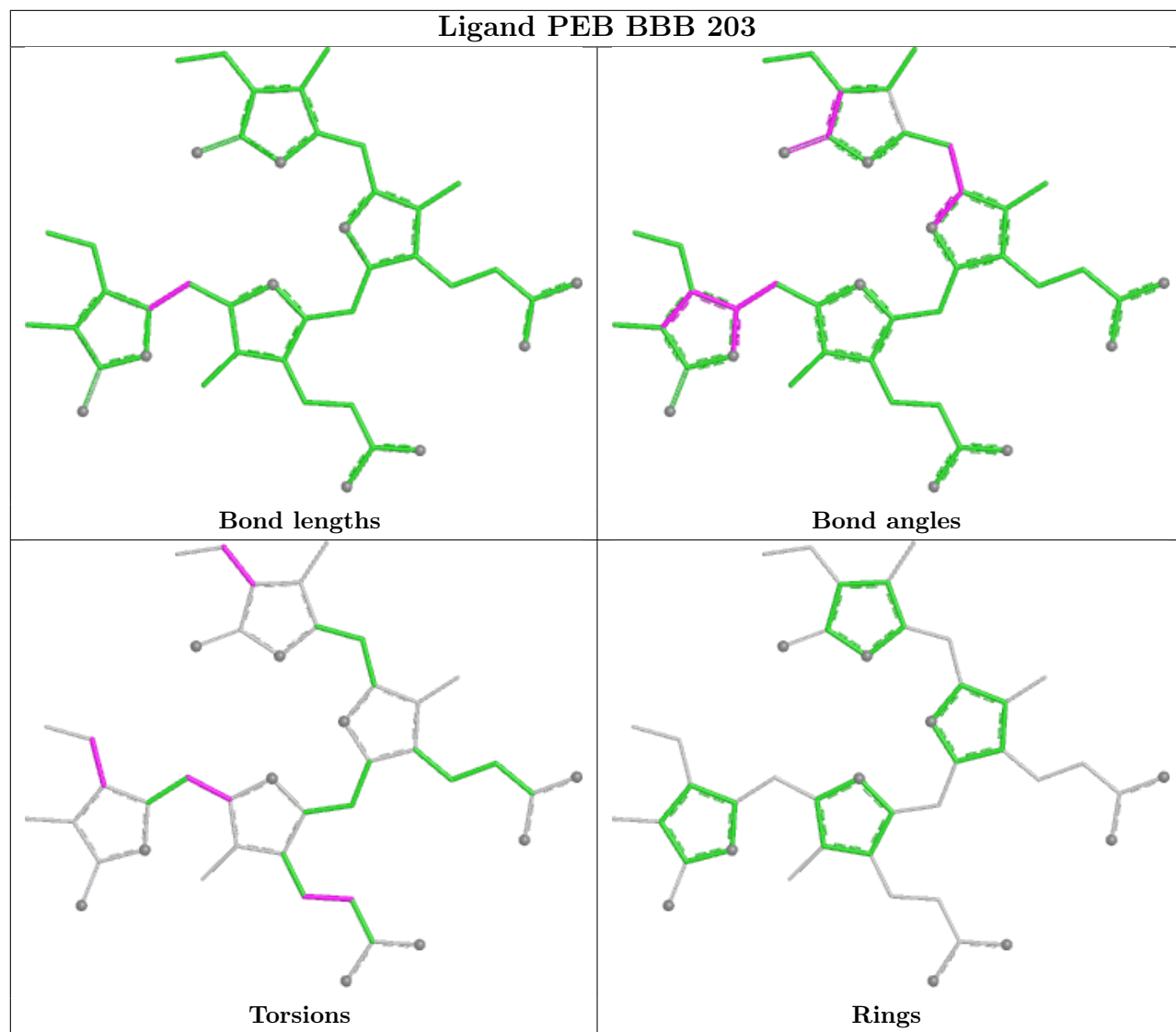


Torsions

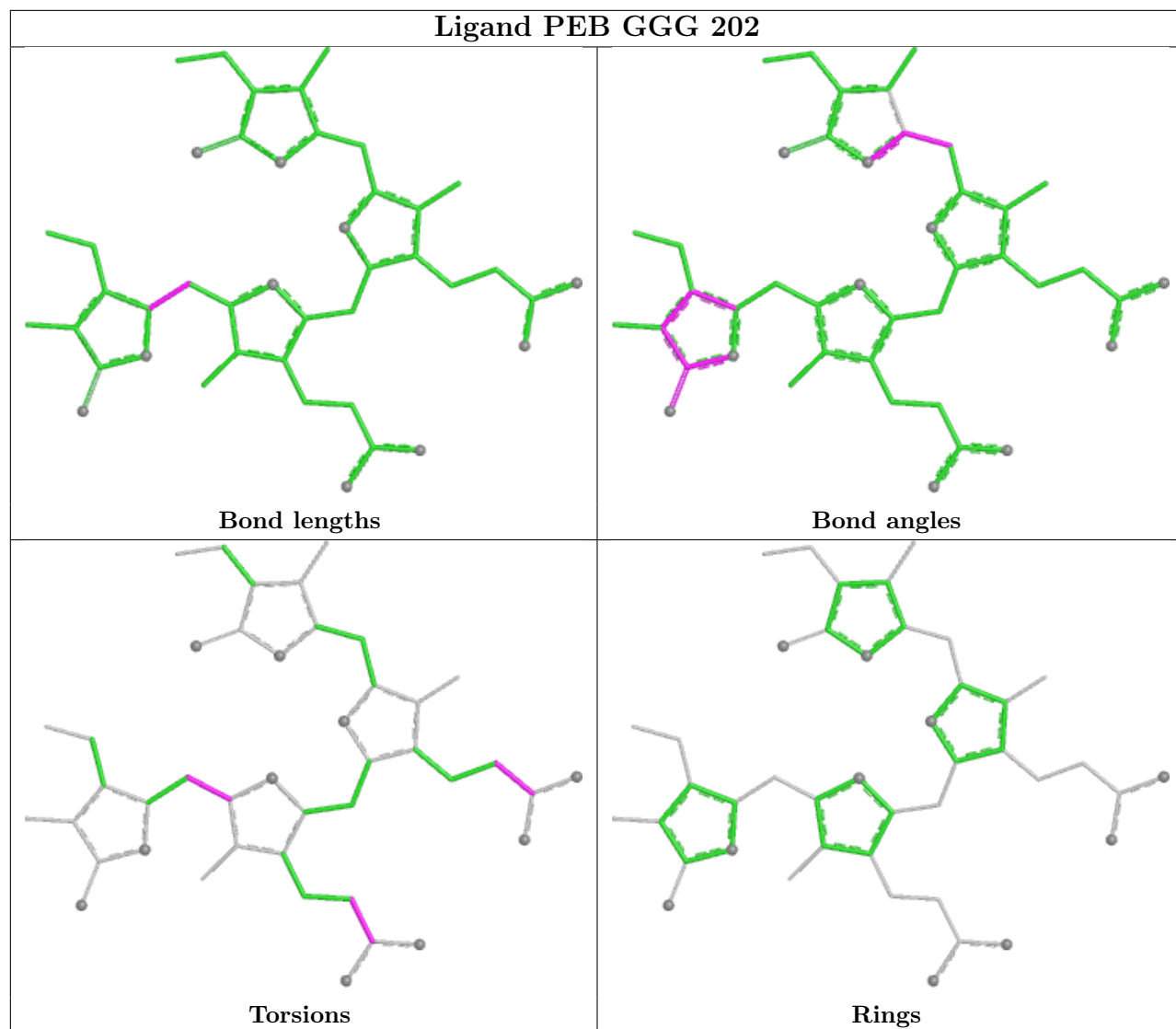


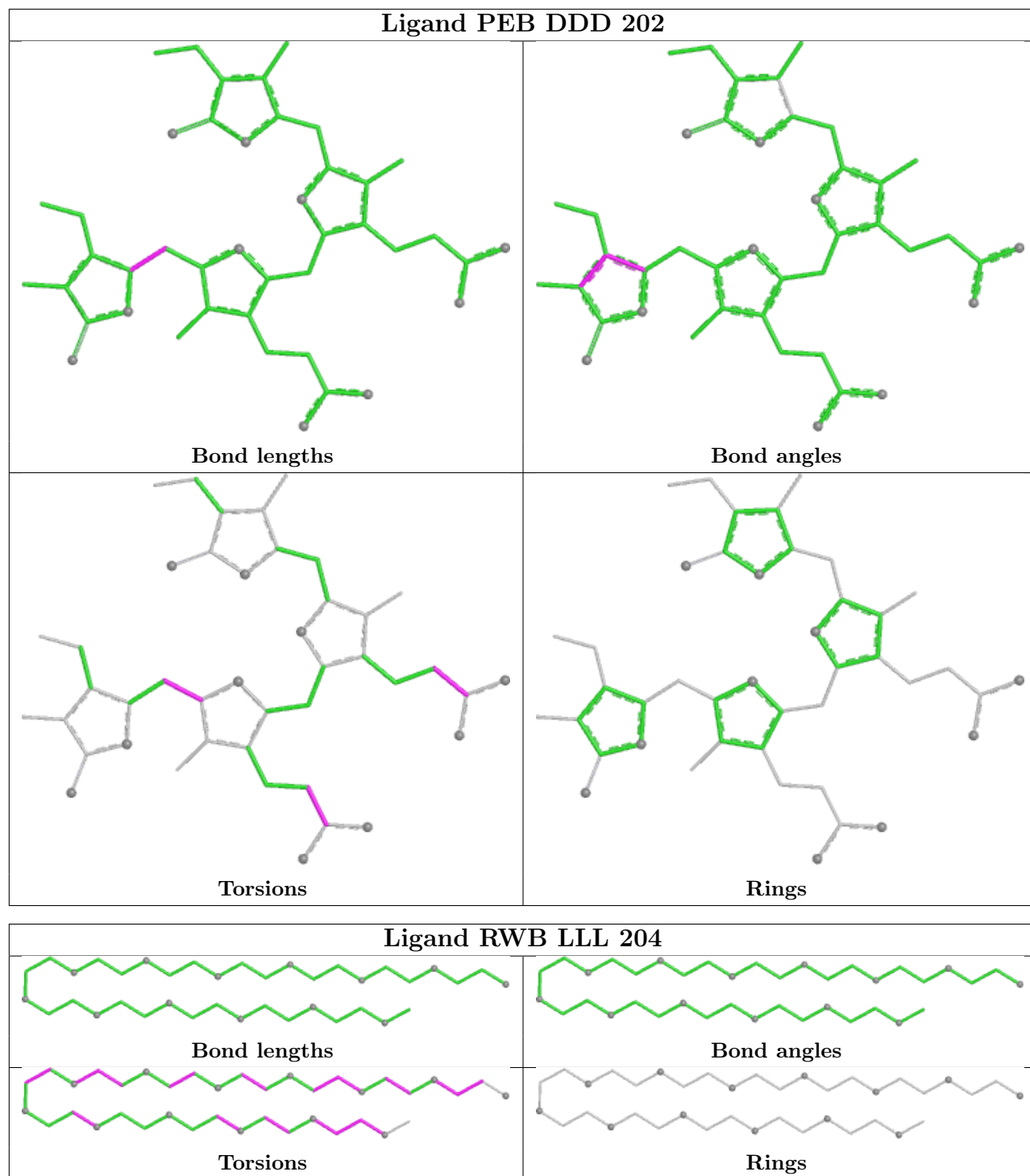
Rings



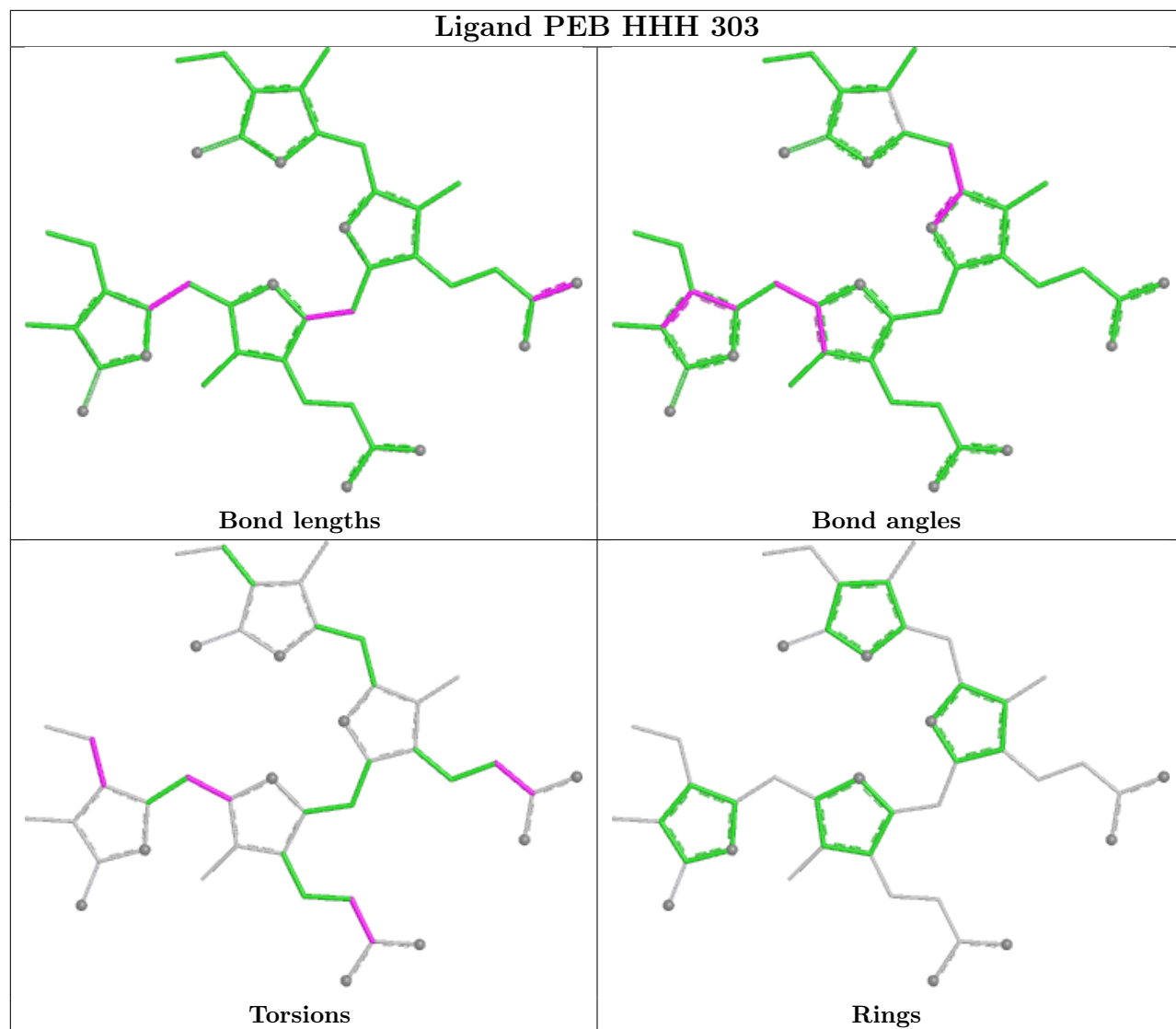


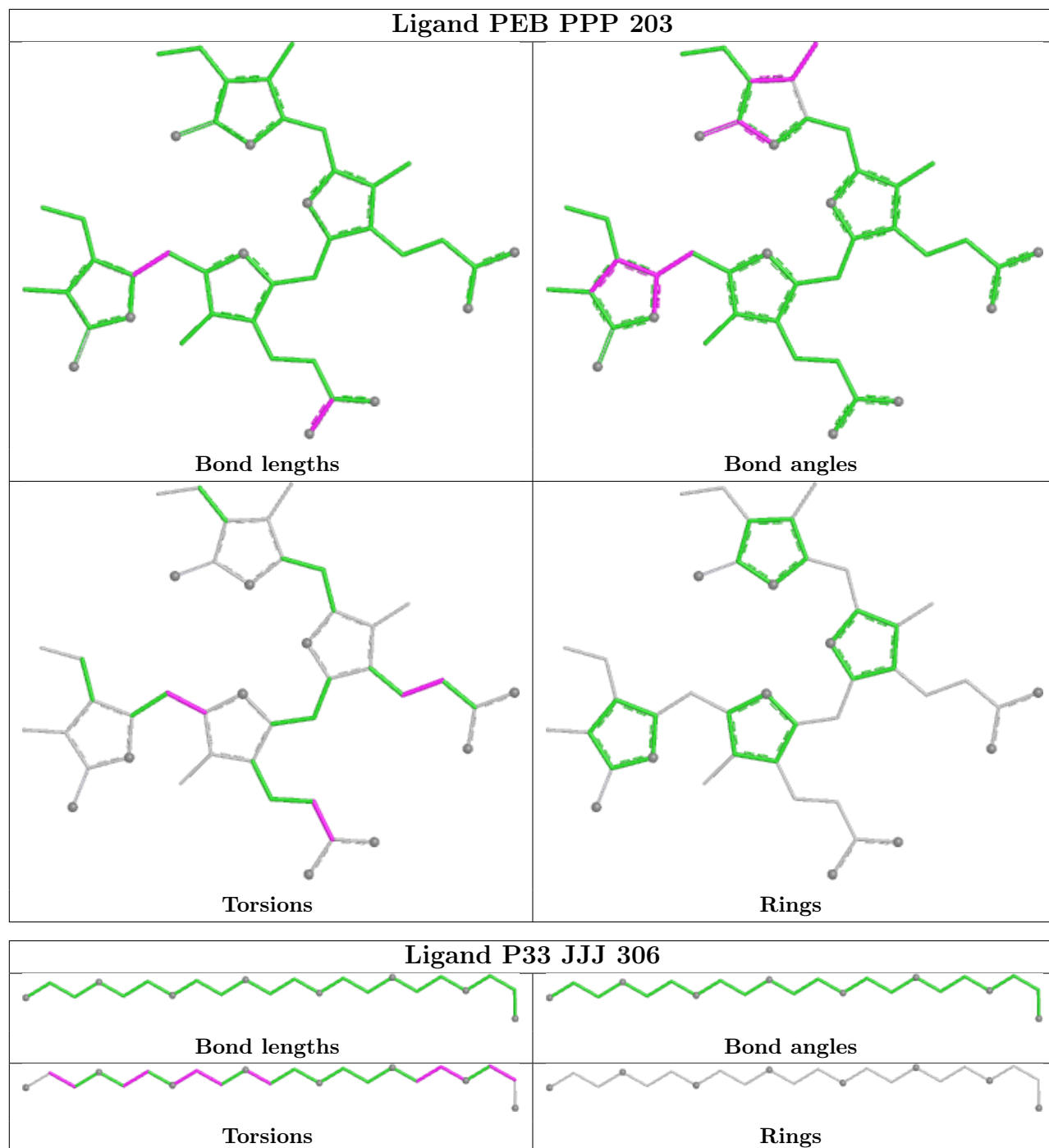
Ligand PEB GGG 202

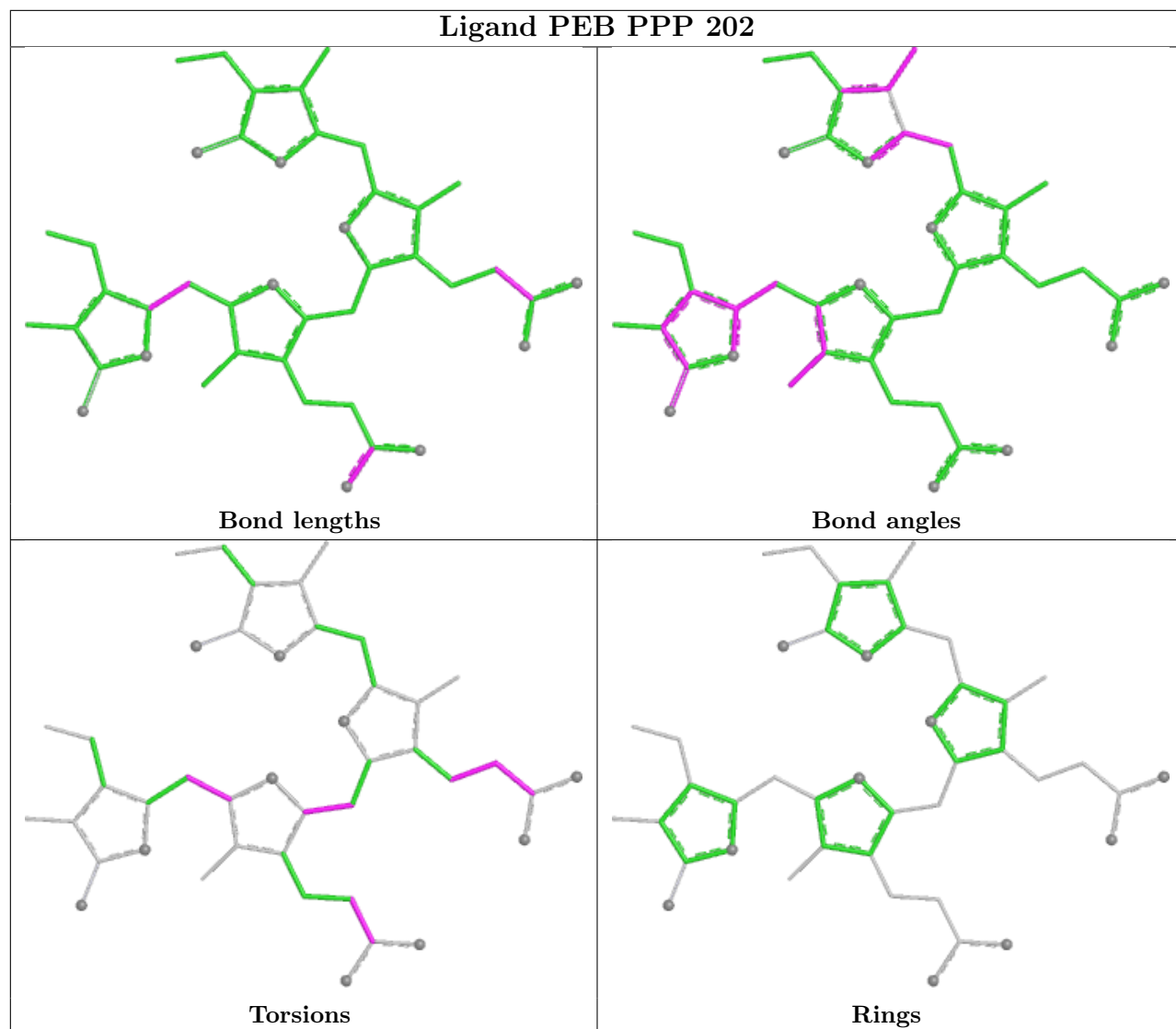




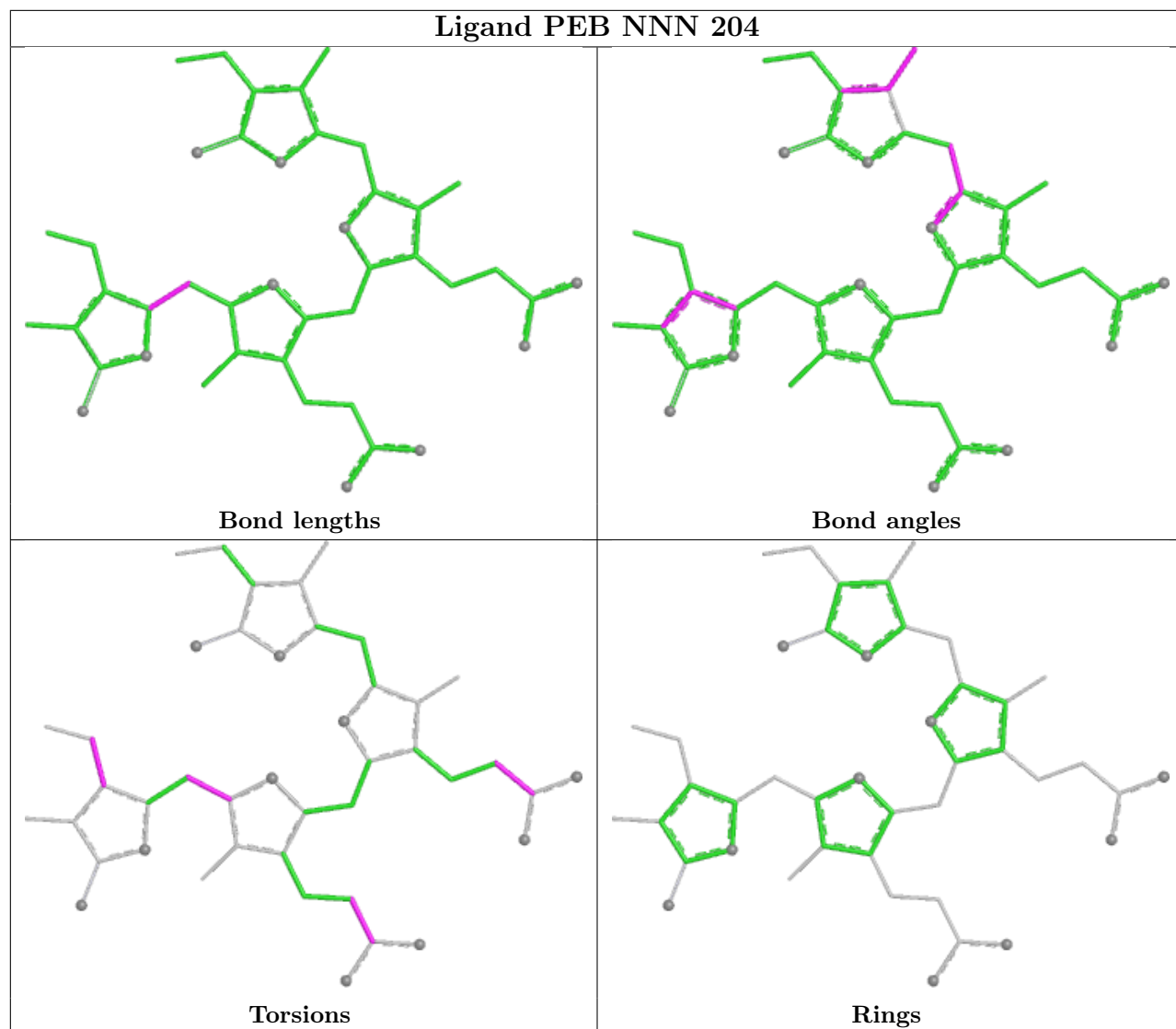
Ligand PEB HHH 303

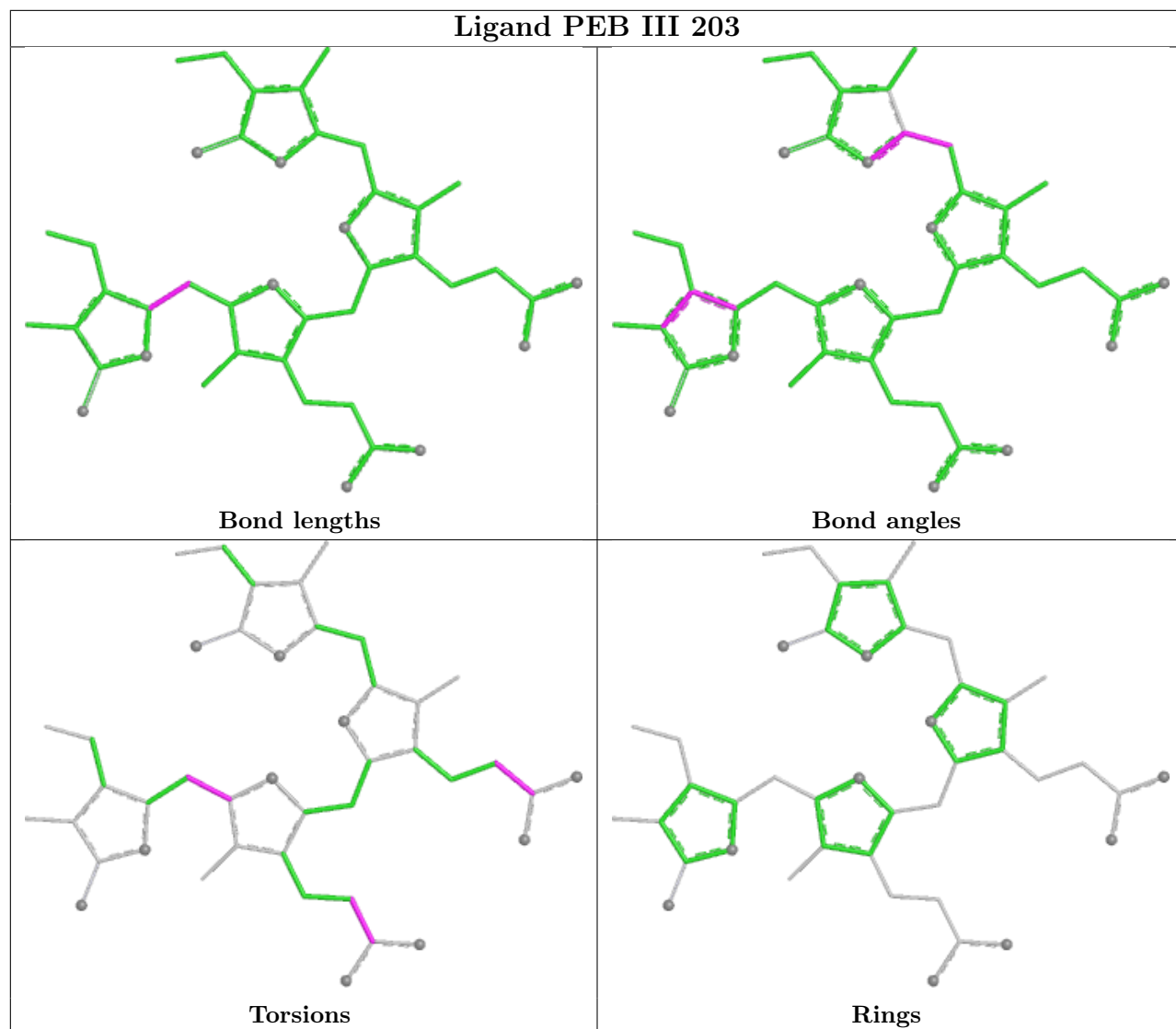




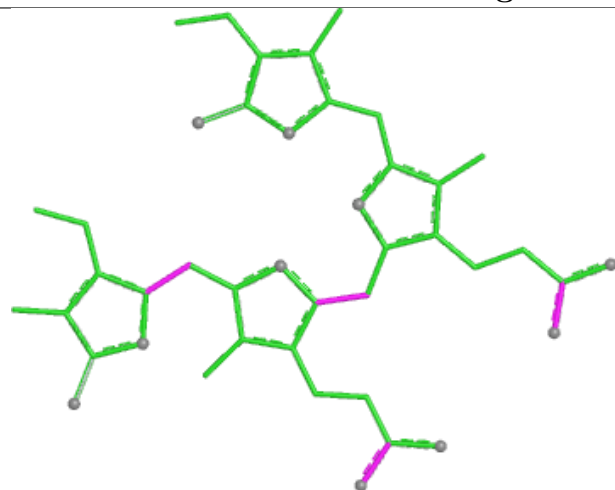


Ligand PEB NNN 204

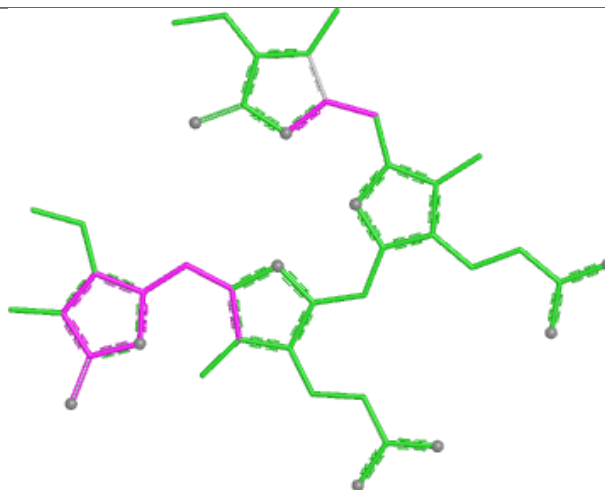




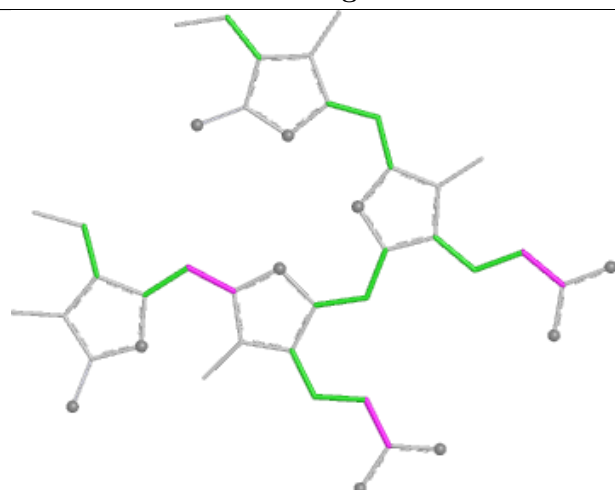
Ligand PEB FFF 204



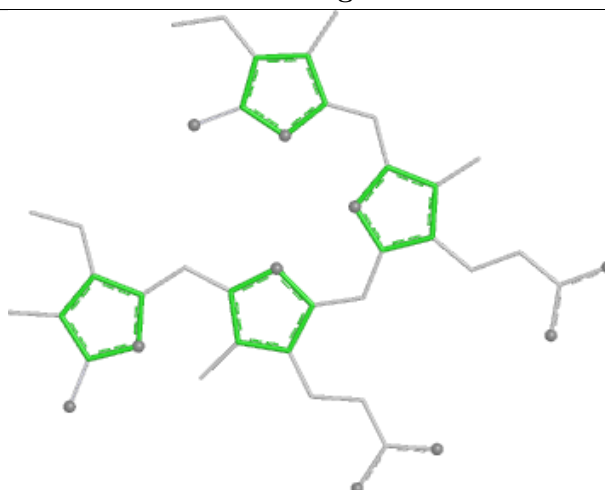
Bond lengths



Bond angles

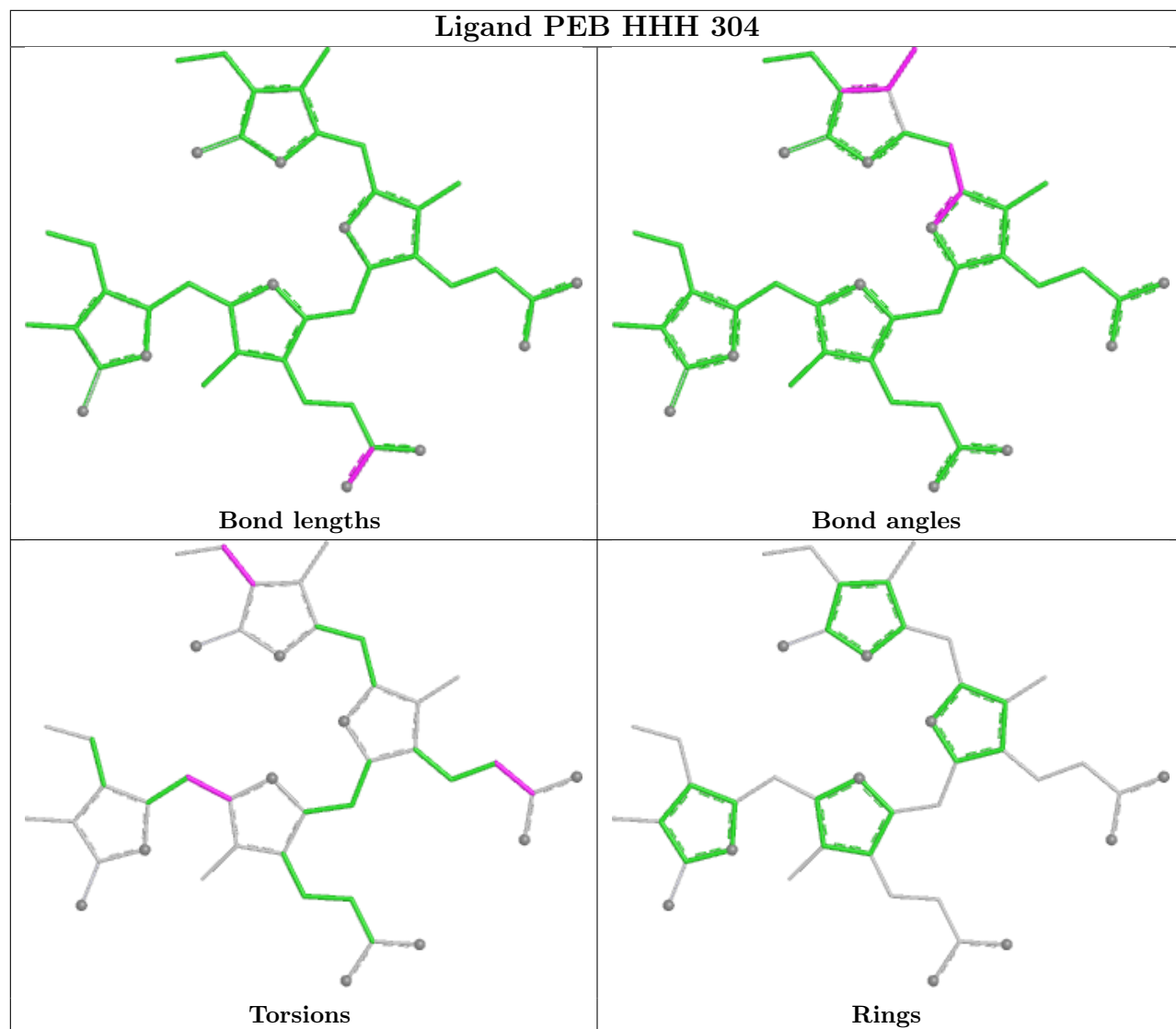


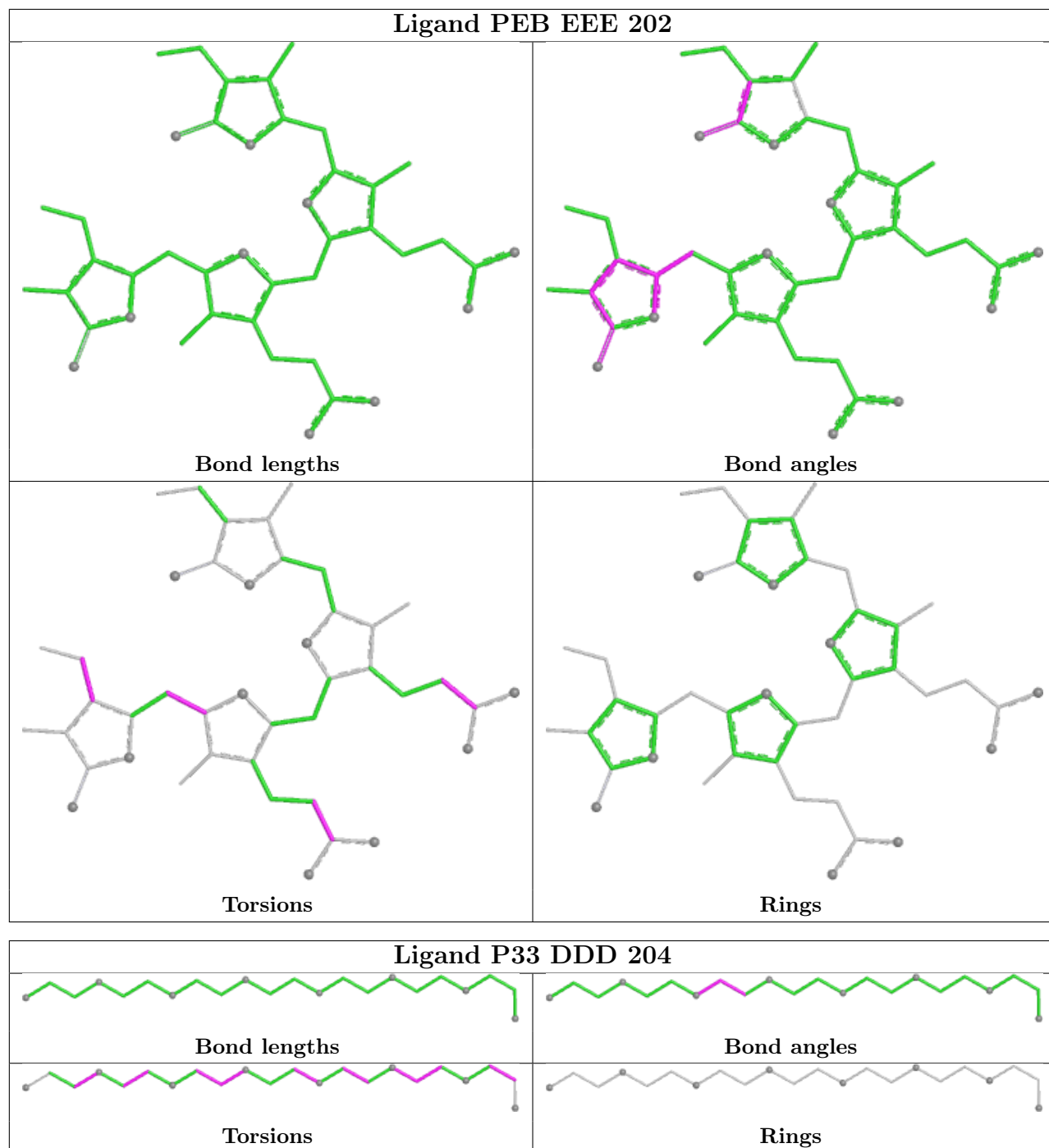
Torsions

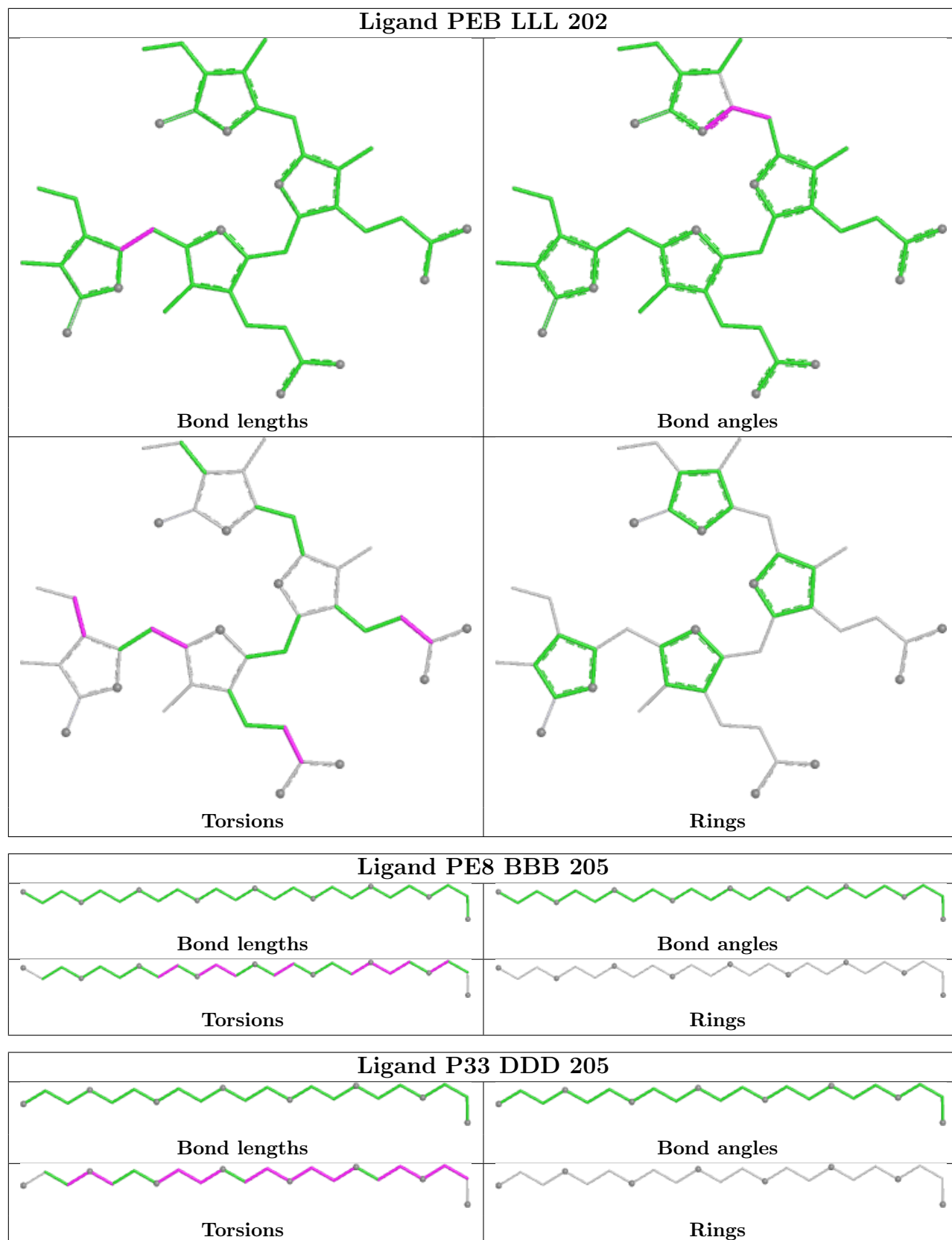


Rings

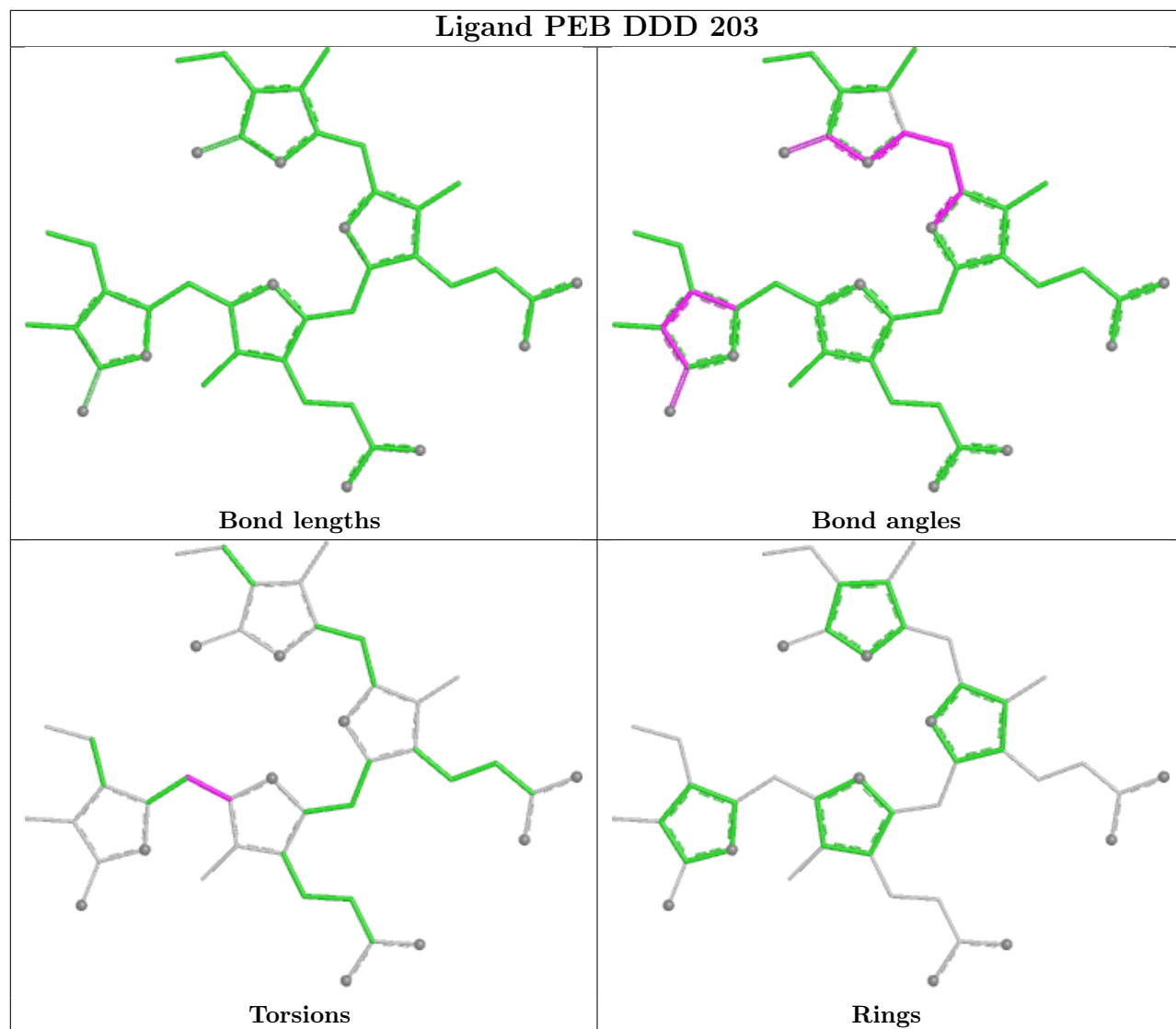
Ligand PEB HHH 304

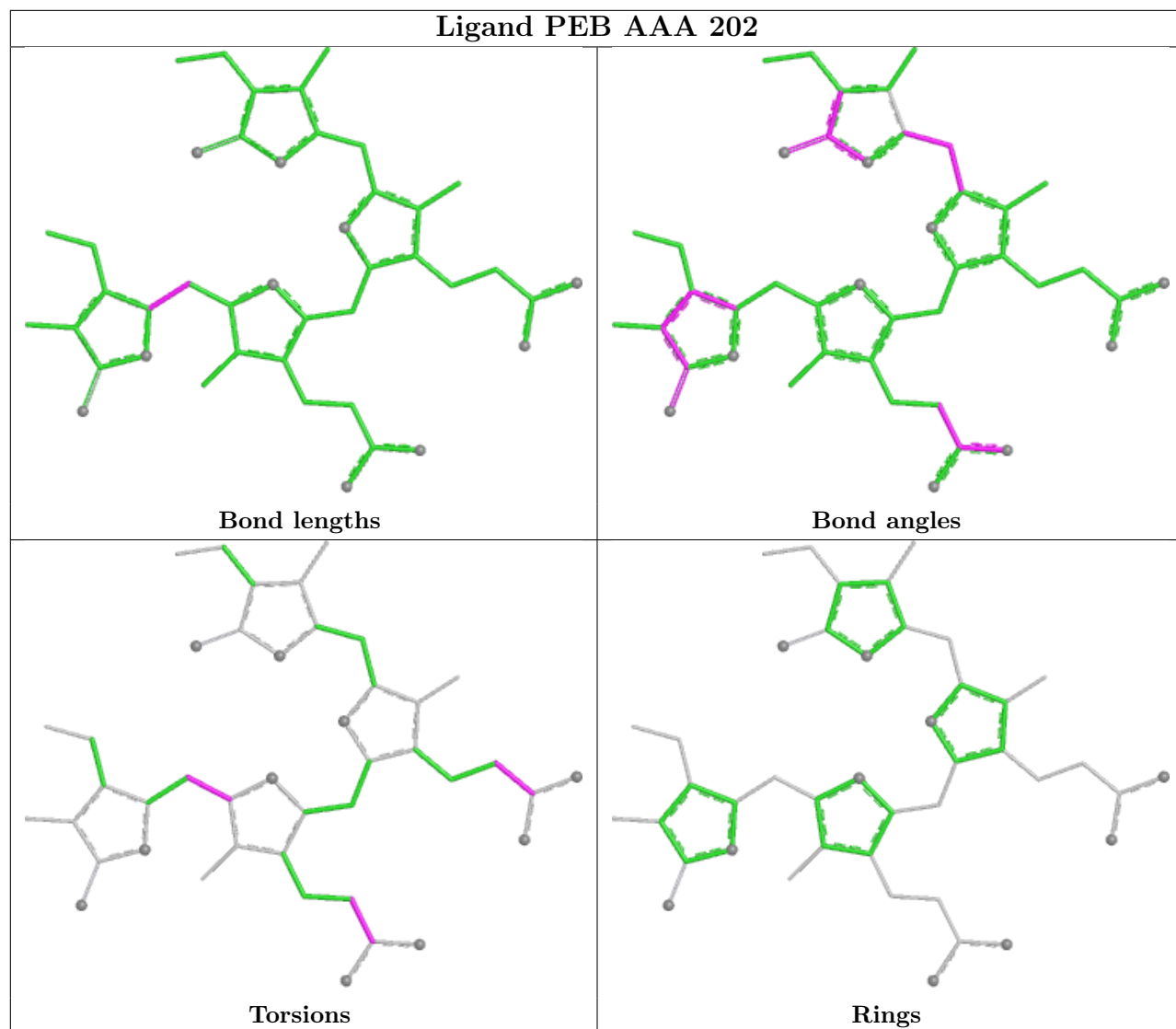


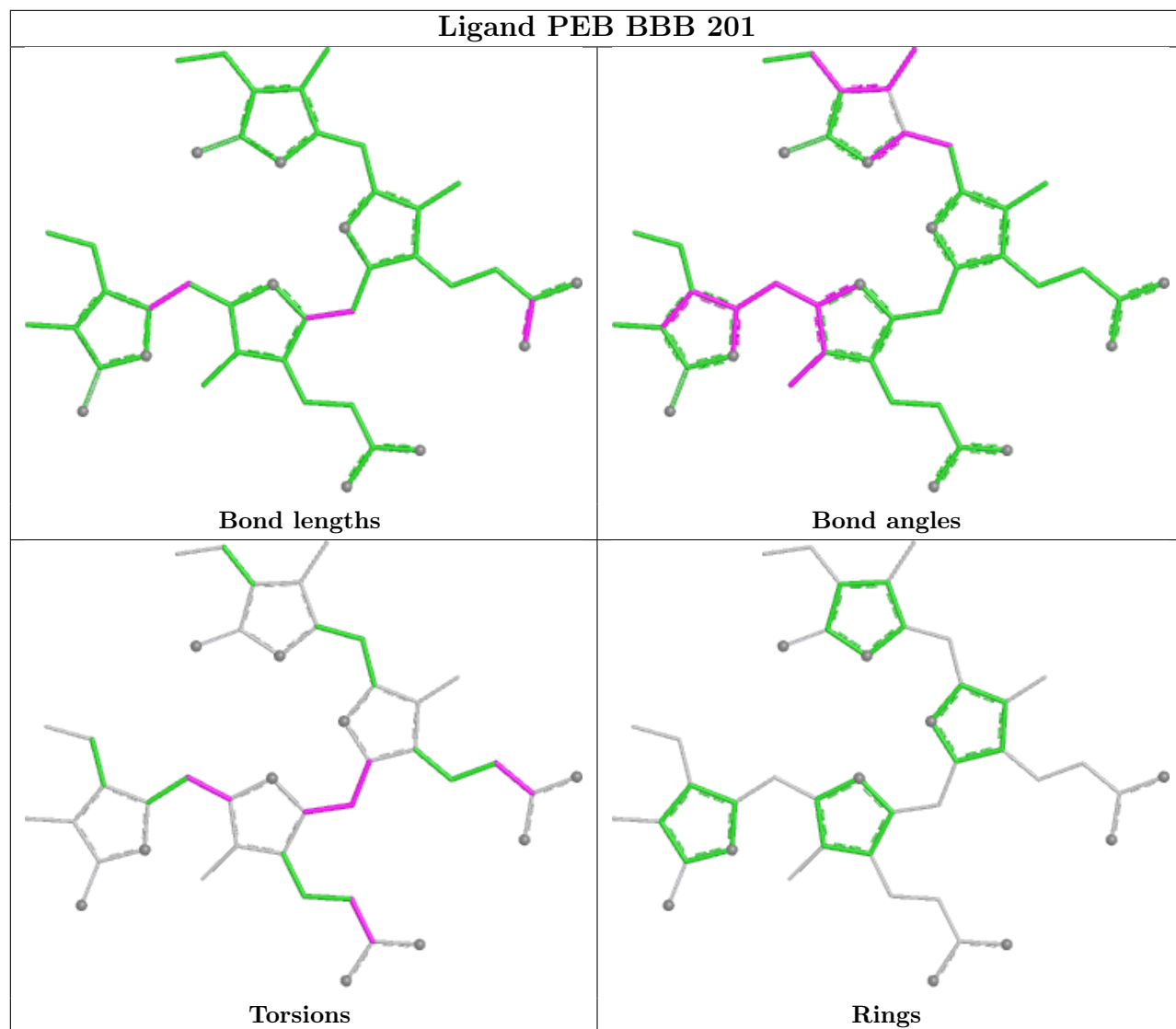




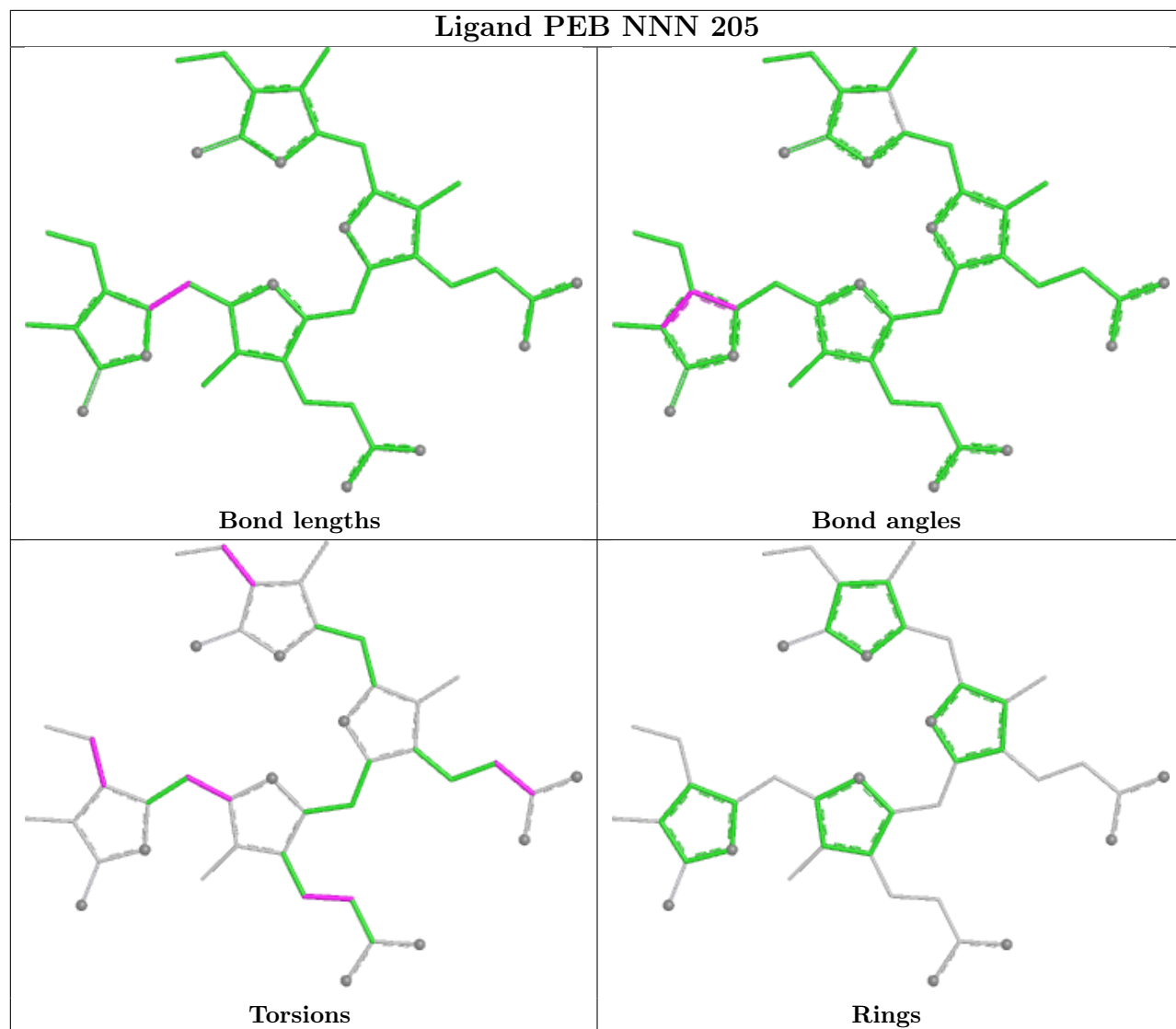
Ligand PEB DDD 203



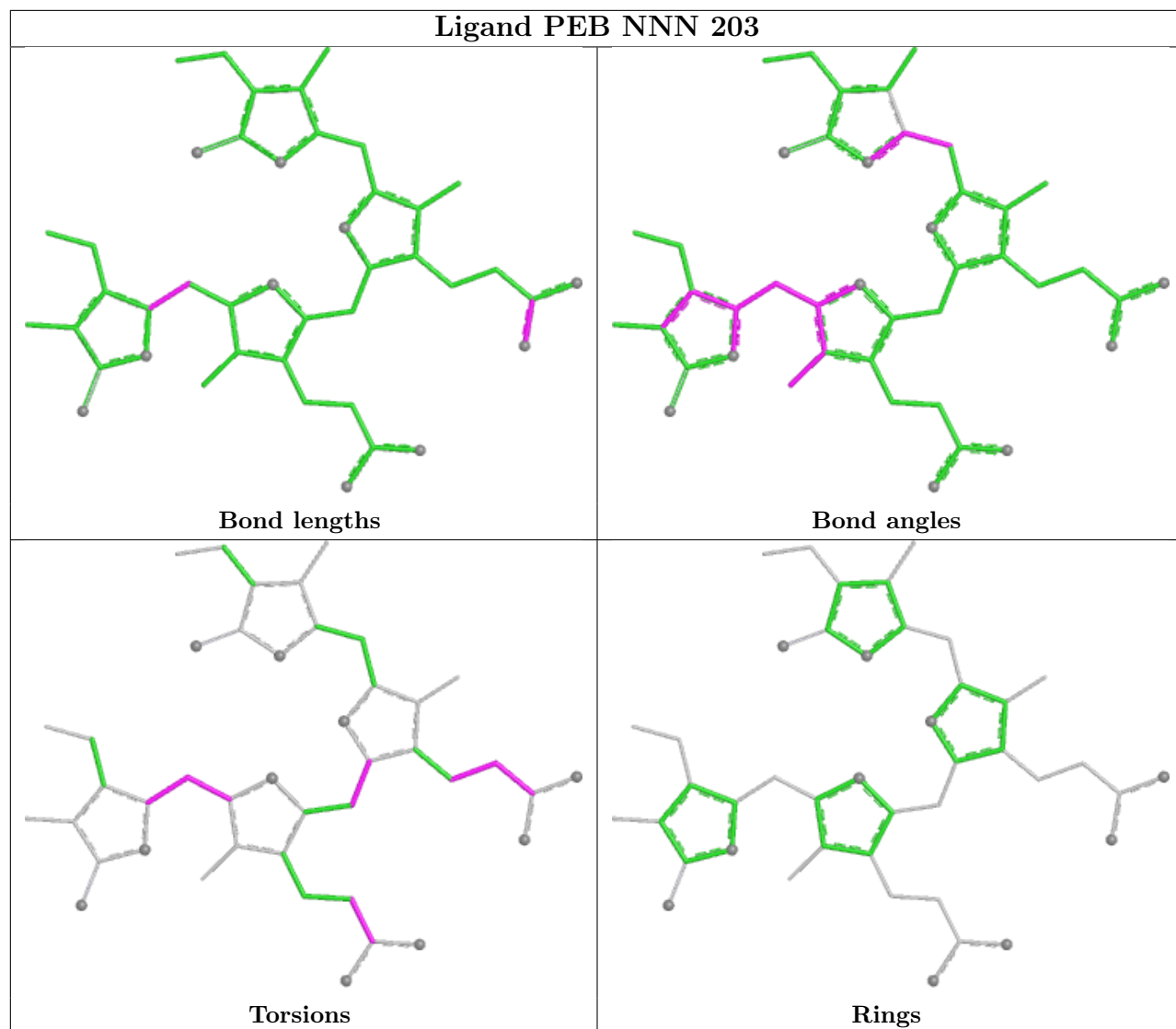




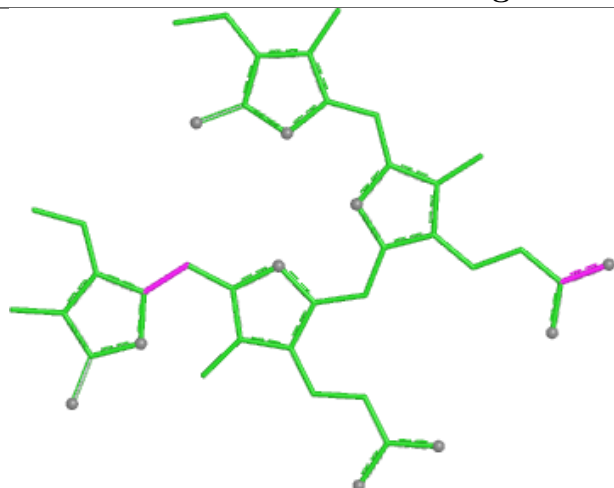
Ligand PEB NNN 205



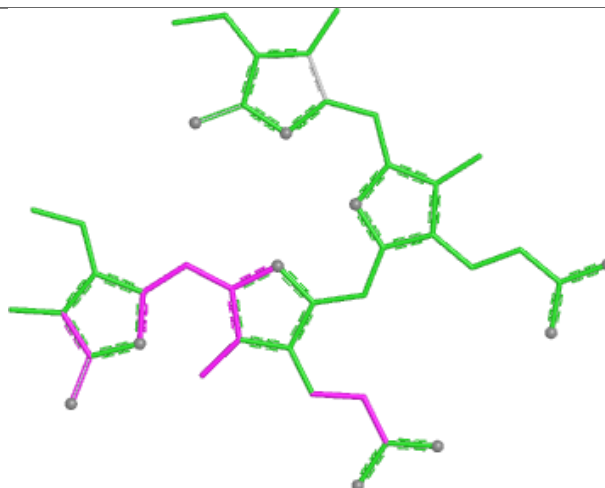
Ligand PEB NNN 203



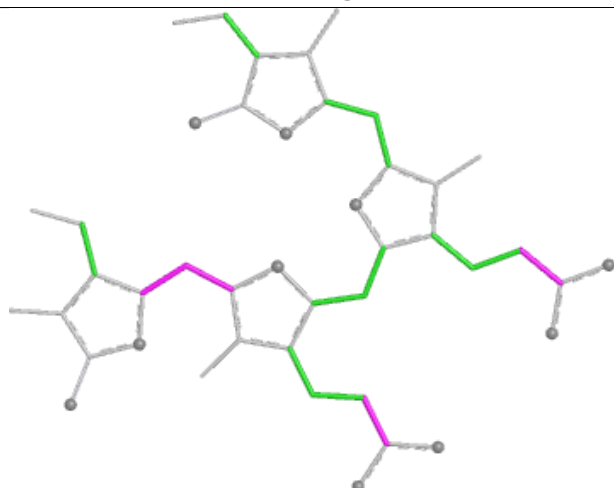
Ligand PEB EEE 201



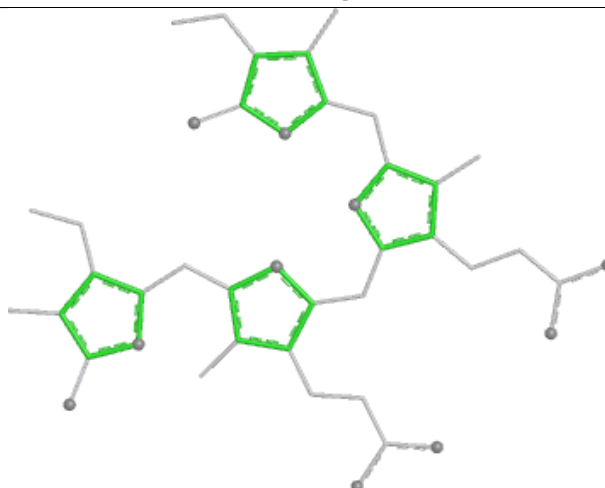
Bond lengths



Bond angles

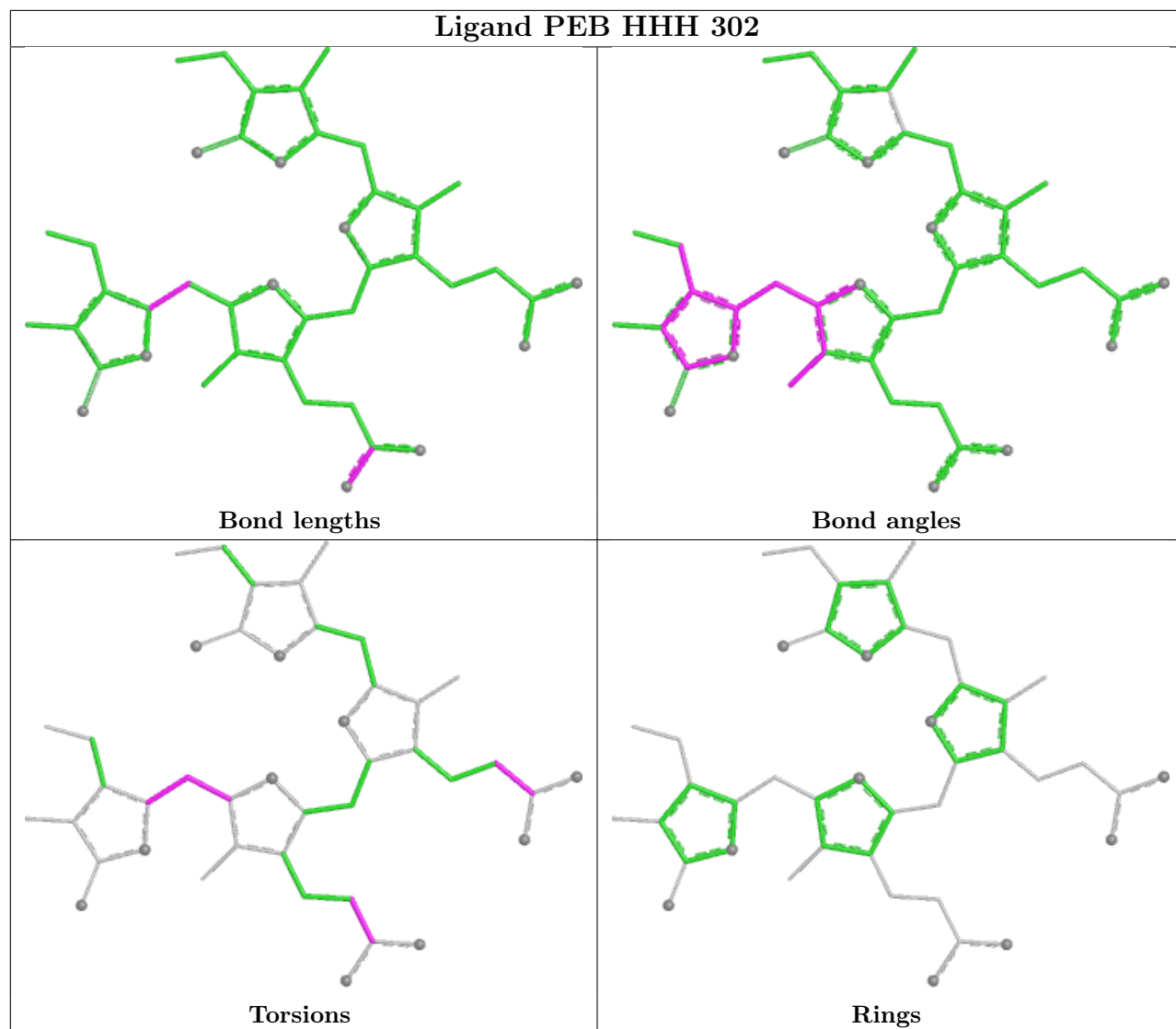


Torsions

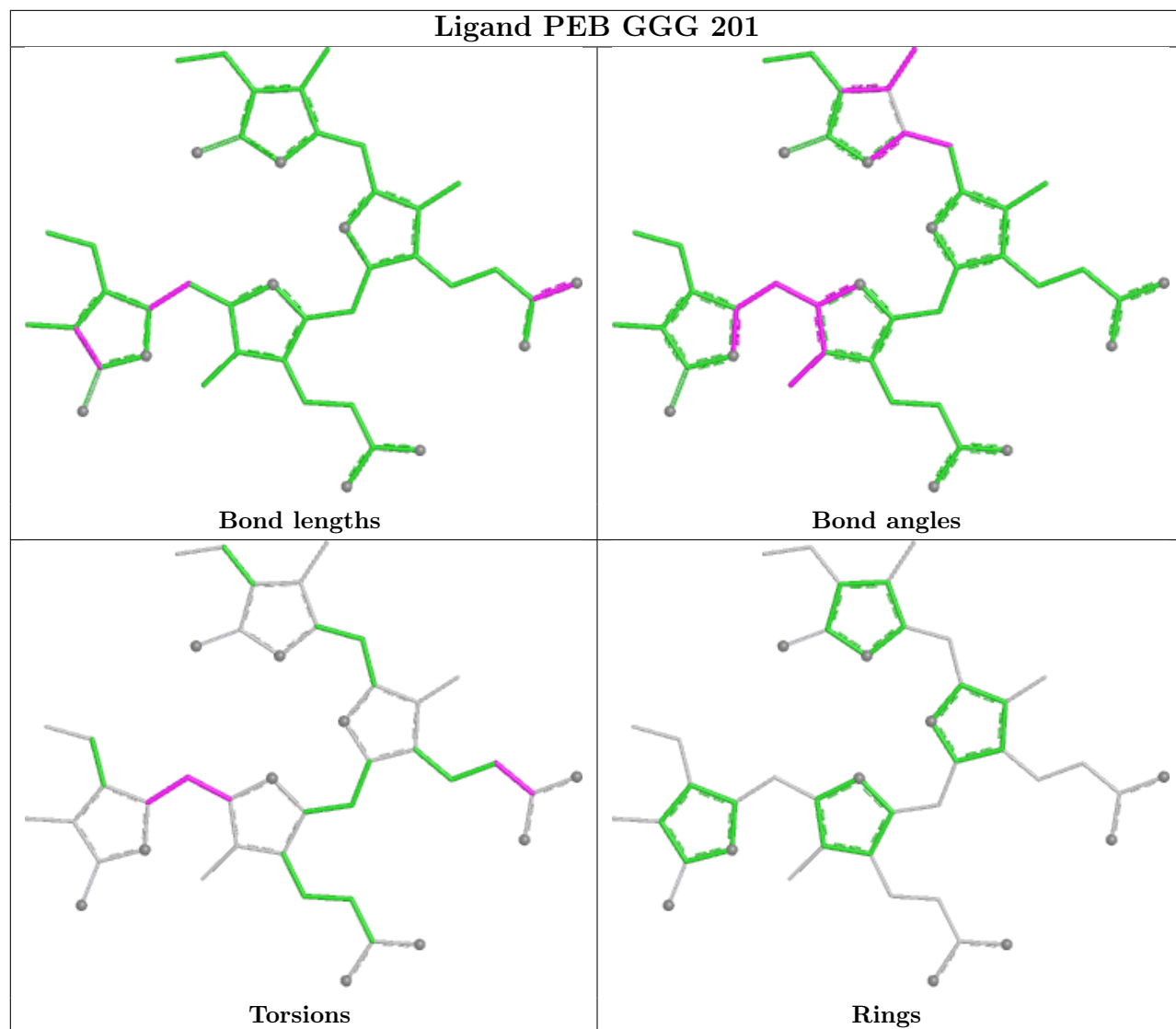


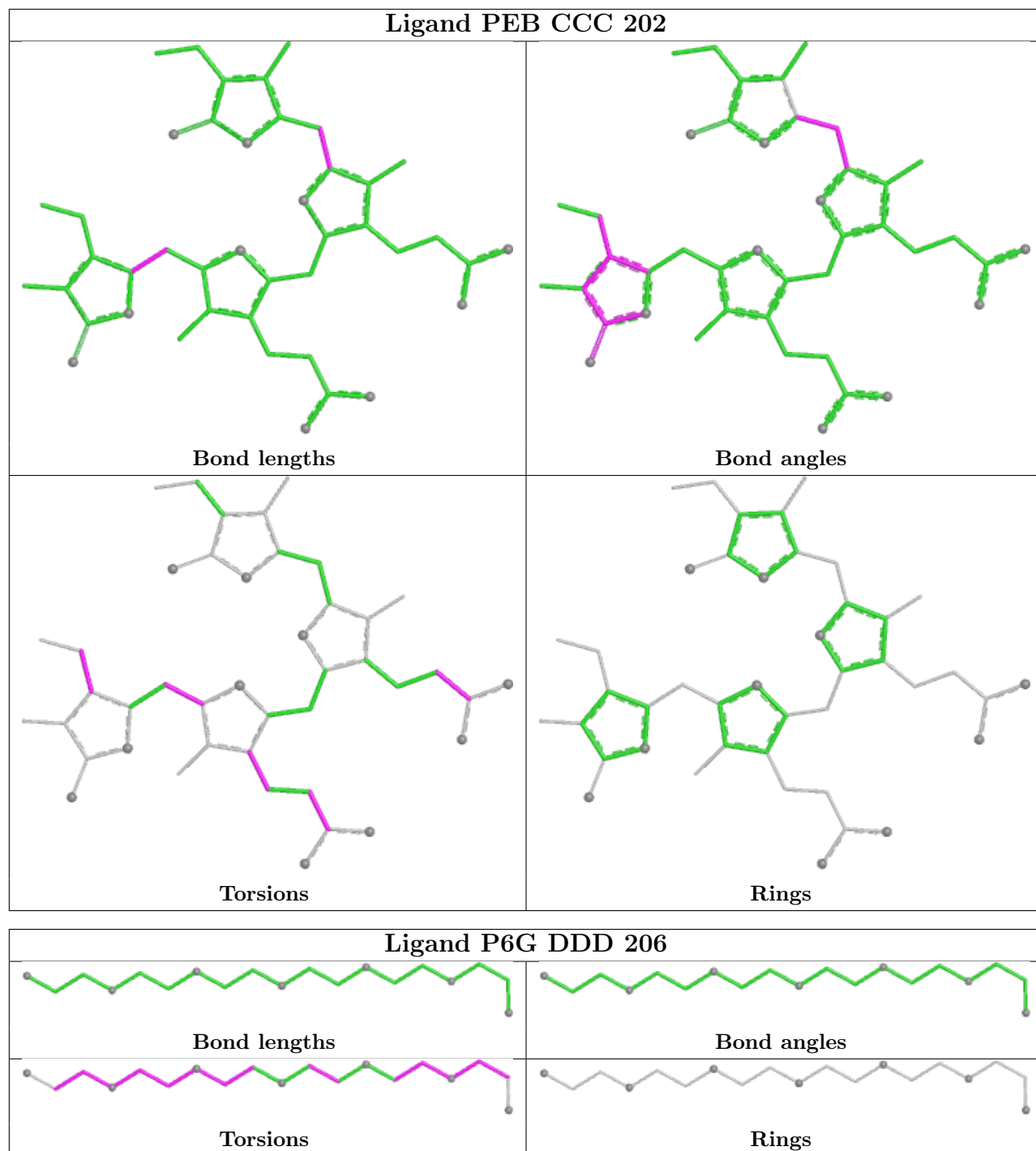
Rings

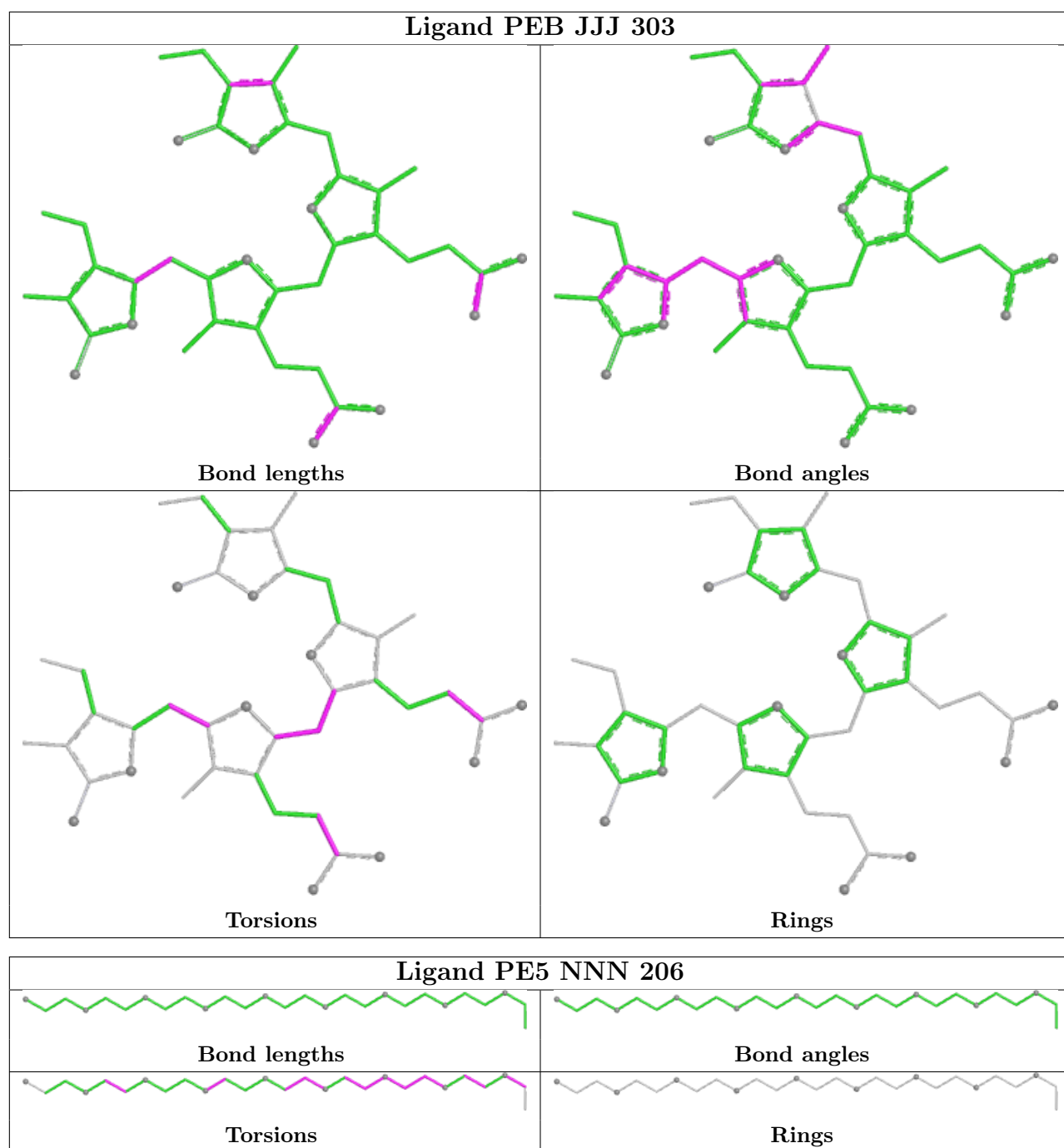
Ligand PEB HHH 302

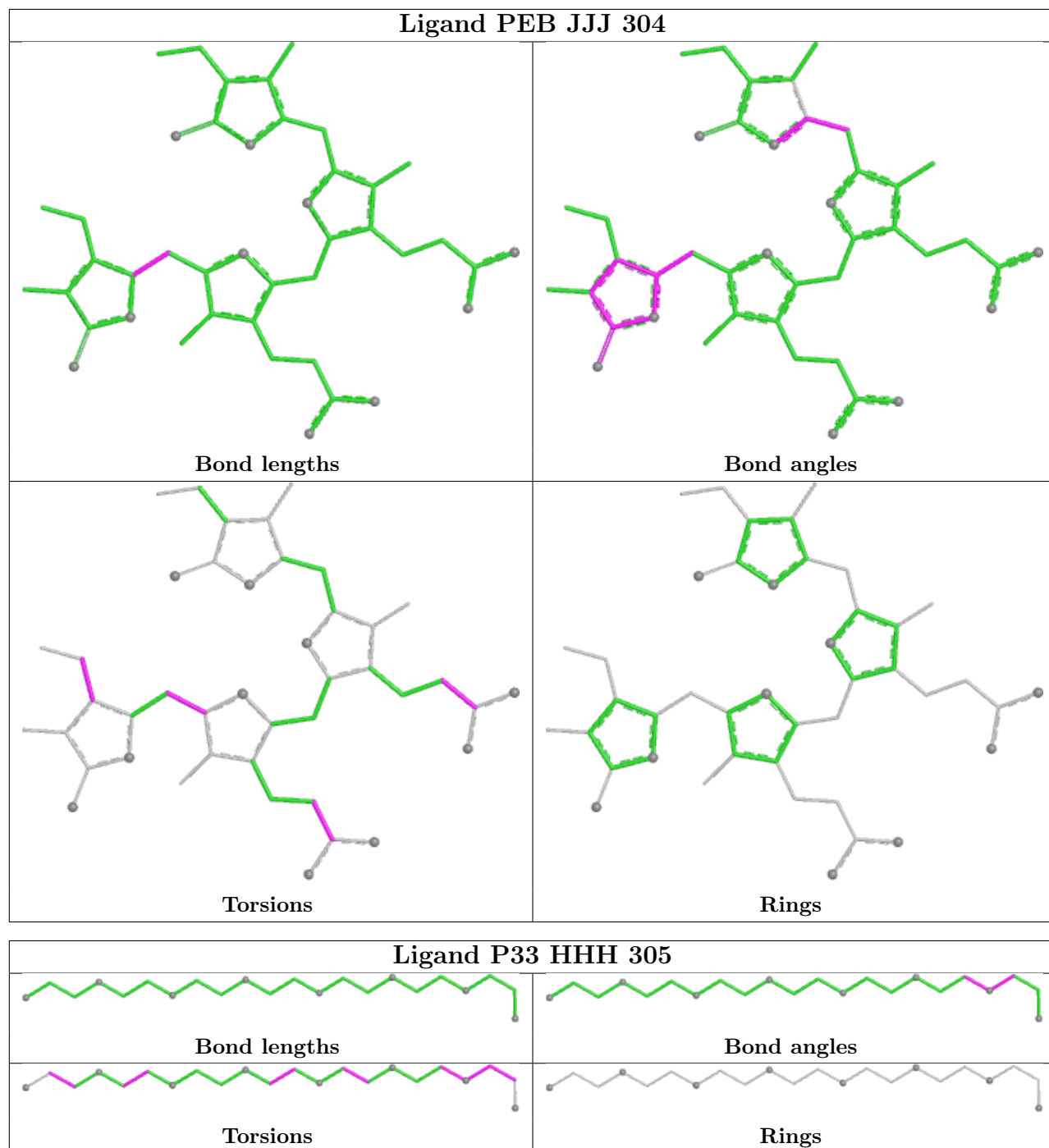


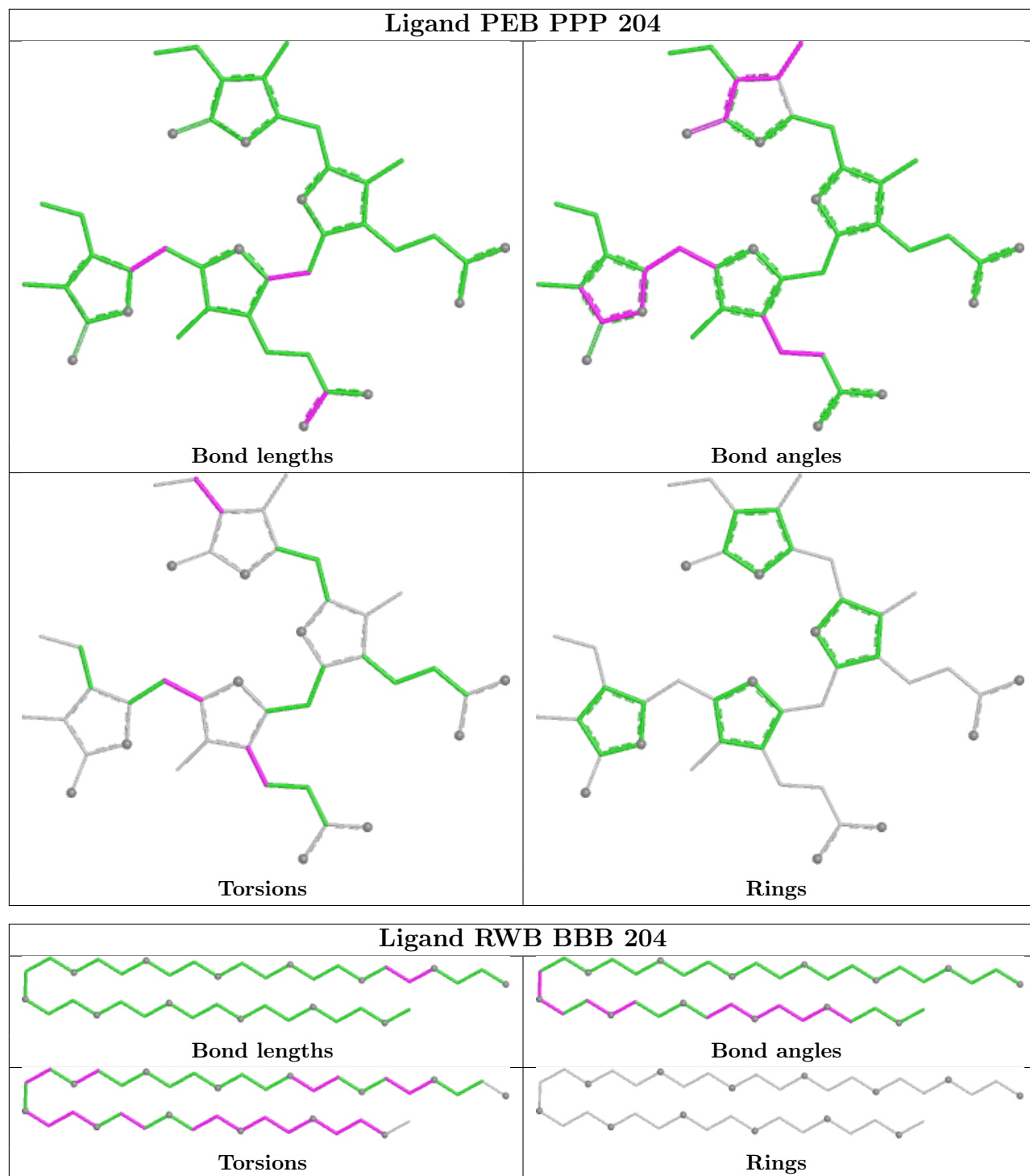
Ligand PEB GGG 201



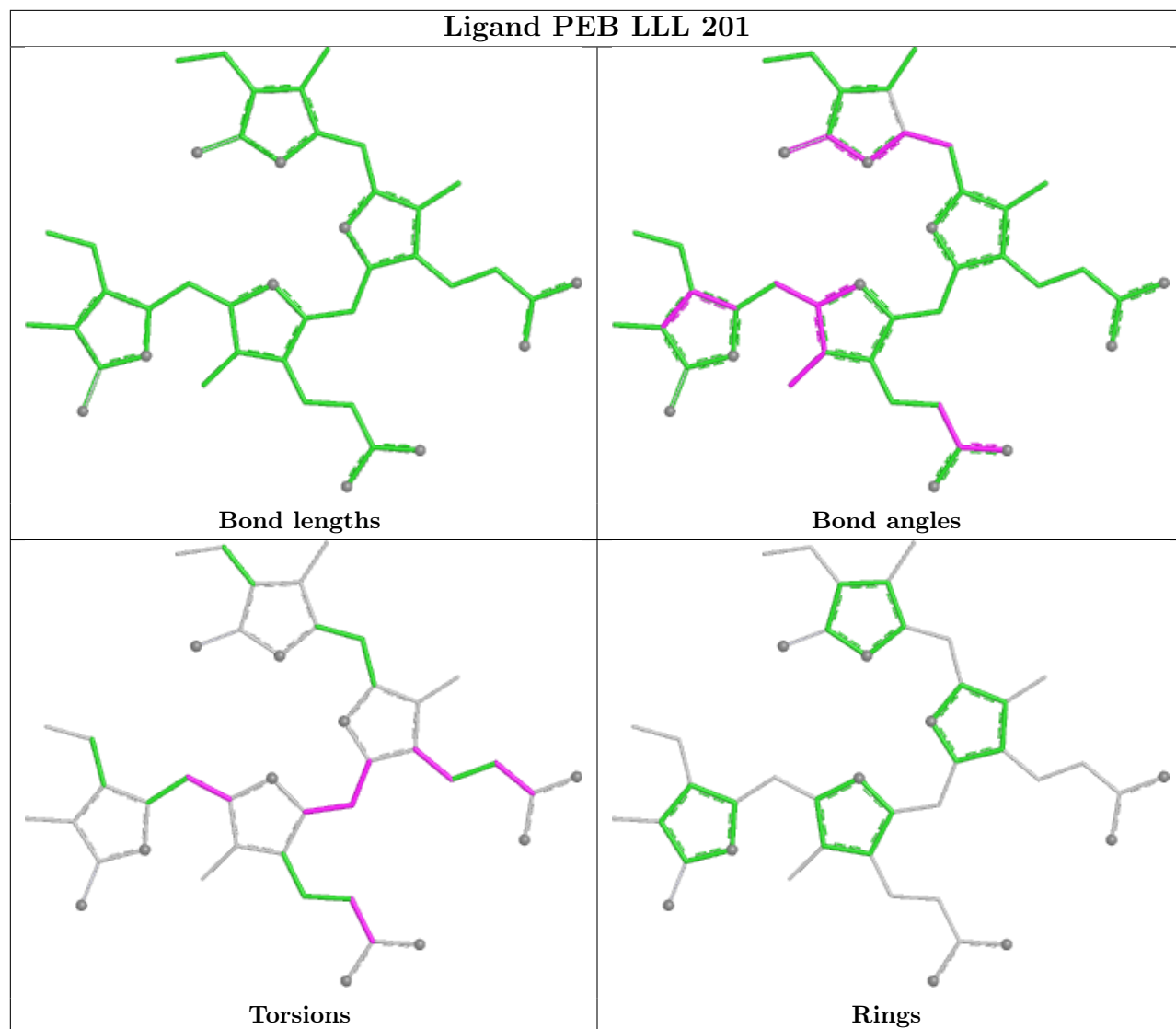




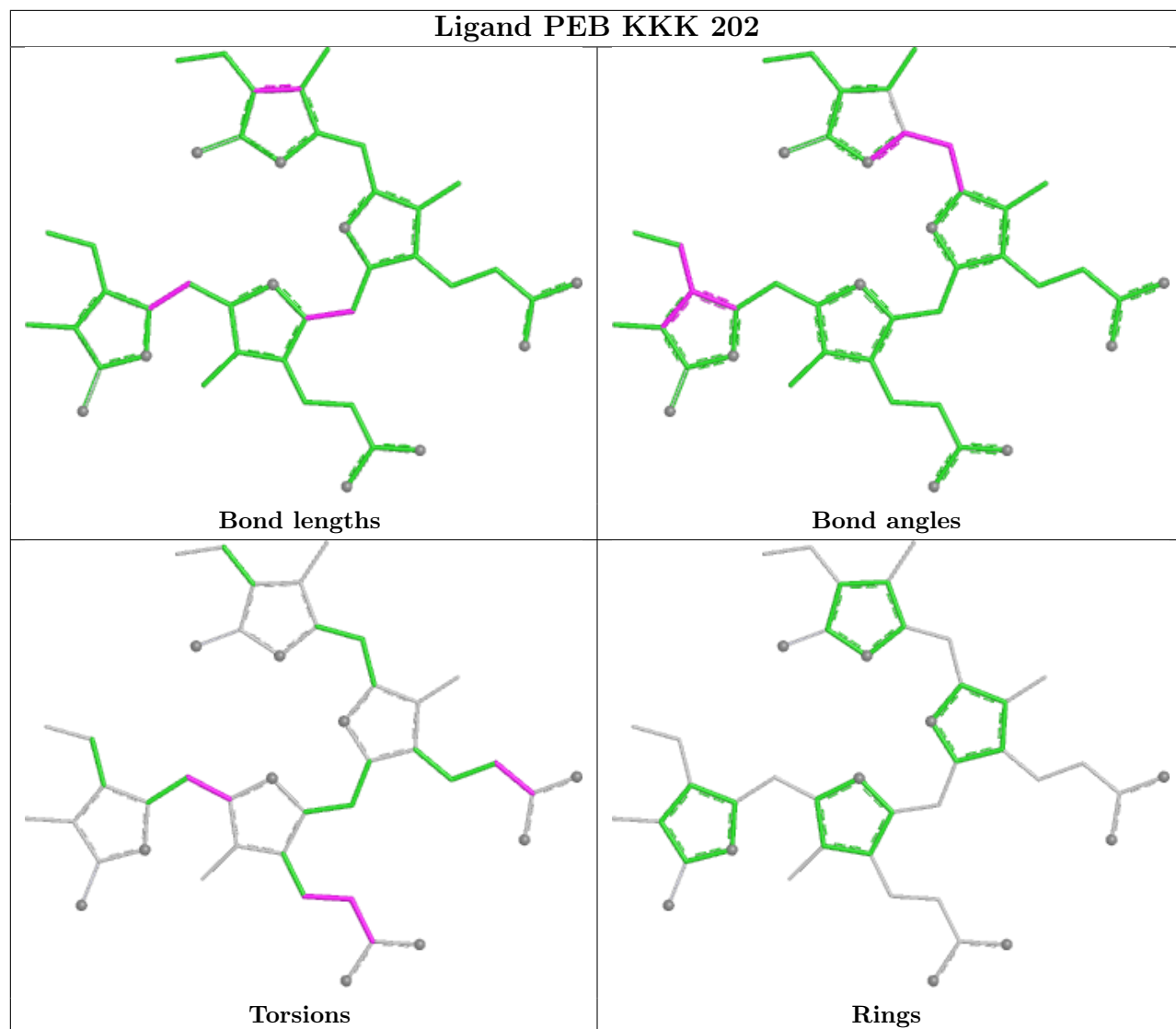




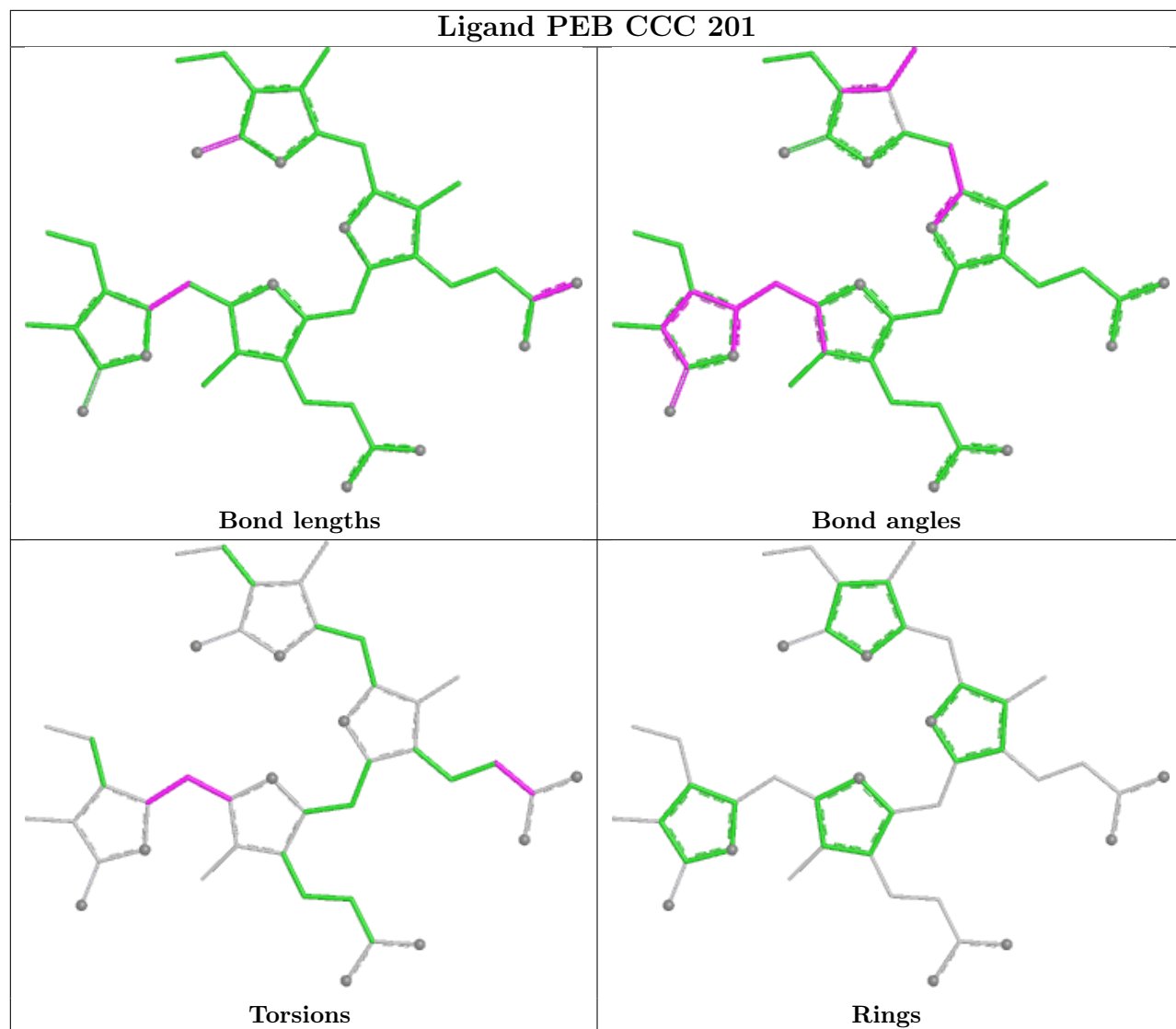
Ligand PEB LLL 201



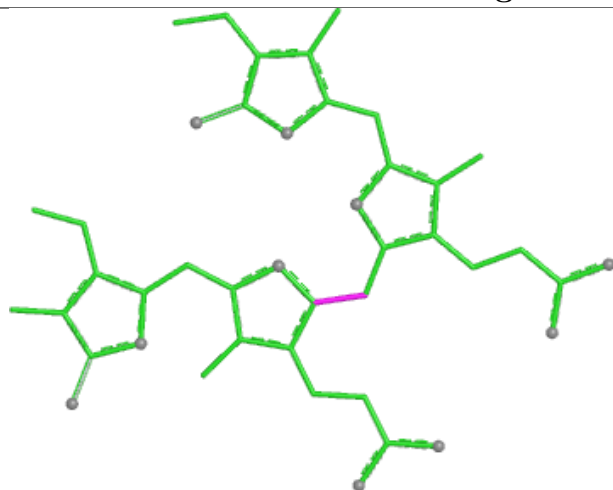
Ligand PEB KKK 202



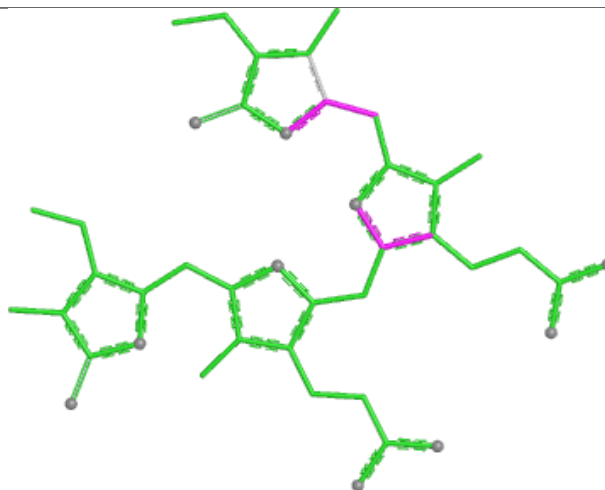
Ligand PEB CCC 201



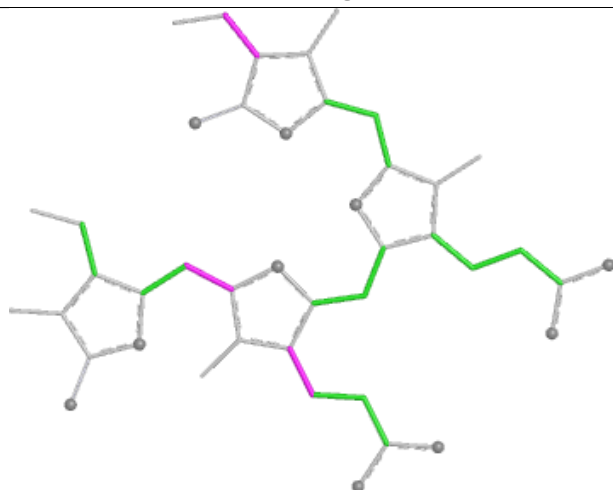
Ligand PEB LLL 203



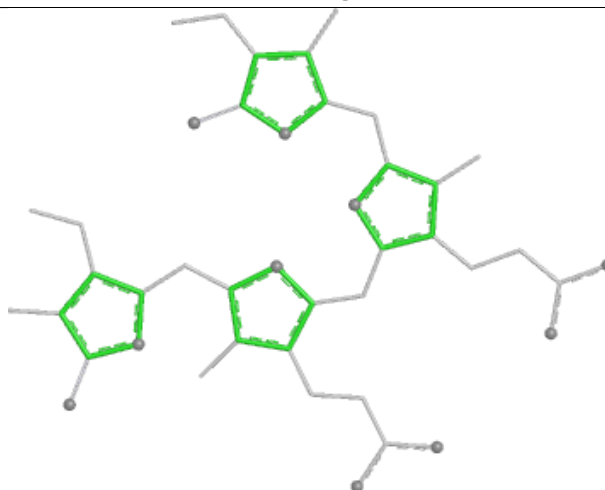
Bond lengths



Bond angles

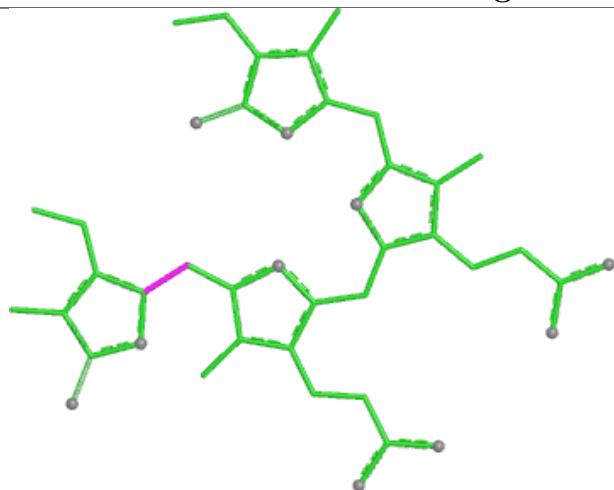


Torsions

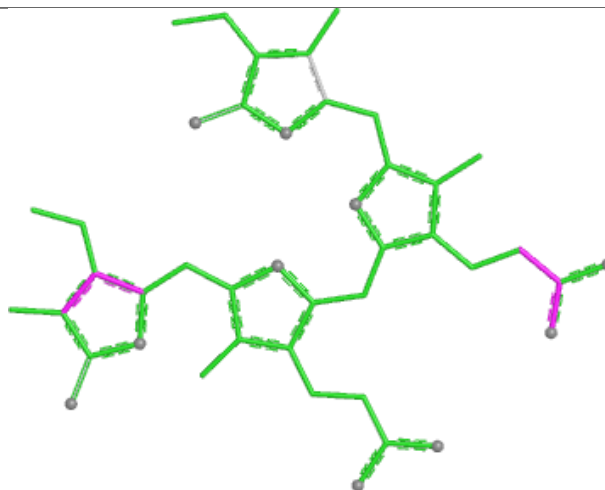


Rings

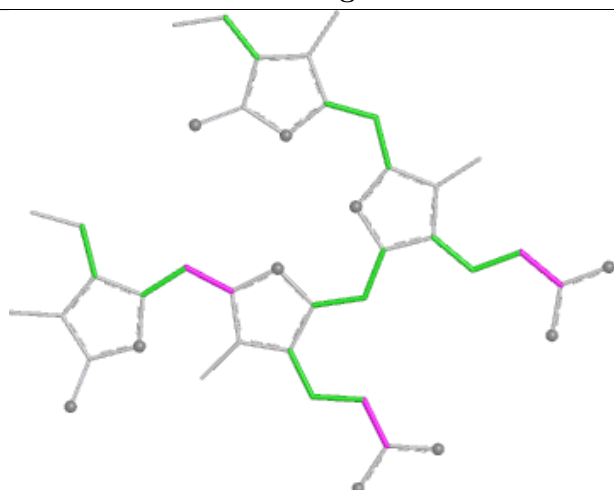
Ligand PEB FFF 205



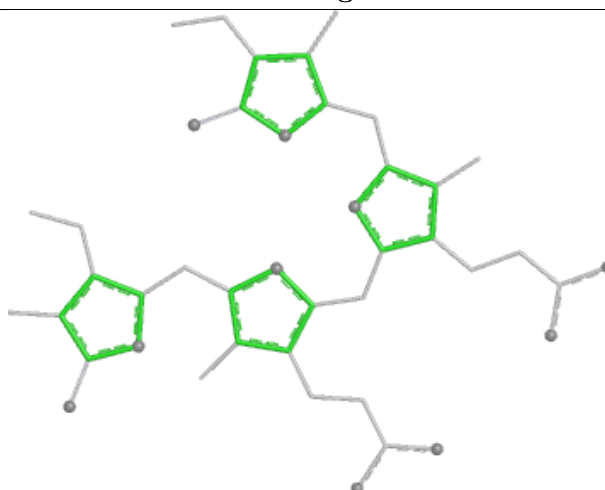
Bond lengths



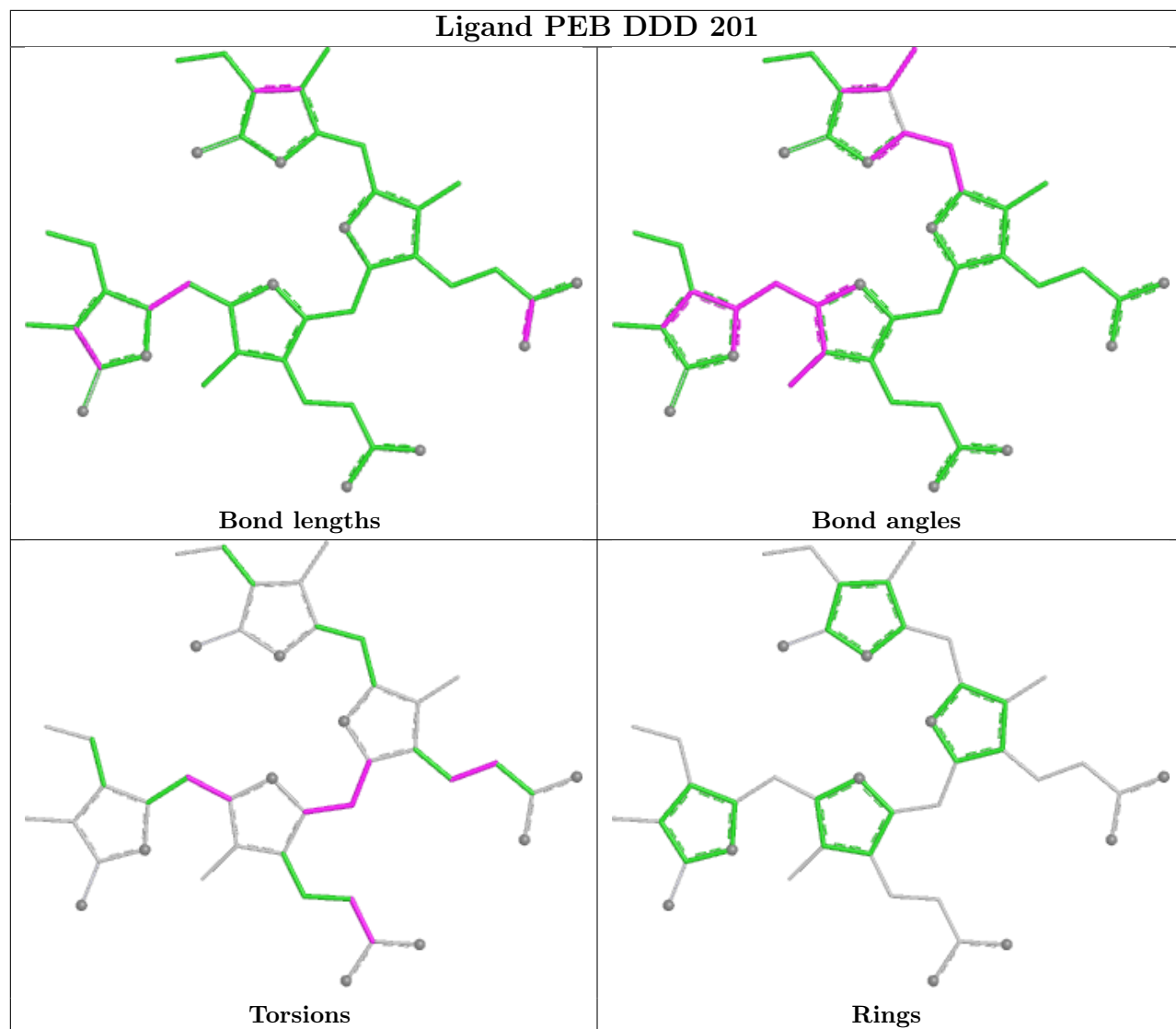
Bond angles

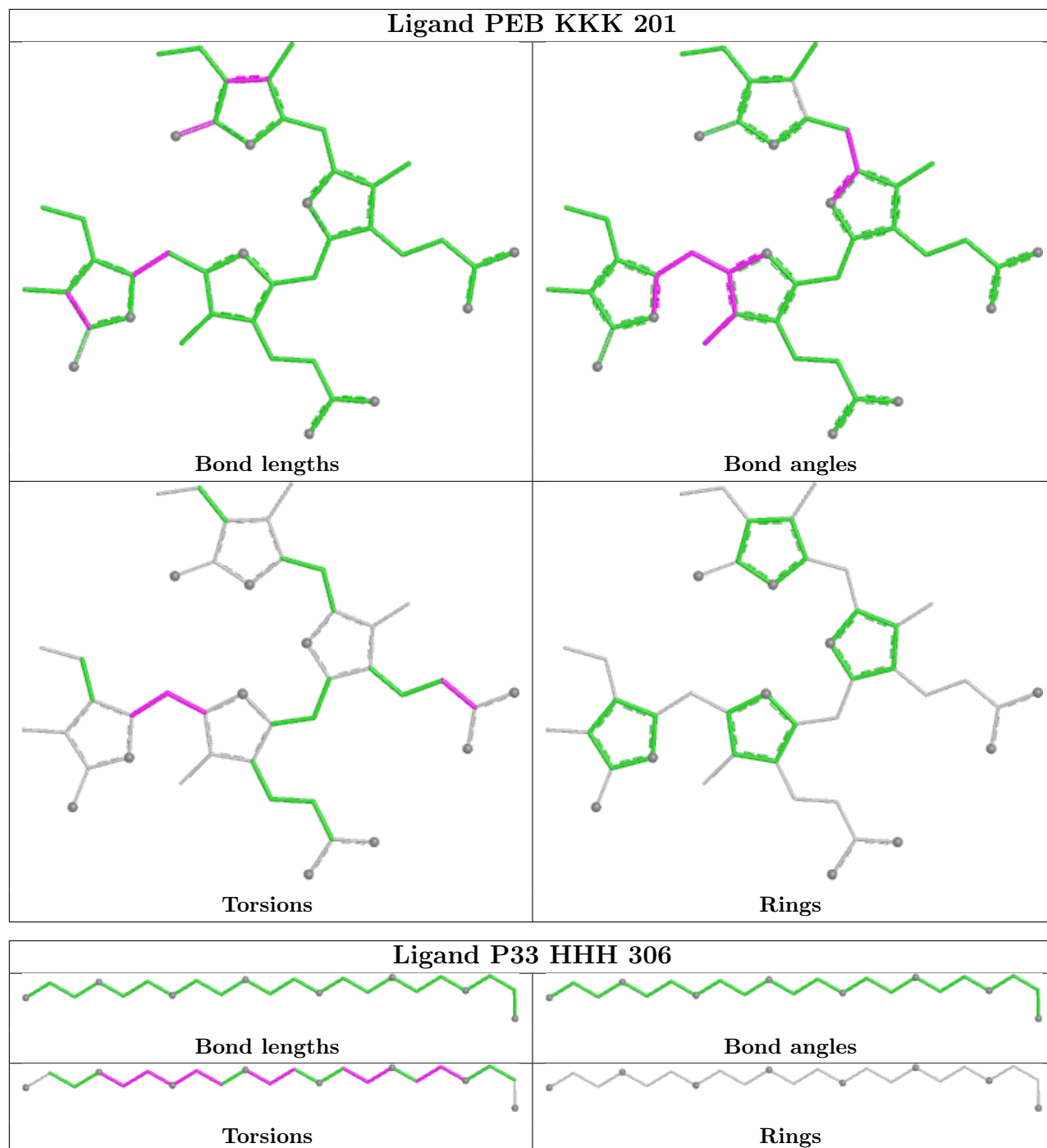


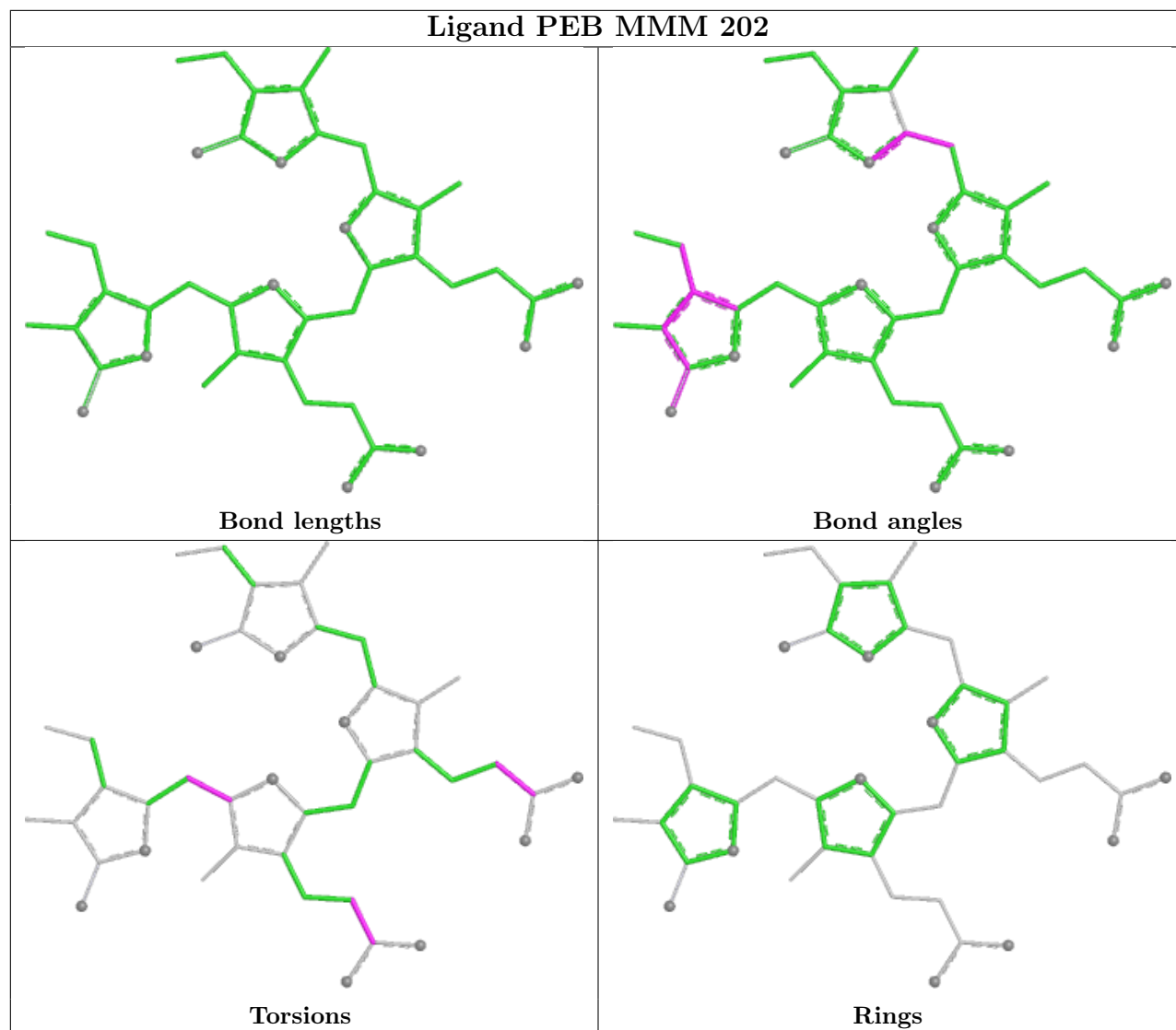
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	164/164 (100%)	-0.16	0 100 100	18, 36, 47, 55	4 (2%)
1	CCC	164/164 (100%)	-0.18	0 100 100	18, 38, 49, 57	4 (2%)
1	EEE	164/164 (100%)	-0.10	0 100 100	18, 39, 52, 59	4 (2%)
1	GGG	164/164 (100%)	-0.09	1 (0%) 85 88	19, 39, 55, 63	2 (1%)
1	III	164/164 (100%)	-0.15	0 100 100	18, 39, 52, 61	2 (1%)
1	KKK	164/164 (100%)	-0.08	0 100 100	22, 40, 52, 59	3 (1%)
1	MMM	164/164 (100%)	-0.06	2 (1%) 76 80	26, 39, 54, 65	3 (1%)
1	OOO	164/164 (100%)	0.91	16 (9%) 13 15	45, 58, 80, 92	1 (0%)
2	BBB	183/184 (99%)	-0.19	0 100 100	14, 35, 48, 74	6 (3%)
2	DDD	183/184 (99%)	-0.12	0 100 100	22, 36, 51, 77	9 (4%)
2	FFF	183/184 (99%)	-0.11	3 (1%) 70 74	23, 37, 51, 75	6 (3%)
2	HHH	183/184 (99%)	-0.12	1 (0%) 87 89	23, 38, 52, 78	7 (3%)
2	JJJ	183/184 (99%)	-0.11	2 (1%) 78 81	22, 37, 54, 67	8 (4%)
2	LLL	183/184 (99%)	-0.12	3 (1%) 70 74	15, 37, 51, 67	7 (3%)
2	NNN	183/184 (99%)	0.05	3 (1%) 70 74	26, 41, 56, 73	3 (1%)
2	PPP	183/184 (99%)	0.86	23 (12%) 8 9	32, 54, 137, 182	5 (2%)
All	All	2776/2784 (99%)	0.01	54 (1%) 66 70	14, 39, 61, 182	74 (2%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	PPP	152	LYS	6.1
2	PPP	153	LEU	5.1
2	PPP	147	ALA	5.0
2	PPP	151	ALA	4.7
2	PPP	159	PRO	4.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MEN	PPP	70	9/10	0.93	0.10	44,45,47,50	0
2	MEN	LLL	70	9/10	0.95	0.09	29,31,35,36	0
2	MEN	FFF	70	9/10	0.95	0.08	33,36,37,39	0
2	MEN	BBB	70	9/10	0.96	0.06	31,33,34,35	0
2	MEN	NNN	70	9/10	0.96	0.07	38,40,42,45	0
2	MEN	JJJ	70	9/10	0.96	0.08	30,33,37,37	0
2	MEN	DDD	70	9/10	0.97	0.07	31,33,37,38	0
2	MEN	HHH	70	9/10	0.98	0.06	31,33,35,36	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PO4	OOO	211	5/5	0.46	0.13	125,128,132,132	0
7	PO4	DDD	224	5/5	0.47	0.17	58,59,60,62	5
14	EDO	FFF	203	4/4	0.48	0.44	51,51,51,53	4
14	EDO	HHH	320	4/4	0.53	0.37	51,52,52,52	4
14	EDO	NNN	217	4/4	0.54	0.31	48,49,50,51	4
8	NO3	JJJ	320	4/4	0.61	0.22	54,55,60,62	4
8	NO3	CCC	218	4/4	0.62	0.20	47,48,51,57	4
8	NO3	DDD	226	4/4	0.63	0.20	43,43,44,46	4
7	PO4	III	216	5/5	0.64	0.30	49,51,55,58	5
8	NO3	AAA	216	4/4	0.65	0.21	38,39,42,47	4
8	NO3	EEE	211	4/4	0.65	0.24	40,41,42,45	4
14	EDO	NNN	218	4/4	0.65	0.30	44,44,45,45	4
6	PEG	III	211	7/7	0.66	0.28	37,39,40,41	7
8	NO3	JJJ	322	4/4	0.68	0.14	41,45,46,46	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	EDO	NNN	219	4/4	0.68	0.27	48,49,50,51	4
7	PO4	PPP	218	5/5	0.69	0.25	46,47,49,51	5
7	PO4	KKK	214	5/5	0.69	0.26	50,50,52,56	5
6	PEG	CCC	215	7/7	0.69	0.20	35,38,38,38	7
8	NO3	AAA	217	4/4	0.70	0.19	45,48,55,57	4
7	PO4	CCC	217	5/5	0.70	0.19	55,56,58,59	5
8	NO3	MMM	211	4/4	0.70	0.20	40,46,49,53	4
8	NO3	HHH	325	4/4	0.70	0.15	38,42,43,46	4
7	PO4	KKK	213	5/5	0.71	0.21	42,46,49,49	5
14	EDO	FFF	219	4/4	0.71	0.28	49,50,53,53	4
5	PGE	OOO	206	10/10	0.72	0.26	63,68,69,71	10
4	PG4	NNN	208	13/13	0.72	0.24	49,55,58,58	13
7	PO4	NNN	224	5/5	0.72	0.17	62,63,65,71	5
5	PGE	BBB	209	10/10	0.72	0.36	45,47,48,49	10
7	PO4	JJJ	321	5/5	0.72	0.18	41,44,47,53	5
8	NO3	FFF	225	4/4	0.73	0.18	43,43,44,50	4
8	NO3	DDD	225	4/4	0.73	0.13	43,44,46,48	4
14	EDO	III	217	4/4	0.73	0.20	42,43,43,44	4
7	PO4	AAA	215	5/5	0.74	0.16	49,51,53,53	5
8	NO3	LLL	223	4/4	0.74	0.15	48,51,51,53	4
5	PGE	CCC	208	10/10	0.74	0.22	42,50,51,51	10
6	PEG	LLL	217	7/7	0.74	0.22	46,48,50,50	7
7	PO4	FFF	224	5/5	0.74	0.17	51,51,52,54	5
6	PEG	III	210	7/7	0.75	0.20	48,48,49,49	7
7	PO4	NNN	221	5/5	0.75	0.22	49,50,50,52	5
6	PEG	BBB	213	7/7	0.75	0.29	38,44,46,47	7
6	PEG	MMM	209	7/7	0.76	0.27	37,41,42,44	7
14	EDO	DDD	218	4/4	0.76	0.34	38,38,39,39	4
6	PEG	CCC	214	7/7	0.76	0.23	43,49,54,54	7
7	PO4	NNN	223	5/5	0.77	0.23	46,49,51,52	5
8	NO3	BBB	221	4/4	0.77	0.14	41,43,45,48	4
6	PEG	GGG	211	7/7	0.77	0.30	29,31,33,33	7
14	EDO	HHH	319	4/4	0.77	0.38	38,39,41,42	4
7	PO4	AAA	214	5/5	0.77	0.24	47,47,49,49	5
7	PO4	HHH	324	5/5	0.77	0.32	40,42,45,47	5
7	PO4	DDD	220	5/5	0.77	0.19	44,48,52,53	5
8	NO3	OOO	212	4/4	0.77	0.14	44,47,49,49	4
8	NO3	PPP	219	4/4	0.77	0.14	39,40,41,42	4
6	PEG	LLL	218[B]	7/7	0.78	0.28	45,48,50,50	7
6	PEG	HHH	316	7/7	0.78	0.19	40,48,53,53	7
6	PEG	III	201	7/7	0.78	0.23	35,36,38,39	7
14	EDO	DDD	217	4/4	0.78	0.27	37,38,38,39	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PGE	DDD	212	10/10	0.78	0.23	39,53,55,56	10
7	PO4	BBB	218	5/5	0.78	0.23	43,45,48,51	5
4	PG4	MMM	205	13/13	0.78	0.24	48,49,53,53	13
6	PEG	III	212	7/7	0.78	0.23	34,37,41,42	7
5	PGE	AAA	210	10/10	0.78	0.31	50,57,57,58	10
8	NO3	III	218	4/4	0.78	0.14	41,41,46,48	4
7	PO4	FFF	222	5/5	0.78	0.25	46,46,47,50	5
6	PEG	LLL	218[A]	7/7	0.78	0.28	40,44,46,46	7
7	PO4	HHH	322	5/5	0.78	0.23	37,39,41,41	5
14	EDO	PPP	215	4/4	0.78	0.26	51,52,52,53	4
8	NO3	KKK	216	4/4	0.79	0.16	42,42,49,49	4
6	PEG	DDD	216	7/7	0.79	0.26	47,48,50,51	7
6	PEG	PPP	211	7/7	0.79	0.27	48,48,51,51	7
5	PGE	KKK	206	10/10	0.79	0.22	47,51,54,55	10
6	PEG	HHH	317	7/7	0.80	0.21	43,48,52,52	7
7	PO4	GGG	215	5/5	0.80	0.25	43,46,47,49	5
6	PEG	CCC	219	7/7	0.80	0.20	46,48,49,50	7
6	PEG	LLL	212	7/7	0.80	0.24	43,46,49,49	7
6	PEG	NNN	214	7/7	0.80	0.26	38,50,57,57	7
6	PEG	NNN	215	7/7	0.80	0.31	41,44,49,50	7
11	1PE	LLL	205	16/16	0.80	0.22	38,56,63,63	16
6	PEG	OOO	207	7/7	0.80	0.30	43,45,47,47	7
5	PGE	HHH	310	10/10	0.80	0.30	48,52,55,55	10
4	PG4	AAA	205	13/13	0.81	0.24	46,48,49,49	13
4	PG4	GGG	205	13/13	0.81	0.21	50,53,56,56	13
5	PGE	HHH	312	10/10	0.81	0.20	41,47,49,49	10
6	PEG	LLL	213	7/7	0.81	0.20	46,49,52,53	7
5	PGE	HHH	313	10/10	0.81	0.23	41,45,48,49	10
4	PG4	AAA	203	13/13	0.81	0.23	42,46,51,51	13
5	PGE	BBB	210	10/10	0.81	0.20	41,45,50,50	10
14	EDO	LLL	219	4/4	0.81	0.26	33,34,34,35	4
6	PEG	HHH	318	7/7	0.81	0.23	41,44,47,47	7
5	PGE	BBB	222	10/10	0.81	0.23	47,48,49,50	10
11	1PE	BBB	207	16/16	0.81	0.24	41,50,57,58	16
4	PG4	NNN	207	13/13	0.81	0.23	42,47,55,55	13
6	PEG	CCC	213	7/7	0.82	0.25	38,40,44,44	7
6	PEG	GGG	210	7/7	0.82	0.27	48,49,51,51	7
4	PG4	DDD	208	13/13	0.82	0.21	37,49,54,54	13
11	1PE	JJJ	308	16/16	0.82	0.25	42,50,52,52	16
4	PG4	FFF	210	13/13	0.82	0.20	43,51,55,56	13
12	P33	DDD	205	22/22	0.82	0.23	39,51,57,58	22
8	NO3	LLL	224	4/4	0.82	0.11	43,45,45,46	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PEG	BBB	216	7/7	0.82	0.22	39,43,45,45	7
14	EDO	EEE	208	4/4	0.82	0.22	38,39,40,41	4
14	EDO	EEE	209	4/4	0.82	0.27	53,53,54,54	4
5	PGE	FFF	213	10/10	0.83	0.19	41,42,53,53	10
5	PGE	HHH	309	10/10	0.83	0.20	46,49,52,52	10
6	PEG	JJJ	314	7/7	0.83	0.23	51,53,56,57	7
7	PO4	DDD	222	5/5	0.83	0.26	48,49,51,52	5
6	PEG	LLL	211	7/7	0.83	0.18	41,44,49,50	7
4	PG4	CCC	203	13/13	0.83	0.20	43,46,50,51	13
6	PEG	OOO	208	7/7	0.83	0.24	51,54,56,56	7
6	PEG	CCC	221	7/7	0.83	0.21	41,42,44,46	7
6	PEG	PPP	212	7/7	0.83	0.32	45,47,48,48	7
4	PG4	AAA	204	13/13	0.83	0.23	46,51,60,61	13
4	PG4	HHH	308	13/13	0.83	0.24	49,51,54,55	13
6	PEG	GGG	212	7/7	0.84	0.20	41,42,44,44	7
4	PG4	MMM	212	13/13	0.84	0.19	42,47,60,60	13
11	1PE	DDD	207	16/16	0.84	0.21	46,52,53,54	16
5	PGE	JJJ	310	10/10	0.84	0.21	38,42,46,47	10
5	PGE	GGG	208	10/10	0.84	0.18	34,50,56,57	10
5	PGE	OOO	204	10/10	0.84	0.25	49,54,57,57	10
12	P33	HHH	306	22/22	0.84	0.24	47,51,58,59	22
5	PGE	OOO	205	10/10	0.84	0.25	45,47,49,50	10
4	PG4	OOO	203	13/13	0.84	0.29	49,51,55,56	13
6	PEG	EEE	212	7/7	0.84	0.26	45,47,47,48	7
7	PO4	III	215	5/5	0.84	0.21	48,51,52,53	5
8	NO3	GGG	216	4/4	0.84	0.13	41,42,44,44	4
6	PEG	PPP	201	7/7	0.84	0.26	43,47,51,52	7
7	PO4	JJJ	317	5/5	0.84	0.15	43,44,45,49	5
6	PEG	JJJ	313	7/7	0.84	0.15	41,44,46,47	7
6	PEG	EEE	213	7/7	0.84	0.22	46,49,50,50	7
6	PEG	FFF	218	7/7	0.84	0.19	40,43,46,47	7
4	PG4	PPP	206	13/13	0.84	0.20	40,48,50,51	13
5	PGE	EEE	205	10/10	0.84	0.23	44,46,51,52	10
7	PO4	CCC	216	5/5	0.84	0.18	46,47,51,52	5
6	PEG	LLL	214	7/7	0.84	0.22	48,49,50,51	7
5	PGE	HHH	311	10/10	0.85	0.22	47,54,60,61	10
6	PEG	FFF	215	7/7	0.85	0.15	43,50,52,54	7
4	PG4	LLL	208	13/13	0.85	0.21	40,42,49,50	13
6	PEG	OOO	210	7/7	0.85	0.20	40,42,43,43	7
8	NO3	EEE	210	4/4	0.85	0.12	40,42,45,49	4
6	PEG	III	209	7/7	0.85	0.23	49,51,54,54	7
9	RWB	BBB	204	38/38	0.85	0.20	34,48,59,61	38

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PEG	LLL	216	7/7	0.85	0.17	49,52,54,57	7
5	PGE	DDD	211	10/10	0.85	0.23	47,53,55,56	10
5	PGE	AAA	209	10/10	0.85	0.23	50,53,57,58	10
4	PG4	KKK	204	13/13	0.85	0.27	40,48,54,54	13
6	PEG	HHH	314	7/7	0.85	0.22	46,47,48,50	7
5	PGE	NNN	210	10/10	0.85	0.18	42,49,51,51	10
13	P6G	DDD	206	19/19	0.85	0.18	35,37,54,54	19
5	PGE	AAA	208	10/10	0.86	0.18	41,43,45,46	10
11	1PE	BBB	208	16/16	0.86	0.19	37,48,54,55	16
6	PEG	BBB	211	7/7	0.86	0.25	46,48,52,52	7
11	1PE	HHH	301	16/16	0.86	0.22	43,48,51,52	16
6	PEG	BBB	212	7/7	0.86	0.14	40,42,51,51	7
4	PG4	GGG	203	13/13	0.86	0.21	50,52,55,55	13
11	1PE	PPP	205	16/16	0.86	0.28	47,53,56,57	16
6	PEG	BBB	214	7/7	0.86	0.17	43,44,46,47	7
4	PG4	NNN	209	13/13	0.86	0.21	44,49,57,58	13
6	PEG	HHH	315	7/7	0.86	0.19	42,45,46,48	7
6	PEG	CCC	209	7/7	0.86	0.21	40,43,46,47	7
6	PEG	CCC	211	7/7	0.86	0.21	42,42,46,47	7
5	PGE	EEE	207	10/10	0.86	0.17	47,49,55,56	10
4	PG4	NNN	202	13/13	0.86	0.23	47,53,57,59	13
6	PEG	III	208	7/7	0.86	0.16	44,44,45,46	7
5	PGE	KKK	207	10/10	0.86	0.18	40,43,46,46	10
4	PG4	HHH	307	13/13	0.86	0.20	39,43,46,48	13
8	NO3	KKK	217	4/4	0.86	0.18	36,39,41,41	4
14	EDO	III	213	4/4	0.86	0.20	43,43,45,45	4
5	PGE	NNN	212	10/10	0.86	0.20	46,51,54,57	10
6	PEG	DDD	214	7/7	0.86	0.17	45,48,50,51	7
6	PEG	DDD	215	7/7	0.86	0.17	53,56,57,59	7
5	PGE	NNN	213	10/10	0.86	0.17	42,48,53,54	10
4	PG4	PPP	207	13/13	0.86	0.19	44,46,52,53	13
5	PGE	AAA	207	10/10	0.86	0.15	45,47,51,53	10
7	PO4	FFF	223	5/5	0.87	0.20	42,46,47,47	5
12	P33	FFF	207	22/22	0.87	0.18	43,46,65,69	22
6	PEG	LLL	215	7/7	0.87	0.19	47,48,51,51	7
5	PGE	III	207	10/10	0.87	0.17	42,48,49,50	10
4	PG4	FFF	202	13/13	0.87	0.16	42,44,46,46	13
4	PG4	KKK	205	13/13	0.87	0.18	39,47,52,53	13
5	PGE	EEE	204	10/10	0.87	0.18	40,45,49,49	10
6	PEG	FFF	214	7/7	0.87	0.17	40,43,48,48	7
7	PO4	BBB	220	5/5	0.87	0.15	46,47,52,53	5
10	PE8	BBB	205	25/25	0.87	0.20	44,50,68,71	25

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PEG	MMM	210	7/7	0.87	0.17	50,51,54,54	7
6	PEG	KKK	209	7/7	0.87	0.16	42,52,55,55	7
7	PO4	CCC	220	5/5	0.87	0.16	43,47,49,50	5
5	PGE	LLL	209	10/10	0.87	0.20	47,51,53,53	10
11	1PE	JJJ	302	16/16	0.87	0.19	37,45,48,49	16
11	1PE	JJJ	307	16/16	0.87	0.15	41,43,48,48	16
5	PGE	CCC	204	10/10	0.87	0.16	43,53,58,58	10
5	PGE	CCC	207	10/10	0.87	0.17	46,51,57,59	10
4	PG4	LLL	206	13/13	0.87	0.19	45,49,64,66	13
5	PGE	GGG	206	10/10	0.88	0.18	45,52,54,54	10
5	PGE	GGG	207	10/10	0.88	0.17	41,46,49,50	10
4	PG4	LLL	207	13/13	0.88	0.18	39,42,48,48	13
5	PGE	GGG	217	10/10	0.88	0.19	51,53,58,60	10
6	PEG	CCC	212	7/7	0.88	0.18	54,56,58,59	7
4	PG4	KKK	203	13/13	0.88	0.15	41,55,66,67	13
6	PEG	KKK	208	7/7	0.88	0.16	39,41,41,42	7
4	PG4	FFF	209	13/13	0.88	0.18	41,44,48,51	13
6	PEG	OOO	209	7/7	0.88	0.18	53,55,56,56	7
6	PEG	KKK	211	7/7	0.88	0.18	43,44,46,47	7
4	PG4	DDD	209	13/13	0.88	0.17	48,52,53,55	13
5	PGE	EEE	206	10/10	0.88	0.15	43,50,56,57	10
7	PO4	III	214	5/5	0.88	0.16	45,48,56,59	5
4	PG4	JJJ	309	13/13	0.88	0.21	44,47,60,61	13
5	PGE	PPP	208	10/10	0.88	0.17	45,50,51,51	10
5	PGE	III	206	10/10	0.88	0.17	47,49,50,51	10
7	PO4	JJJ	318	5/5	0.88	0.17	43,44,45,49	5
5	PGE	FFF	212	10/10	0.88	0.20	43,46,49,52	10
5	PGE	AAA	211	10/10	0.88	0.21	27,28,29,31	10
6	PEG	KKK	212	7/7	0.89	0.15	41,42,43,43	7
7	PO4	PPP	216	5/5	0.89	0.14	48,48,51,52	5
5	PGE	NNN	211	10/10	0.89	0.19	43,43,48,49	10
8	NO3	LLL	222	4/4	0.89	0.16	43,46,46,47	4
5	PGE	JJJ	311	10/10	0.89	0.18	47,53,59,59	10
12	P33	JJJ	306	22/22	0.89	0.17	44,48,73,75	22
5	PGE	III	204	10/10	0.89	0.16	44,47,55,59	10
5	PGE	DDD	210	10/10	0.89	0.19	39,48,57,58	10
4	PG4	FFF	208	13/13	0.89	0.15	40,43,45,45	13
5	PGE	MMM	206	10/10	0.89	0.15	44,48,51,52	10
6	PEG	FFF	216	7/7	0.89	0.17	43,44,45,45	7
9	RWB	LLL	204	38/38	0.89	0.17	38,47,69,70	38
7	PO4	JJJ	319	5/5	0.89	0.12	62,62,65,67	5
11	1PE	BBB	206	16/16	0.89	0.16	40,44,49,50	16

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PEG	DDD	213	7/7	0.89	0.16	42,43,54,58	7
7	PO4	DDD	223	5/5	0.89	0.18	45,52,53,53	5
6	PEG	PPP	209	7/7	0.89	0.17	47,47,50,51	7
11	1PE	EEE	203	16/16	0.89	0.17	47,60,64,67	16
4	PG4	GGG	204	13/13	0.89	0.15	30,35,56,59	13
8	NO3	HHH	326	4/4	0.89	0.10	47,47,49,51	4
6	PEG	MMM	208	7/7	0.89	0.18	42,46,49,50	7
6	PEG	PPP	214	7/7	0.89	0.19	42,48,50,50	7
15	PE5	NNN	206	27/27	0.89	0.17	33,43,71,74	27
11	1PE	FFF	201	16/16	0.90	0.17	38,51,63,64	16
6	PEG	GGG	213	7/7	0.90	0.14	46,47,50,52	7
7	PO4	KKK	215	5/5	0.90	0.14	45,47,50,51	5
5	PGE	III	205	10/10	0.90	0.13	42,43,45,45	10
4	PG4	MMM	203	13/13	0.90	0.15	38,44,55,57	13
3	PEB	OOO	202	43/43	0.90	0.11	56,63,73,74	0
6	PEG	FFF	217	7/7	0.90	0.15	43,45,46,46	7
5	PGE	LLL	210	10/10	0.90	0.17	43,45,47,48	10
6	PEG	KKK	210	7/7	0.90	0.15	43,45,49,50	7
6	PEG	PPP	210	7/7	0.90	0.16	49,52,54,54	7
6	PEG	GGG	209	7/7	0.90	0.15	43,47,57,59	7
5	PGE	AAA	206	10/10	0.90	0.17	37,42,55,56	10
5	PGE	FFF	211	10/10	0.90	0.17	42,43,48,49	10
6	PEG	BBB	223	7/7	0.90	0.20	42,46,51,51	7
7	PO4	PPP	217	5/5	0.91	0.16	31,33,35,35	5
5	PGE	LLL	226	10/10	0.91	0.14	46,49,50,50	10
4	PG4	MMM	204	13/13	0.91	0.14	44,49,51,52	13
5	PGE	MMM	207	10/10	0.91	0.15	41,42,43,45	10
6	PEG	AAA	213	7/7	0.91	0.21	37,37,38,40	7
6	PEG	PPP	213	7/7	0.91	0.16	43,47,50,50	7
7	PO4	FFF	221	5/5	0.91	0.15	39,42,44,45	5
3	PEB	PPP	204	43/43	0.91	0.11	49,60,81,87	0
5	PGE	CCC	206	10/10	0.91	0.12	45,48,58,58	10
6	PEG	JJJ	312	7/7	0.91	0.15	43,44,46,46	7
12	P33	DDD	204	22/22	0.91	0.16	44,47,65,67	22
7	PO4	GGG	214	5/5	0.91	0.14	42,49,49,52	5
3	PEB	PPP	202	43/43	0.91	0.11	49,55,74,88	0
5	PGE	HHH	327	10/10	0.91	0.15	44,50,66,67	10
6	PEG	BBB	215	7/7	0.91	0.15	46,49,49,50	7
5	PGE	LLL	225	10/10	0.91	0.14	41,47,62,64	10
6	PEG	AAA	212	7/7	0.92	0.16	44,45,47,48	7
4	PG4	NNN	201	13/13	0.92	0.14	43,48,62,62	13
3	PEB	PPP	203	43/43	0.92	0.11	55,65,80,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEB	III	203	43/43	0.92	0.09	47,52,58,60	0
7	PO4	FFF	220	5/5	0.92	0.11	44,47,48,51	5
12	P33	HHH	305	22/22	0.93	0.14	45,48,56,57	22
6	PEG	NNN	216	7/7	0.93	0.15	42,46,46,48	7
3	PEB	KKK	202	43/43	0.93	0.09	45,54,59,63	0
5	PGE	JJJ	301	10/10	0.93	0.13	37,44,56,56	10
7	PO4	HHH	321	5/5	0.93	0.12	35,37,40,40	5
7	PO4	LLL	220	5/5	0.94	0.10	46,47,48,51	5
7	PO4	NNN	220	5/5	0.94	0.15	41,46,47,48	5
7	PO4	JJJ	316	5/5	0.94	0.10	43,43,46,49	5
3	PEB	OOO	201	43/43	0.94	0.09	45,51,56,60	0
5	PGE	CCC	205	10/10	0.94	0.10	45,46,55,63	0
3	PEB	FFF	206	43/43	0.94	0.08	33,37,44,51	0
7	PO4	DDD	219	5/5	0.94	0.10	37,39,40,41	5
3	PEB	BBB	202	43/43	0.94	0.08	32,36,44,55	0
6	PEG	DDD	227	7/7	0.94	0.12	45,46,51,54	7
3	PEB	EEE	202	43/43	0.94	0.09	45,55,60,64	0
3	PEB	LLL	202	43/43	0.95	0.08	36,41,52,72	0
3	PEB	LLL	203	43/43	0.95	0.07	30,35,48,51	0
7	PO4	BBB	217	5/5	0.95	0.09	42,43,44,45	5
3	PEB	MMM	202	43/43	0.95	0.08	44,50,56,58	0
7	PO4	BBB	219	5/5	0.95	0.10	41,41,44,45	5
3	PEB	NNN	203	43/43	0.95	0.08	40,47,58,72	0
3	PEB	NNN	205	43/43	0.95	0.08	37,42,46,50	0
3	PEB	EEE	201	43/43	0.95	0.08	33,36,42,45	0
7	PO4	JJJ	315	5/5	0.95	0.12	48,51,52,53	5
3	PEB	BBB	201	43/43	0.95	0.07	32,37,49,64	0
3	PEB	FFF	204	43/43	0.95	0.07	32,38,51,73	0
3	PEB	AAA	202	43/43	0.95	0.08	41,45,52,64	0
7	PO4	DDD	221	5/5	0.95	0.10	47,51,53,53	5
3	PEB	GGG	202	43/43	0.95	0.08	45,51,57,60	0
3	PEB	HHH	302	43/43	0.95	0.07	33,37,44,63	0
3	PEB	HHH	303	43/43	0.95	0.08	37,41,51,58	0
3	PEB	CCC	202	43/43	0.95	0.07	34,41,47,50	0
3	PEB	JJJ	303	43/43	0.95	0.07	34,38,49,75	0
3	PEB	JJJ	304	43/43	0.95	0.08	36,39,46,59	0
6	PEG	CCC	210	7/7	0.95	0.12	41,42,43,43	7
7	PO4	NNN	222	5/5	0.95	0.11	40,42,42,46	5
3	PEB	DDD	201	43/43	0.95	0.08	30,35,55,69	0
3	PEB	NNN	204	43/43	0.96	0.07	34,40,53,68	0
3	PEB	BBB	203	43/43	0.96	0.07	31,36,42,46	0
3	PEB	JJJ	305	43/43	0.96	0.06	32,36,41,42	0

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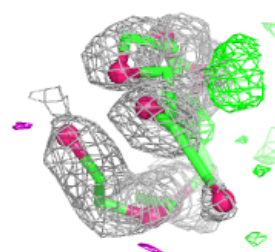
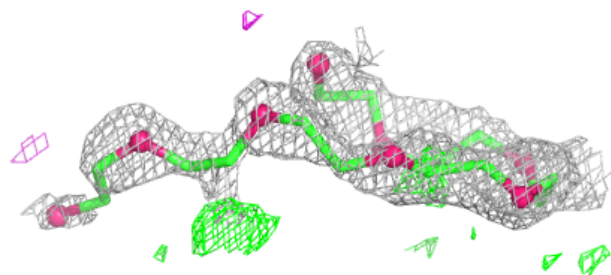
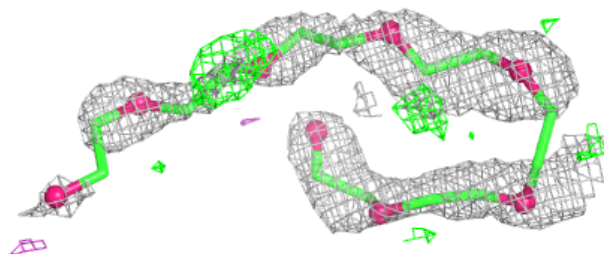
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEB	KKK	201	43/43	0.96	0.07	32,37,40,42	0
7	PO4	HHH	323	5/5	0.96	0.09	40,41,43,45	5
3	PEB	DDD	202	43/43	0.96	0.07	37,40,47,60	0
3	PEB	LLL	201	43/43	0.96	0.07	32,36,47,68	0
7	PO4	LLL	221	5/5	0.96	0.10	42,43,46,48	5
3	PEB	FFF	205	43/43	0.96	0.07	36,41,47,58	0
3	PEB	HHH	304	43/43	0.96	0.06	31,38,43,50	0
3	PEB	MMM	201	43/43	0.96	0.07	36,39,43,49	0
3	PEB	AAA	201	43/43	0.96	0.07	32,35,41,43	0
3	PEB	GGG	201	43/43	0.96	0.07	33,37,41,49	0
3	PEB	CCC	201	43/43	0.97	0.06	32,37,40,42	0
3	PEB	DDD	203	43/43	0.97	0.06	33,36,42,48	0
3	PEB	III	202	43/43	0.97	0.06	31,35,41,43	0

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

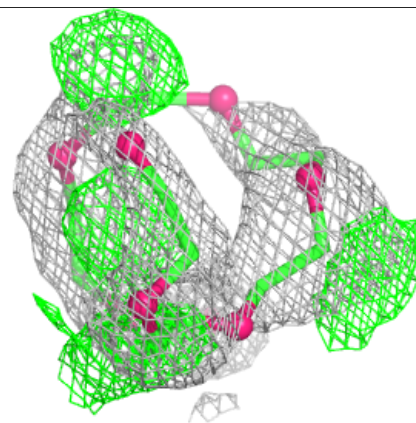
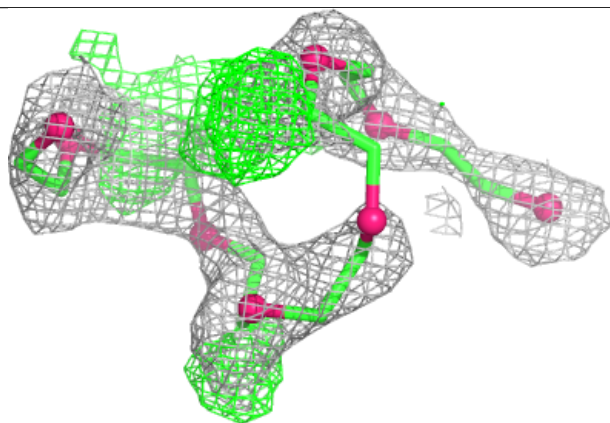
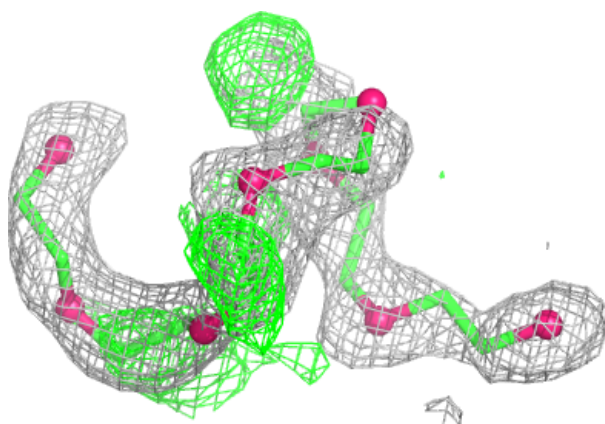
Electron density around P33 DDD 205:

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

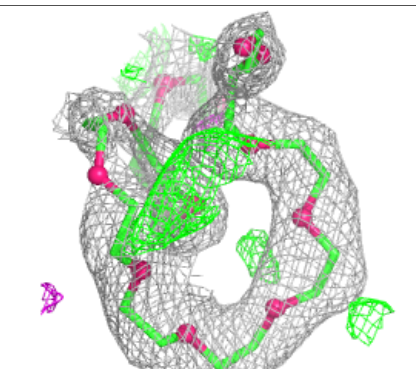
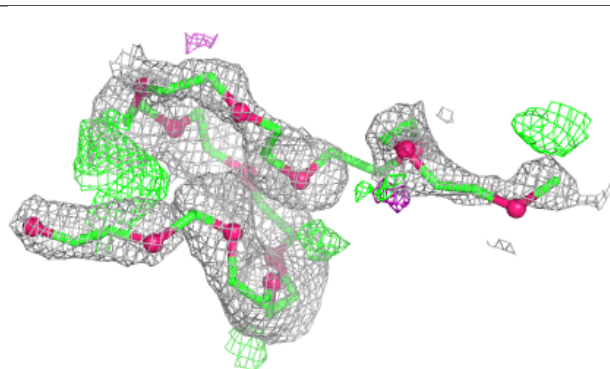
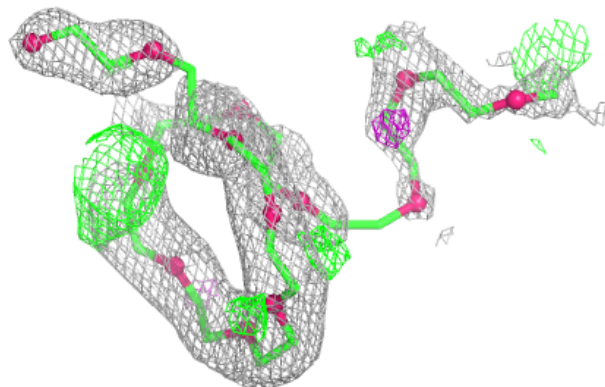


Electron density around P33 HHH 306:

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

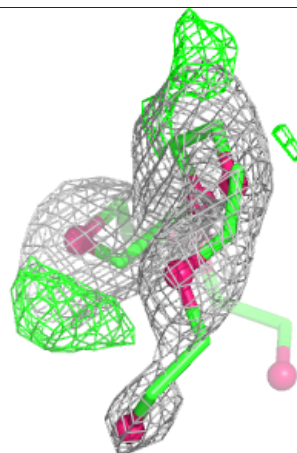
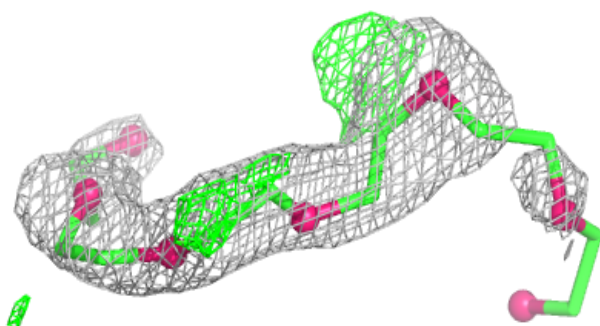
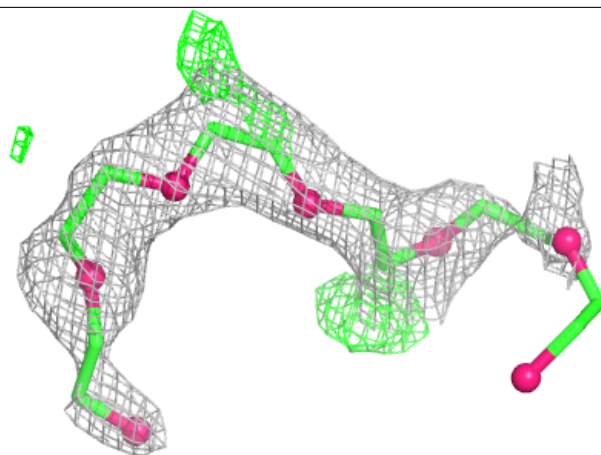
**Electron density around RWB BBB 204:**

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



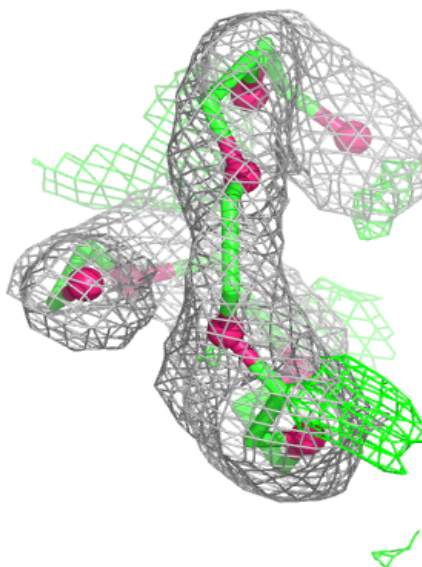
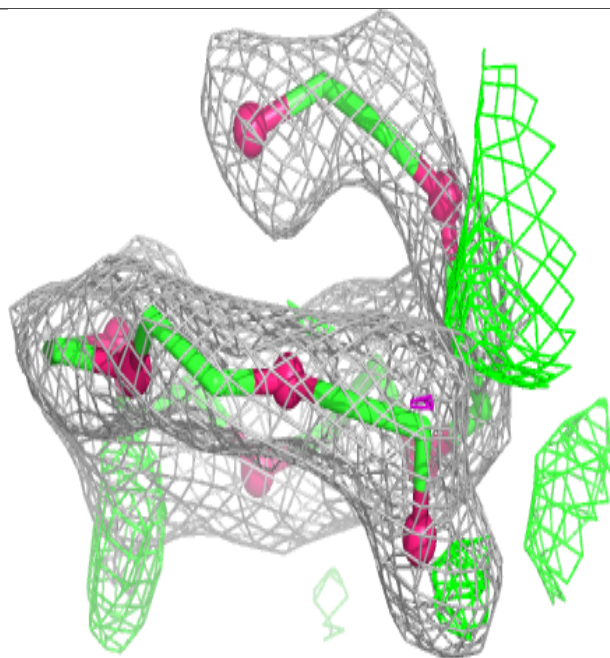
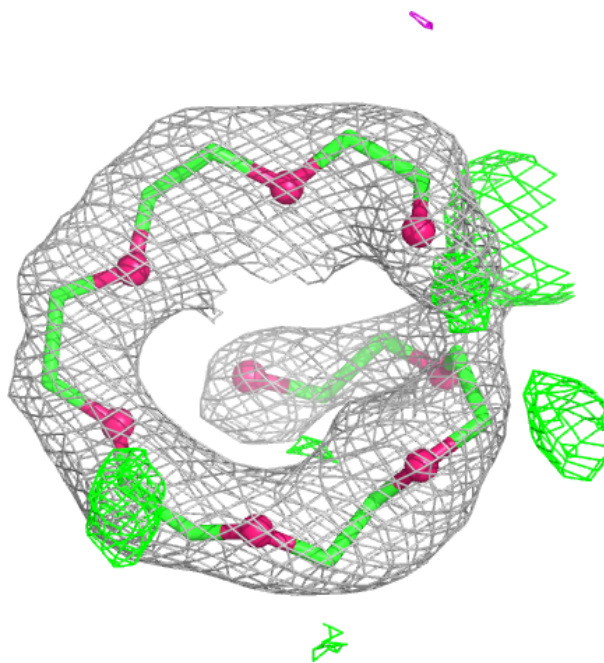
Electron density around P6G DDD 206:

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



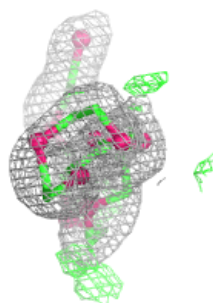
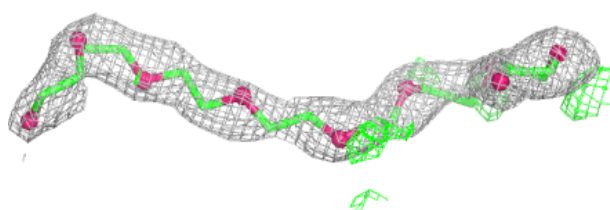
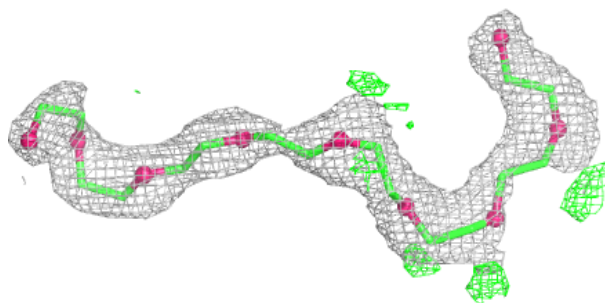
Electron density around P33 FFF 207:

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

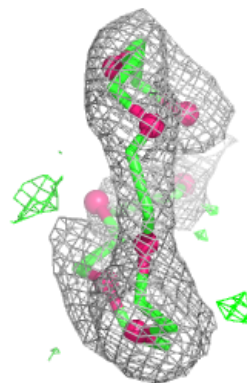
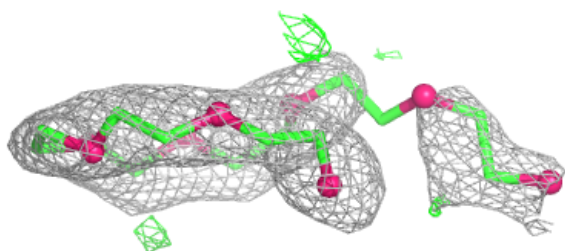
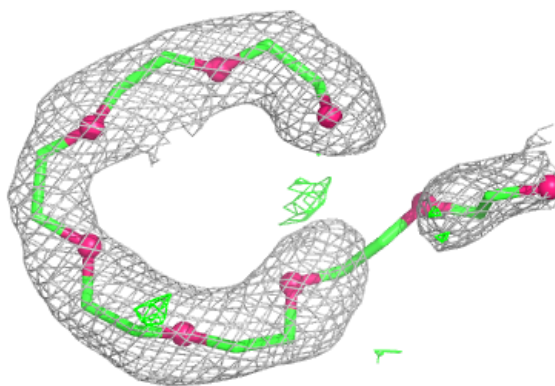


Electron density around PE8 BBB 205:

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

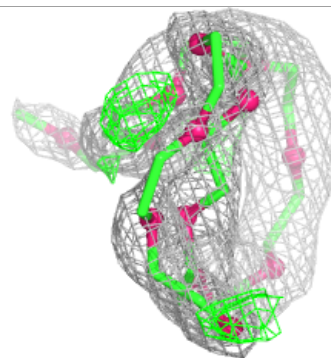
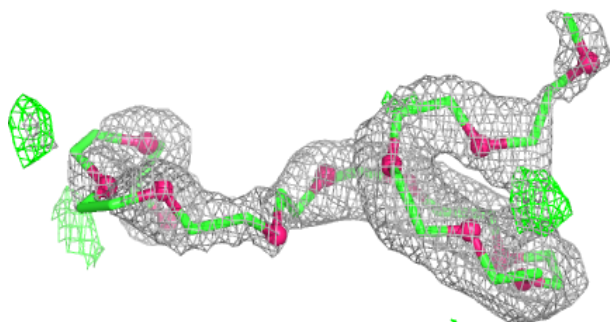
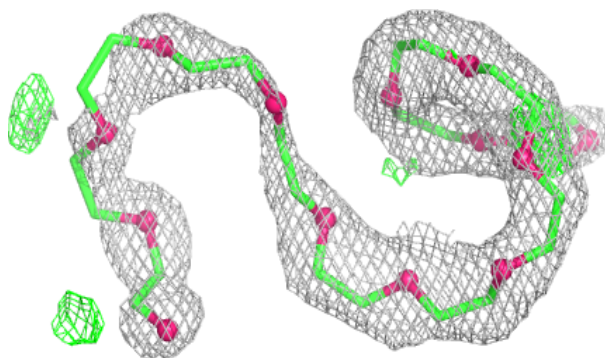
**Electron density around P33 JJJ 306:**

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

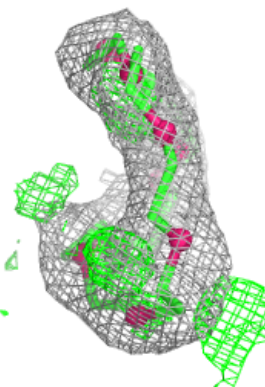
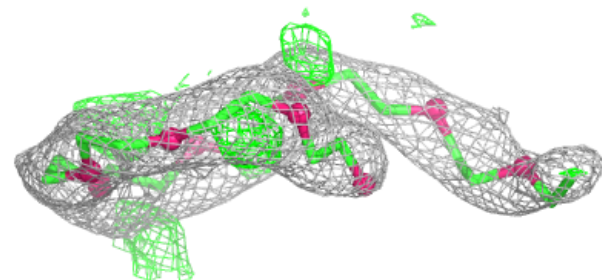
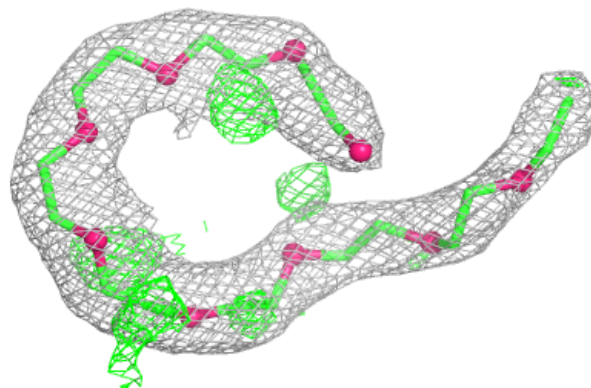


Electron density around RWB LLL 204:

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

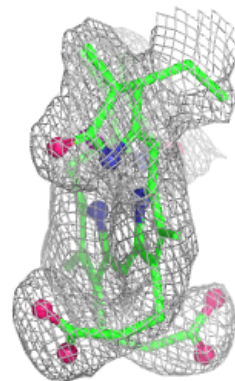
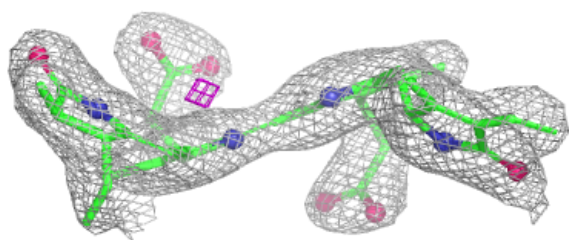
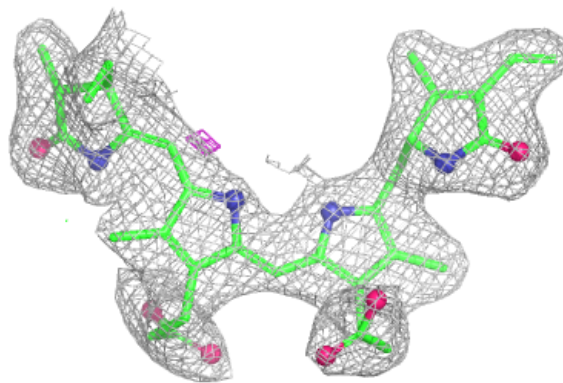
**Electron density around PE5 NNN 206:**

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



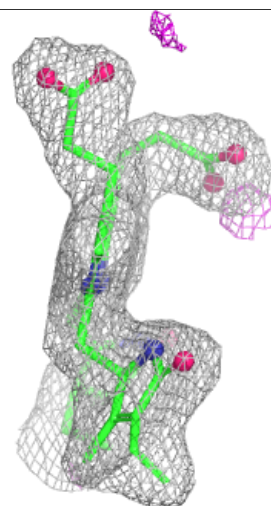
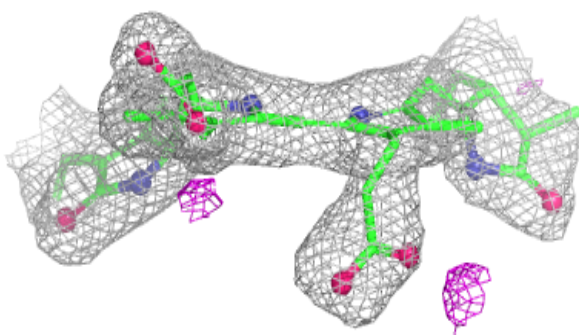
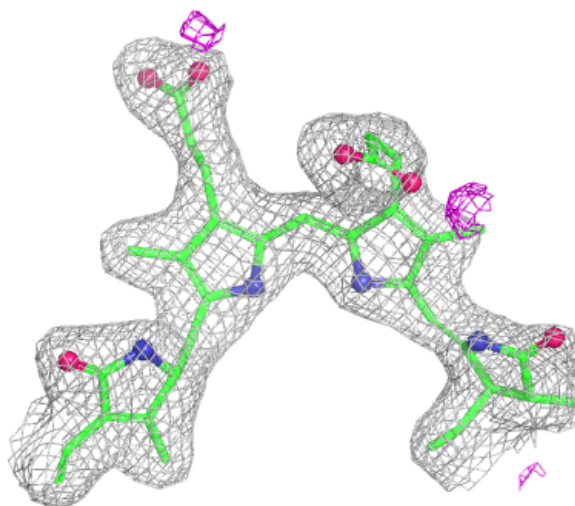
Electron density around PEB OOO 202:

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



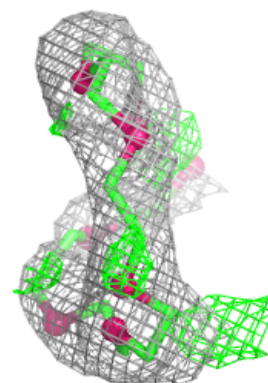
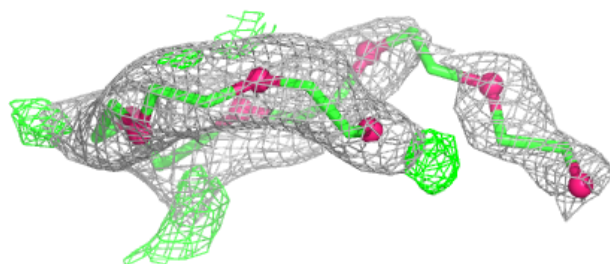
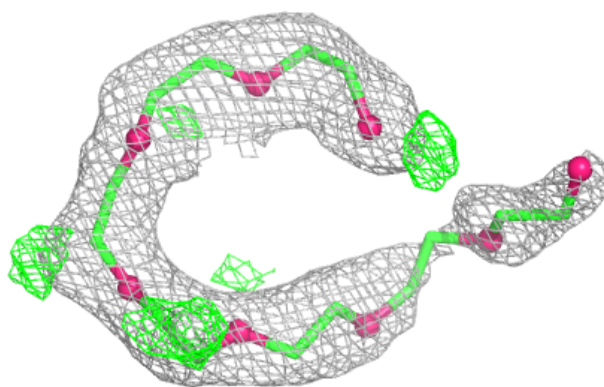
Electron density around PEB PPP 204:

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



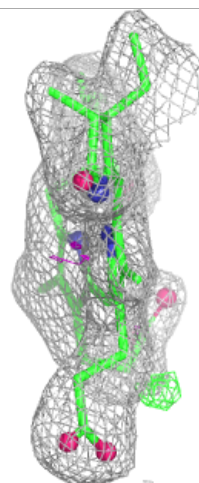
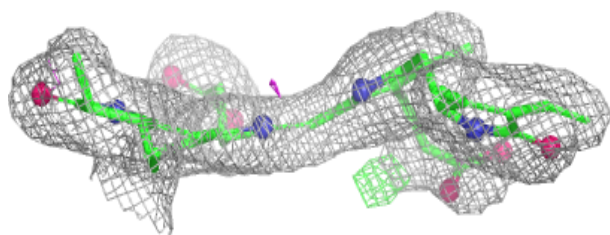
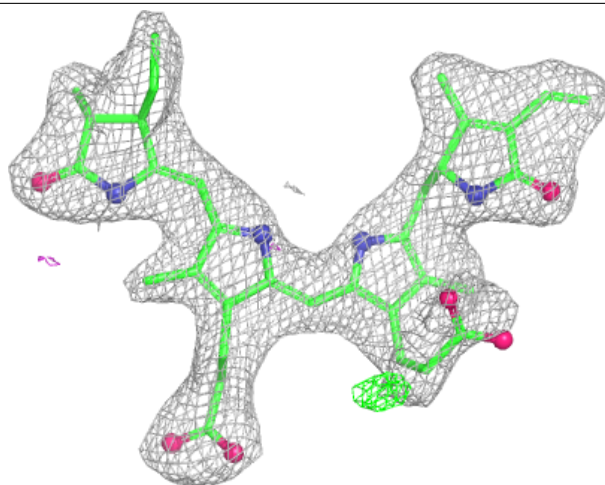
Electron density around P33 DDD 204:

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



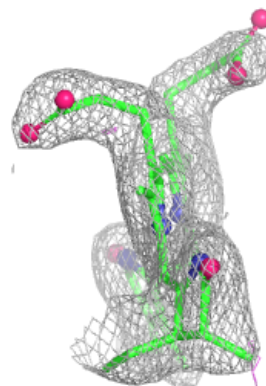
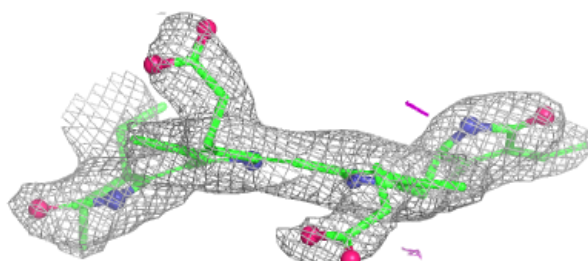
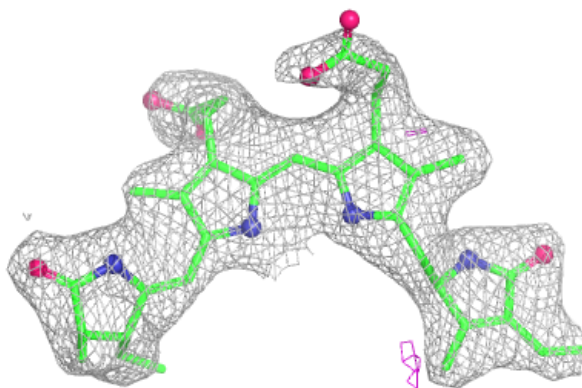
Electron density around PEB PPP 202:

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

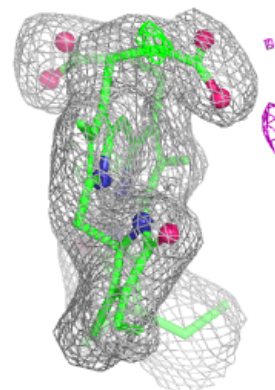
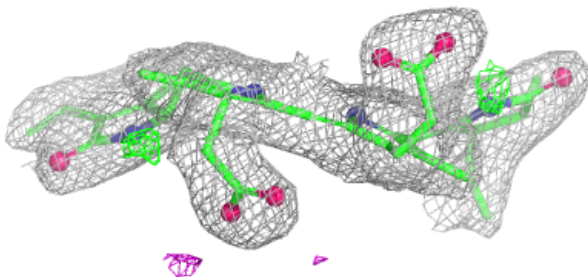
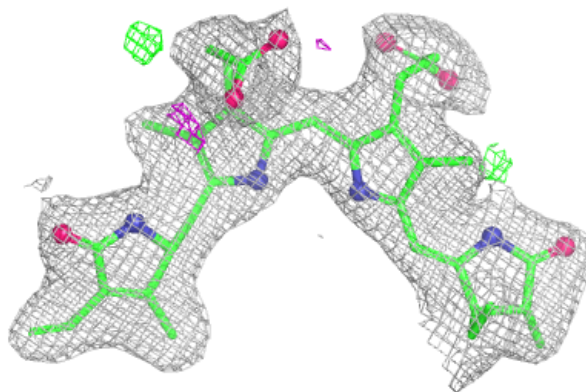


Electron density around PEB PPP 203:

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

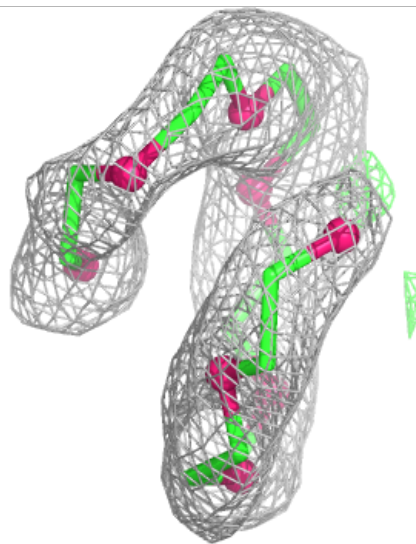
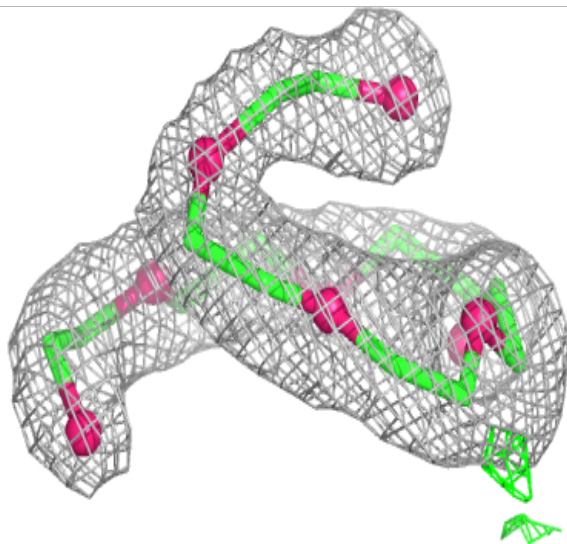
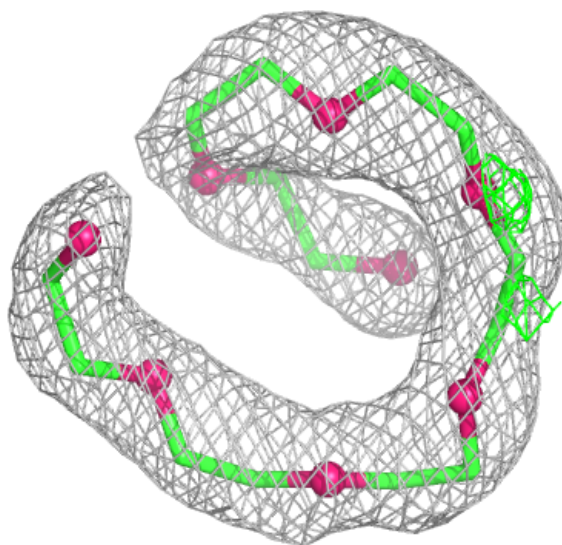
**Electron density around PEB III 203:**

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



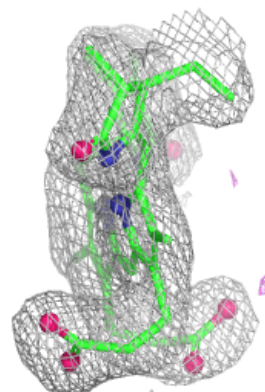
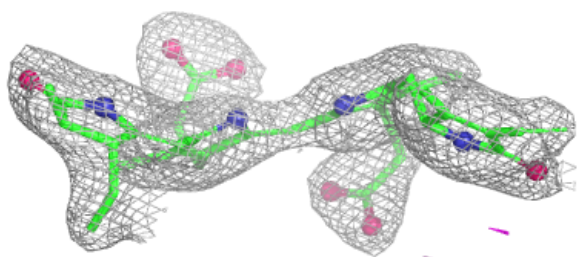
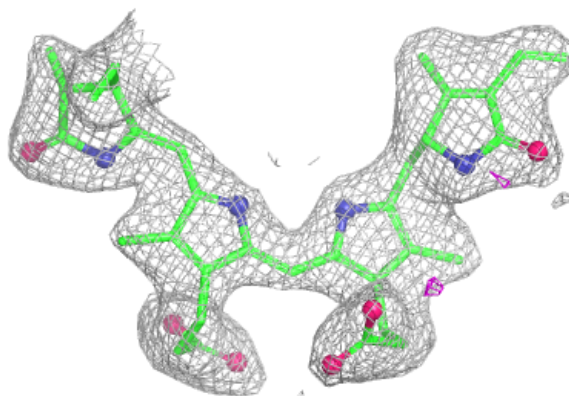
Electron density around P33 HHH 305:

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



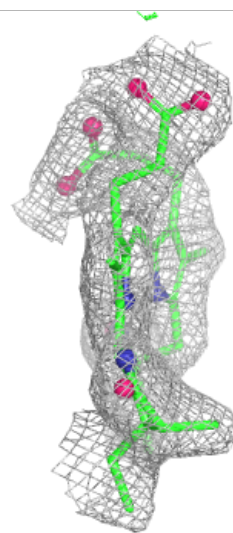
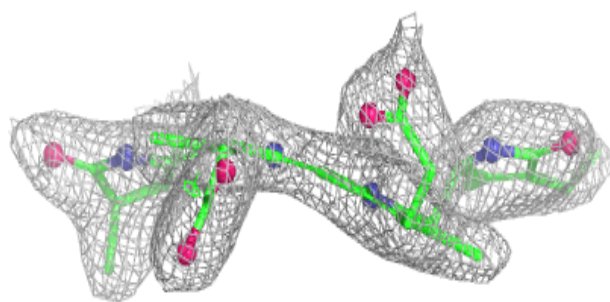
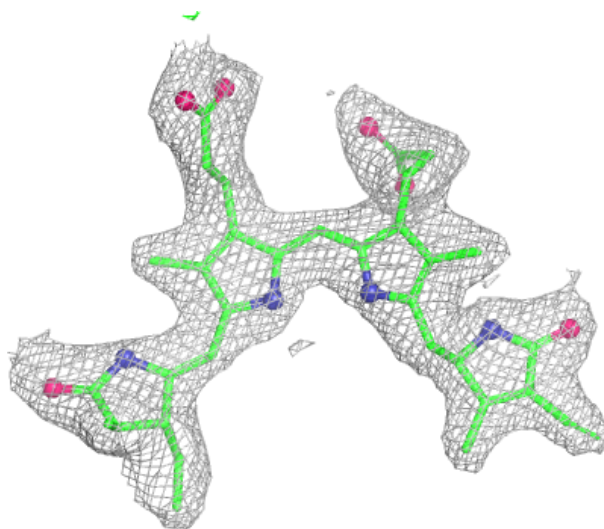
Electron density around PEB KKK 202:

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



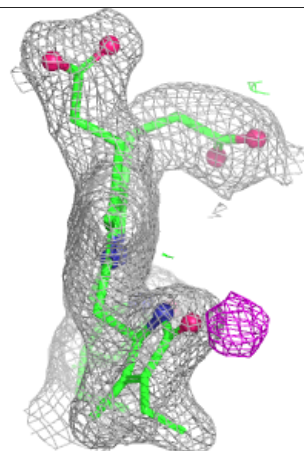
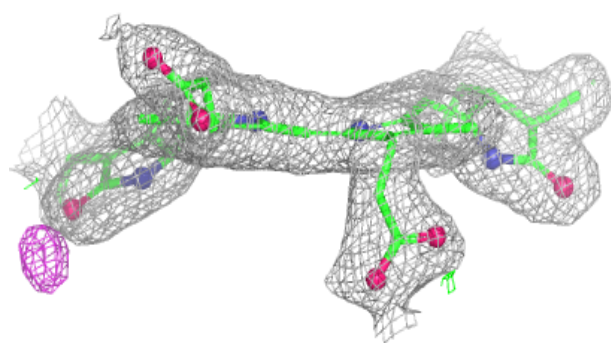
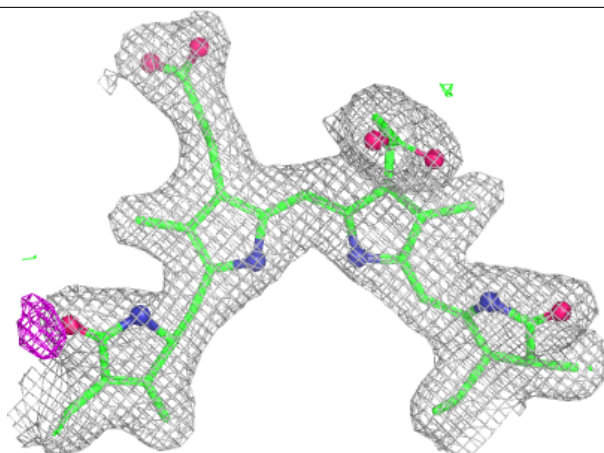
Electron density around PEB OOO 201:

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

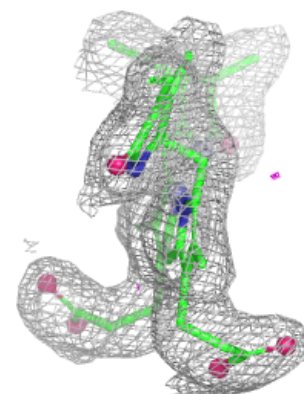
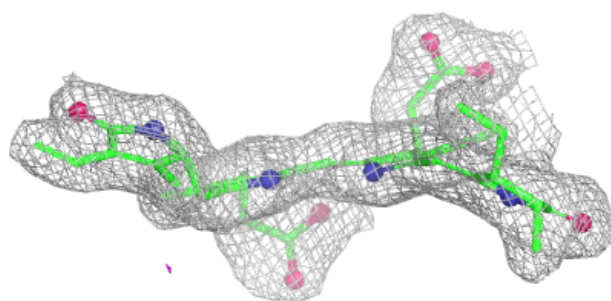
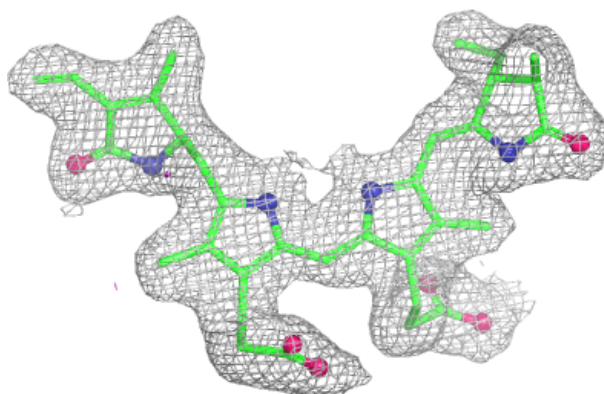


Electron density around PEB FFF 206:

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

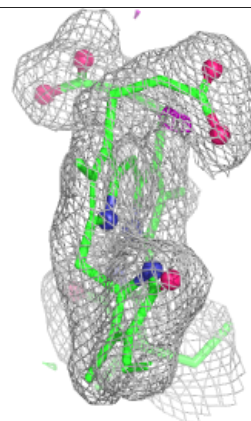
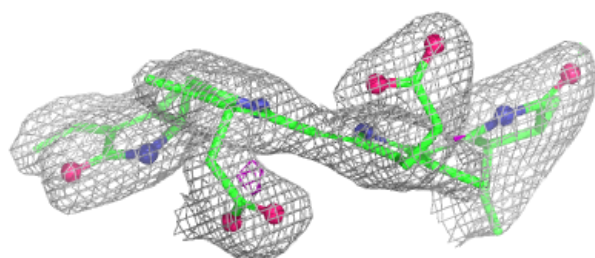
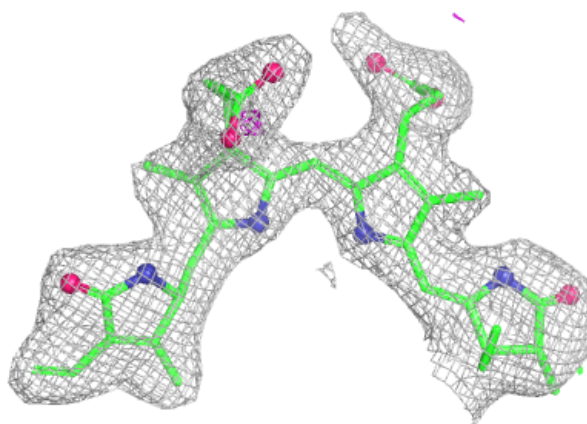
**Electron density around PEB BBB 202:**

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

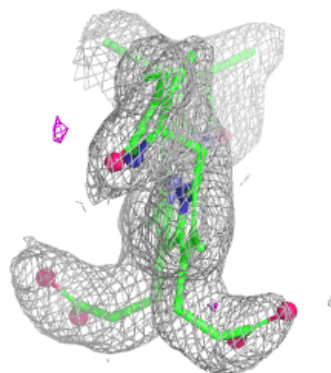
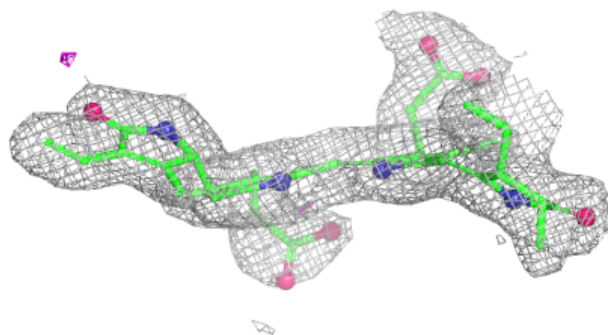
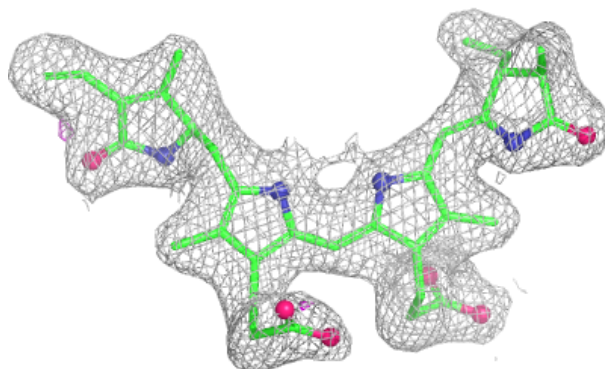


Electron density around PEB EEE 202:

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

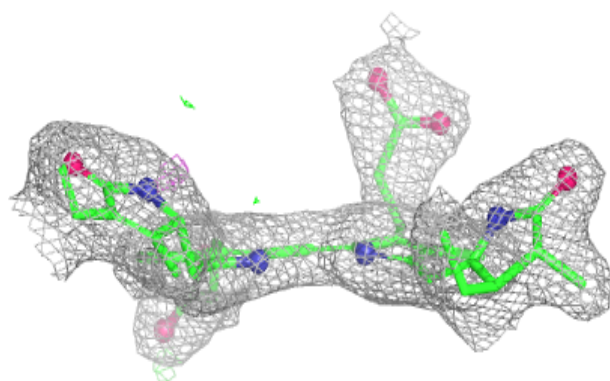
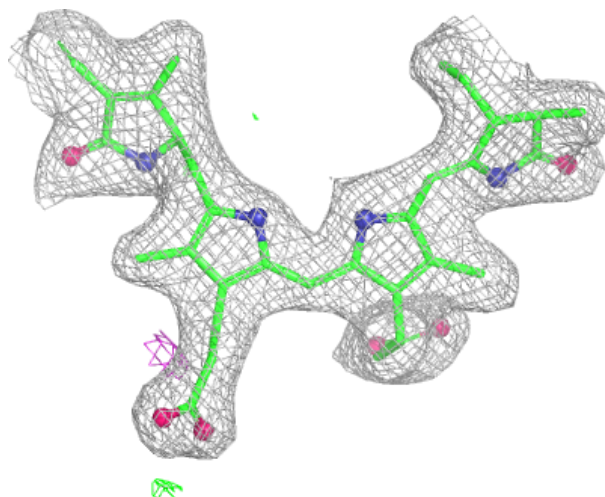
**Electron density around PEB LLL 202:**

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



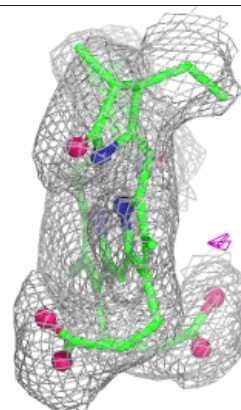
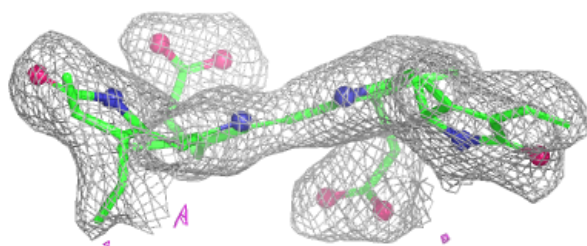
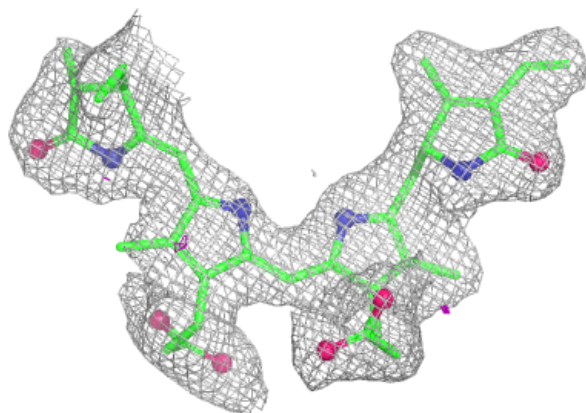
Electron density around PEB LLL 203:

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



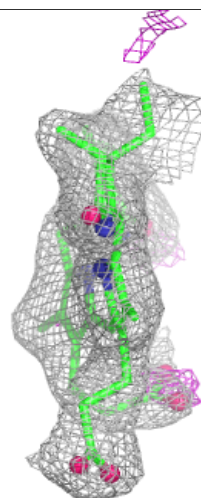
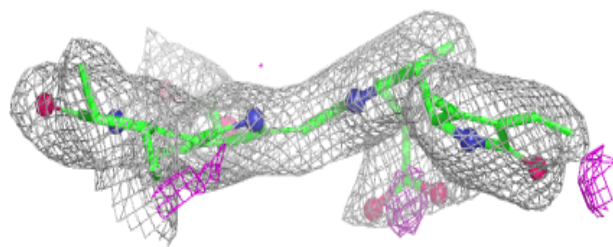
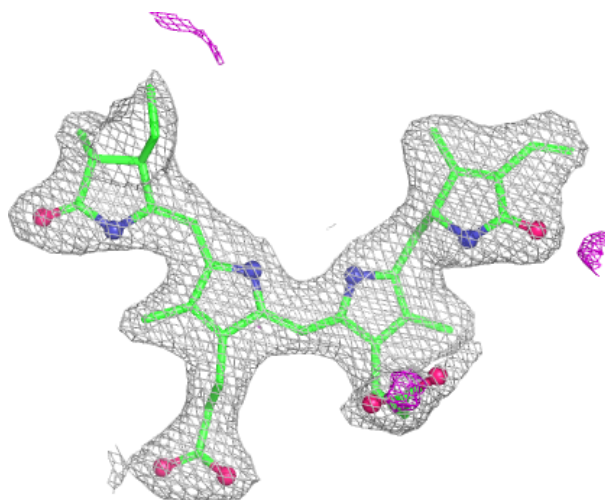
Electron density around PEB MMM 202:

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



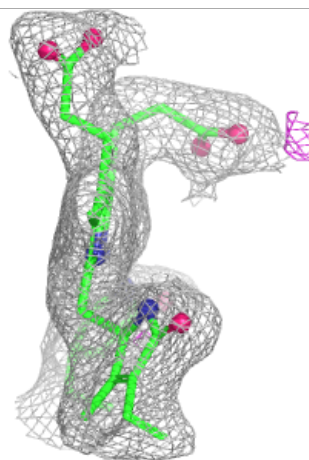
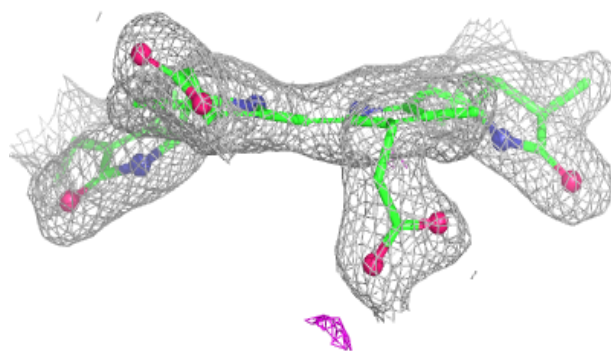
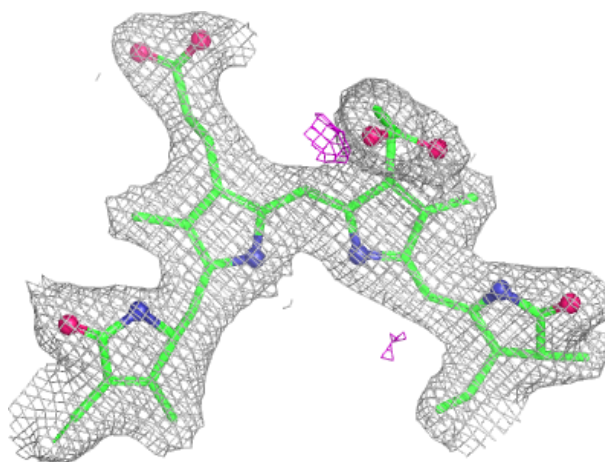
Electron density around PEB NNN 203:

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



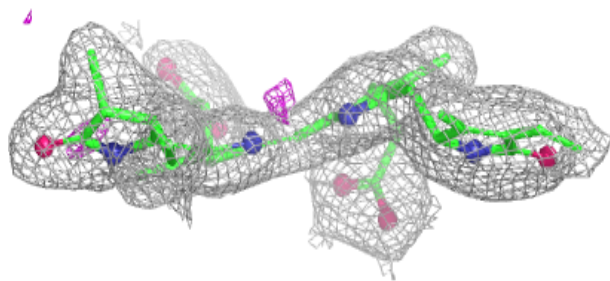
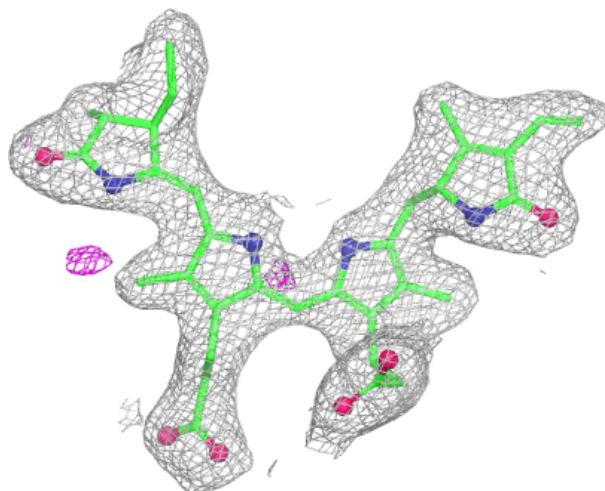
Electron density around PEB NNN 205:

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



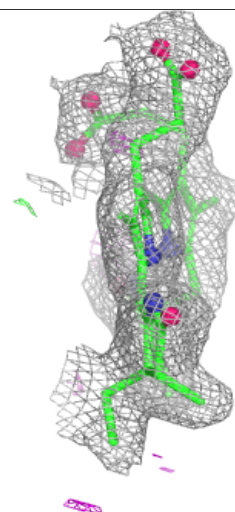
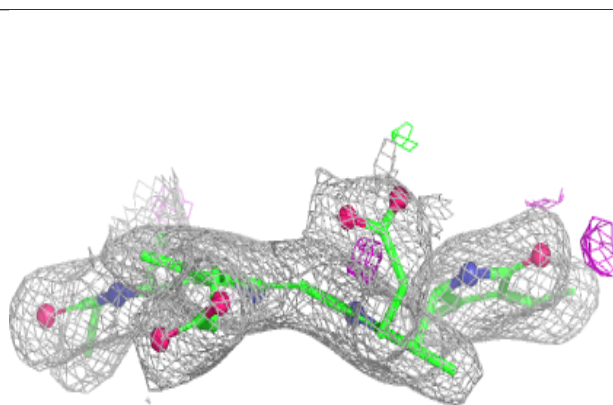
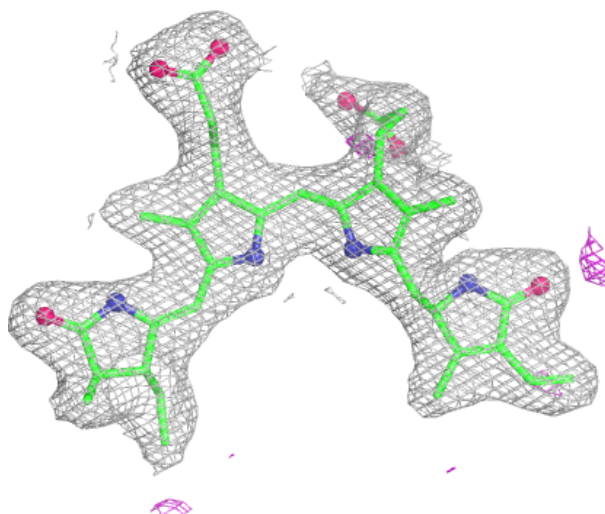
Electron density around PEB EEE 201:

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



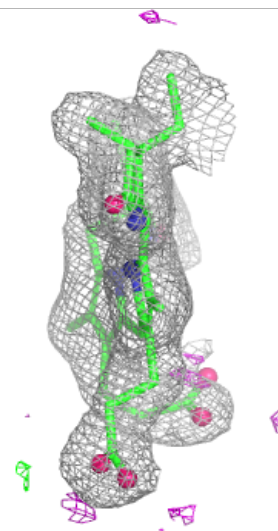
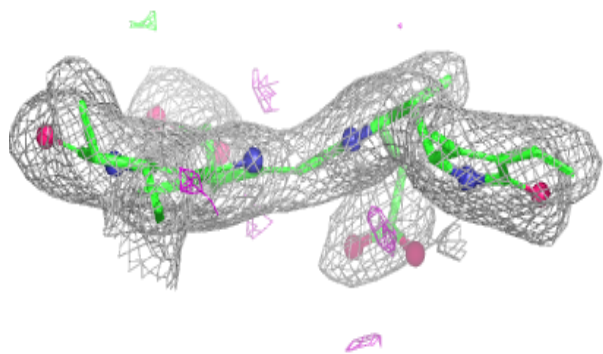
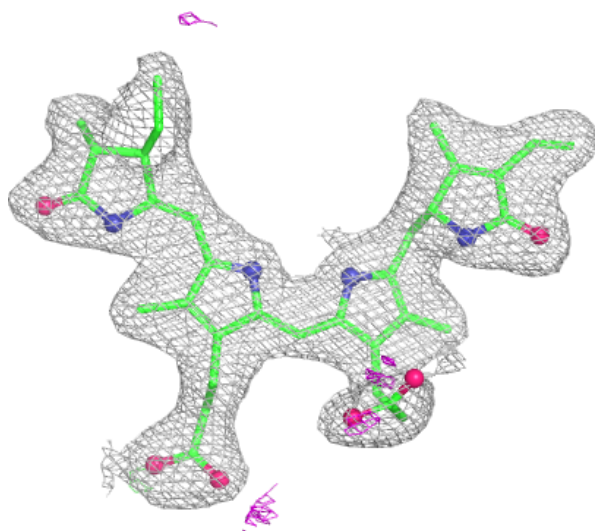
Electron density around PEB BBB 201:

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



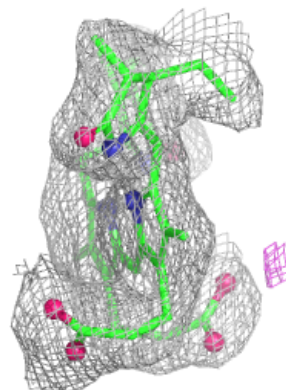
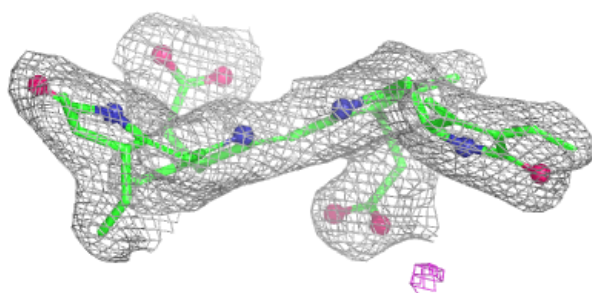
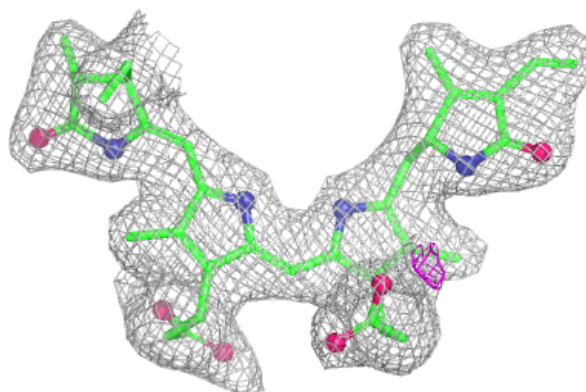
Electron density around PEB FFF 204:

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

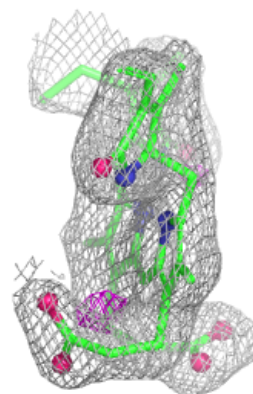
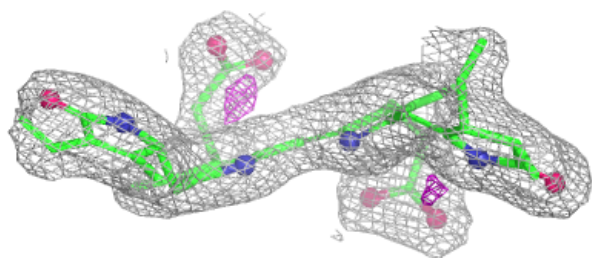
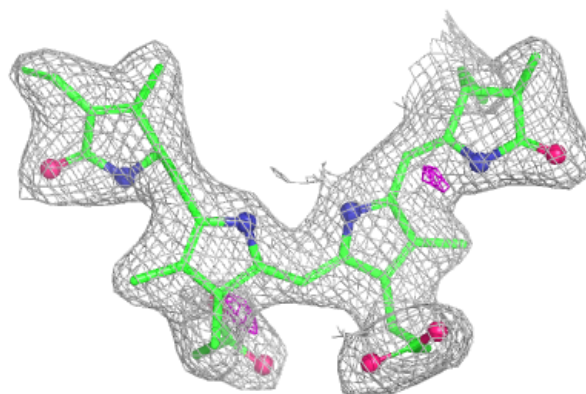


Electron density around PEB AAA 202:

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

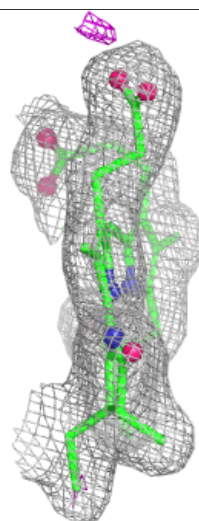
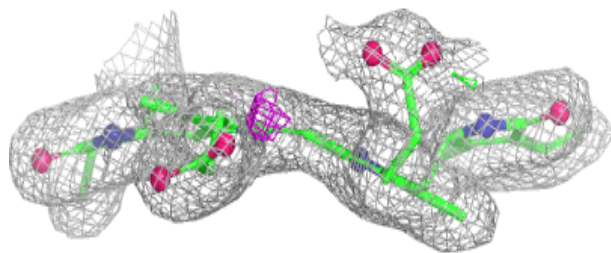
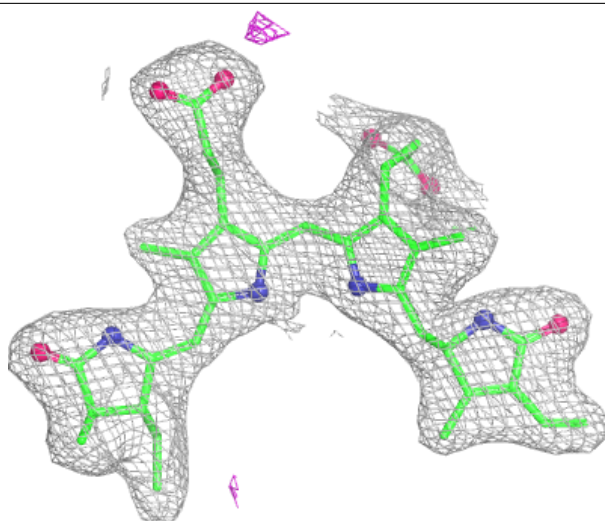
**Electron density around PEB GGG 202:**

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



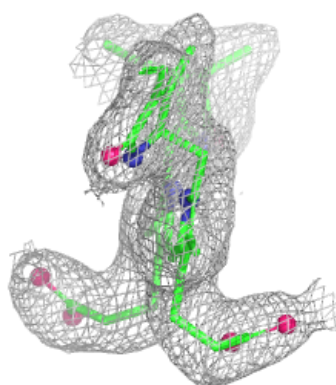
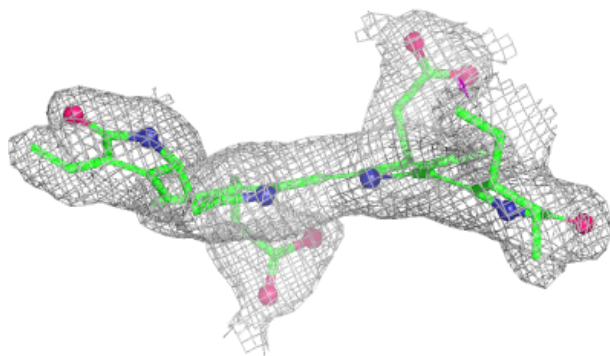
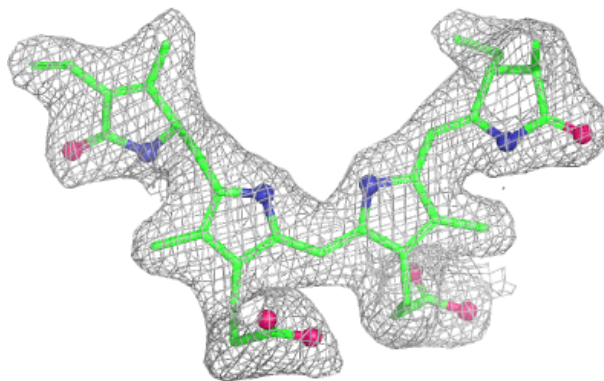
Electron density around PEB HHH 302:

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

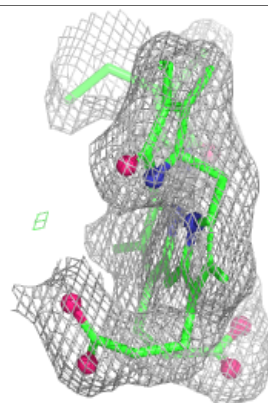
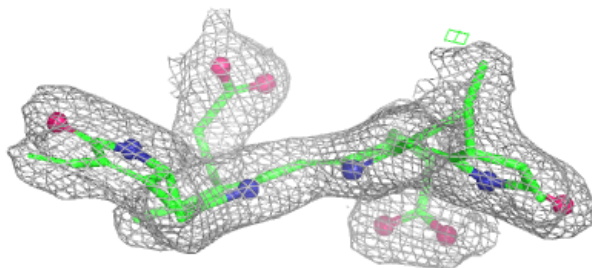
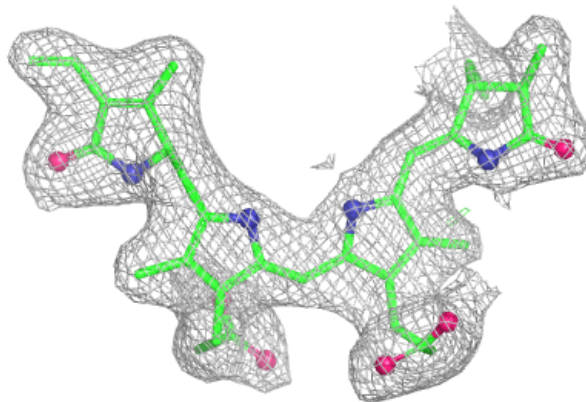


Electron density around PEB HHH 303:

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

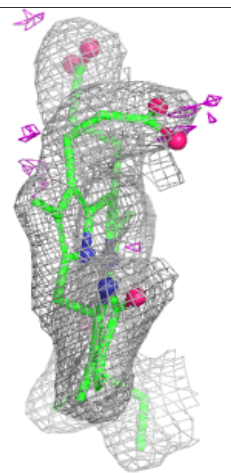
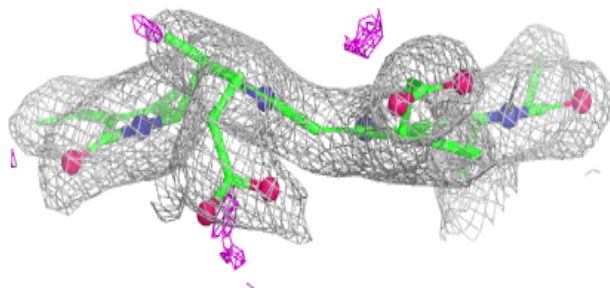
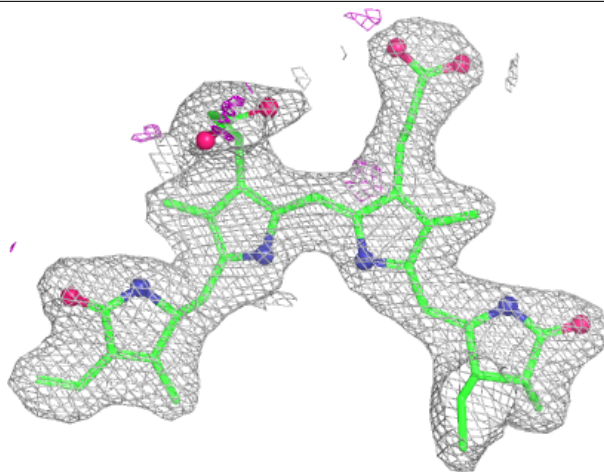
**Electron density around PEB CCC 202:**

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



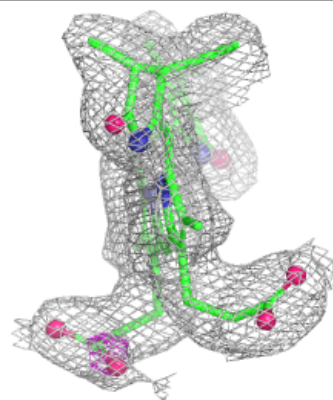
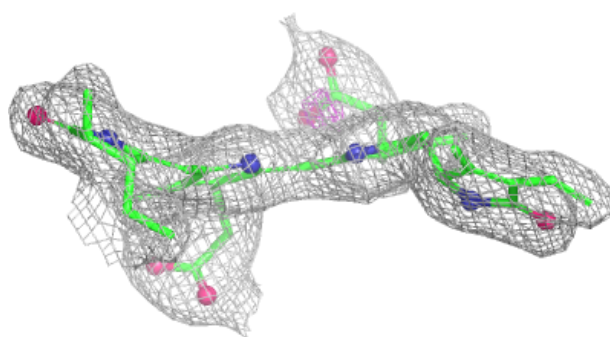
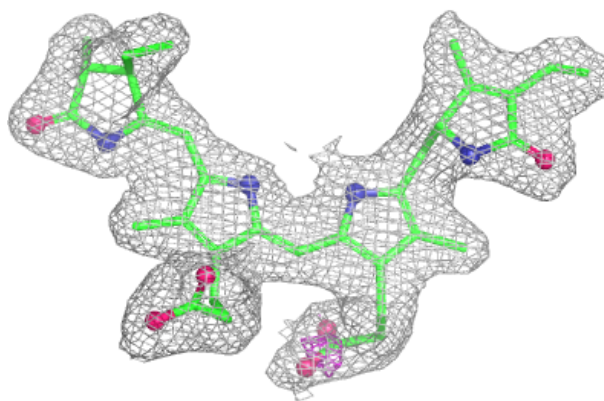
Electron density around PEB JJJ 303:

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



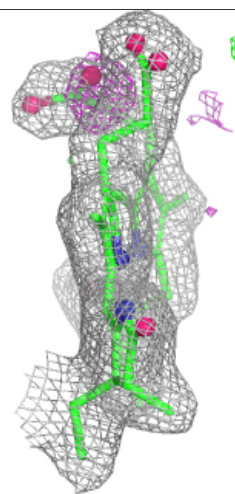
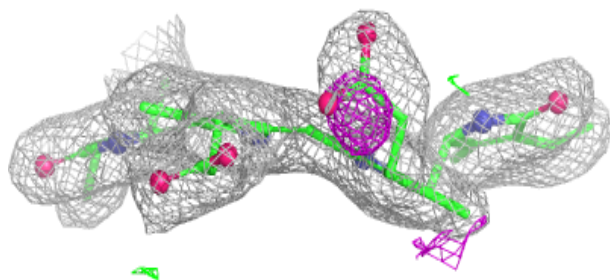
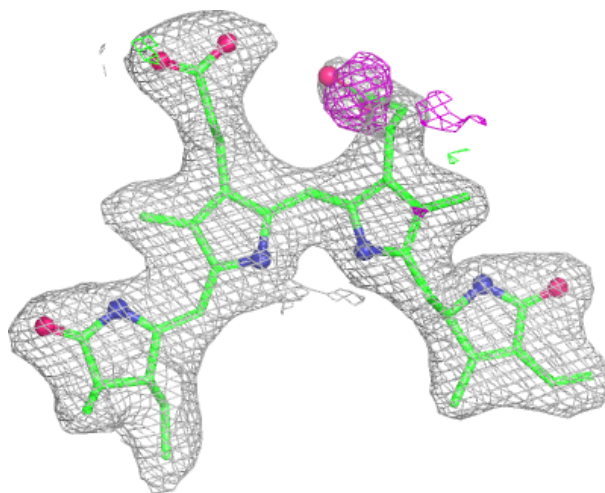
Electron density around PEB JJJ 304:

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



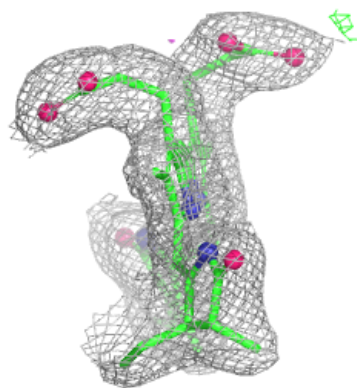
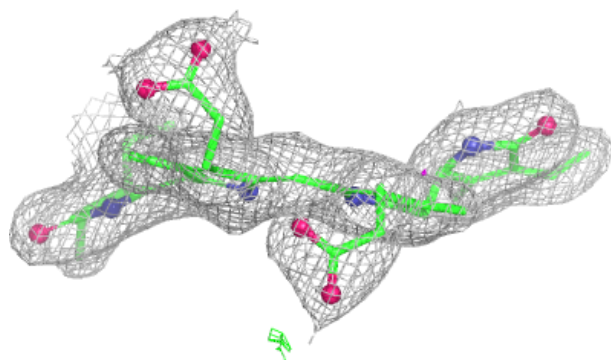
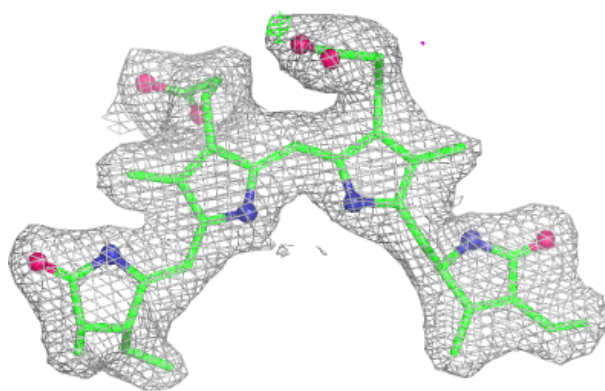
Electron density around PEB DDD 201:

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



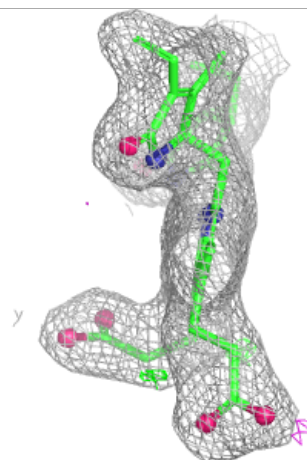
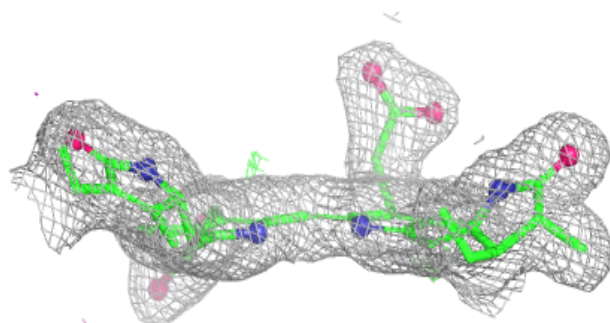
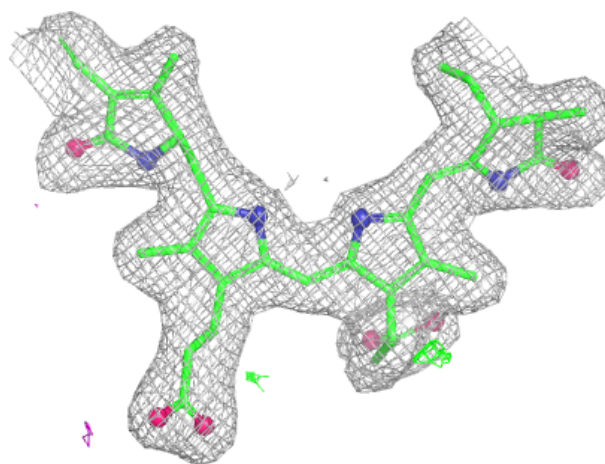
Electron density around PEB NNN 204:

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



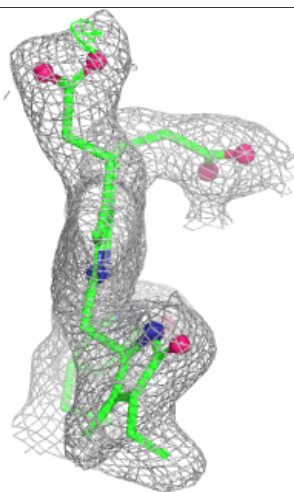
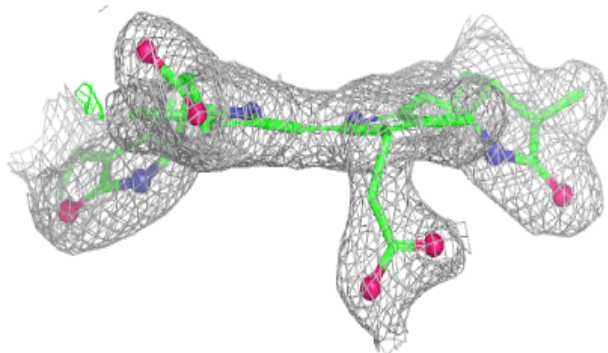
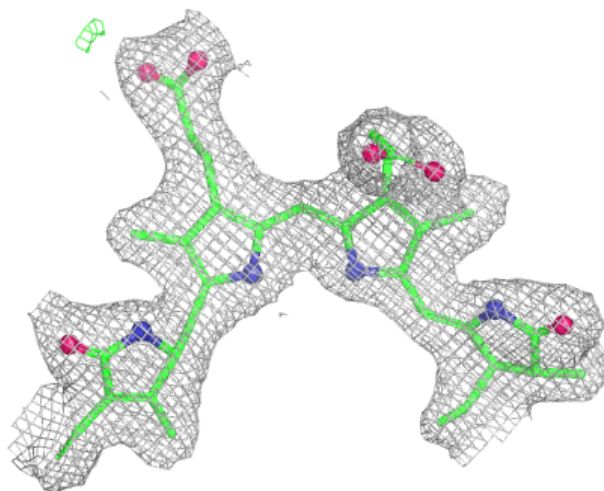
Electron density around PEB BBB 203:

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



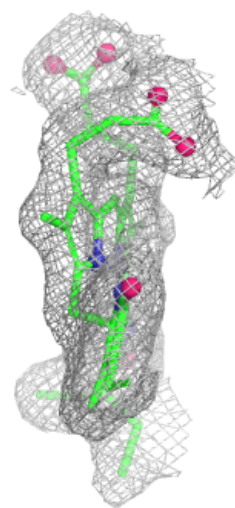
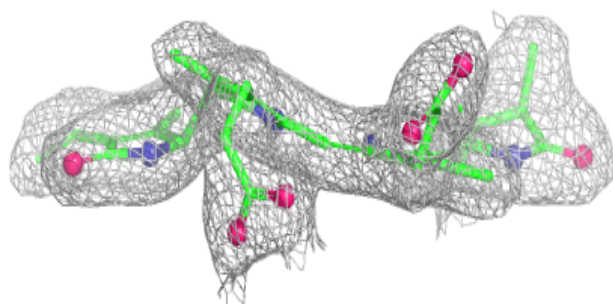
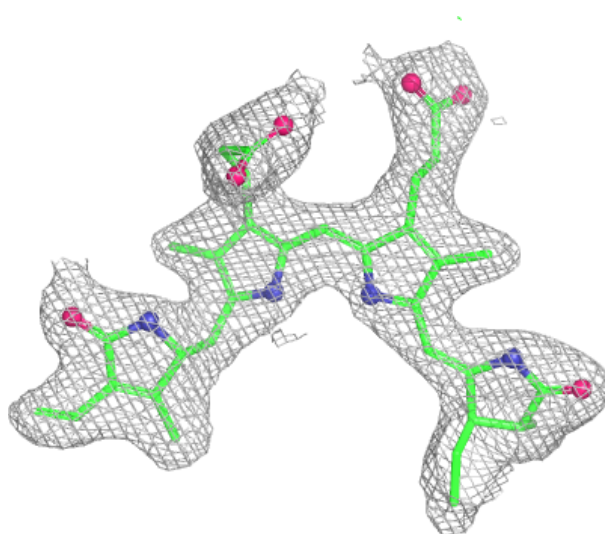
Electron density around PEB JJJ 305:

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



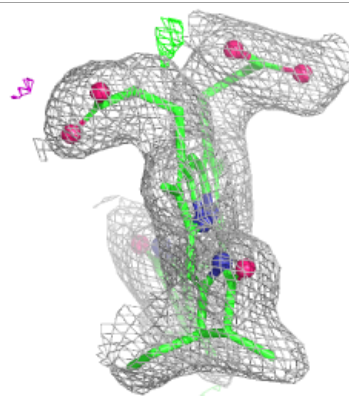
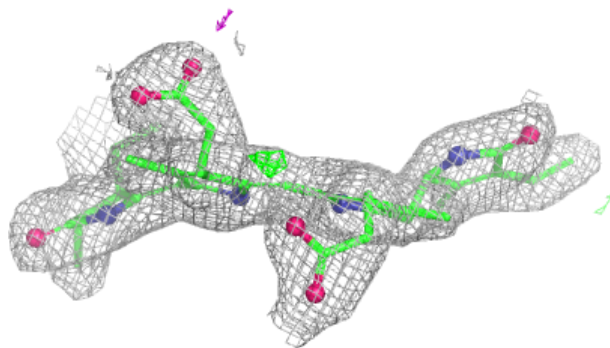
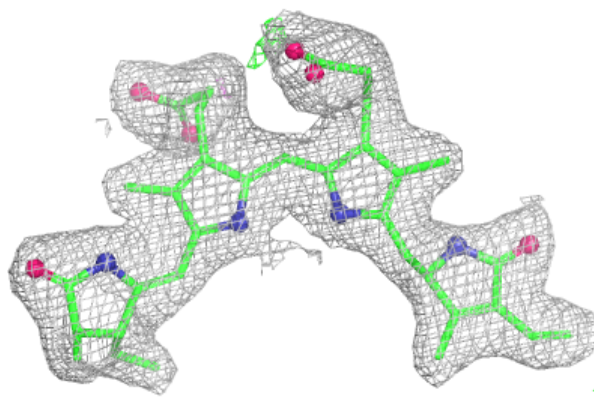
Electron density around PEB KKK 201:

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



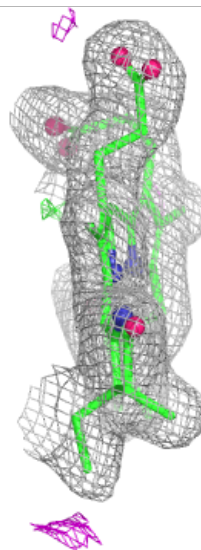
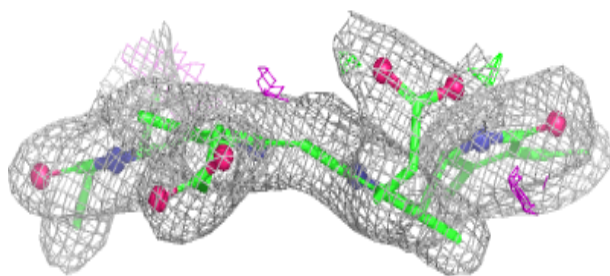
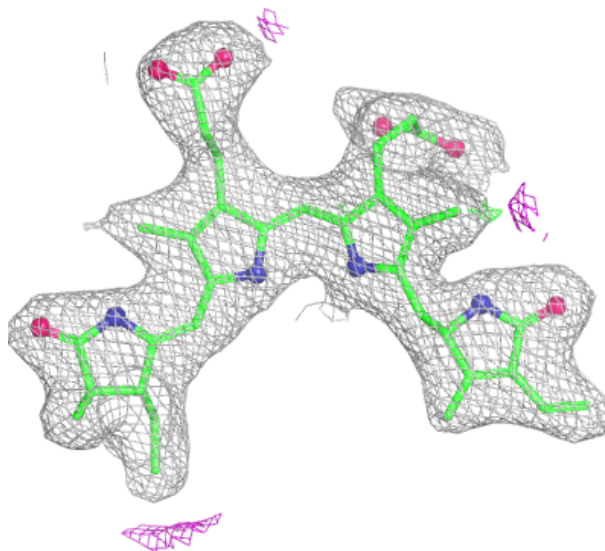
Electron density around PEB DDD 202:

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



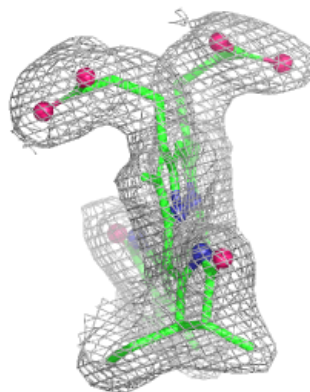
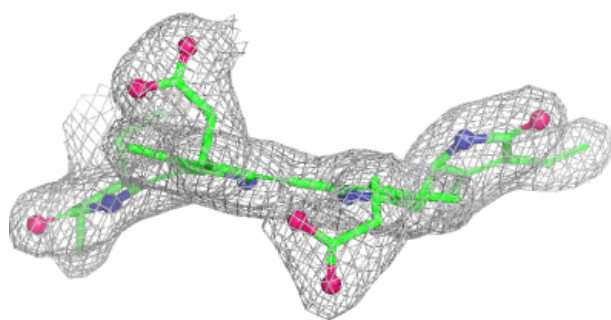
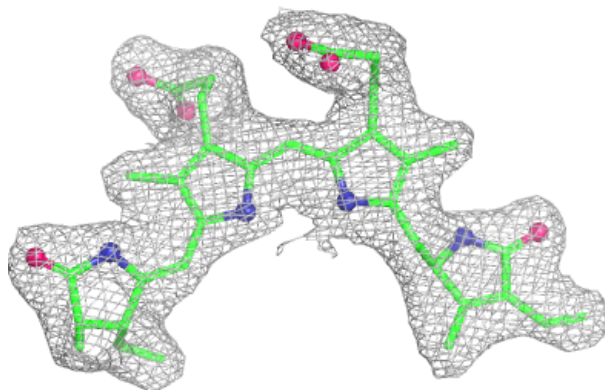
Electron density around PEB LLL 201:

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



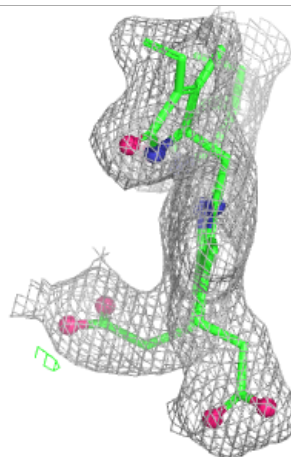
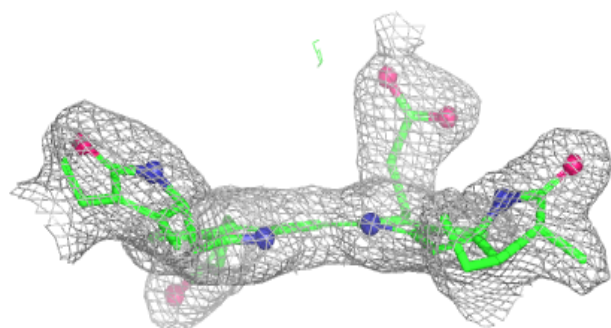
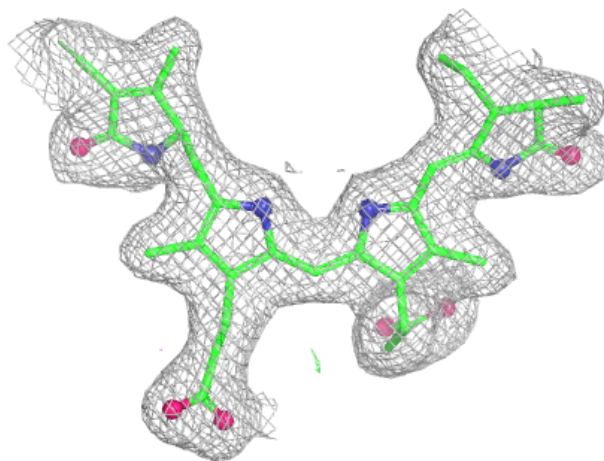
Electron density around PEB FFF 205:

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



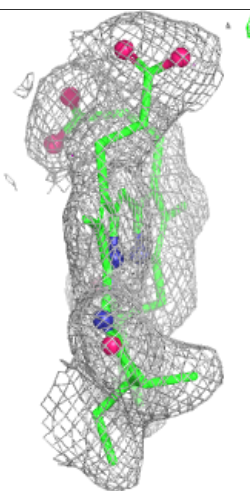
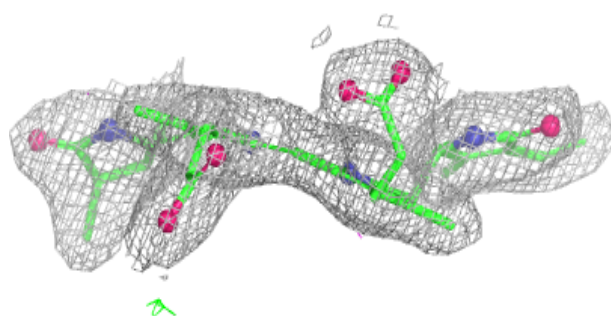
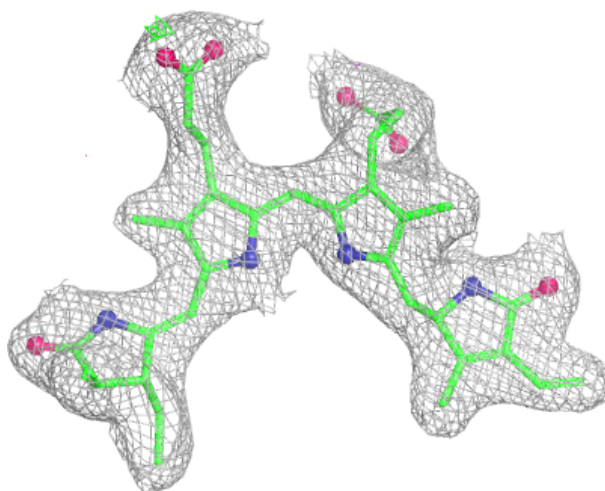
Electron density around PEB HHH 304:

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



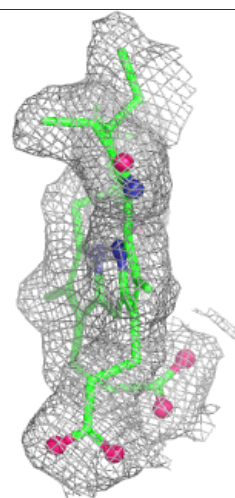
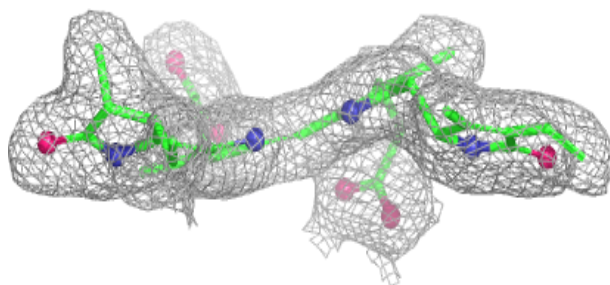
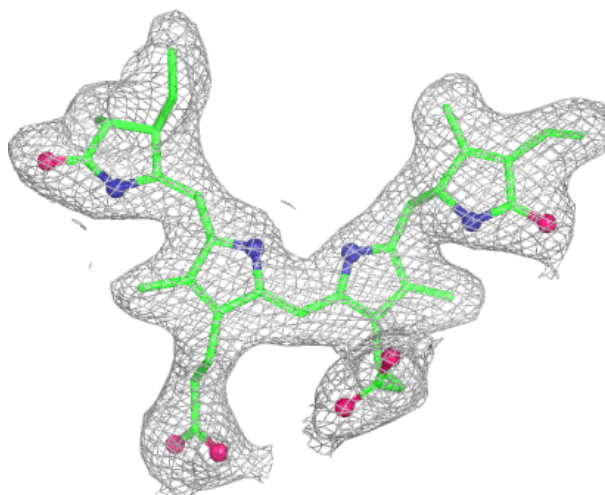
Electron density around PEB MMM 201:

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



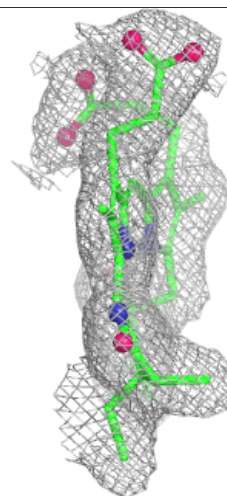
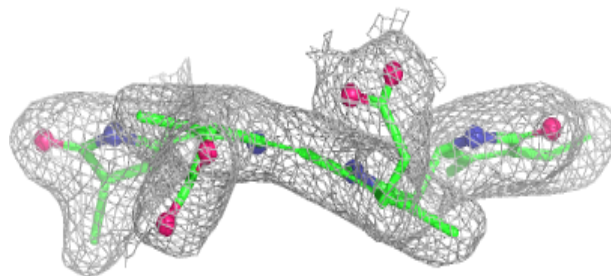
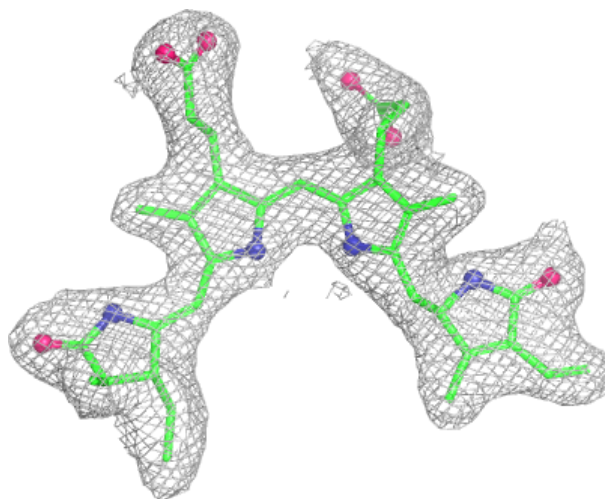
Electron density around PEB AAA 201:

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



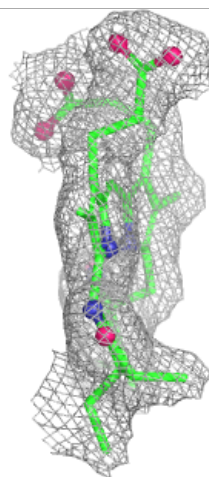
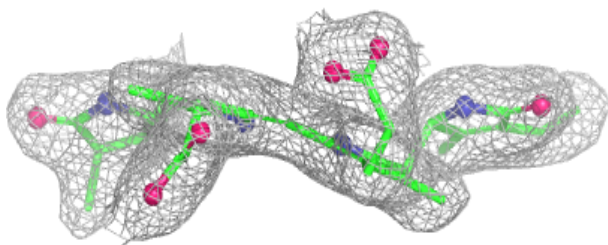
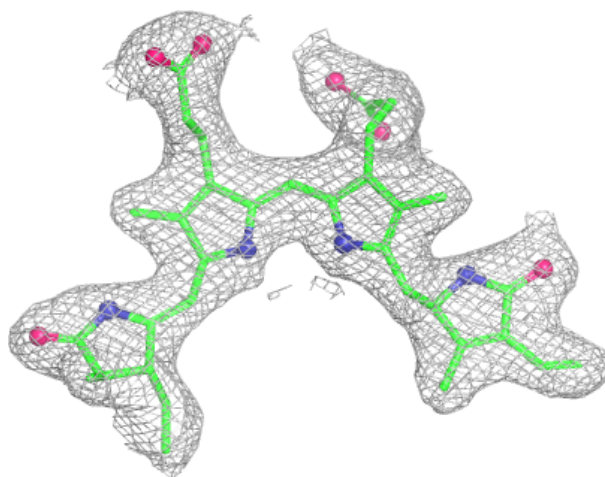
Electron density around PEB GGG 201:

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



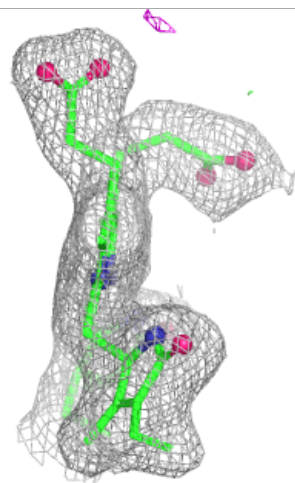
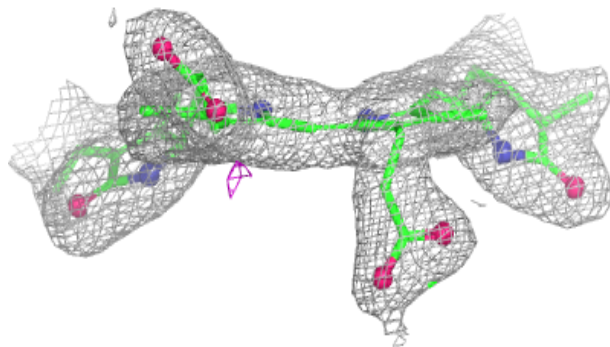
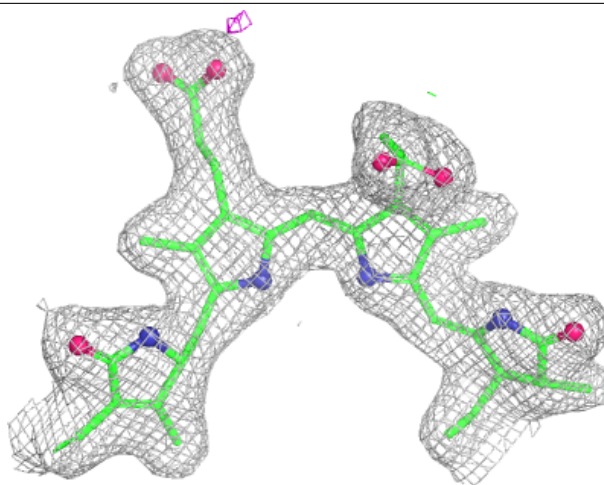
Electron density around PEB CCC 201:

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



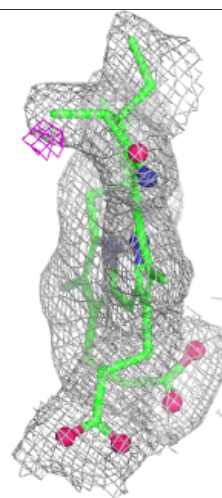
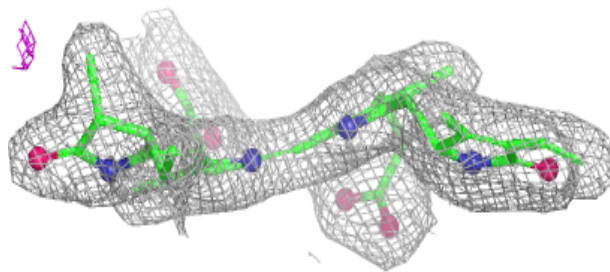
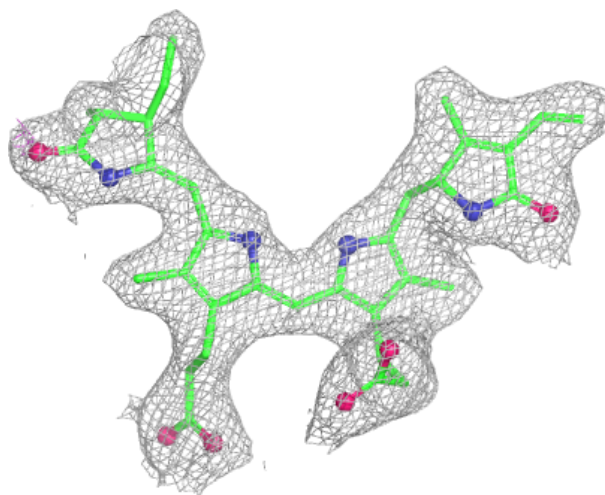
Electron density around PEB DDD 203:

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



Electron density around PEB III 202:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.