



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:58 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

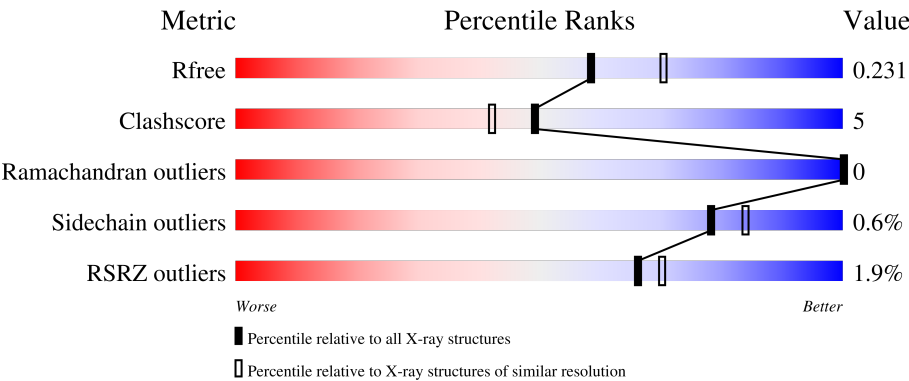
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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.



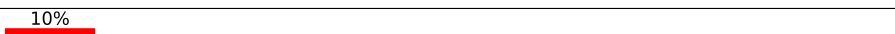
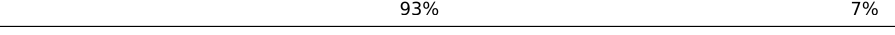
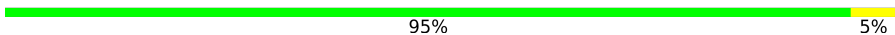
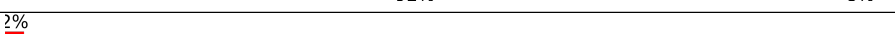
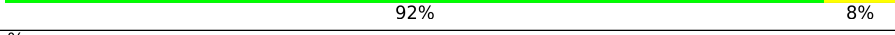
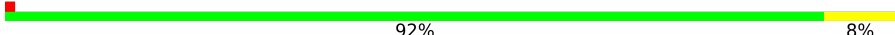
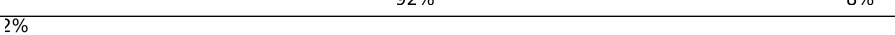
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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%
1	OOO	164	 93% 7%
2	BBB	184	 95% 5%
2	DDD	184	 92% 8%
2	FFF	184	 92% 8%
2	HHH	184	 92% 8%
2	JJJ	184	 92% 8%
2	LLL	184	 90% 10%
2	NNN	184	 93% 7%
2	PPP	184	 91% 9%

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.

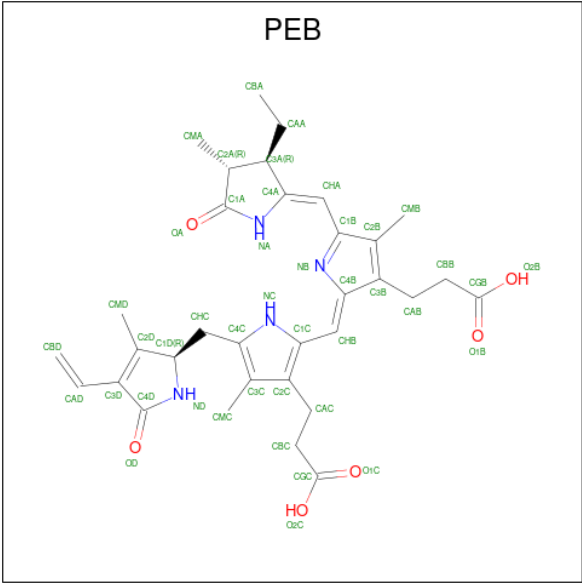
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	184	Total	C	N	O	S	0	6	0
			1378	845	253	268	12			
2	DDD	184	Total	C	N	O	S	0	9	0
			1382	849	251	270	12			
2	FFF	184	Total	C	N	O	S	0	6	0
			1370	840	250	268	12			
2	HHH	184	Total	C	N	O	S	0	7	0
			1368	839	247	270	12			
2	JJJ	184	Total	C	N	O	S	0	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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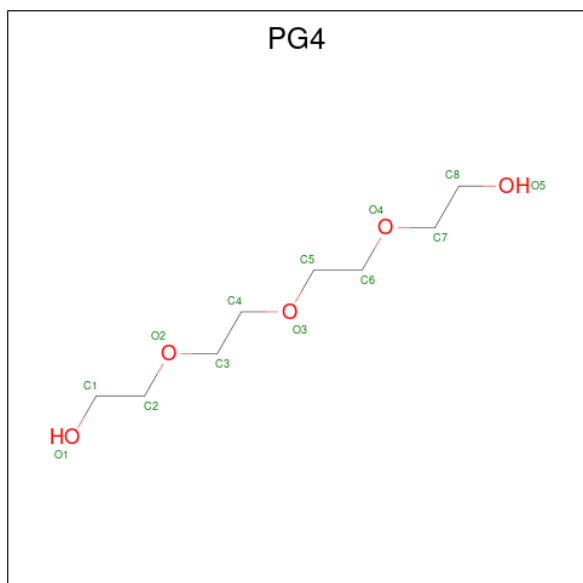
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	DDD	1	Total	C	N	O	0	0
			43	33	4	6		
3	EEE	1	Total	C	N	O	0	0
			43	33	4	6		
3	EEE	1	Total	C	N	O	0	0
			43	33	4	6		
3	FFF	1	Total	C	N	O	0	0
			43	33	4	6		
3	FFF	1	Total	C	N	O	0	0
			43	33	4	6		
3	FFF	1	Total	C	N	O	0	0
			43	33	4	6		
3	GGG	1	Total	C	N	O	0	0
			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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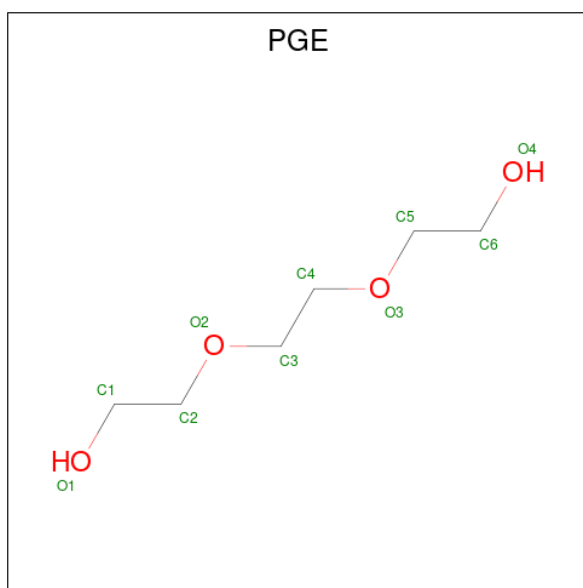
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			13	8	5		
4	AAA	1	Total	C	O	0	0
			13	8	5		
4	CCC	1	Total	C	O	0	0
			13	8	5		
4	DDD	1	Total	C	O	0	0
			13	8	5		
4	DDD	1	Total	C	O	0	0
			13	8	5		
4	FFF	1	Total	C	O	0	0
			13	8	5		
4	FFF	1	Total	C	O	0	0
			13	8	5		
4	FFF	1	Total	C	O	0	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 10 6 4	0	0
5	AAA	1	Total C O 10 6 4	0	0
5	AAA	1	Total C O 10 6 4	0	0
5	AAA	1	Total C O 10 6 4	0	0
5	AAA	1	Total C O 10 6 4	0	0
5	AAA	1	Total C O 10 6 4	0	0
5	BBB	1	Total C O 10 6 4	0	0
5	BBB	1	Total C O 10 6 4	0	0
5	BBB	1	Total C O 10 6 4	0	0
5	CCC	1	Total C O 10 6 4	0	0
5	CCC	1	Total C O 10 6 4	0	0
5	CCC	1	Total C O 10 6 4	0	0
5	CCC	1	Total C O 10 6 4	0	0
5	CCC	1	Total C O 10 6 4	0	0
5	DDD	1	Total C O 10 6 4	0	0
5	DDD	1	Total C O 10 6 4	0	0
5	DDD	1	Total C O 10 6 4	0	0
5	EEE	1	Total C O 10 6 4	0	0
5	EEE	1	Total C O 10 6 4	0	0
5	EEE	1	Total C O 10 6 4	0	0
5	EEE	1	Total C O 10 6 4	0	0
5	FFF	1	Total C O 10 6 4	0	0

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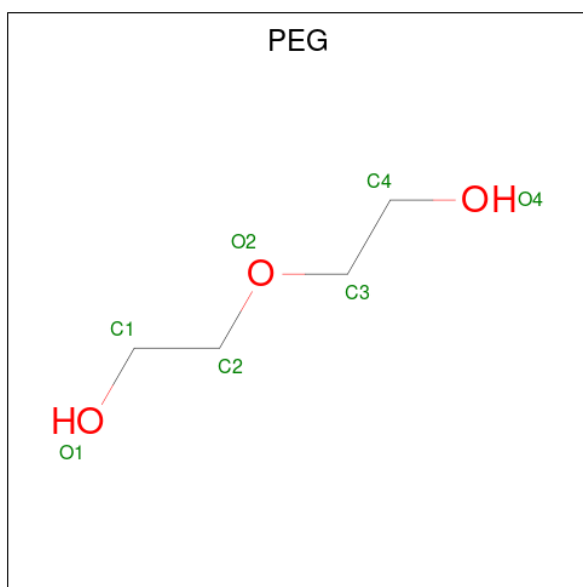
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	FFF	1	Total	C	O	0	0
			10	6	4		
5	FFF	1	Total	C	O	0	0
			10	6	4		
5	GGG	1	Total	C	O	0	0
			10	6	4		
5	GGG	1	Total	C	O	0	0
			10	6	4		
5	GGG	1	Total	C	O	0	0
			10	6	4		
5	GGG	1	Total	C	O	0	0
			10	6	4		
5	HHH	1	Total	C	O	0	0
			10	6	4		
5	HHH	1	Total	C	O	0	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		
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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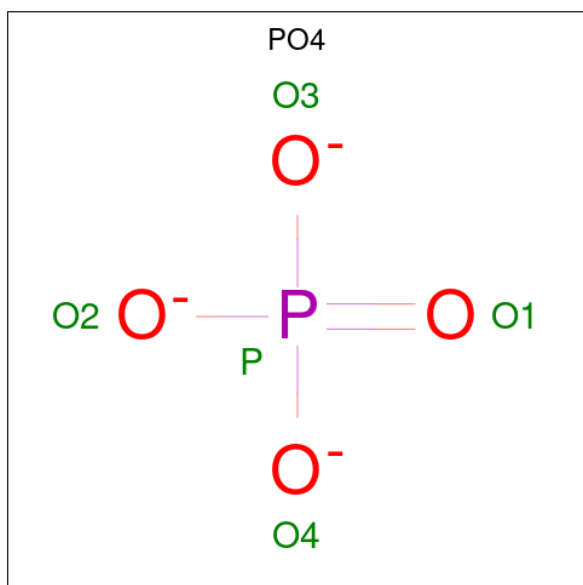
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	0
			7	4	3		
6	LLL	1	Total	C	O	0	1
			14	8	6		
6	MMM	1	Total	C	O	0	0
			7	4	3		
6	MMM	1	Total	C	O	0	0
			7	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: O_4P).



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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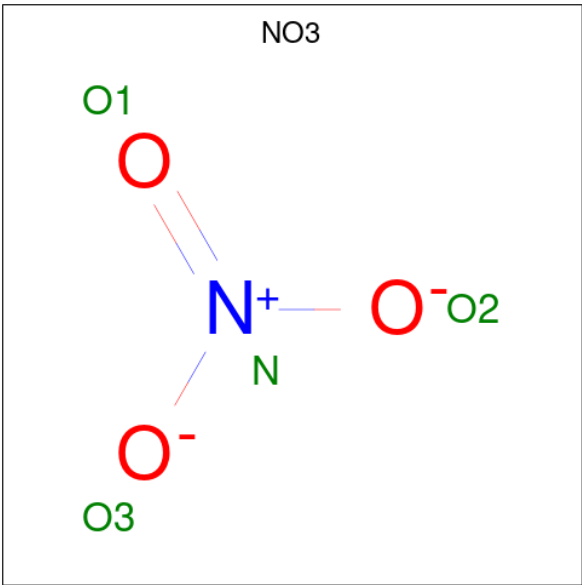
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	DDD	1	Total	O	P	0	0
			5	4	1		
7	FFF	1	Total	O	P	0	0
			5	4	1		
7	FFF	1	Total	O	P	0	0
			5	4	1		
7	FFF	1	Total	O	P	0	0
			5	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).



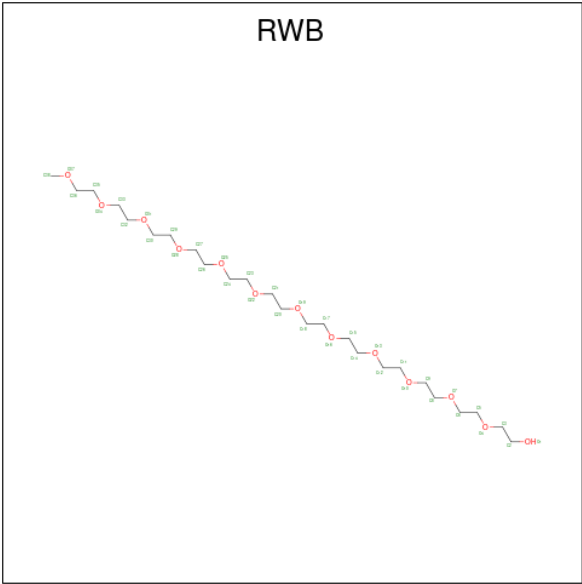
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	AAA	1	Total	N	O	0	0
			4	1	3		
8	AAA	1	Total	N	O	0	0
			4	1	3		
8	BBB	1	Total	N	O	0	0
			4	1	3		
8	CCC	1	Total	N	O	0	0
			4	1	3		
8	DDD	1	Total	N	O	0	0
			4	1	3		
8	DDD	1	Total	N	O	0	0
			4	1	3		
8	EEE	1	Total	N	O	0	0
			4	1	3		
8	EEE	1	Total	N	O	0	0
			4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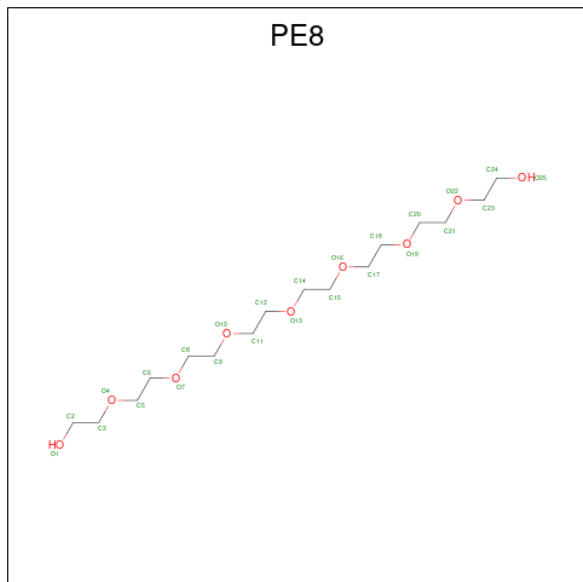
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	JJJ	1	Total	N	O	0	0
			4	1	3		
8	KKK	1	Total	N	O	0	0
			4	1	3		
8	KKK	1	Total	N	O	0	0
			4	1	3		
8	LLL	1	Total	N	O	0	0
			4	1	3		
8	LLL	1	Total	N	O	0	0
			4	1	3		
8	LLL	1	Total	N	O	0	0
			4	1	3		
8	MMM	1	Total	N	O	0	0
			4	1	3		
8	OOO	1	Total	N	O	0	0
			4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

- Molecule 9 is dodecaethylene glycol monomethyl ether (CCD ID: RWB) (formula: C₂₅H₅₂O₁₃).



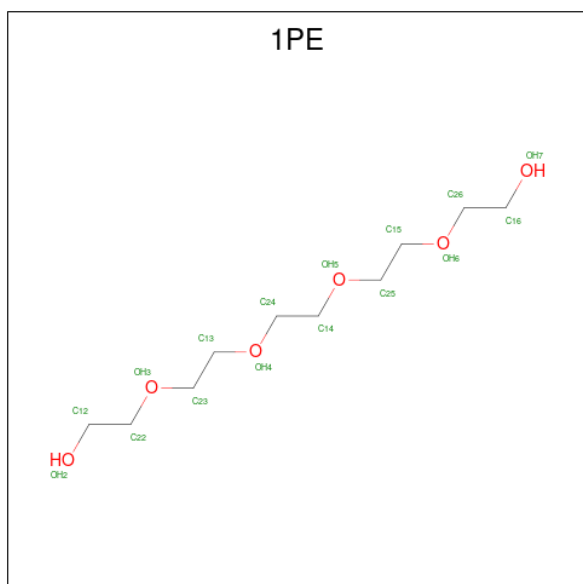
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	BBB	1	Total	C	O	0	0
			38	25	13		
9	LLL	1	Total	C	O	0	0
			38	25	13		

- Molecule 10 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: $C_{16}H_{34}O_9$).



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: $C_{10}H_{22}O_6$).



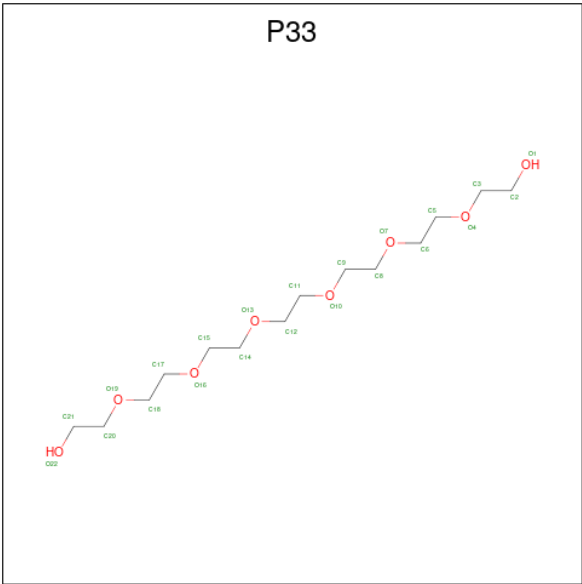
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	BBB	1	Total	C	O	0	0
			16	10	6		

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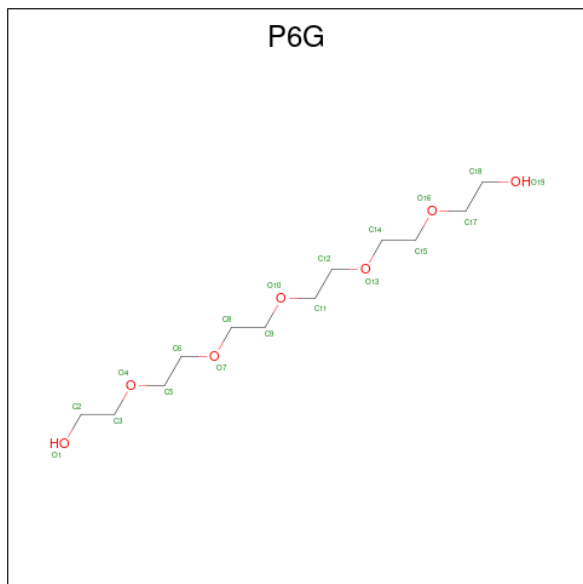
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	BBB	1	Total	C	O	0	0
			16	10	6		
11	BBB	1	Total	C	O	0	0
			16	10	6		
11	DDD	1	Total	C	O	0	0
			16	10	6		
11	EEE	1	Total	C	O	0	0
			16	10	6		
11	FFF	1	Total	C	O	0	0
			16	10	6		
11	HHH	1	Total	C	O	0	0
			16	10	6		
11	JJJ	1	Total	C	O	0	0
			16	10	6		
11	JJJ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



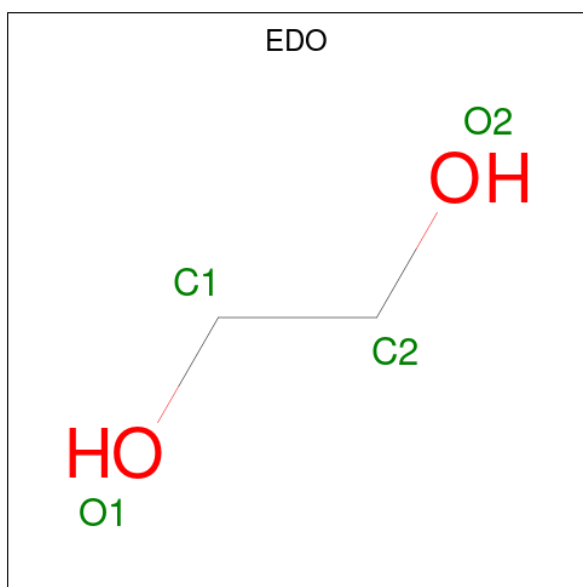
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	DDD	1	Total	C	O	0	0
			22	14	8		
12	DDD	1	Total	C	O	0	0
			22	14	8		
12	FFF	1	Total	C	O	0	0
			22	14	8		
12	HHH	1	Total	C	O	0	0
			22	14	8		
12	HHH	1	Total	C	O	0	0
			22	14	8		
12	JJJ	1	Total	C	O	0	0
			22	14	8		

- 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: $C_2H_6O_2$).



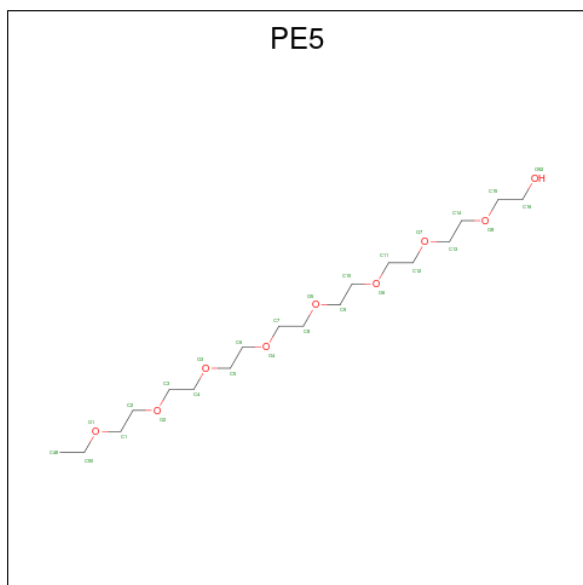
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	DDD	1	Total	C	O	0	0
			4	2	2		
14	DDD	1	Total	C	O	0	0
			4	2	2		
14	EEE	1	Total	C	O	0	0
			4	2	2		
14	EEE	1	Total	C	O	0	0
			4	2	2		
14	FFF	1	Total	C	O	0	0
			4	2	2		
14	FFF	1	Total	C	O	0	0
			4	2	2		
14	HHH	1	Total	C	O	0	0
			4	2	2		
14	HHH	1	Total	C	O	0	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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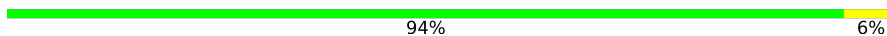
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	HHH	92	Total 92	O 92	0	0
16	III	79	Total 79	O 79	0	0
16	JJJ	106	Total 106	O 106	0	0
16	KKK	86	Total 86	O 86	0	0
16	LLL	97	Total 97	O 97	0	0
16	MMM	76	Total 76	O 76	0	0
16	NNN	76	Total 76	O 76	0	0
16	OOO	57	Total 57	O 57	0	0
16	PPP	57	Total 57	O 57	0	0

3 Residue-property plots [i](#)

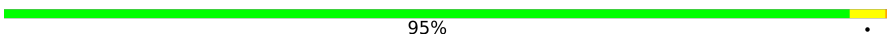
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

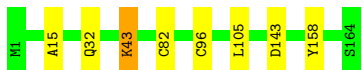
- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain AAA:  94% 6%

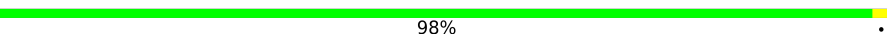


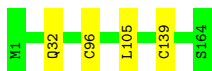
- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain CCC:  95% ..

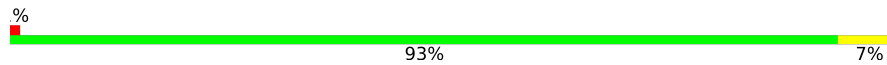


- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain EEE:  98% .



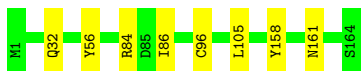
- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain GGG:  93% 7%

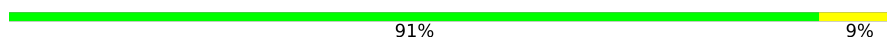


- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

Chain III:  95% 5%

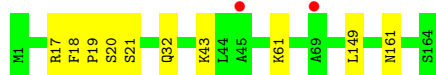


- Molecule 1: Alpha subunit of cyanobacterial protein phycoerythrin

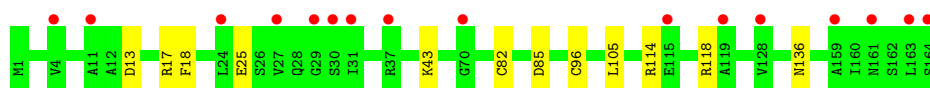
Chain KKK:  91% 9%



- 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

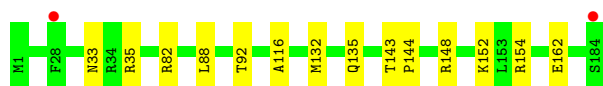


- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin

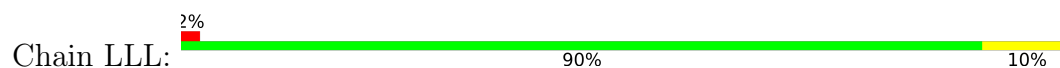


- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin





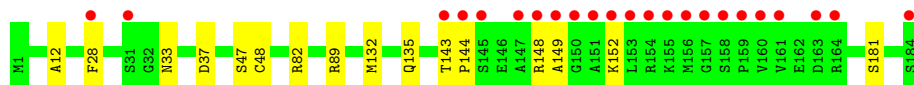
- Molecule 2: Beta subunit of cyanobacterial protein phycoerythrin



- 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.

All (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
1:AAA:47:ASN:CA	4:AAA:203:PG4:H52	2.05	0.86
2:HHH:148[B]:ARG:HG2	2:HHH:148[B]:ARG:HH11	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KKK:32:GLN:HG3	1:MMM:32:GLN:HG3	1.57	0.86
1:KKK:115:GLU:OE2	7:KKK:215:PO4:O1	1.98	0.82
2:FFF:116:ALA:HA	5:FFF:212:PGE:H5	1.61	0.82
2:JJJ:88:LEU:O	2:JJJ:92[B]:THR:HG23	1.81	0.81
2:PPP:28:PHE:HB3	4:PPP:207:PG4:H51	1.62	0.80
1:AAA:47:ASN:HA	4:AAA:203:PG4:C5	2.11	0.80
2:HHH:89:ARG:HH22	5:HHH:312:PGE:H22	1.48	0.77
2:PPP:148[A]:ARG:HD2	3:PPP:204:PEB:O2B	1.86	0.74
2:JJJ:116:ALA:HB2	4:JJJ:309:PG4:H52	1.68	0.74
5:FFF:213:PGE:H12	11:HHH:301:1PE:H132	1.69	0.74
2:JJJ:116:ALA:HB2	4:JJJ:309:PG4:C5	2.19	0.73
2:NNN:113:GLU:OE1	16:NNN:301:HOH:O	2.05	0.72
1:AAA:49:ASP:CB	4:AAA:203:PG4:H61	2.19	0.72
1:GGG:49:ASP:CB	5:GGG:208:PGE:H1	2.15	0.72
3:FFF:204:PEB:HNA	3:FFF:204:PEB:HMB3	1.55	0.71
3:NNN:204:PEB:HMB2	3:NNN:204:PEB:HNA	1.56	0.70
6:NNN:214:PEG:H41	16:NNN:365:HOH:O	1.92	0.69
2:LLL:152:LYS:NZ	9:LLL:204:RWB:O19	2.26	0.68
1:MMM:21[A]:SER:H	4:MMM:203:PG4:H81	1.59	0.67
2:PPP:12:ALA:HB2	6:PPP:214:PEG:H42	1.75	0.67
15:NNN:206:PE5:C16	15:NNN:206:PE5:H31	2.25	0.66
2:DDD:116:ALA:HB2	13:DDD:206:P6G:H91	1.77	0.65
3:OOO:201:PEB:HNA	3:OOO:201:PEB:HMB3	1.62	0.65
2:PPP:148[A]:ARG:CD	3:PPP:204:PEB:O2B	2.45	0.65
1:MMM:20:SER:HB2	4:MMM:203:PG4:H82	1.78	0.64
1:AAA:47:ASN:C	4:AAA:203:PG4:H52	2.22	0.64
1:AAA:114:ARG:HG3	4:AAA:204:PG4:H12	1.80	0.64
1:MMM:19:PRO:O	4:MMM:203:PG4:H52	1.97	0.64
1:KKK:145:SER:HB2	6:KKK:209:PEG:H12	1.79	0.64
1:MMM:61:LYS:NZ	4:MMM:205:PG4:O2	2.30	0.64
5:FFF:213:PGE:C4	2:HHH:130:GLN:HG2	2.27	0.63
16:KKK:832:HOH:O	4:MMM:203:PG4:H31	1.98	0.63
2:LLL:82[B]:ARG:NH2	16:LLL:301:HOH:O	2.28	0.63
1:KKK:115:GLU:OE2	7:KKK:215:PO4:P	2.57	0.63
3:BBB:202:PEB:HMB2	3:BBB:202:PEB:HNA	1.62	0.63
1:MMM:18:PHE:O	4:MMM:203:PG4:H41	1.99	0.62
1:MMM:21[B]:SER:H	4:MMM:203:PG4:H81	1.61	0.62
2:LLL:157:GLY:HA3	5:LLL:225:PGE:C2	2.30	0.62
3:FFF:204:PEB:HNA	3:FFF:204:PEB:CMB	2.12	0.62
1:AAA:114:ARG:CG	4:AAA:204:PG4:H12	2.31	0.61
1:MMM:18:PHE:N	4:MMM:203:PG4:O2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GGG:39:GLU:O	1:GGG:43:LYS:HG2	1.99	0.60
1:MMM:19:PRO:O	4:MMM:203:PG4:C5	2.49	0.60
2:FFF:28:PHE:HB3	4:FFF:209:PG4:H51	1.83	0.60
3:DDD:202:PEB:HMB2	3:DDD:202:PEB:HNA	1.66	0.59
1:III:161:ASN:HB3	5:III:204:PGE:H1	1.84	0.59
1:KKK:161:ASN:HB3	6:KKK:208:PEG:H22	1.84	0.58
1:MMM:43:LYS:HG2	3:MMM:202:PEB:HBD1	1.84	0.58
1:CCC:82:CYS:HA	3:CCC:201:PEB:HHA1	1.86	0.58
1:GGG:32:GLN:CG	1:III:32:GLN:HG3	2.30	0.58
2:LLL:157:GLY:HA3	5:LLL:225:PGE:H2	1.85	0.58
1:KKK:32:GLN:CG	1:MMM:32:GLN:HG3	2.31	0.58
5:FFF:213:PGE:H42	2:HHH:130:GLN:HG2	1.86	0.58
5:LLL:226:PGE:H3	1:MMM:161:ASN:HB3	1.86	0.57
1:OOO:136:ASN:ND2	7:OOO:211:PO4:O1	2.36	0.57
1:GGG:32:GLN:HG3	1:III:32:GLN:CG	2.31	0.57
2:PPP:149:ALA:HB2	3:PPP:204:PEB:C1A	2.34	0.57
1:OOO:82:CYS:HA	3:OOO:201:PEB:HHA1	1.85	0.57
3:CCC:201:PEB:HNA	3:CCC:201:PEB:HMB3	1.70	0.57
5:FFF:213:PGE:H2	2:HHH:180:ILE:HG21	1.86	0.57
6:JJJ:312:PEG:H42	16:JJJ:437:HOH:O	2.05	0.56
1:OOO:17:ARG:HG3	1:OOO:18:PHE:O	2.05	0.56
16:KKK:811:HOH:O	4:MMM:203:PG4:H62	2.04	0.56
3:BBB:202:PEB:HMB2	3:BBB:202:PEB:NA	2.20	0.56
1:CCC:143:ASP:HA	6:CCC:210:PEG:H22	1.88	0.56
5:LLL:225:PGE:H1	1:MMM:149:LEU:HD23	1.87	0.56
1:III:84:ARG:HG3	11:JJJ:302:1PE:H241	1.87	0.56
2:NNN:152:LYS:HE3	15:NNN:206:PE5:H61	1.87	0.56
2:FFF:4:ALA:HB2	4:FFF:209:PG4:H41	1.88	0.56
1:MMM:21[A]:SER:H	4:MMM:203:PG4:C8	2.18	0.56
2:LLL:118:LEU:HD11	3:LLL:201:PEB:HAC1	1.87	0.55
2:FFF:28:PHE:HB3	4:FFF:209:PG4:C5	2.37	0.55
5:FFF:213:PGE:H4	2:HHH:130:GLN:HG2	1.88	0.55
1:CCC:15:ALA:HB2	5:CCC:208:PGE:H4	1.89	0.55
1:KKK:32:GLN:HG3	1:MMM:32:GLN:CG	2.33	0.55
1:MMM:20:SER:CB	4:MMM:203:PG4:H82	2.36	0.55
2:JJJ:154:ARG:NH2	12:JJJ:306:P33:H52	2.23	0.54
2:BBB:113:GLU:OE2	11:BBB:206:1PE:H161	2.07	0.54
1:KKK:18:PHE:CD1	5:LLL:226:PGE:H5	2.43	0.54
1:MMM:20:SER:HB3	4:MMM:203:PG4:H42	1.89	0.54
2:NNN:28:PHE:CE1	5:NNN:212:PGE:H5	2.42	0.54
1:CCC:32[A]:GLN:CG	1:EEE:32[A]:GLN:HG3	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MMM:21[B]:SER:H	4:MMM:203:PG4:C8	2.20	0.54
2:PPP:135:GLN:HG2	3:PPP:204:PEB:C1B	2.38	0.54
3:LLL:201:PEB:CMB	3:LLL:201:PEB:HNA	2.22	0.53
3:HHH:302:PEB:CMB	3:HHH:302:PEB:HNA	2.21	0.53
2:HHH:148[B]:ARG:HH11	2:HHH:148[B]:ARG:CG	2.18	0.52
3:HHH:302:PEB:HNA	3:HHH:302:PEB:HMB3	1.73	0.52
1:MMM:17:ARG:HA	4:MMM:203:PG4:H11	1.92	0.52
2:NNN:152:LYS:HG2	15:NNN:206:PE5:H151	1.91	0.52
1:AAA:115:GLU:OE2	4:AAA:204:PG4:O2	2.28	0.52
2:PPP:149:ALA:CB	3:PPP:204:PEB:C1A	2.88	0.52
1:AAA:115:GLU:OE2	4:AAA:204:PG4:C3	2.57	0.52
2:FFF:157:GLY:O	11:FFF:201:1PE:H232	2.10	0.52
6:PPP:214:PEG:H41	16:PPP:337:HOH:O	2.10	0.52
1:MMM:18:PHE:C	4:MMM:203:PG4:H41	2.34	0.52
3:HHH:304:PEB:HNA	3:HHH:304:PEB:HMB3	1.75	0.51
6:KKK:208:PEG:H32	4:MMM:203:PG4:H32	1.93	0.51
1:MMM:43:LYS:HG2	3:MMM:202:PEB:CBD	2.39	0.51
3:EEE:202:PEB:HBD1	3:EEE:202:PEB:OD	2.10	0.51
2:LLL:88:LEU:O	2:LLL:92[B]:THR:HG23	2.09	0.51
2:NNN:170:ALA:HB1	4:NNN:208:PG4:H81	1.91	0.51
3:CCC:202:PEB:C4D	6:CCC:210:PEG:H21	2.40	0.51
3:BBB:201:PEB:CMB	3:BBB:201:PEB:HNA	2.24	0.51
3:DDD:201:PEB:CMB	3:DDD:201:PEB:HNA	2.24	0.51
2:LLL:116:ALA:HB2	4:LLL:207:PG4:H32	1.93	0.51
1:CCC:32[A]:GLN:HG3	1:EEE:32[A]:GLN:CG	2.33	0.50
2:DDD:28:PHE:HB3	6:DDD:213:PEG:H12	1.92	0.50
2:JJJ:152:LYS:HE3	12:JJJ:306:P33:H141	1.93	0.50
1:AAA:112:GLY:H	4:AAA:204:PG4:C4	2.25	0.50
1:CCC:143:ASP:HA	6:CCC:210:PEG:C2	2.42	0.50
3:FFF:204:PEB:HMB3	3:FFF:204:PEB:NA	2.24	0.50
2:LLL:86:ILE:HG21	3:LLL:201:PEB:CAD	2.41	0.50
2:PPP:152:LYS:O	3:PPP:204:PEB:HMA2	2.12	0.50
3:PPP:202:PEB:CMB	3:PPP:202:PEB:HNA	2.25	0.50
3:EEE:201:PEB:HNA	3:EEE:201:PEB:HMB3	1.75	0.49
3:NNN:203:PEB:HMB2	3:NNN:203:PEB:HNA	1.76	0.49
3:DDD:202:PEB:HMB2	3:DDD:202:PEB:NA	2.27	0.49
3:KKK:201:PEB:HNA	3:KKK:201:PEB:HMB3	1.77	0.49
1:AAA:113:GLN:N	4:AAA:204:PG4:H21	2.28	0.49
1:AAA:115:GLU:OE2	4:AAA:204:PG4:H32	2.12	0.49
1:KKK:128:VAL:HG12	15:NNN:206:PE5:H141	1.94	0.49
1:GGG:2:LYS:HD2	6:III:201:PEG:H11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KKK:158:TYR:HD1	4:MMM:203:PG4:H61	1.77	0.49
3:NNN:204:PEB:HMB2	3:NNN:204:PEB:NA	2.26	0.48
1:CCC:143:ASP:CA	6:CCC:210:PEG:H22	2.43	0.48
2:HHH:98:GLY:HA3	5:HHH:309:PGE:H6	1.95	0.48
2:FFF:153:LEU:HB3	4:FFF:202:PG4:H72	1.95	0.48
1:AAA:114:ARG:H	4:AAA:204:PG4:H21	1.78	0.48
12:DDD:205:P33:H112	12:DDD:205:P33:H182	1.95	0.48
2:PPP:149:ALA:HB2	3:PPP:204:PEB:OA	2.12	0.48
1:AAA:57:ASN:HB3	5:AAA:207:PGE:H6	1.94	0.48
2:FFF:152:LYS:HE3	12:FFF:207:P33:O13	2.13	0.48
1:GGG:48:ILE:N	5:GGG:208:PGE:H22	2.29	0.48
1:GGG:115:GLU:OE2	7:GGG:214:PO4:O1	2.31	0.48
2:BBB:148[B]:ARG:CD	16:BBB:364:HOH:O	2.61	0.48
2:BBB:148[B]:ARG:HD2	16:BBB:364:HOH:O	2.15	0.47
16:KKK:811:HOH:O	4:MMM:203:PG4:C6	2.60	0.47
2:HHH:27:ALA:HA	5:HHH:311:PGE:H32	1.96	0.47
2:HHH:35:ARG:CZ	5:HHH:309:PGE:H62	2.45	0.47
2:FFF:163:ASP:OD1	16:FFF:301:HOH:O	2.20	0.46
2:JJJ:152:LYS:HE3	12:JJJ:306:P33:C14	2.45	0.46
2:FFF:35:ARG:NH2	4:FFF:209:PG4:H42	2.29	0.46
3:HHH:304:PEB:HMB3	3:HHH:304:PEB:NA	2.31	0.46
12:HHH:305:P33:O22	12:HHH:305:P33:H112	2.16	0.46
3:NNN:204:PEB:HBD1	3:NNN:204:PEB:OD	2.15	0.46
1:AAA:49:ASP:HB2	4:AAA:203:PG4:H31	1.97	0.46
2:LLL:46:ALA:HB3	5:LLL:226:PGE:H62	1.97	0.46
5:NNN:212:PGE:H1	16:NNN:362:HOH:O	2.15	0.46
2:HHH:112:LYS:HG2	4:HHH:307:PG4:H71	1.98	0.46
3:LLL:203:PEB:NA	3:LLL:203:PEB:HMB3	2.29	0.46
1:KKK:83:ALA:HB3	6:KKK:212:PEG:H12	1.98	0.46
3:NNN:203:PEB:HBD1	3:NNN:203:PEB:OD	2.15	0.46
3:DDD:201:PEB:OD	3:DDD:201:PEB:HBD1	2.16	0.46
3:GGG:201:PEB:HNA	3:GGG:201:PEB:HMB3	1.81	0.45
3:FFF:206:PEB:HMB3	3:FFF:206:PEB:NA	2.31	0.45
2:PPP:33:ASN:HB3	3:PPP:203:PEB:C1C	2.45	0.45
2:LLL:157:GLY:HA3	5:LLL:225:PGE:H22	1.99	0.45
2:PPP:48:CYS:SG	3:PPP:204:PEB:HMA1	2.56	0.45
1:AAA:49:ASP:HB2	4:AAA:203:PG4:C6	2.33	0.45
5:GGG:207:PGE:H22	5:III:204:PGE:H62	1.98	0.45
2:NNN:168:LEU:HG	6:NNN:214:PEG:C1	2.46	0.45
1:AAA:112:GLY:H	4:AAA:204:PG4:H41	1.81	0.45
2:DDD:7:ARG:HH22	11:DDD:207:1PE:H261	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FFF:152:LYS:NZ	12:FFF:207:P33:O4	2.45	0.45
1:III:161:ASN:CB	5:III:204:PGE:H32	2.47	0.45
2:BBB:33:ASN:HB3	3:BBB:202:PEB:C1C	2.47	0.45
3:LLL:203:PEB:HMB3	3:LLL:203:PEB:HNA	1.82	0.45
1:CCC:43:LYS:HG3	6:CCC:210:PEG:O1	2.17	0.44
2:HHH:152:LYS:HE3	12:HHH:305:P33:H141	1.99	0.44
2:HHH:181[A]:SER:OG	11:HHH:301:1PE:H141	2.17	0.44
2:FFF:164:ARG:NH2	16:FFF:307:HOH:O	2.41	0.44
2:HHH:148[B]:ARG:HG2	16:HHH:420:HOH:O	2.17	0.44
1:OOO:13:ASP:OD1	2:PPP:89:ARG:NH1	2.45	0.44
2:DDD:152:LYS:NZ	12:DDD:204:P33:O4	2.49	0.44
3:DDD:201:PEB:HNA	3:DDD:201:PEB:HMB3	1.81	0.44
3:MMM:202:PEB:NA	3:MMM:202:PEB:HMB2	2.33	0.44
15:NNN:206:PE5:H31	15:NNN:206:PE5:H161	1.96	0.44
2:PPP:28:PHE:HB3	4:PPP:207:PG4:C5	2.42	0.44
6:HHH:316:PEG:C4	6:HHH:316:PEG:H11	2.48	0.44
2:PPP:132:MET:HA	2:PPP:135:GLN:OE1	2.18	0.44
2:BBB:132:MET:HA	2:BBB:135:GLN:OE1	2.18	0.43
2:JJJ:152:LYS:HZ2	12:JJJ:306:P33:C6	2.31	0.43
1:MMM:20:SER:HA	4:MMM:203:PG4:C8	2.47	0.43
3:AAA:202:PEB:HBD1	3:AAA:202:PEB:OD	2.18	0.43
2:FFF:132:MET:HA	2:FFF:135:GLN:OE1	2.19	0.43
2:HHH:177:ASP:CG	11:HHH:301:1PE:H232	2.43	0.43
2:LLL:33:ASN:HB3	3:LLL:202:PEB:C1C	2.49	0.43
1:OOO:96:CYS:SG	1:OOO:105:LEU:HB2	2.57	0.43
2:DDD:33:ASN:HB3	3:DDD:202:PEB:C1C	2.49	0.43
1:EEE:96:CYS:SG	1:EEE:105:LEU:HB2	2.59	0.43
1:KKK:149:LEU:HD23	4:NNN:201:PG4:H41	2.00	0.43
1:KKK:61:LYS:NZ	5:KKK:206:PGE:O2	2.44	0.43
1:AAA:110:ILE:O	4:AAA:204:PG4:H22	2.19	0.43
6:CCC:210:PEG:H21	6:CCC:210:PEG:H42	1.77	0.43
2:DDD:31[B]:SER:OG	16:DDD:302:HOH:O	2.21	0.43
2:HHH:82:ARG:HH22	3:HHH:302:PEB:C1C	2.32	0.43
2:JJJ:116:ALA:HB2	4:JJJ:309:PG4:H51	1.96	0.43
2:JJJ:132:MET:HA	2:JJJ:135:GLN:OE1	2.19	0.43
1:KKK:10:ALA:HB1	4:KKK:204:PG4:H81	2.00	0.43
2:LLL:152:LYS:HE3	9:LLL:204:RWB:C27	2.49	0.43
3:MMM:202:PEB:HBB1	3:MMM:202:PEB:HMB1	2.00	0.43
3:MMM:201:PEB:HNA	3:MMM:201:PEB:HMB3	1.83	0.43
2:PPP:28:PHE:CB	4:PPP:207:PG4:H51	2.42	0.43
2:BBB:37:ASP:OD2	3:BBB:202:PEB:NB	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:158:TYR:CD1	5:CCC:205:PGE:H42	2.54	0.42
1:GGG:56:TYR:HB2	1:GGG:86:ILE:HD12	2.01	0.42
1:MMM:19:PRO:O	4:MMM:203:PG4:H51	2.18	0.42
2:BBB:143:THR:N	2:BBB:144:PRO:CD	2.83	0.42
2:HHH:27:ALA:N	5:HHH:311:PGE:H22	2.33	0.42
2:LLL:132:MET:HA	2:LLL:135:GLN:OE1	2.19	0.42
2:LLL:47:SER:OG	6:MMM:209:PEG:H21	2.19	0.42
1:OOO:85:ASP:OD1	3:OOO:201:PEB:H1D1	2.19	0.42
1:GGG:96:CYS:SG	1:GGG:105:LEU:HB2	2.59	0.42
1:III:56:TYR:HB2	1:III:86:ILE:HD12	2.01	0.42
2:JJJ:35:ARG:CZ	11:JJJ:307:1PE:H141	2.50	0.42
2:JJJ:82[A]:ARG:HH22	3:JJJ:303:PEB:C1C	2.32	0.42
2:DDD:132:MET:HA	2:DDD:135:GLN:OE1	2.19	0.42
2:LLL:47:SER:OG	6:MMM:209:PEG:C2	2.67	0.42
2:NNN:132:MET:HA	2:NNN:135:GLN:OE1	2.20	0.42
2:NNN:143:THR:N	2:NNN:144:PRO:CD	2.83	0.42
3:NNN:205:PEB:HMB2	3:NNN:205:PEB:HNA	1.85	0.42
2:PPP:82[A]:ARG:NH2	3:PPP:202:PEB:O1C	2.52	0.42
2:BBB:82[A]:ARG:HH22	3:BBB:201:PEB:C1C	2.32	0.42
2:FFF:82[A]:ARG:HH22	3:FFF:204:PEB:C1C	2.33	0.42
3:JJJ:303:PEB:HBD1	3:JJJ:303:PEB:OD	2.18	0.42
15:NNN:206:PE5:C16	15:NNN:206:PE5:C3	2.94	0.42
1:MMM:61:LYS:HE2	6:MMM:210:PEG:H42	2.02	0.42
2:HHH:132:MET:HA	2:HHH:135:GLN:OE1	2.19	0.41
5:CCC:204:PGE:H22	6:CCC:210:PEG:H12	2.02	0.41
1:III:96:CYS:SG	1:III:105:LEU:HB2	2.60	0.41
1:III:161:ASN:HB2	5:III:204:PGE:H32	2.02	0.41
3:AAA:201:PEB:HNA	3:AAA:201:PEB:HMB1	1.86	0.41
2:DDD:113:GLU:HA	13:DDD:206:P6G:H142	2.01	0.41
3:PPP:202:PEB:HNA	3:PPP:202:PEB:HMB2	1.84	0.41
1:KKK:96:CYS:SG	1:KKK:105:LEU:HB2	2.60	0.41
6:KKK:208:PEG:H21	4:MMM:203:PG4:H21	2.03	0.41
2:DDD:143:THR:N	2:DDD:144:PRO:CD	2.84	0.41
2:HHH:89:ARG:NH2	5:HHH:312:PGE:H22	2.25	0.41
2:HHH:112:LYS:HE3	4:HHH:307:PG4:H71	2.03	0.41
2:HHH:152:LYS:HE3	12:HHH:305:P33:C14	2.51	0.41
1:CCC:96:CYS:SG	1:CCC:105:LEU:HB2	2.60	0.41
3:KKK:202:PEB:NA	3:KKK:202:PEB:HMB2	2.36	0.41
2:LLL:82[A]:ARG:HH22	3:LLL:201:PEB:C1C	2.34	0.41
2:LLL:143:THR:N	2:LLL:144:PRO:CD	2.84	0.41
4:MMM:203:PG4:H51	2:NNN:43:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:NNN:205:PEB:HNA	3:NNN:205:PEB:CMB	2.34	0.41
2:PPP:143:THR:N	2:PPP:144:PRO:CD	2.84	0.41
2:BBB:152:LYS:HZ2	9:BBB:204:RWB:C17	2.34	0.41
2:DDD:70:MEN:O	2:DDD:76:ARG:HB3	2.21	0.41
1:III:158:TYR:CD1	5:III:204:PGE:H4	2.56	0.41
2:JJJ:143:THR:N	2:JJJ:144:PRO:CD	2.84	0.41
2:LLL:98:GLY:HA3	4:LLL:206:PG4:C3	2.51	0.41
2:PPP:37:ASP:OD2	3:PPP:203:PEB:NB	2.54	0.41
1:AAA:96:CYS:SG	1:AAA:105:LEU:HB2	2.61	0.40
1:KKK:10:ALA:CB	4:KKK:204:PG4:H81	2.51	0.40
2:FFF:143:THR:N	2:FFF:144:PRO:CD	2.84	0.40
2:JJJ:33:ASN:HB3	3:JJJ:304:PEB:C1C	2.52	0.40
1:KKK:84:ARG:HA	6:KKK:212:PEG:H21	2.02	0.40
2:LLL:70:MEN:O	2:LLL:76:ARG:HB3	2.22	0.40
2:DDD:37:ASP:OD2	3:DDD:202:PEB:NB	2.54	0.40
2:NNN:70:MEN:O	2:NNN:76:ARG:HB3	2.22	0.40
3:BBB:201:PEB:HNA	3:BBB:201:PEB:HMB3	1.85	0.40
1:EEE:139:CYS:SG	3:EEE:202:PEB:HHA1	2.62	0.40
2:NNN:168:LEU:HG	6:NNN:214:PEG:H12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	43	LYS
2	DDD	155[A]	LYS
2	DDD	155[B]	LYS
1	GGG	1[A]	MET
1	GGG	1[B]	MET
2	JJJ	148[A]	ARG
2	JJJ	148[B]	ARG
2	JJJ	162	GLU
1	KKK	43	LYS
2	NNN	167	SER
1	OOO	25	GLU
1	OOO	43	LYS
1	OOO	114	ARG
1	OOO	118	ARG
2	PPP	47	SER
2	PPP	181	SER

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.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	DDD	70	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
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
2	NNN	70	MEN	CA-CB-CG-ND2
2	PPP	70	MEN	CA-CB-CG-ND2
2	JJJ	70	MEN	CA-CB-CG-OD1
2	LLL	70	MEN	CA-CB-CG-OD1
2	NNN	70	MEN	CA-CB-CG-OD1
2	PPP	70	MEN	CA-CB-CG-OD1
2	BBB	70	MEN	CA-CB-CG-ND2
2	BBB	70	MEN	CA-CB-CG-OD1
2	DDD	70	MEN	CA-CB-CG-OD1
2	FFF	70	MEN	CA-CB-CG-OD1
2	HHH	70	MEN	CA-CB-CG-OD1

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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	FFF	211	-	-	3/7/7/7	-

All (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
3	BBB	201	PEB	CHA-C4A	4.32	1.43	1.36
3	CCC	201	PEB	CHA-C4A	4.10	1.43	1.36
3	AAA	201	PEB	CHA-C4A	4.03	1.43	1.36
3	KKK	201	PEB	CHA-C4A	3.95	1.43	1.36
3	OOO	201	PEB	CHB-C4B	3.80	1.45	1.38
3	AAA	202	PEB	CHA-C4A	3.80	1.42	1.36
3	LLL	202	PEB	CHA-C4A	3.78	1.42	1.36
3	JJJ	303	PEB	CHA-C4A	3.70	1.42	1.36
3	JJJ	305	PEB	CHA-C4A	3.60	1.42	1.36
3	PPP	203	PEB	CHA-C4A	3.45	1.42	1.36
3	BBB	202	PEB	CHA-C4A	3.42	1.42	1.36
3	CCC	202	PEB	CHA-C4A	3.33	1.42	1.36
3	BBB	203	PEB	CHA-C4A	3.32	1.42	1.36
3	HHH	302	PEB	CHA-C4A	3.20	1.41	1.36
3	JJJ	304	PEB	CHA-C4A	3.17	1.41	1.36
3	DDD	202	PEB	CHA-C4A	3.15	1.41	1.36
3	NNN	204	PEB	CHA-C4A	3.08	1.41	1.36
3	KKK	202	PEB	CHA-C4A	3.08	1.41	1.36
3	LLL	203	PEB	CHB-C4B	3.03	1.44	1.38
3	NNN	205	PEB	CHA-C4A	3.03	1.41	1.36
3	NNN	203	PEB	CHA-C4A	3.02	1.41	1.36
3	III	202	PEB	CHB-C4B	2.90	1.44	1.38
3	JJJ	303	PEB	O2B-CGB	-2.88	1.21	1.30
3	DDD	201	PEB	C2D-C3D	-2.83	1.31	1.34
3	GGG	202	PEB	CHA-C4A	2.79	1.41	1.36
3	PPP	202	PEB	O2B-CGB	-2.75	1.21	1.30
3	JJJ	303	PEB	C2D-C3D	-2.75	1.31	1.34
3	HHH	302	PEB	O2B-CGB	-2.71	1.21	1.30
3	CCC	201	PEB	O2C-CGC	-2.69	1.21	1.30
3	HHH	303	PEB	CHA-C4A	2.68	1.41	1.36
3	FFF	204	PEB	CHA-C4A	2.67	1.40	1.36
3	DDD	201	PEB	C2A-C1A	-2.63	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	OOO	202	PEB	CHA-C4A	2.61	1.40	1.36
7	III	214	PO4	P-O1	2.59	1.56	1.50
3	DDD	201	PEB	O1C-CGC	2.57	1.30	1.22
3	KKK	202	PEB	C2D-C3D	-2.56	1.31	1.34
3	FFF	206	PEB	CHA-C4A	2.55	1.40	1.36
3	PPP	204	PEB	CHA-C4A	2.54	1.40	1.36
3	FFF	204	PEB	CHB-C4B	2.52	1.43	1.38
3	DDD	201	PEB	CHA-C4A	2.51	1.40	1.36
3	BBB	202	PEB	C4D-ND	2.50	1.38	1.35
7	JJJ	321	PO4	P-O1	2.46	1.56	1.50
3	KKK	202	PEB	CHB-C4B	2.46	1.43	1.38
3	AAA	201	PEB	O2B-CGB	-2.43	1.22	1.30
3	EEE	201	PEB	CHA-C4A	2.41	1.40	1.36
3	GGG	201	PEB	O2C-CGC	-2.40	1.22	1.30
3	MMM	201	PEB	OD-C4D	2.39	1.28	1.23
3	FFF	205	PEB	CHA-C4A	2.39	1.40	1.36
3	HHH	303	PEB	CHB-C4B	2.34	1.43	1.38
3	JJJ	303	PEB	O1C-CGC	2.32	1.29	1.22
3	III	203	PEB	CHA-C4A	2.31	1.40	1.36
3	AAA	201	PEB	CHB-C4B	2.28	1.43	1.38
3	PPP	204	PEB	CHB-C4B	2.26	1.43	1.38
3	KKK	201	PEB	OD-C4D	2.26	1.27	1.23
3	PPP	203	PEB	O2B-CGB	-2.25	1.23	1.30
3	NNN	203	PEB	O1C-CGC	2.23	1.29	1.22
3	KKK	201	PEB	C2D-C3D	-2.22	1.31	1.34
3	FFF	204	PEB	O1C-CGC	2.22	1.29	1.22
3	CCC	201	PEB	OD-C4D	2.21	1.27	1.23
3	CCC	202	PEB	CHC-C4C	-2.20	1.47	1.50
3	AAA	201	PEB	O1B-CGB	2.19	1.29	1.22
3	III	202	PEB	CHA-C1B	2.19	1.45	1.40
3	BBB	202	PEB	C4A-NA	2.19	1.41	1.37
3	KKK	201	PEB	C2A-C1A	-2.16	1.50	1.52
3	EEE	201	PEB	O2C-CGC	-2.16	1.23	1.30
3	FFF	204	PEB	O2B-CGB	-2.14	1.23	1.30
3	MMM	201	PEB	C2A-C1A	-2.13	1.50	1.52
9	BBB	204	RWB	C5-C6	2.13	1.59	1.49
3	BBB	201	PEB	O1C-CGC	2.12	1.29	1.22
7	CCC	220	PO4	P-O1	2.11	1.55	1.50
3	HHH	304	PEB	O2B-CGB	-2.11	1.23	1.30
3	MMM	201	PEB	O2C-CGC	-2.08	1.23	1.30
3	BBB	201	PEB	CHB-C4B	2.06	1.42	1.38
3	PPP	202	PEB	CBC-CGC	2.06	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	OOO	201	PEB	O2C-CGC	-2.05	1.24	1.30
9	BBB	204	RWB	O4-C5	2.05	1.51	1.42
3	OOO	201	PEB	O1B-CGB	2.04	1.28	1.22
3	GGG	201	PEB	C2A-C1A	-2.04	1.50	1.52
3	PPP	204	PEB	O2B-CGB	-2.02	1.24	1.30
3	HHH	303	PEB	O2C-CGC	-2.01	1.24	1.30

All (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
3	JJJ	303	PEB	CHA-C4A-NA	4.91	131.76	125.63
3	JJJ	304	PEB	CHC-C1D-ND	-4.80	107.84	113.73
3	DDD	201	PEB	CHC-C1D-ND	-4.72	107.94	113.73
3	FFF	204	PEB	CHC-C1D-ND	-4.60	108.09	113.73
3	EEE	201	PEB	CHA-C4A-NA	4.24	130.92	125.63
3	PPP	204	PEB	C1A-NA-C4A	-4.14	108.21	113.41
3	MMM	202	PEB	CHC-C1D-ND	-4.01	108.81	113.73
3	NNN	203	PEB	CMB-C2B-C1B	3.98	131.28	125.10
3	JJJ	304	PEB	OA-C1A-C2A	-3.98	123.01	126.17
3	MMM	201	PEB	CHA-C4A-NA	3.88	130.48	125.63
3	NNN	204	PEB	CMD-C2D-C3D	-3.85	124.48	129.95
3	CCC	202	PEB	C1D-CHC-C4C	-3.84	106.85	113.32
3	GGG	201	PEB	CHA-C4A-NA	3.64	130.18	125.63
3	BBB	201	PEB	CHA-C4A-NA	3.63	130.16	125.63
3	OOO	201	PEB	CHA-C4A-NA	3.62	130.15	125.63
9	BBB	204	RWB	C23-O22-C21	3.59	128.95	113.26
3	AAA	201	PEB	CMB-C2B-C1B	3.54	130.59	125.10
3	KKK	202	PEB	C1D-CHC-C4C	-3.49	107.45	113.32
3	GGG	201	PEB	CHC-C1D-ND	-3.47	109.47	113.73
3	III	203	PEB	CHC-C1D-ND	-3.44	109.51	113.73
3	NNN	203	PEB	CHA-C4A-NA	3.43	129.92	125.63
3	III	202	PEB	CHA-C1B-C2B	3.40	133.60	124.87
3	DDD	201	PEB	CMD-C2D-C3D	-3.38	125.15	129.95
3	III	202	PEB	C1B-CHA-C4A	3.38	134.11	127.25
9	BBB	204	RWB	C24-O25-C26	3.37	128.00	113.26
3	PPP	204	PEB	CMD-C2D-C3D	-3.27	125.30	129.95
3	BBB	201	PEB	CHC-C1D-ND	-3.25	109.74	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	FFF	204	PEB	CHA-C4A-NA	3.20	129.62	125.63
3	KKK	201	PEB	CHA-C1B-NB	-3.18	118.09	124.95
3	GGG	202	PEB	OA-C1A-C2A	-3.13	123.68	126.17
3	DDD	201	PEB	CHA-C4A-NA	3.12	129.53	125.63
3	KKK	201	PEB	CHA-C1B-C2B	3.12	132.87	124.87
3	CCC	202	PEB	OA-C1A-C2A	-3.10	123.70	126.17
3	JJJ	303	PEB	C1B-CHA-C4A	3.09	133.54	127.25
3	JJJ	303	PEB	CHA-C1B-C2B	3.05	132.71	124.87
3	HHH	303	PEB	C2A-C3A-C4A	3.05	105.90	101.34
3	EEE	201	PEB	CHA-C1B-C2B	3.04	132.67	124.87
3	EEE	201	PEB	CHA-C1B-NB	-3.04	118.40	124.95
3	AAA	202	PEB	C2A-C3A-C4A	3.02	105.86	101.34
3	HHH	302	PEB	CHA-C4A-NA	3.01	129.39	125.63
3	BBB	201	PEB	C2A-C3A-C4A	3.01	105.85	101.34
3	MMM	201	PEB	CMD-C2D-C3D	-3.01	125.68	129.95
3	PPP	202	PEB	CHA-C4A-NA	2.97	129.34	125.63
3	BBB	201	PEB	CMD-C2D-C3D	-2.96	125.74	129.95
3	III	202	PEB	CHA-C1B-NB	-2.90	118.69	124.95
3	GGG	201	PEB	CHA-C1B-C2B	2.87	132.26	124.87
3	KKK	201	PEB	CHA-C4A-NA	2.87	129.22	125.63
3	EEE	202	PEB	C2A-C3A-C4A	2.87	105.63	101.34
3	GGG	201	PEB	C1B-CHA-C4A	2.85	133.05	127.25
3	LLL	201	PEB	CMB-C2B-C1B	2.85	129.53	125.10
3	JJJ	303	PEB	C2A-C3A-C4A	2.83	105.58	101.34
3	AAA	201	PEB	CHA-C1B-NB	-2.82	118.86	124.95
3	AAA	201	PEB	CHA-C1B-C2B	2.81	132.10	124.87
3	JJJ	303	PEB	CMD-C2D-C3D	-2.80	125.98	129.95
3	FFF	206	PEB	CHC-C1D-ND	-2.79	110.30	113.73
11	EEE	203	1PE	C26-OH6-C15	2.79	125.47	113.26
3	HHH	304	PEB	CHC-C4C-NC	2.78	124.82	121.10
3	KKK	201	PEB	CMB-C2B-C1B	2.77	129.40	125.10
3	CCC	202	PEB	C2A-C3A-C4A	2.76	105.48	101.34
3	JJJ	303	PEB	CHA-C1B-NB	-2.74	119.05	124.95
3	AAA	201	PEB	OA-C1A-C2A	-2.73	124.00	126.17
3	NNN	203	PEB	C2A-C3A-C4A	2.73	105.42	101.34
3	PPP	202	PEB	C2A-C3A-C4A	2.71	105.40	101.34
3	AAA	202	PEB	OD-C4D-C3D	-2.71	123.17	129.71
3	DDD	202	PEB	C2A-C3A-C4A	2.70	105.39	101.34
3	MMM	201	PEB	OA-C1A-C2A	-2.69	124.03	126.17
3	AAA	201	PEB	C1B-CHA-C4A	2.69	132.72	127.25
3	LLL	201	PEB	CHC-C1D-ND	-2.68	110.44	113.73
3	EEE	202	PEB	CHA-C4A-NA	2.67	128.96	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	KKK	202	PEB	CHC-C1D-ND	-2.66	110.47	113.73
3	FFF	204	PEB	C2A-C3A-C4A	2.65	105.31	101.34
3	FFF	206	PEB	C2A-C3A-C4A	2.64	105.30	101.34
3	FFF	206	PEB	C1D-CHC-C4C	2.64	117.76	113.32
3	DDD	203	PEB	CHC-C1D-ND	-2.63	110.50	113.73
3	OOO	201	PEB	CMD-C2D-C3D	-2.61	126.24	129.95
3	CCC	201	PEB	CHA-C4A-NA	2.61	128.89	125.63
3	HHH	304	PEB	CMD-C2D-C3D	-2.60	126.25	129.95
12	DDD	204	P33	O7-C8-C9	2.60	122.21	110.35
3	BBB	201	PEB	CMB-C2B-C1B	2.60	129.14	125.10
3	GGG	201	PEB	CHA-C1B-NB	-2.60	119.34	124.95
3	GGG	202	PEB	C2A-C3A-C4A	2.59	105.22	101.34
3	BBB	203	PEB	C2A-C3A-C4A	2.58	105.21	101.34
3	NNN	204	PEB	CHC-C4C-NC	2.58	124.55	121.10
3	BBB	203	PEB	OD-C4D-C3D	-2.57	123.50	129.71
3	FFF	204	PEB	C2A-C1A-NA	2.57	110.42	108.29
3	NNN	205	PEB	C2A-C3A-C4A	2.56	105.17	101.34
3	MMM	201	PEB	CHA-C1B-C2B	2.55	131.43	124.87
3	HHH	302	PEB	CHA-C1B-C2B	2.55	131.42	124.87
3	LLL	201	PEB	CHA-C1B-NB	-2.55	119.45	124.95
3	JJJ	305	PEB	CMB-C2B-C1B	2.54	129.04	125.10
3	GGG	201	PEB	CMD-C2D-C3D	-2.54	126.35	129.95
3	LLL	201	PEB	C2A-C3A-C4A	2.53	105.13	101.34
3	KKK	202	PEB	CAA-C3A-C4A	2.53	119.17	112.67
3	EEE	202	PEB	OA-C1A-C2A	-2.52	124.17	126.17
3	DDD	201	PEB	C2A-C3A-C4A	2.52	105.11	101.34
3	LLL	201	PEB	CHA-C1B-C2B	2.50	131.28	124.87
3	AAA	202	PEB	OA-C1A-C2A	-2.48	124.20	126.17
3	KKK	201	PEB	C1B-CHA-C4A	2.47	132.27	127.25
3	OOO	201	PEB	OD-C4D-C3D	-2.47	123.74	129.71
3	DDD	203	PEB	OA-C1A-C2A	-2.46	124.22	126.17
3	CCC	201	PEB	CMD-C2D-C3D	-2.46	126.46	129.95
3	III	203	PEB	C2A-C3A-C4A	2.44	105.00	101.34
3	DDD	203	PEB	OD-C4D-ND	-2.44	122.67	126.02
3	EEE	201	PEB	C1B-CHA-C4A	2.43	132.19	127.25
3	AAA	202	PEB	OD-C4D-ND	2.43	129.35	126.02
3	EEE	201	PEB	CMB-C2B-C1B	2.42	128.85	125.10
3	CCC	201	PEB	OA-C1A-C2A	-2.41	124.26	126.17
3	MMM	202	PEB	OA-C1A-C2A	-2.41	124.26	126.17
9	BBB	204	RWB	C30-O31-C32	2.40	123.77	113.26
3	HHH	302	PEB	C2A-C1A-NA	2.39	110.28	108.29
3	KKK	202	PEB	C2A-C3A-C4A	2.39	104.92	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	MMM	201	PEB	C1B-CHA-C4A	2.39	132.10	127.25
3	FFF	204	PEB	OA-C1A-C2A	-2.39	124.28	126.17
3	EEE	202	PEB	OD-C4D-C3D	-2.38	123.95	129.71
3	HHH	303	PEB	CHC-C4C-NC	2.38	124.29	121.10
3	AAA	201	PEB	C2A-C1A-NA	2.38	110.27	108.29
3	MMM	201	PEB	CMB-C2B-C1B	2.37	128.78	125.10
3	EEE	201	PEB	OA-C1A-C2A	-2.36	124.29	126.17
3	JJJ	303	PEB	CHC-C1D-ND	-2.36	110.84	113.73
3	CCC	201	PEB	CHC-C4C-NC	2.35	124.24	121.10
3	AAA	201	PEB	OD-C4D-C3D	-2.33	124.08	129.71
3	HHH	302	PEB	CHA-C1B-NB	-2.32	119.94	124.95
3	CCC	202	PEB	C2A-C1A-NA	2.31	110.21	108.29
3	MMM	201	PEB	CHA-C1B-NB	-2.31	119.95	124.95
3	AAA	201	PEB	C2C-C1C-NC	-2.31	104.67	107.57
3	HHH	302	PEB	CMB-C2B-C1B	2.31	128.69	125.10
3	LLL	203	PEB	CHC-C1D-ND	-2.31	110.90	113.73
3	PPP	203	PEB	C2A-C3A-C4A	2.30	104.79	101.34
3	HHH	302	PEB	C2A-C3A-C4A	2.30	104.79	101.34
3	NNN	204	PEB	C2A-C3A-C4A	2.29	104.77	101.34
3	HHH	302	PEB	CAA-C3A-C4A	2.29	118.55	112.67
3	PPP	203	PEB	CMD-C2D-C3D	-2.27	126.72	129.95
3	III	202	PEB	CMB-C2B-C1B	2.27	128.62	125.10
3	FFF	205	PEB	O1C-CGC-CBC	-2.27	115.91	123.09
3	HHH	302	PEB	C1B-CHA-C4A	2.26	131.84	127.25
3	DDD	203	PEB	C2A-C3A-C4A	2.25	104.71	101.34
3	GGG	201	PEB	CMB-C2B-C1B	2.25	128.59	125.10
3	JJJ	305	PEB	C2A-C3A-C4A	2.25	104.70	101.34
3	PPP	204	PEB	C2A-C1A-NA	-2.24	106.42	108.29
3	MMM	202	PEB	CAA-C3A-C4A	2.23	118.41	112.67
3	MMM	202	PEB	C2A-C3A-C4A	2.23	104.68	101.34
3	MMM	201	PEB	C2A-C3A-C4A	2.22	104.67	101.34
3	AAA	202	PEB	C1D-CHC-C4C	-2.22	109.58	113.32
3	BBB	202	PEB	OA-C1A-C2A	-2.22	124.41	126.17
3	PPP	203	PEB	OD-C4D-ND	-2.21	122.98	126.02
3	KKK	201	PEB	CHC-C4C-NC	2.21	124.06	121.10
3	JJJ	304	PEB	C2A-C1A-NA	2.21	110.12	108.29
3	BBB	202	PEB	C2A-C3A-C4A	2.20	104.64	101.34
3	DDD	201	PEB	CHA-C1B-NB	-2.20	120.20	124.95
3	MMM	201	PEB	CHC-C1D-ND	-2.20	111.04	113.73
3	GGG	202	PEB	OA-C1A-NA	2.19	127.51	124.93
3	FFF	205	PEB	C2A-C3A-C4A	2.19	104.62	101.34
3	EEE	201	PEB	CAB-CBB-CGB	2.18	119.44	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	PPP	202	PEB	CMB-C2B-C1B	2.18	128.48	125.10
3	BBB	203	PEB	CHA-C4A-NA	2.17	128.35	125.63
3	BBB	203	PEB	CHC-C4C-NC	2.17	124.01	121.10
3	DDD	201	PEB	CHA-C1B-C2B	2.17	130.45	124.87
3	DDD	201	PEB	CMB-C2B-C1B	2.17	128.47	125.10
3	PPP	203	PEB	CHA-C4A-NA	2.17	128.33	125.63
9	BBB	204	RWB	C33-O34-C35	2.16	122.70	113.26
3	PPP	204	PEB	OD-C4D-C3D	-2.16	124.50	129.71
3	BBB	201	PEB	CHA-C1B-NB	-2.16	120.30	124.95
3	FFF	206	PEB	CHC-C4C-NC	2.15	123.98	121.10
3	AAA	202	PEB	O1B-CGB-CBB	-2.15	116.27	123.09
3	GGG	202	PEB	CHC-C1D-ND	-2.14	111.11	113.73
3	III	202	PEB	C2C-C1C-NC	-2.14	104.89	107.57
9	BBB	204	RWB	O31-C30-C29	2.14	120.09	110.35
3	BBB	201	PEB	CHA-C1B-C2B	2.14	130.36	124.87
3	LLL	201	PEB	OD-C4D-ND	-2.13	123.09	126.02
3	NNN	203	PEB	CHA-C1B-C2B	2.12	130.31	124.87
12	HHH	305	P33	C18-O19-C20	2.11	122.50	113.26
3	CCC	202	PEB	CAA-C3A-C4A	2.11	118.08	112.67
3	FFF	204	PEB	CHA-C1B-C2B	2.09	130.24	124.87
3	PPP	204	PEB	CBB-CAB-C3B	2.09	118.30	112.53
11	EEE	203	1PE	OH6-C26-C16	2.08	119.29	110.11
3	DDD	201	PEB	C1D-CHC-C4C	-2.08	109.82	113.32
3	PPP	202	PEB	CMD-C2D-C3D	-2.08	127.00	129.95
3	CCC	201	PEB	CHA-C1B-C2B	2.07	130.20	124.87
3	OOO	202	PEB	C1D-CHC-C4C	-2.07	109.84	113.32
3	HHH	303	PEB	CHA-C1B-C2B	2.06	130.17	124.87
3	NNN	203	PEB	CHA-C1B-NB	-2.06	120.51	124.95
3	OOO	202	PEB	C2A-C3A-C4A	2.05	104.41	101.34
3	LLL	201	PEB	O1B-CGB-CBB	-2.05	116.60	123.09
3	PPP	204	PEB	C1B-CHA-C4A	-2.05	123.10	127.25
3	PPP	202	PEB	OA-C1A-C2A	-2.04	124.55	126.17
3	BBB	201	PEB	CAD-C3D-C2D	-2.04	121.81	128.43
3	JJJ	305	PEB	CAB-CBB-CGB	2.03	119.05	113.67
3	JJJ	304	PEB	C2A-C3A-C4A	2.03	104.38	101.34
3	LLL	202	PEB	CHC-C1D-ND	2.03	116.23	113.73
3	OOO	201	PEB	C2A-C3A-C4A	2.02	104.37	101.34
3	LLL	203	PEB	C2C-C1C-NC	-2.02	105.03	107.57
9	BBB	204	RWB	O34-C33-C32	2.02	119.56	110.35
3	AAA	201	PEB	C2A-C3A-C4A	2.02	104.36	101.34
3	BBB	202	PEB	O1C-CGC-CBC	-2.01	116.72	123.09
3	DDD	203	PEB	CHC-C4C-NC	2.00	123.78	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	201	PEB	C2A-C3A-C4A	2.00	104.34	101.34
11	EEE	203	1PE	C23-OH3-C22	2.00	122.03	113.26

There are no chirality outliers.

All (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
3	BBB	202	PEB	NB-C1B-CHA-C4A
3	BBB	202	PEB	C2B-C1B-CHA-C4A
3	BBB	203	PEB	C2D-C3D-CAD-CBD
3	BBB	203	PEB	NB-C1B-CHA-C4A
3	BBB	203	PEB	C2B-C1B-CHA-C4A
3	CCC	201	PEB	NA-C4A-CHA-C1B
3	CCC	201	PEB	C3A-C4A-CHA-C1B
3	CCC	201	PEB	NB-C1B-CHA-C4A
3	CCC	201	PEB	C2B-C1B-CHA-C4A
3	CCC	202	PEB	NB-C1B-CHA-C4A
3	CCC	202	PEB	C2B-C1B-CHA-C4A
3	DDD	201	PEB	NB-C1B-CHA-C4A
3	DDD	201	PEB	C2B-C1B-CHA-C4A
3	DDD	202	PEB	NB-C1B-CHA-C4A
3	DDD	202	PEB	C2B-C1B-CHA-C4A
3	DDD	203	PEB	NB-C1B-CHA-C4A
3	DDD	203	PEB	C2B-C1B-CHA-C4A
3	EEE	201	PEB	NA-C4A-CHA-C1B
3	EEE	201	PEB	C3A-C4A-CHA-C1B
3	EEE	202	PEB	NB-C1B-CHA-C4A
3	EEE	202	PEB	C2B-C1B-CHA-C4A
3	FFF	204	PEB	NB-C1B-CHA-C4A
3	FFF	204	PEB	C2B-C1B-CHA-C4A
3	FFF	205	PEB	NB-C1B-CHA-C4A
3	FFF	205	PEB	C2B-C1B-CHA-C4A
3	FFF	206	PEB	C2D-C3D-CAD-CBD
3	FFF	206	PEB	NB-C1B-CHA-C4A
3	FFF	206	PEB	C2B-C1B-CHA-C4A
3	GGG	201	PEB	NA-C4A-CHA-C1B
3	GGG	201	PEB	C3A-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
3	GGG	201	PEB	NB-C1B-CHA-C4A
3	GGG	201	PEB	C2B-C1B-CHA-C4A
3	GGG	202	PEB	NB-C1B-CHA-C4A
3	GGG	202	PEB	C2B-C1B-CHA-C4A
3	HHH	302	PEB	NA-C4A-CHA-C1B
3	HHH	302	PEB	NB-C1B-CHA-C4A
3	HHH	302	PEB	C2B-C1B-CHA-C4A
3	HHH	303	PEB	NB-C1B-CHA-C4A
3	HHH	303	PEB	C2B-C1B-CHA-C4A
3	HHH	304	PEB	NB-C1B-CHA-C4A
3	HHH	304	PEB	C2B-C1B-CHA-C4A
3	III	202	PEB	NB-C1B-CHA-C4A
3	III	202	PEB	C2B-C1B-CHA-C4A
3	III	203	PEB	NB-C1B-CHA-C4A
3	III	203	PEB	C2B-C1B-CHA-C4A
3	JJJ	304	PEB	NB-C1B-CHA-C4A
3	JJJ	304	PEB	C2B-C1B-CHA-C4A
3	JJJ	305	PEB	C2D-C3D-CAD-CBD
3	JJJ	305	PEB	NB-C1B-CHA-C4A
3	JJJ	305	PEB	C2B-C1B-CHA-C4A
3	KKK	201	PEB	NA-C4A-CHA-C1B
3	KKK	201	PEB	C3A-C4A-CHA-C1B
3	KKK	201	PEB	NB-C1B-CHA-C4A
3	KKK	201	PEB	C2B-C1B-CHA-C4A
3	KKK	202	PEB	NB-C1B-CHA-C4A
3	KKK	202	PEB	C2B-C1B-CHA-C4A
3	LLL	201	PEB	NB-C1B-CHA-C4A
3	LLL	201	PEB	C2B-C1B-CHA-C4A
3	LLL	202	PEB	NB-C1B-CHA-C4A
3	LLL	202	PEB	C2B-C1B-CHA-C4A
3	LLL	203	PEB	C2D-C3D-CAD-CBD
3	LLL	203	PEB	NB-C1B-CHA-C4A
3	LLL	203	PEB	C2B-C1B-CHA-C4A
3	MMM	201	PEB	NA-C4A-CHA-C1B
3	MMM	201	PEB	C3A-C4A-CHA-C1B
3	MMM	201	PEB	NB-C1B-CHA-C4A
3	MMM	201	PEB	C2B-C1B-CHA-C4A
3	MMM	202	PEB	NB-C1B-CHA-C4A
3	MMM	202	PEB	C2B-C1B-CHA-C4A
3	NNN	203	PEB	NB-C1B-CHA-C4A
3	NNN	203	PEB	C2B-C1B-CHA-C4A
3	NNN	204	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
3	NNN	204	PEB	C2B-C1B-CHA-C4A
3	NNN	205	PEB	NB-C1B-CHA-C4A
3	NNN	205	PEB	C2B-C1B-CHA-C4A
3	OOO	201	PEB	C2D-C3D-CAD-CBD
3	OOO	201	PEB	NA-C4A-CHA-C1B
3	OOO	201	PEB	C3A-C4A-CHA-C1B
3	OOO	201	PEB	NB-C1B-CHA-C4A
3	OOO	201	PEB	C2B-C1B-CHA-C4A
3	OOO	202	PEB	NB-C1B-CHA-C4A
3	OOO	202	PEB	C2B-C1B-CHA-C4A
3	PPP	202	PEB	NB-C1B-CHA-C4A
3	PPP	202	PEB	C2B-C1B-CHA-C4A
3	PPP	203	PEB	NB-C1B-CHA-C4A
3	PPP	203	PEB	C2B-C1B-CHA-C4A
3	PPP	204	PEB	C2D-C3D-CAD-CBD
3	PPP	204	PEB	C4D-C3D-CAD-CBD
3	PPP	204	PEB	NB-C1B-CHA-C4A
3	PPP	204	PEB	C2B-C1B-CHA-C4A
4	GGG	205	PG4	C3-C4-O3-C5
4	HHH	308	PG4	C4-C3-O2-C2
6	MMM	208	PEG	C1-C2-O2-C3
11	DDD	207	1PE	C25-C15-OH6-C26
11	EEE	203	1PE	C16-C26-OH6-C15
4	FFF	210	PG4	C1-C2-O2-C3
5	BBB	209	PGE	C4-C3-O2-C2
5	BBB	222	PGE	C3-C4-O3-C5
5	KKK	207	PGE	C3-C4-O3-C5
5	LLL	210	PGE	C6-C5-O3-C4
6	CCC	215	PEG	C4-C3-O2-C2
6	DDD	215	PEG	C1-C2-O2-C3
11	BBB	208	1PE	C25-C15-OH6-C26
4	FFF	202	PG4	C4-C3-O2-C2
4	PPP	206	PG4	C3-C4-O3-C5
6	LLL	212	PEG	C4-C3-O2-C2
6	OOO	207	PEG	C1-C2-O2-C3
6	PPP	210	PEG	C4-C3-O2-C2
11	LLL	205	1PE	C12-C22-OH3-C23
12	DDD	204	P33	C18-C17-O16-C15
4	NNN	208	PG4	C8-C7-O4-C6
5	III	206	PGE	C4-C3-O2-C2
6	KKK	208	PEG	C4-C3-O2-C2
12	HHH	305	P33	C17-C18-O19-C20

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Mol	Chain	Res	Type	Atoms
12	HHH	306	P33	C6-C5-O4-C3
4	CCC	203	PG4	C5-C6-O4-C7
4	KKK	205	PG4	C6-C5-O3-C4
4	OOO	203	PG4	C6-C5-O3-C4
6	CCC	212	PEG	C1-C2-O2-C3
11	BBB	208	1PE	C24-C14-OH5-C25
11	DDD	207	1PE	C24-C14-OH5-C25
12	HHH	306	P33	C9-C8-O7-C6
4	CCC	203	PG4	C1-C2-O2-C3
5	GGG	206	PGE	C1-C2-O2-C3
6	BBB	223	PEG	C4-C3-O2-C2
11	JJJ	302	1PE	C15-C25-OH5-C14
12	DDD	205	P33	C17-C18-O19-C20
13	DDD	206	P6G	C11-C12-O13-C14
6	EEE	213	PEG	C4-C3-O2-C2
4	FFF	210	PG4	C5-C6-O4-C7
5	BBB	222	PGE	C4-C3-O2-C2
6	HHH	314	PEG	C4-C3-O2-C2
9	BBB	204	RWB	C29-C30-O31-C32
12	DDD	205	P33	C2-C3-O4-C5
6	HHH	318	PEG	C1-C2-O2-C3
6	KKK	210	PEG	C4-C3-O2-C2
9	LLL	204	RWB	C36-C35-O34-C33
5	JJJ	310	PGE	C3-C4-O3-C5
6	CCC	212	PEG	C4-C3-O2-C2
4	FFF	209	PG4	C6-C5-O3-C4
5	CCC	206	PGE	C3-C4-O3-C5
5	NNN	213	PGE	C4-C3-O2-C2
11	JJJ	307	1PE	C25-C15-OH6-C26
3	PPP	202	PEB	C2C-CAC-CBC-CGC
4	HHH	307	PG4	O3-C5-C6-O4
5	HHH	313	PGE	O2-C3-C4-O3
5	MMM	207	PGE	O2-C3-C4-O3
5	PPP	208	PGE	O2-C3-C4-O3
9	LLL	204	RWB	O34-C35-C36-O37
10	BBB	205	PE8	O10-C11-C12-O13
12	HHH	305	P33	O10-C11-C12-O13
12	HHH	306	P33	O7-C8-C9-O10
13	DDD	206	P6G	O13-C14-C15-O16
15	NNN	206	PE5	O7-C13-C14-O8
6	CCC	210	PEG	C4-C3-O2-C2
4	LLL	206	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
4	MMM	204	PG4	O3-C5-C6-O4
5	BBB	222	PGE	O2-C3-C4-O3
5	CCC	208	PGE	O2-C3-C4-O3
3	AAA	201	PEB	C2B-C1B-CHA-C4A
3	BBB	201	PEB	C2B-C1B-CHA-C4A
3	EEE	201	PEB	C2B-C1B-CHA-C4A
4	GGG	203	PG4	O2-C3-C4-O3
4	DDD	209	PG4	O2-C3-C4-O3
5	GGG	217	PGE	O2-C3-C4-O3
11	DDD	207	1PE	OH6-C15-C25-OH5
11	EEE	203	1PE	OH6-C15-C25-OH5
12	DDD	205	P33	O13-C14-C15-O16
4	DDD	208	PG4	O2-C3-C4-O3
4	FFF	209	PG4	O2-C3-C4-O3
4	FFF	210	PG4	O2-C3-C4-O3
4	PPP	207	PG4	O4-C7-C8-O5
5	DDD	211	PGE	O3-C5-C6-O4
5	EEE	204	PGE	O1-C1-C2-O2
5	GGG	206	PGE	O3-C5-C6-O4
5	MMM	206	PGE	O1-C1-C2-O2
6	GGG	212	PEG	O1-C1-C2-O2
12	HHH	305	P33	O19-C20-C21-O22
6	GGG	212	PEG	C1-C2-O2-C3
4	DDD	209	PG4	O3-C5-C6-O4
5	CCC	207	PGE	O2-C3-C4-O3
5	HHH	312	PGE	O2-C3-C4-O3
12	HHH	306	P33	O13-C14-C15-O16
9	BBB	204	RWB	C36-C35-O34-C33
4	DDD	208	PG4	O3-C5-C6-O4
5	FFF	212	PGE	O2-C3-C4-O3
5	FFF	213	PGE	O2-C3-C4-O3
11	JJJ	307	1PE	OH5-C14-C24-OH4
4	MMM	205	PG4	C6-C5-O3-C4
4	LLL	207	PG4	O2-C3-C4-O3
5	LLL	209	PGE	O2-C3-C4-O3
12	HHH	306	P33	O4-C5-C6-O7
9	BBB	204	RWB	O28-C29-C30-O31
12	DDD	204	P33	O16-C17-C18-O19
4	GGG	205	PG4	C1-C2-O2-C3
4	FFF	208	PG4	O2-C3-C4-O3
9	BBB	204	RWB	O4-C5-C6-O7
5	AAA	209	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
5	III	204	PGE	O2-C3-C4-O3
11	BBB	208	1PE	OH5-C14-C24-OH4
15	NNN	206	PE5	O3-C5-C6-O4
15	NNN	206	PE5	O4-C7-C8-O5
9	BBB	204	RWB	C33-C32-O31-C30
5	NNN	211	PGE	O2-C3-C4-O3
11	LLL	205	1PE	OH4-C13-C23-OH3
4	MMM	205	PG4	O2-C3-C4-O3
11	JJJ	307	1PE	OH6-C15-C25-OH5
12	DDD	204	P33	O13-C14-C15-O16
12	DDD	204	P33	O7-C8-C9-O10
12	DDD	205	P33	O7-C8-C9-O10
13	DDD	206	P6G	O10-C11-C12-O13
4	NNN	201	PG4	O3-C5-C6-O4
9	BBB	204	RWB	O22-C23-C24-O25
12	FFF	207	P33	O10-C11-C12-O13
4	OOO	203	PG4	O2-C3-C4-O3
9	BBB	204	RWB	O31-C32-C33-O34
12	JJJ	306	P33	O4-C5-C6-O7
4	FFF	202	PG4	C3-C4-O3-C5
5	AAA	208	PGE	C3-C4-O3-C5
5	FFF	213	PGE	C1-C2-O2-C3
6	BBB	213	PEG	C1-C2-O2-C3
4	NNN	209	PG4	O2-C3-C4-O3
5	III	207	PGE	O2-C3-C4-O3
11	JJJ	308	1PE	C14-C24-OH4-C13
9	LLL	204	RWB	O10-C11-C12-O13
12	HHH	306	P33	O16-C17-C18-O19
11	PPP	205	1PE	OH5-C14-C24-OH4
4	FFF	208	PG4	O4-C7-C8-O5
4	FFF	210	PG4	O1-C1-C2-O2
4	HHH	308	PG4	O1-C1-C2-O2
4	MMM	205	PG4	O4-C7-C8-O5
4	NNN	201	PG4	O4-C7-C8-O5
4	NNN	207	PG4	O4-C7-C8-O5
5	DDD	212	PGE	O1-C1-C2-O2
5	FFF	213	PGE	O3-C5-C6-O4
5	HHH	310	PGE	O3-C5-C6-O4
5	JJJ	310	PGE	O1-C1-C2-O2
5	LLL	225	PGE	O1-C1-C2-O2
6	BBB	215	PEG	O2-C3-C4-O4
6	GGG	213	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
6	HHH	314	PEG	O1-C1-C2-O2
6	KKK	212	PEG	O2-C3-C4-O4
6	NNN	215	PEG	O2-C3-C4-O4
6	OOO	210	PEG	O2-C3-C4-O4
6	PPP	209	PEG	O1-C1-C2-O2
6	PPP	209	PEG	O2-C3-C4-O4
9	LLL	204	RWB	O1-C2-C3-O4
13	DDD	206	P6G	O1-C2-C3-O4
11	BBB	208	1PE	OH6-C15-C25-OH5
4	AAA	205	PG4	O3-C5-C6-O4
11	BBB	206	1PE	OH6-C15-C25-OH5
4	PPP	206	PG4	O3-C5-C6-O4
5	NNN	210	PGE	O2-C3-C4-O3
3	JJJ	303	PEB	C2B-C1B-CHA-C4A
5	OOO	205	PGE	O2-C3-C4-O3
10	BBB	205	PE8	O4-C5-C6-O7
9	BBB	204	RWB	O19-C20-C21-O22
11	BBB	207	1PE	OH5-C14-C24-OH4
9	LLL	204	RWB	O13-C14-C15-O16
4	MMM	203	PG4	O3-C5-C6-O4
5	KKK	207	PGE	O2-C3-C4-O3
12	DDD	205	P33	O10-C11-C12-O13
5	CCC	204	PGE	O2-C3-C4-O3
4	AAA	204	PG4	O4-C7-C8-O5
4	CCC	203	PG4	O1-C1-C2-O2
4	FFF	202	PG4	O1-C1-C2-O2
4	MMM	203	PG4	O1-C1-C2-O2
4	MMM	204	PG4	O1-C1-C2-O2
4	NNN	207	PG4	O1-C1-C2-O2
4	NNN	208	PG4	O4-C7-C8-O5
4	PPP	207	PG4	O1-C1-C2-O2
5	AAA	208	PGE	O1-C1-C2-O2
5	AAA	208	PGE	O3-C5-C6-O4
5	AAA	209	PGE	O3-C5-C6-O4
5	BBB	222	PGE	O3-C5-C6-O4
5	DDD	212	PGE	O3-C5-C6-O4
5	GGG	217	PGE	O3-C5-C6-O4
5	HHH	309	PGE	O3-C5-C6-O4
5	HHH	310	PGE	O1-C1-C2-O2
5	HHH	311	PGE	O3-C5-C6-O4
5	HHH	312	PGE	O1-C1-C2-O2
5	III	205	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
5	III	206	PGE	O3-C5-C6-O4
5	KKK	206	PGE	O3-C5-C6-O4
5	LLL	225	PGE	O3-C5-C6-O4
5	MMM	206	PGE	O3-C5-C6-O4
5	MMM	207	PGE	O1-C1-C2-O2
5	NNN	210	PGE	O1-C1-C2-O2
5	NNN	212	PGE	O3-C5-C6-O4
6	AAA	213	PEG	O1-C1-C2-O2
6	DDD	213	PEG	O2-C3-C4-O4
6	DDD	214	PEG	O2-C3-C4-O4
6	FFF	217	PEG	O1-C1-C2-O2
6	FFF	217	PEG	O2-C3-C4-O4
6	HHH	317	PEG	O1-C1-C2-O2
6	HHH	318	PEG	O1-C1-C2-O2
6	III	211	PEG	O1-C1-C2-O2
6	JJJ	312	PEG	O1-C1-C2-O2
6	KKK	210	PEG	O1-C1-C2-O2
6	KKK	211	PEG	O2-C3-C4-O4
6	KKK	212	PEG	O1-C1-C2-O2
6	LLL	215	PEG	O1-C1-C2-O2
6	LLL	217	PEG	O1-C1-C2-O2
6	LLL	218[A]	PEG	O2-C3-C4-O4
6	MMM	210	PEG	O1-C1-C2-O2
6	NNN	215	PEG	O1-C1-C2-O2
6	OOO	208	PEG	O2-C3-C4-O4
6	PPP	212	PEG	O1-C1-C2-O2
11	HHH	301	1PE	OH2-C12-C22-OH3
4	CCC	203	PG4	O3-C5-C6-O4
5	EEE	207	PGE	O2-C3-C4-O3
11	DDD	207	1PE	OH4-C13-C23-OH3
6	LLL	215	PEG	C1-C2-O2-C3
12	HHH	305	P33	O4-C5-C6-O7
5	LLL	210	PGE	O2-C3-C4-O3
9	BBB	204	RWB	O34-C35-C36-O37
11	BBB	207	1PE	OH6-C15-C25-OH5
5	AAA	210	PGE	O2-C3-C4-O3
4	MMM	203	PG4	O2-C3-C4-O3
3	AAA	201	PEB	NB-C1B-CHA-C4A
3	EEE	201	PEB	NB-C1B-CHA-C4A
3	JJJ	303	PEB	NB-C1B-CHA-C4A
4	CCC	203	PG4	O2-C3-C4-O3
5	III	206	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
4	AAA	205	PG4	O1-C1-C2-O2
4	GGG	203	PG4	O4-C7-C8-O5
4	KKK	203	PG4	O1-C1-C2-O2
4	LLL	207	PG4	O1-C1-C2-O2
4	LLL	207	PG4	O4-C7-C8-O5
4	OOO	203	PG4	O4-C7-C8-O5
5	AAA	206	PGE	O1-C1-C2-O2
5	AAA	207	PGE	O3-C5-C6-O4
5	CCC	207	PGE	O3-C5-C6-O4
5	DDD	210	PGE	O1-C1-C2-O2
5	GGG	208	PGE	O3-C5-C6-O4
5	GGG	217	PGE	O1-C1-C2-O2
5	HHH	312	PGE	O3-C5-C6-O4
5	HHH	327	PGE	O3-C5-C6-O4
5	KKK	207	PGE	O3-C5-C6-O4
5	MMM	207	PGE	O3-C5-C6-O4
6	CCC	209	PEG	O2-C3-C4-O4
6	CCC	221	PEG	O1-C1-C2-O2
6	GGG	209	PEG	O1-C1-C2-O2
6	GGG	213	PEG	O1-C1-C2-O2
6	III	210	PEG	O1-C1-C2-O2
6	III	212	PEG	O1-C1-C2-O2
6	JJJ	312	PEG	O2-C3-C4-O4
6	JJJ	313	PEG	O2-C3-C4-O4
6	JJJ	314	PEG	O1-C1-C2-O2
6	KKK	209	PEG	O1-C1-C2-O2
6	LLL	213	PEG	O1-C1-C2-O2
6	LLL	218[B]	PEG	O1-C1-C2-O2
6	PPP	214	PEG	O2-C3-C4-O4
11	JJJ	302	1PE	OH7-C16-C26-OH6
11	PPP	205	1PE	OH2-C12-C22-OH3
12	FFF	207	P33	O19-C20-C21-O22
4	PPP	207	PG4	O2-C3-C4-O3
15	NNN	206	PE5	O2-C3-C4-O3
11	BBB	207	1PE	C16-C26-OH6-C15
5	III	205	PGE	O2-C3-C4-O3
12	HHH	306	P33	O10-C11-C12-O13
5	CCC	206	PGE	O2-C3-C4-O3
4	GGG	204	PG4	O2-C3-C4-O3
11	BBB	208	1PE	OH4-C13-C23-OH3
12	JJJ	306	P33	O16-C17-C18-O19
4	DDD	208	PG4	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	GGG	205	PG4	O4-C7-C8-O5
4	MMM	212	PG4	O1-C1-C2-O2
4	PPP	206	PG4	O4-C7-C8-O5
5	BBB	209	PGE	O1-C1-C2-O2
5	CCC	204	PGE	O1-C1-C2-O2
5	DDD	210	PGE	O3-C5-C6-O4
5	EEE	204	PGE	O3-C5-C6-O4
5	FFF	212	PGE	O1-C1-C2-O2
5	HHH	311	PGE	O1-C1-C2-O2
5	JJJ	311	PGE	O3-C5-C6-O4
5	NNN	213	PGE	O1-C1-C2-O2
5	NNN	213	PGE	O3-C5-C6-O4
6	BBB	214	PEG	O2-C3-C4-O4
6	CCC	210	PEG	O2-C3-C4-O4
6	CCC	213	PEG	O2-C3-C4-O4
6	EEE	213	PEG	O2-C3-C4-O4
6	FFF	216	PEG	O1-C1-C2-O2
6	III	201	PEG	O2-C3-C4-O4
6	JJJ	314	PEG	O2-C3-C4-O4
6	LLL	212	PEG	O2-C3-C4-O4
6	PPP	211	PEG	O1-C1-C2-O2
11	DDD	207	1PE	OH2-C12-C22-OH3
11	JJJ	302	1PE	OH2-C12-C22-OH3
11	JJJ	308	1PE	OH2-C12-C22-OH3
11	LLL	205	1PE	OH2-C12-C22-OH3
12	DDD	205	P33	O19-C20-C21-O22
5	III	204	PGE	C1-C2-O2-C3
14	DDD	217	EDO	O1-C1-C2-O2
14	PPP	215	EDO	O1-C1-C2-O2
4	MMM	204	PG4	O2-C3-C4-O3
3	PPP	204	PEB	C2B-C3B-CAB-CBB
3	NNN	203	PEB	C2C-CAC-CBC-CGC
11	FFF	201	1PE	OH6-C15-C25-OH5
12	DDD	205	P33	O16-C17-C18-O19
11	EEE	203	1PE	C14-C24-OH4-C13
9	LLL	204	RWB	O31-C32-C33-O34
4	KKK	203	PG4	O2-C3-C4-O3
4	KKK	203	PG4	O4-C7-C8-O5
5	CCC	207	PGE	O1-C1-C2-O2
5	EEE	205	PGE	O1-C1-C2-O2
5	EEE	206	PGE	O1-C1-C2-O2
5	JJJ	301	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	KKK	207	PGE	O1-C1-C2-O2
5	NNN	211	PGE	O1-C1-C2-O2
6	FFF	214	PEG	O2-C3-C4-O4
6	HHH	315	PEG	O1-C1-C2-O2
6	HHH	318	PEG	O2-C3-C4-O4
6	III	208	PEG	O1-C1-C2-O2
6	MMM	209	PEG	O1-C1-C2-O2
6	OOO	208	PEG	O1-C1-C2-O2
11	JJJ	308	1PE	OH7-C16-C26-OH6
11	PPP	205	1PE	OH7-C16-C26-OH6
12	DDD	204	P33	O19-C20-C21-O22
5	HHH	311	PGE	O2-C3-C4-O3
4	LLL	208	PG4	O3-C5-C6-O4
5	GGG	206	PGE	O2-C3-C4-O3
9	LLL	204	RWB	O7-C8-C9-O10
3	HHH	304	PEB	C2D-C3D-CAD-CBD
3	NNN	205	PEB	C2D-C3D-CAD-CBD
9	BBB	204	RWB	C6-C5-O4-C3
4	NNN	208	PG4	O3-C5-C6-O4
11	BBB	207	1PE	OH4-C13-C23-OH3
12	FFF	207	P33	O7-C8-C9-O10
5	HHH	310	PGE	C6-C5-O3-C4
11	PPP	205	1PE	OH4-C13-C23-OH3
9	LLL	204	RWB	O4-C5-C6-O7
11	JJJ	302	1PE	OH5-C14-C24-OH4
3	JJJ	303	PEB	NB-C4B-CHB-C1C
4	AAA	203	PG4	O4-C7-C8-O5
4	AAA	205	PG4	O4-C7-C8-O5
4	KKK	204	PG4	O4-C7-C8-O5
4	LLL	206	PG4	O4-C7-C8-O5
4	NNN	209	PG4	O1-C1-C2-O2
4	PPP	206	PG4	O1-C1-C2-O2
5	CCC	206	PGE	O1-C1-C2-O2
5	CCC	208	PGE	O1-C1-C2-O2
5	HHH	309	PGE	O1-C1-C2-O2
5	III	204	PGE	O1-C1-C2-O2
5	III	206	PGE	O1-C1-C2-O2
5	JJJ	310	PGE	O3-C5-C6-O4
5	LLL	209	PGE	O3-C5-C6-O4
6	AAA	212	PEG	O1-C1-C2-O2
6	BBB	211	PEG	O2-C3-C4-O4
6	BBB	212	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	BBB	216	PEG	O1-C1-C2-O2
6	CCC	210	PEG	O1-C1-C2-O2
6	CCC	211	PEG	O1-C1-C2-O2
6	CCC	221	PEG	O2-C3-C4-O4
6	DDD	215	PEG	O1-C1-C2-O2
6	FFF	215	PEG	O1-C1-C2-O2
6	III	209	PEG	O2-C3-C4-O4
6	KKK	208	PEG	O2-C3-C4-O4
6	LLL	214	PEG	O1-C1-C2-O2
6	LLL	216	PEG	O2-C3-C4-O4
6	LLL	218[B]	PEG	O2-C3-C4-O4
6	OOO	209	PEG	O1-C1-C2-O2
11	BBB	207	1PE	OH7-C16-C26-OH6
13	DDD	206	P6G	O16-C17-C18-O19
4	MMM	212	PG4	O3-C5-C6-O4
5	DDD	211	PGE	O2-C3-C4-O3
5	HHH	327	PGE	O2-C3-C4-O3
5	MMM	206	PGE	O2-C3-C4-O3
6	LLL	214	PEG	C4-C3-O2-C2
11	LLL	205	1PE	OH6-C15-C25-OH5
4	LLL	208	PG4	C6-C5-O3-C4
11	JJJ	302	1PE	OH4-C13-C23-OH3
3	PPP	204	PEB	C4B-C3B-CAB-CBB
5	AAA	209	PGE	O1-C1-C2-O2
6	CCC	212	PEG	O1-C1-C2-O2
6	HHH	316	PEG	O2-C3-C4-O4
6	LLL	217	PEG	O2-C3-C4-O4
11	EEE	203	1PE	OH7-C16-C26-OH6
14	NNN	218	EDO	O1-C1-C2-O2
10	BBB	205	PE8	O13-C14-C15-O16
11	HHH	301	1PE	OH4-C13-C23-OH3
5	DDD	212	PGE	O2-C3-C4-O3
5	DDD	211	PGE	C1-C2-O2-C3
5	EEE	207	PGE	C4-C3-O2-C2
4	KKK	205	PG4	O1-C1-C2-O2
5	OOO	204	PGE	O1-C1-C2-O2
5	BBB	210	PGE	C1-C2-O2-C3
5	PPP	208	PGE	C1-C2-O2-C3
6	DDD	214	PEG	C4-C3-O2-C2
4	FFF	202	PG4	O2-C3-C4-O3
5	OOO	204	PGE	O2-C3-C4-O3
4	FFF	210	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
3	CCC	202	PEB	C4B-C3B-CAB-CBB
6	III	211	PEG	C4-C3-O2-C2
4	MMM	212	PG4	O4-C7-C8-O5
5	III	207	PGE	O3-C5-C6-O4
6	CCC	213	PEG	O1-C1-C2-O2
12	JJJ	306	P33	O1-C2-C3-O4
4	FFF	209	PG4	O3-C5-C6-O4
4	MMM	212	PG4	O2-C3-C4-O3
15	NNN	206	PE5	C48-C50-O1-C1
4	KKK	204	PG4	O3-C5-C6-O4
4	AAA	204	PG4	O3-C5-C6-O4
5	OOO	206	PGE	O2-C3-C4-O3
4	KKK	204	PG4	O2-C3-C4-O3
5	BBB	210	PGE	O2-C3-C4-O3
6	BBB	214	PEG	O1-C1-C2-O2
6	LLL	213	PEG	O2-C3-C4-O4
6	MMM	209	PEG	O2-C3-C4-O4
11	EEE	203	1PE	OH5-C14-C24-OH4
3	JJJ	303	PEB	NC-C1C-CHB-C4B
14	EEE	208	EDO	O1-C1-C2-O2
14	EEE	209	EDO	O1-C1-C2-O2
14	III	213	EDO	O1-C1-C2-O2
3	NNN	205	PEB	C3B-CAB-CBB-CGB
4	HHH	307	PG4	O2-C3-C4-O3
5	AAA	211	PGE	O2-C3-C4-O3
4	GGG	205	PG4	O1-C1-C2-O2
6	HHH	317	PEG	O2-C3-C4-O4
5	AAA	206	PGE	O2-C3-C4-O3
12	HHH	305	P33	O13-C14-C15-O16
12	HHH	306	P33	C17-C18-O19-C20
5	CCC	208	PGE	C4-C3-O2-C2
11	JJJ	308	1PE	C25-C15-OH6-C26
4	KKK	205	PG4	O3-C5-C6-O4
5	LLL	226	PGE	C3-C4-O3-C5
6	PPP	209	PEG	C4-C3-O2-C2
3	BBB	203	PEB	C4D-C3D-CAD-CBD
3	FFF	206	PEB	C4D-C3D-CAD-CBD
3	HHH	304	PEB	C4D-C3D-CAD-CBD
3	LLL	203	PEB	C4D-C3D-CAD-CBD
3	OOO	201	PEB	C4D-C3D-CAD-CBD
3	LLL	203	PEB	C2B-C3B-CAB-CBB
4	KKK	205	PG4	C5-C6-O4-C7

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Mol	Chain	Res	Type	Atoms
3	BBB	203	PEB	C4A-C3A-CAA-CBA
3	CCC	202	PEB	C4A-C3A-CAA-CBA
3	EEE	202	PEB	C4A-C3A-CAA-CBA
3	NNN	204	PEB	C4A-C3A-CAA-CBA
5	KKK	206	PGE	O2-C3-C4-O3
9	LLL	204	RWB	O16-C17-C18-O19
4	NNN	207	PG4	C3-C4-O3-C5
4	NNN	208	PG4	C5-C6-O4-C7
4	NNN	209	PG4	C4-C3-O2-C2
6	III	212	PEG	C1-C2-O2-C3
6	PPP	213	PEG	C1-C2-O2-C3
4	KKK	204	PG4	C8-C7-O4-C6
15	NNN	206	PE5	C3-C4-O3-C5
3	LLL	201	PEB	NC-C1C-CHB-C4B
3	NNN	203	PEB	NC-C1C-CHB-C4B
4	HHH	307	PG4	O1-C1-C2-O2
5	JJJ	301	PGE	O3-C5-C6-O4
5	NNN	211	PGE	O3-C5-C6-O4
6	DDD	216	PEG	O1-C1-C2-O2
6	JJJ	313	PEG	O1-C1-C2-O2
6	OOO	207	PEG	O1-C1-C2-O2
4	DDD	208	PG4	C5-C6-O4-C7
4	HHH	307	PG4	C5-C6-O4-C7
5	DDD	212	PGE	C6-C5-O3-C4
11	JJJ	302	1PE	C12-C22-OH3-C23
5	HHH	309	PGE	O2-C3-C4-O3
4	AAA	203	PG4	C5-C6-O4-C7
4	GGG	204	PG4	C3-C4-O3-C5
4	NNN	201	PG4	C5-C6-O4-C7
5	LLL	226	PGE	C6-C5-O3-C4
6	FFF	218	PEG	C1-C2-O2-C3
6	LLL	213	PEG	C4-C3-O2-C2
6	PPP	212	PEG	C1-C2-O2-C3
6	KKK	211	PEG	C1-C2-O2-C3
6	PPP	213	PEG	C4-C3-O2-C2
5	AAA	209	PGE	C3-C4-O3-C5
4	NNN	202	PG4	C1-C2-O2-C3
4	NNN	207	PG4	C6-C5-O3-C4
5	DDD	210	PGE	C6-C5-O3-C4
5	EEE	206	PGE	C6-C5-O3-C4
6	LLL	218[B]	PEG	C4-C3-O2-C2
9	BBB	204	RWB	O7-C8-C9-O10

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Mol	Chain	Res	Type	Atoms
5	GGG	206	PGE	C3-C4-O3-C5
6	CCC	213	PEG	C4-C3-O2-C2
6	LLL	212	PEG	C1-C2-O2-C3
11	HHH	301	1PE	C13-C23-OH3-C22
4	FFF	209	PG4	C5-C6-O4-C7
6	CCC	221	PEG	C1-C2-O2-C3
11	FFF	201	1PE	C12-C22-OH3-C23
3	DDD	201	PEB	C2C-CAC-CBC-CGC
4	LLL	208	PG4	O2-C3-C4-O3
4	GGG	203	PG4	C8-C7-O4-C6
4	PPP	207	PG4	C4-C3-O2-C2
5	HHH	310	PGE	C4-C3-O2-C2
5	III	206	PGE	C3-C4-O3-C5
6	EEE	212	PEG	C4-C3-O2-C2
6	FFF	214	PEG	C1-C2-O2-C3
6	OOO	209	PEG	C4-C3-O2-C2
9	BBB	204	RWB	C24-C23-O22-C21
11	BBB	208	1PE	C14-C24-OH4-C13
12	DDD	204	P33	C8-C9-O10-C11
12	FFF	207	P33	C21-C20-O19-C18
4	MMM	203	PG4	C4-C3-O2-C2
5	JJJ	301	PGE	C3-C4-O3-C5
6	CCC	219	PEG	C1-C2-O2-C3
11	PPP	205	1PE	C23-C13-OH4-C24
12	HHH	306	P33	C5-C6-O7-C8
4	MMM	205	PG4	C4-C3-O2-C2
5	BBB	209	PGE	C3-C4-O3-C5
5	NNN	211	PGE	C1-C2-O2-C3
6	GGG	209	PEG	C1-C2-O2-C3
11	DDD	207	1PE	C14-C24-OH4-C13
4	CCC	203	PG4	C4-C3-O2-C2
4	GGG	205	PG4	C8-C7-O4-C6
5	BBB	210	PGE	C3-C4-O3-C5
5	HHH	311	PGE	C4-C3-O2-C2
5	III	204	PGE	C6-C5-O3-C4
6	FFF	216	PEG	C1-C2-O2-C3
11	BBB	207	1PE	C12-C22-OH3-C23
11	DDD	207	1PE	C23-C13-OH4-C24
5	OOO	204	PGE	C1-C2-O2-C3
4	JJJ	309	PG4	C1-C2-O2-C3
4	MMM	203	PG4	C5-C6-O4-C7
4	NNN	209	PG4	C8-C7-O4-C6

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Mol	Chain	Res	Type	Atoms
5	CCC	208	PGE	C6-C5-O3-C4
5	HHH	313	PGE	C3-C4-O3-C5
5	III	204	PGE	C4-C3-O2-C2
6	CCC	221	PEG	C4-C3-O2-C2
9	BBB	204	RWB	C23-C24-O25-C26
15	NNN	206	PE5	C9-C10-O6-C11
4	MMM	203	PG4	C1-C2-O2-C3
5	OOO	205	PGE	C1-C2-O2-C3
11	JJJ	308	1PE	C16-C26-OH6-C15
5	AAA	211	PGE	C3-C4-O3-C5
4	LLL	206	PG4	O1-C1-C2-O2
5	AAA	210	PGE	O3-C5-C6-O4
5	EEE	207	PGE	O3-C5-C6-O4
5	FFF	213	PGE	O1-C1-C2-O2
5	GGG	207	PGE	O1-C1-C2-O2
6	BBB	213	PEG	O2-C3-C4-O4
6	CCC	219	PEG	O2-C3-C4-O4
6	EEE	213	PEG	O1-C1-C2-O2
6	HHH	314	PEG	O2-C3-C4-O4
6	MMM	208	PEG	O2-C3-C4-O4
6	PPP	210	PEG	O1-C1-C2-O2
12	JJJ	306	P33	O19-C20-C21-O22
5	MMM	207	PGE	C6-C5-O3-C4
4	PPP	206	PG4	C8-C7-O4-C6
11	EEE	203	1PE	C25-C15-OH6-C26
12	JJJ	306	P33	C17-C18-O19-C20
3	III	202	PEB	NA-C4A-CHA-C1B
3	NNN	203	PEB	NA-C4A-CHA-C1B
5	FFF	213	PGE	C3-C4-O3-C5
12	HHH	306	P33	C14-C15-O16-C17
13	DDD	206	P6G	C6-C5-O4-C3
6	III	208	PEG	C1-C2-O2-C3
9	LLL	204	RWB	C9-C8-O7-C6
4	HHH	307	PG4	C8-C7-O4-C6
4	MMM	212	PG4	C4-C3-O2-C2
5	GGG	208	PGE	C3-C4-O3-C5
4	OOO	203	PG4	C4-C3-O2-C2
5	LLL	209	PGE	C4-C3-O2-C2
13	DDD	206	P6G	C15-C14-O13-C12
4	LLL	207	PG4	C1-C2-O2-C3
5	BBB	222	PGE	C1-C2-O2-C3
5	FFF	211	PGE	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
6	PPP	211	PEG	C4-C3-O2-C2
4	MMM	205	PG4	C3-C4-O3-C5
5	III	205	PGE	C4-C3-O2-C2
6	FFF	218	PEG	C4-C3-O2-C2
6	LLL	218[A]	PEG	C4-C3-O2-C2
4	GGG	204	PG4	C1-C2-O2-C3
6	DDD	214	PEG	C1-C2-O2-C3
6	OOO	210	PEG	C1-C2-O2-C3
4	LLL	208	PG4	C3-C4-O3-C5
6	FFF	217	PEG	C4-C3-O2-C2
6	GGG	211	PEG	C4-C3-O2-C2
3	PPP	203	PEB	C2C-CAC-CBC-CGC
4	AAA	203	PG4	O1-C1-C2-O2
5	AAA	207	PGE	O1-C1-C2-O2
4	LLL	207	PG4	C8-C7-O4-C6
5	NNN	210	PGE	C1-C2-O2-C3
6	FFF	215	PEG	C1-C2-O2-C3
5	CCC	204	PGE	C3-C4-O3-C5
5	OOO	206	PGE	C1-C2-O2-C3
12	FFF	207	P33	O13-C14-C15-O16
5	GGG	217	PGE	C1-C2-O2-C3
4	AAA	203	PG4	O3-C5-C6-O4
4	FFF	202	PG4	C8-C7-O4-C6
4	GGG	205	PG4	C4-C3-O2-C2
6	MMM	209	PEG	C1-C2-O2-C3
5	PPP	208	PGE	C4-C3-O2-C2
9	BBB	204	RWB	C17-C18-O19-C20
9	BBB	204	RWB	C8-C9-O10-C11
5	CCC	206	PGE	C4-C3-O2-C2
6	KKK	209	PEG	C1-C2-O2-C3
4	DDD	209	PG4	O4-C7-C8-O5
4	MMM	204	PG4	O4-C7-C8-O5
4	NNN	202	PG4	O4-C7-C8-O5
5	FFF	211	PGE	O1-C1-C2-O2
6	BBB	215	PEG	O1-C1-C2-O2
6	DDD	227	PEG	O1-C1-C2-O2
6	DDD	227	PEG	O2-C3-C4-O4
6	MMM	210	PEG	O2-C3-C4-O4
6	NNN	216	PEG	O2-C3-C4-O4
11	BBB	207	1PE	C15-C25-OH5-C14
15	NNN	206	PE5	C6-C5-O3-C4
11	EEE	203	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
3	JJJ	303	PEB	C3B-C4B-CHB-C1C
5	LLL	225	PGE	O2-C3-C4-O3
4	FFF	209	PG4	C3-C4-O3-C5
5	III	206	PGE	C1-C2-O2-C3
9	LLL	204	RWB	C17-C18-O19-C20
5	BBB	209	PGE	C6-C5-O3-C4
5	III	207	PGE	C1-C2-O2-C3
12	DDD	205	P33	C21-C20-O19-C18
3	LLL	201	PEB	NB-C4B-CHB-C1C
6	LLL	211	PEG	C1-C2-O2-C3
5	GGG	206	PGE	C4-C3-O2-C2
6	BBB	214	PEG	C1-C2-O2-C3
12	DDD	205	P33	C8-C9-O10-C11
6	HHH	317	PEG	C1-C2-O2-C3
12	FFF	207	P33	C8-C9-O10-C11
4	FFF	202	PG4	C6-C5-O3-C4
4	NNN	208	PG4	C3-C4-O3-C5
4	NNN	208	PG4	C6-C5-O3-C4
6	NNN	214	PEG	C4-C3-O2-C2
5	EEE	207	PGE	O1-C1-C2-O2
6	BBB	212	PEG	O2-C3-C4-O4
6	BBB	216	PEG	O2-C3-C4-O4
6	DDD	215	PEG	O2-C3-C4-O4
11	BBB	206	1PE	OH7-C16-C26-OH6
5	JJJ	311	PGE	C4-C3-O2-C2
4	KKK	203	PG4	O3-C5-C6-O4
5	LLL	226	PGE	C4-C3-O2-C2
11	PPP	205	1PE	C25-C15-OH6-C26
14	LLL	219	EDO	O1-C1-C2-O2
5	GGG	217	PGE	C6-C5-O3-C4
11	EEE	203	1PE	C15-C25-OH5-C14
5	AAA	209	PGE	C4-C3-O2-C2
5	DDD	211	PGE	C6-C5-O3-C4
5	HHH	312	PGE	C6-C5-O3-C4
5	NNN	210	PGE	C3-C4-O3-C5
5	DDD	211	PGE	C4-C3-O2-C2
5	GGG	206	PGE	O1-C1-C2-O2
6	HHH	315	PEG	O2-C3-C4-O4
6	LLL	218[A]	PEG	O1-C1-C2-O2
4	DDD	208	PG4	C4-C3-O2-C2
4	FFF	209	PG4	C1-C2-O2-C3
6	FFF	214	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
4	NNN	202	PG4	C3-C4-O3-C5
5	KKK	206	PGE	C6-C5-O3-C4
12	HHH	305	P33	C21-C20-O19-C18
5	FFF	211	PGE	C4-C3-O2-C2
5	JJJ	311	PGE	C3-C4-O3-C5
5	HHH	309	PGE	C1-C2-O2-C3
11	BBB	207	1PE	C24-C14-OH5-C25
6	OOO	208	PEG	C1-C2-O2-C3
6	III	210	PEG	C4-C3-O2-C2
4	LLL	208	PG4	O1-C1-C2-O2
4	NNN	208	PG4	O1-C1-C2-O2
6	CCC	211	PEG	O2-C3-C4-O4
3	JJJ	305	PEB	C4D-C3D-CAD-CBD
3	NNN	205	PEB	C4D-C3D-CAD-CBD
4	CCC	203	PG4	C8-C7-O4-C6
6	HHH	315	PEG	C4-C3-O2-C2
4	GGG	203	PG4	C3-C4-O3-C5
5	NNN	210	PGE	C6-C5-O3-C4
11	JJJ	307	1PE	C13-C23-OH3-C22
12	DDD	204	P33	C11-C12-O13-C14
11	BBB	208	1PE	C23-C13-OH4-C24
4	FFF	208	PG4	C4-C3-O2-C2
5	LLL	210	PGE	C4-C3-O2-C2
10	BBB	205	PE8	C9-C8-O7-C6
11	BBB	207	1PE	C25-C15-OH6-C26
15	NNN	206	PE5	C4-C3-O2-C2
5	EEE	204	PGE	O2-C3-C4-O3
6	EEE	213	PEG	C1-C2-O2-C3
6	JJJ	313	PEG	C4-C3-O2-C2
6	LLL	217	PEG	C1-C2-O2-C3
6	NNN	214	PEG	C1-C2-O2-C3
9	LLL	204	RWB	C2-C3-O4-C5
5	BBB	222	PGE	C6-C5-O3-C4
5	DDD	210	PGE	C3-C4-O3-C5
9	BBB	204	RWB	C35-C36-O37-C38
11	JJJ	308	1PE	C15-C25-OH5-C14
4	GGG	203	PG4	O3-C5-C6-O4
3	DDD	201	PEB	NC-C1C-CHB-C4B
5	JJJ	301	PGE	C1-C2-O2-C3
6	FFF	218	PEG	O1-C1-C2-O2
11	BBB	207	1PE	OH2-C12-C22-OH3
4	PPP	206	PG4	C5-C6-O4-C7

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Mol	Chain	Res	Type	Atoms
6	III	212	PEG	C4-C3-O2-C2
9	LLL	204	RWB	C23-C24-O25-C26
12	DDD	205	P33	C9-C8-O7-C6
4	KKK	203	PG4	C6-C5-O3-C4
5	AAA	207	PGE	O2-C3-C4-O3
5	AAA	208	PGE	O2-C3-C4-O3
5	EEE	204	PGE	C1-C2-O2-C3
11	BBB	206	1PE	OH5-C14-C24-OH4
4	NNN	202	PG4	C4-C3-O2-C2
5	EEE	205	PGE	C6-C5-O3-C4
14	III	217	EDO	O1-C1-C2-O2
13	DDD	206	P6G	O4-C5-C6-O7
5	EEE	206	PGE	O2-C3-C4-O3
5	BBB	209	PGE	C1-C2-O2-C3
4	FFF	209	PG4	O4-C7-C8-O5
10	BBB	205	PE8	C5-C6-O7-C8
9	LLL	204	RWB	C35-C36-O37-C38
4	OOO	203	PG4	C5-C6-O4-C7
11	JJJ	307	1PE	C16-C26-OH6-C15
6	BBB	213	PEG	C4-C3-O2-C2
12	JJJ	306	P33	O7-C8-C9-O10
6	JJJ	312	PEG	C4-C3-O2-C2
4	MMM	205	PG4	O3-C5-C6-O4
5	NNN	213	PGE	O2-C3-C4-O3
4	NNN	207	PG4	C1-C2-O2-C3
6	BBB	216	PEG	C1-C2-O2-C3
6	OOO	208	PEG	C4-C3-O2-C2
5	CCC	207	PGE	C3-C4-O3-C5
9	BBB	204	RWB	O25-C26-C27-O28
6	CCC	210	PEG	C1-C2-O2-C3
11	BBB	206	1PE	C25-C15-OH6-C26
6	BBB	211	PEG	C4-C3-O2-C2
5	OOO	206	PGE	O3-C5-C6-O4
6	HHH	316	PEG	O1-C1-C2-O2
6	III	212	PEG	O2-C3-C4-O4
4	NNN	202	PG4	O3-C5-C6-O4
3	CCC	202	PEB	CAC-CBC-CGC-O2C
5	AAA	207	PGE	C1-C2-O2-C3
5	HHH	311	PGE	C6-C5-O3-C4
5	LLL	226	PGE	O2-C3-C4-O3
3	BBB	201	PEB	CAC-CBC-CGC-O1C
3	GGG	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
3	KKK	202	PEB	CAB-CBB-CGB-O2B
3	MMM	202	PEB	CAC-CBC-CGC-O1C
4	MMM	204	PG4	C4-C3-O2-C2
5	AAA	210	PGE	C4-C3-O2-C2
3	KKK	201	PEB	CAC-CBC-CGC-O1C
3	KKK	202	PEB	CAB-CBB-CGB-O1B
3	OOO	202	PEB	CAC-CBC-CGC-O1C
12	FFF	207	P33	C18-C17-O16-C15
11	BBB	208	1PE	C13-C23-OH3-C22
11	JJJ	307	1PE	C23-C13-OH4-C24
11	PPP	205	1PE	C13-C23-OH3-C22
4	MMM	204	PG4	C5-C6-O4-C7
12	DDD	205	P33	C15-C14-O13-C12
13	DDD	206	P6G	C14-C15-O16-C17
5	III	207	PGE	C4-C3-O2-C2
4	DDD	208	PG4	C8-C7-O4-C6
3	AAA	202	PEB	CAC-CBC-CGC-O1C
3	DDD	202	PEB	CAB-CBB-CGB-O1B
3	FFF	204	PEB	CAB-CBB-CGB-O2B
3	JJJ	303	PEB	CAB-CBB-CGB-O2B
3	MMM	201	PEB	CAC-CBC-CGC-O1C
3	BBB	201	PEB	NB-C4B-CHB-C1C
4	NNN	202	PG4	C6-C5-O3-C4
5	LLL	209	PGE	C6-C5-O3-C4
5	MMM	206	PGE	C4-C3-O2-C2
11	HHH	301	1PE	C12-C22-OH3-C23
4	HHH	308	PG4	C6-C5-O3-C4
6	LLL	216	PEG	C1-C2-O2-C3
3	BBB	202	PEB	CAB-CBB-CGB-O1B
3	BBB	202	PEB	CAB-CBB-CGB-O2B
3	DDD	201	PEB	CAB-CBB-CGB-O1B
3	FFF	204	PEB	CAC-CBC-CGC-O1C
3	III	202	PEB	CAC-CBC-CGC-O1C
5	CCC	207	PGE	C6-C5-O3-C4
5	OOO	204	PGE	C4-C3-O2-C2
3	CCC	201	PEB	CAC-CBC-CGC-O1C
3	CCC	202	PEB	CAC-CBC-CGC-O1C
3	EEE	201	PEB	CAC-CBC-CGC-O2C
3	FFF	204	PEB	CAB-CBB-CGB-O1B
3	III	203	PEB	CAC-CBC-CGC-O1C
3	JJJ	304	PEB	CAB-CBB-CGB-O1B
3	LLL	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
3	NNN	203	PEB	CAC-CBC-CGC-O1C
3	BBB	201	PEB	NC-C1C-CHB-C4B
4	CCC	203	PG4	C3-C4-O3-C5
11	DDD	207	1PE	C16-C26-OH6-C15
3	DDD	202	PEB	CAB-CBB-CGB-O2B
3	FFF	205	PEB	CAC-CBC-CGC-O1C
3	LLL	202	PEB	CAB-CBB-CGB-O2B
14	HHH	319	EDO	O1-C1-C2-O2
14	NNN	217	EDO	O1-C1-C2-O2
4	KKK	205	PG4	C8-C7-O4-C6
4	AAA	205	PG4	C8-C7-O4-C6
3	HHH	302	PEB	CAC-CBC-CGC-O1C
3	KKK	201	PEB	CAC-CBC-CGC-O2C
3	LLL	201	PEB	CAB-CBB-CGB-O1B
3	MMM	202	PEB	CAC-CBC-CGC-O2C
3	AAA	201	PEB	CAC-CBC-CGC-O1C
3	HHH	302	PEB	CAC-CBC-CGC-O2C
3	NNN	204	PEB	CAB-CBB-CGB-O1B
3	OOO	202	PEB	CAC-CBC-CGC-O2C
4	HHH	307	PG4	C3-C4-O3-C5
4	KKK	203	PG4	C4-C3-O2-C2
3	BBB	201	PEB	CAB-CBB-CGB-O2B
3	DDD	201	PEB	CAB-CBB-CGB-O2B
3	III	203	PEB	CAC-CBC-CGC-O2C
3	JJJ	303	PEB	CAB-CBB-CGB-O1B
3	NNN	203	PEB	CAC-CBC-CGC-O2C
3	OOO	201	PEB	CAC-CBC-CGC-O1C
3	OOO	201	PEB	CAC-CBC-CGC-O2C
4	DDD	209	PG4	C6-C5-O3-C4
6	LLL	218[A]	PEG	C1-C2-O2-C3
3	BBB	201	PEB	CAB-CBB-CGB-O1B
3	CCC	202	PEB	CAB-CBB-CGB-O2B
3	HHH	302	PEB	CAB-CBB-CGB-O1B
3	JJJ	304	PEB	CAC-CBC-CGC-O1C
3	LLL	202	PEB	CAB-CBB-CGB-O1B
12	JJJ	306	P33	C9-C8-O7-C6
3	BBB	201	PEB	CAC-CBC-CGC-O2C
3	CCC	201	PEB	CAC-CBC-CGC-O2C
3	FFF	205	PEB	CAB-CBB-CGB-O1B
3	LLL	202	PEB	CAC-CBC-CGC-O2C
3	MMM	201	PEB	CAC-CBC-CGC-O2C
3	NNN	203	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
12	DDD	204	P33	C2-C3-O4-C5
3	DDD	202	PEB	CAC-CBC-CGC-O1C
3	GGG	202	PEB	CAC-CBC-CGC-O2C
3	PPP	203	PEB	CAB-CBB-CGB-O1B
3	NNN	204	PEB	C2A-C3A-CAA-CBA
4	GGG	205	PG4	C6-C5-O3-C4
4	PPP	206	PG4	C6-C5-O3-C4
11	PPP	205	1PE	C24-C14-OH5-C25
3	AAA	202	PEB	CAC-CBC-CGC-O2C
3	HHH	303	PEB	CAC-CBC-CGC-O1C
3	HHH	303	PEB	CAB-CBB-CGB-O1B
3	JJJ	304	PEB	CAB-CBB-CGB-O2B
13	DDD	206	P6G	C2-C3-O4-C5
6	KKK	209	PEG	O2-C3-C4-O4
3	FFF	204	PEB	CAC-CBC-CGC-O2C
3	MMM	202	PEB	CAB-CBB-CGB-O2B
9	LLL	204	RWB	O19-C20-C21-O22
3	III	202	PEB	CAC-CBC-CGC-O2C
5	EEE	205	PGE	O2-C3-C4-O3
3	AAA	201	PEB	CAC-CBC-CGC-O2C
3	KKK	202	PEB	CAC-CBC-CGC-O2C
3	PPP	202	PEB	CAB-CBB-CGB-O1B
5	OOO	204	PGE	C3-C4-O3-C5
3	NNN	204	PEB	CAB-CBB-CGB-O2B
4	FFF	208	PG4	C6-C5-O3-C4
11	JJJ	302	1PE	C13-C23-OH3-C22
3	DDD	202	PEB	CAC-CBC-CGC-O2C
5	HHH	311	PGE	C3-C4-O3-C5
4	KKK	203	PG4	C8-C7-O4-C6
6	III	211	PEG	C1-C2-O2-C3
6	NNN	215	PEG	C4-C3-O2-C2
4	MMM	203	PG4	O4-C7-C8-O5
6	PPP	201	PEG	O2-C3-C4-O4
3	JJJ	304	PEB	CAC-CBC-CGC-O2C
3	KKK	202	PEB	C3B-CAB-CBB-CGB
3	LLL	201	PEB	C3B-C4B-CHB-C1C
11	BBB	207	1PE	C14-C24-OH4-C13
3	FFF	205	PEB	CAB-CBB-CGB-O2B
3	HHH	303	PEB	CAB-CBB-CGB-O2B
3	LLL	201	PEB	CAB-CBB-CGB-O2B
3	NNN	203	PEB	CAB-CBB-CGB-O2B
3	PPP	203	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
3	HHH	303	PEB	C4A-C3A-CAA-CBA
3	JJJ	304	PEB	C4A-C3A-CAA-CBA
3	LLL	202	PEB	C4A-C3A-CAA-CBA
3	NNN	205	PEB	C4A-C3A-CAA-CBA
5	EEE	207	PGE	C3-C4-O3-C5
11	HHH	301	1PE	C24-C14-OH5-C25
3	AAA	202	PEB	CAB-CBB-CGB-O2B
3	III	203	PEB	CAB-CBB-CGB-O2B
4	FFF	202	PG4	C1-C2-O2-C3
4	AAA	203	PG4	C3-C4-O3-C5
3	PPP	202	PEB	CAB-CBB-CGB-O2B
5	AAA	211	PGE	C4-C3-O2-C2
5	JJJ	311	PGE	O2-C3-C4-O3
13	DDD	206	P6G	C18-C17-O16-C15
3	HHH	302	PEB	CAB-CBB-CGB-O2B
3	HHH	303	PEB	CAC-CBC-CGC-O2C
3	LLL	201	PEB	CAC-CBC-CGC-O2C
3	MMM	202	PEB	CAB-CBB-CGB-O1B
4	PPP	207	PG4	C8-C7-O4-C6
5	CCC	204	PGE	C6-C5-O3-C4
11	PPP	205	1PE	OH6-C15-C25-OH5
3	BBB	202	PEB	CAC-CBC-CGC-O1C
3	OOO	202	PEB	CAB-CBB-CGB-O2B
5	LLL	210	PGE	O1-C1-C2-O2
5	OOO	205	PGE	O3-C5-C6-O4
6	NNN	214	PEG	O1-C1-C2-O2
5	HHH	310	PGE	C1-C2-O2-C3
12	FFF	207	P33	C17-C18-O19-C20
5	NNN	213	PGE	C6-C5-O3-C4
6	HHH	315	PEG	C1-C2-O2-C3
3	EEE	202	PEB	CAC-CBC-CGC-O1C
3	PPP	202	PEB	CAC-CBC-CGC-O2C
5	III	207	PGE	C6-C5-O3-C4
5	JJJ	311	PGE	C1-C2-O2-C3
3	EEE	201	PEB	CAC-CBC-CGC-O1C
4	GGG	203	PG4	C6-C5-O3-C4
11	JJJ	302	1PE	C14-C24-OH4-C13
5	EEE	207	PGE	C1-C2-O2-C3
6	JJJ	314	PEG	C4-C3-O2-C2
3	GGG	201	PEB	CAC-CBC-CGC-O2C
3	JJJ	303	PEB	CAC-CBC-CGC-O2C
3	FFF	205	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
3	GGG	201	PEB	CAC-CBC-CGC-O1C
5	OOO	206	PGE	C3-C4-O3-C5
3	PPP	202	PEB	CAC-CBC-CGC-O1C
6	PPP	201	PEG	O1-C1-C2-O2
15	NNN	206	PE5	O1-C1-C2-O2
3	EEE	202	PEB	CAC-CBC-CGC-O2C
13	DDD	206	P6G	O7-C8-C9-O10
3	OOO	202	PEB	CAB-CBB-CGB-O1B
4	GGG	203	PG4	C5-C6-O4-C7
5	HHH	312	PGE	C4-C3-O2-C2
5	MMM	207	PGE	C1-C2-O2-C3
4	AAA	205	PG4	C5-C6-O4-C7
5	AAA	209	PGE	C1-C2-O2-C3
3	GGG	202	PEB	CAB-CBB-CGB-O2B
10	BBB	205	PE8	C2-C3-O4-C5
12	DDD	205	P33	C11-C12-O13-C14
3	LLL	203	PEB	C4B-C3B-CAB-CBB
3	CCC	202	PEB	CAB-CBB-CGB-O1B
3	KKK	202	PEB	CAC-CBC-CGC-O1C
9	LLL	204	RWB	C29-C30-O31-C32
12	DDD	204	P33	O4-C5-C6-O7
3	III	203	PEB	CAB-CBB-CGB-O1B
5	NNN	211	PGE	C6-C5-O3-C4
6	BBB	212	PEG	C1-C2-O2-C3
3	JJJ	303	PEB	CAC-CBC-CGC-O1C
3	PPP	202	PEB	NB-C4B-CHB-C1C
3	EEE	201	PEB	CAB-CBB-CGB-O1B
3	GGG	202	PEB	CAB-CBB-CGB-O1B
5	NNN	212	PGE	C1-C2-O2-C3
5	HHH	313	PGE	C6-C5-O3-C4
5	OOO	206	PGE	C6-C5-O3-C4
4	AAA	205	PG4	C4-C3-O2-C2
5	NNN	212	PGE	O2-C3-C4-O3
3	LLL	201	PEB	CAC-CBC-CGC-O1C
4	LLL	206	PG4	O2-C3-C4-O3
3	AAA	202	PEB	CAB-CBB-CGB-O1B
4	KKK	205	PG4	O2-C3-C4-O3
4	KKK	205	PG4	C1-C2-O2-C3
5	HHH	327	PGE	C4-C3-O2-C2
5	KKK	207	PGE	C4-C3-O2-C2
5	III	207	PGE	C3-C4-O3-C5
3	FFF	206	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
5	III	204	PGE	C3-C4-O3-C5
5	NNN	212	PGE	C3-C4-O3-C5
10	BBB	205	PE8	C14-C15-O16-C17
11	BBB	208	1PE	C16-C26-OH6-C15
3	JJJ	303	PEB	C2C-C1C-CHB-C4B
3	NNN	204	PEB	CAC-CBC-CGC-O1C
4	LLL	206	PG4	C5-C6-O4-C7
11	JJJ	308	1PE	OH6-C15-C25-OH5
4	HHH	308	PG4	O2-C3-C4-O3
11	BBB	208	1PE	C15-C25-OH5-C14
5	AAA	210	PGE	C6-C5-O3-C4
5	AAA	210	PGE	C1-C2-O2-C3
11	BBB	208	1PE	C12-C22-OH3-C23
12	JJJ	306	P33	C12-C11-O10-C9
4	MMM	205	PG4	O1-C1-C2-O2
6	FFF	216	PEG	O2-C3-C4-O4
6	FFF	218	PEG	O2-C3-C4-O4
12	HHH	305	P33	O1-C2-C3-O4
5	JJJ	310	PGE	C1-C2-O2-C3
11	JJJ	307	1PE	C24-C14-OH5-C25
15	NNN	206	PE5	C8-C7-O4-C6
4	JJJ	309	PG4	C3-C4-O3-C5
3	NNN	204	PEB	CAC-CBC-CGC-O2C
4	GGG	205	PG4	O2-C3-C4-O3
4	DDD	208	PG4	C6-C5-O3-C4
11	JJJ	308	1PE	C23-C13-OH4-C24
11	PPP	205	1PE	C14-C24-OH4-C13
12	DDD	205	P33	C6-C5-O4-C3
3	EEE	201	PEB	CAB-CBB-CGB-O2B
3	EEE	202	PEB	CAB-CBB-CGB-O2B
4	NNN	209	PG4	C5-C6-O4-C7
6	CCC	219	PEG	C4-C3-O2-C2
6	MMM	208	PEG	O1-C1-C2-O2
10	BBB	205	PE8	O16-C17-C18-O19
12	HHH	306	P33	C12-C11-O10-C9
4	JJJ	309	PG4	O3-C5-C6-O4
3	NNN	205	PEB	CAC-CBC-CGC-O1C
4	PPP	207	PG4	O3-C5-C6-O4
12	DDD	205	P33	C14-C15-O16-C17
3	DDD	201	PEB	NB-C4B-CHB-C1C
3	LLL	201	PEB	C1C-C2C-CAC-CBC
5	EEE	205	PGE	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
11	DDD	207	1PE	C13-C23-OH3-C22
3	EEE	202	PEB	CAB-CBB-CGB-O1B
5	LLL	226	PGE	O1-C1-C2-O2
6	DDD	214	PEG	O1-C1-C2-O2
6	III	208	PEG	O2-C3-C4-O4
11	BBB	208	1PE	OH2-C12-C22-OH3
5	OOO	206	PGE	C4-C3-O2-C2
4	AAA	205	PG4	O2-C3-C4-O3
3	BBB	202	PEB	CAC-CBC-CGC-O2C
4	HHH	307	PG4	C1-C2-O2-C3
6	BBB	215	PEG	C4-C3-O2-C2
9	BBB	204	RWB	C32-C33-O34-C35
4	DDD	209	PG4	C5-C6-O4-C7
11	HHH	301	1PE	C15-C25-OH5-C14
3	FFF	206	PEB	CAC-CBC-CGC-O2C
4	LLL	208	PG4	C4-C3-O2-C2
5	BBB	222	PGE	O1-C1-C2-O2
6	CCC	214	PEG	O1-C1-C2-O2
4	NNN	202	PG4	C8-C7-O4-C6
3	BBB	203	PEB	C3B-CAB-CBB-CGB
5	BBB	210	PGE	C4-C3-O2-C2
4	AAA	204	PG4	O1-C1-C2-O2
4	AAA	204	PG4	O2-C3-C4-O3
5	HHH	327	PGE	C6-C5-O3-C4
3	HHH	304	PEB	CAC-CBC-CGC-O1C
3	NNN	205	PEB	CAC-CBC-CGC-O2C
5	LLL	225	PGE	C3-C4-O3-C5

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

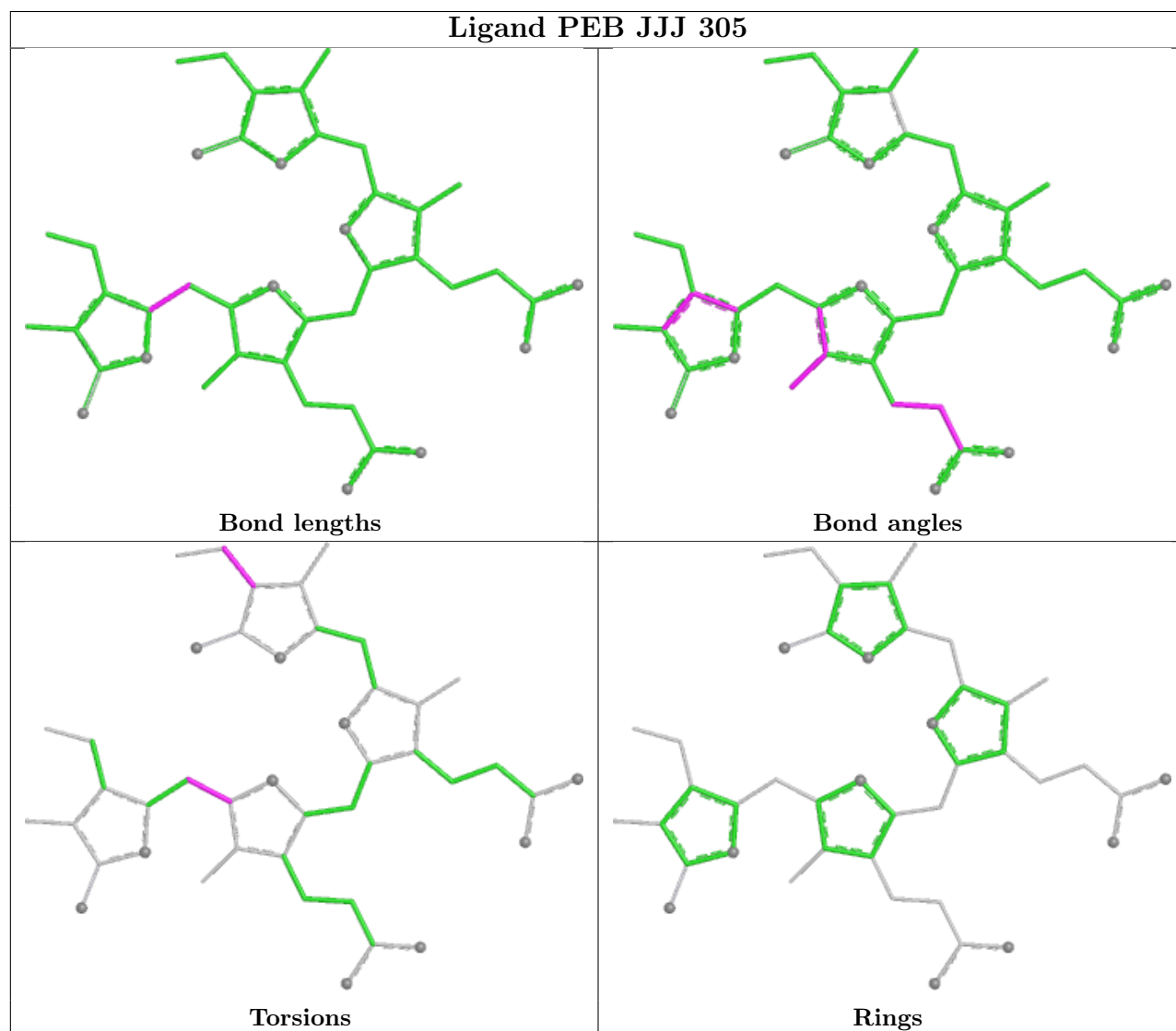
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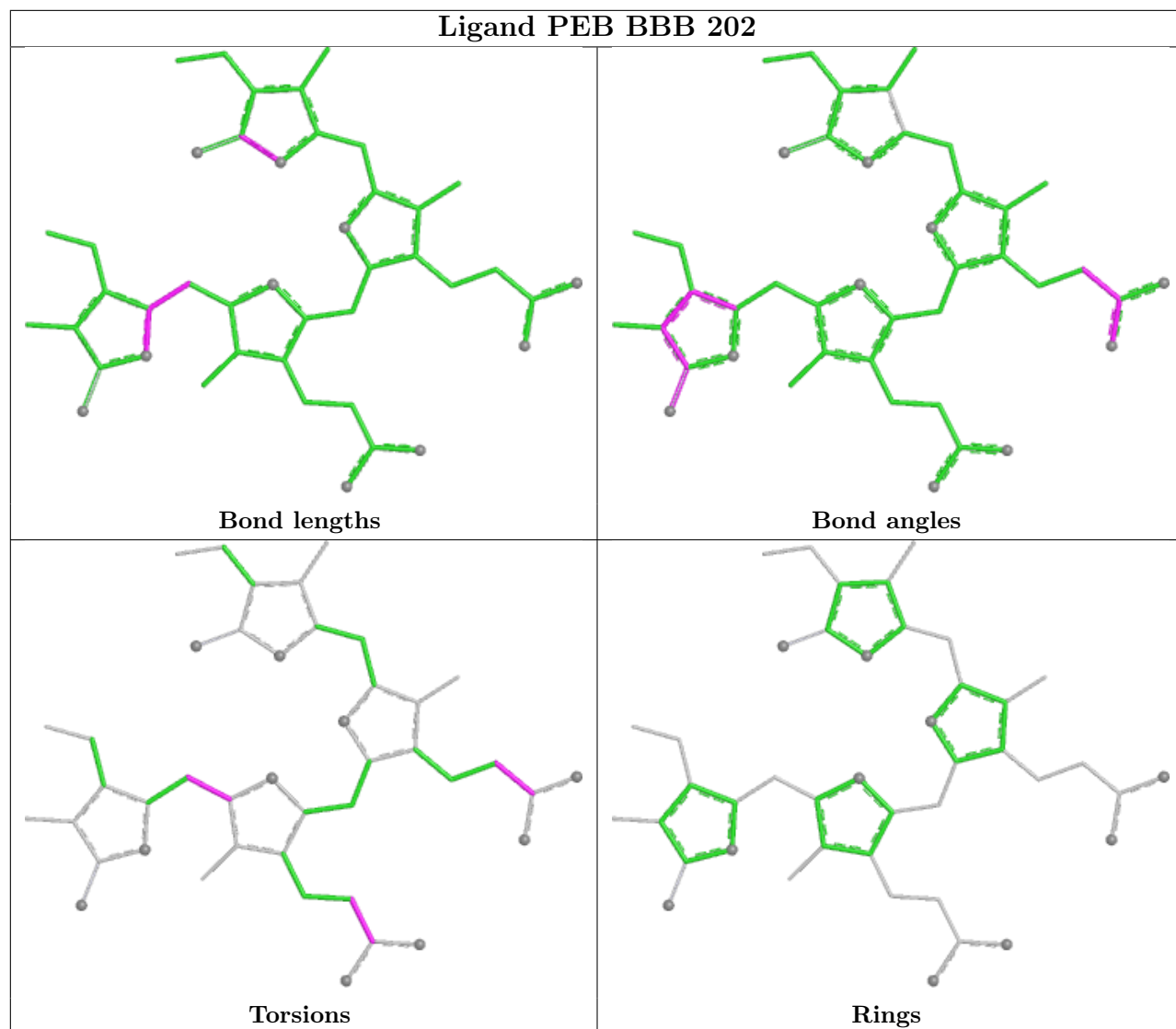
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	JJJ	309	PG4	3	0
3	NNN	205	PEB	2	0
3	NNN	203	PEB	2	0
5	GGG	208	PGE	3	0
3	EEE	201	PEB	1	0
4	MMM	205	PG4	1	0
11	FFF	201	1PE	1	0
3	HHH	302	PEB	3	0
3	GGG	201	PEB	1	0
3	CCC	202	PEB	1	0
6	KKK	208	PEG	3	0
13	DDD	206	P6G	2	0
3	JJJ	303	PEB	2	0
15	NNN	206	PE5	6	0
11	BBB	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

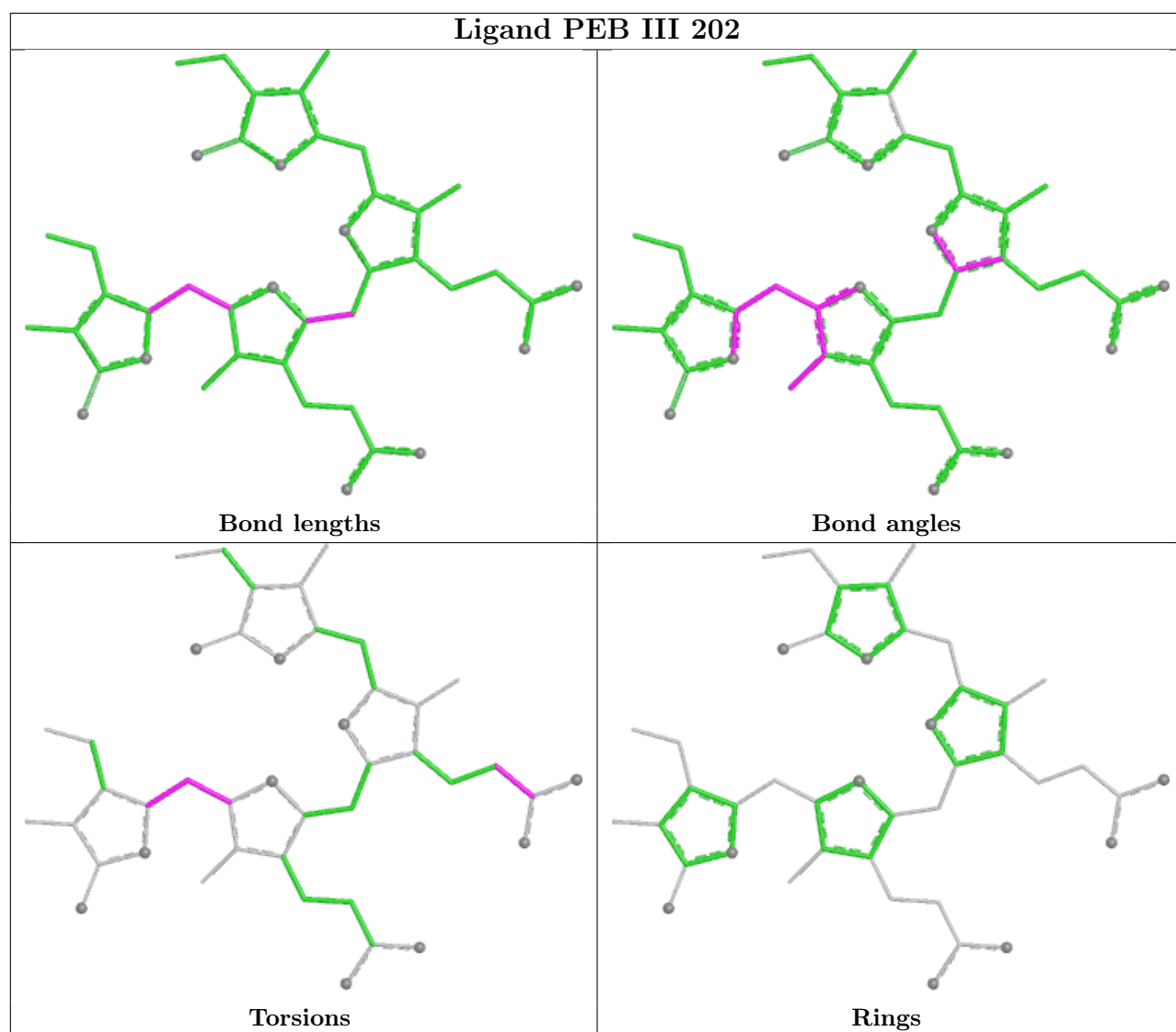
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

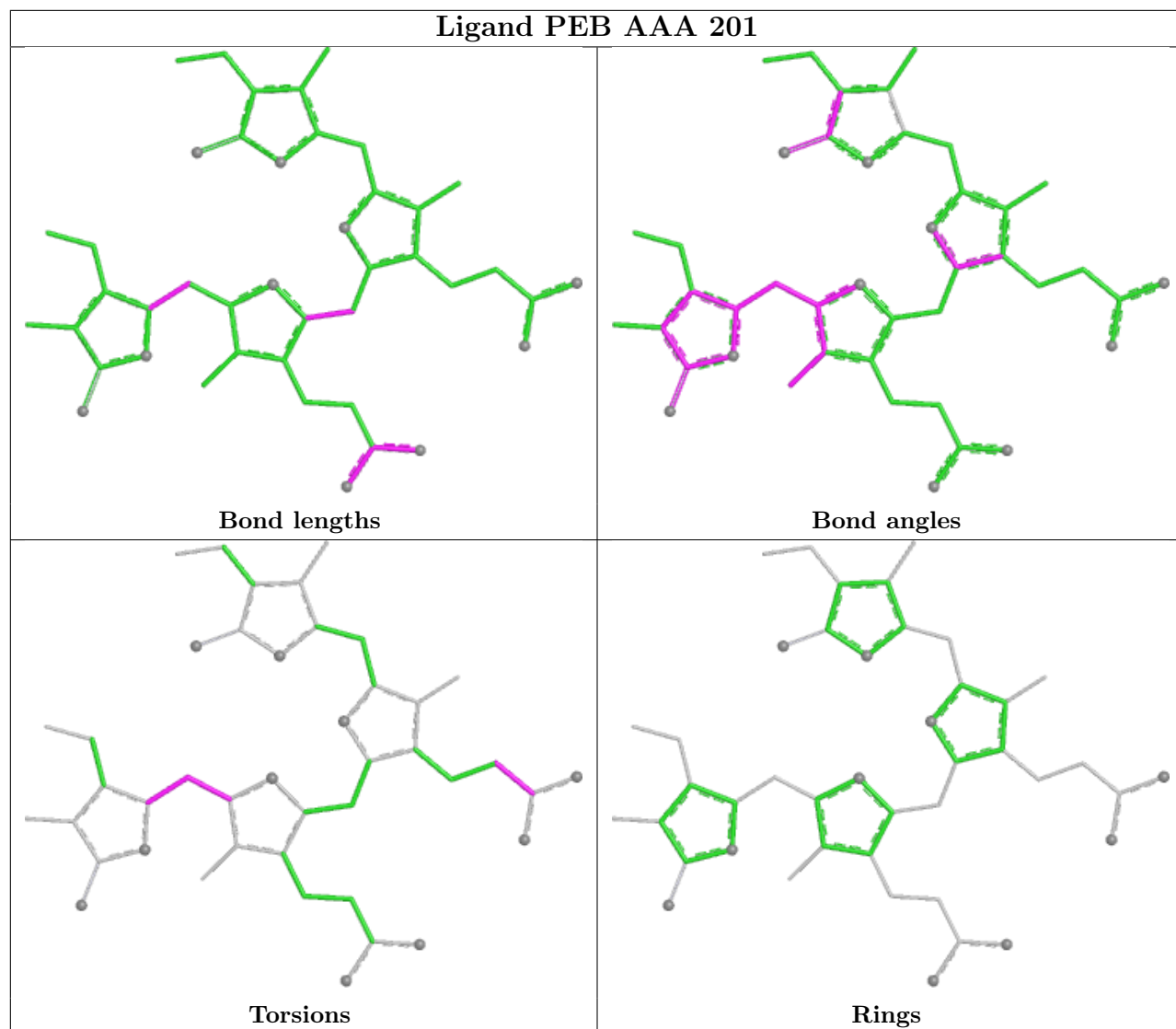
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



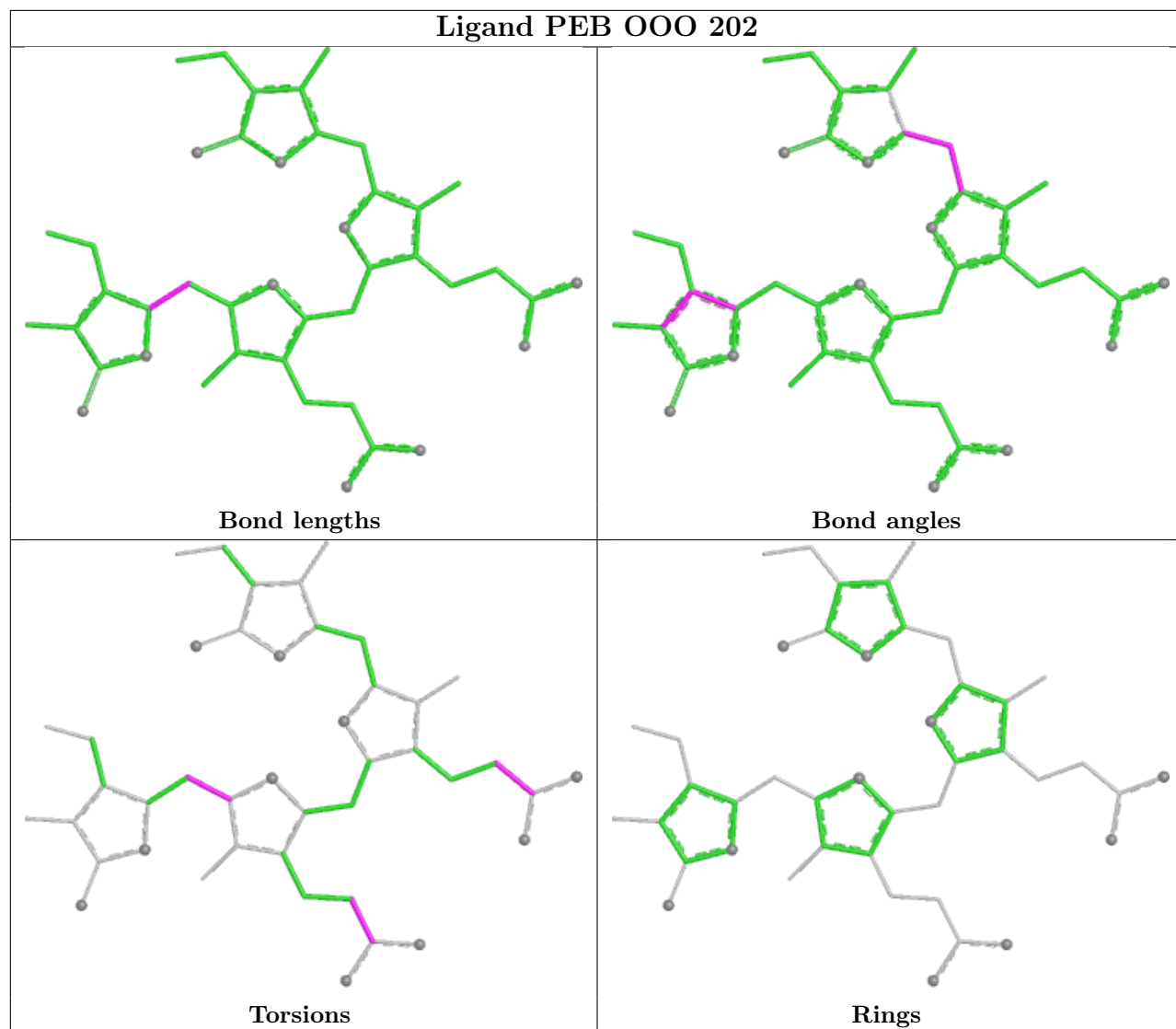
Ligand PEB BBB 202



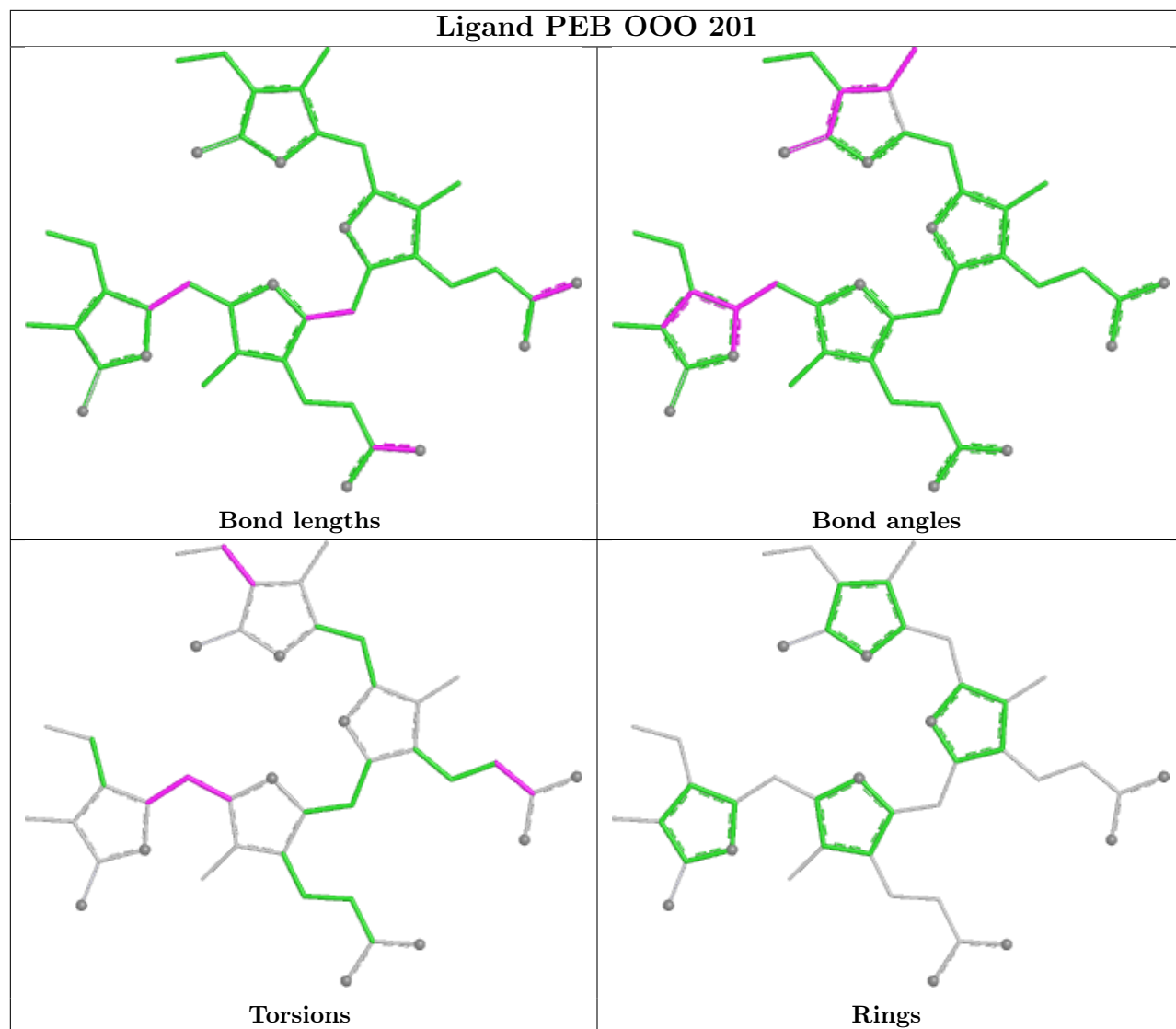




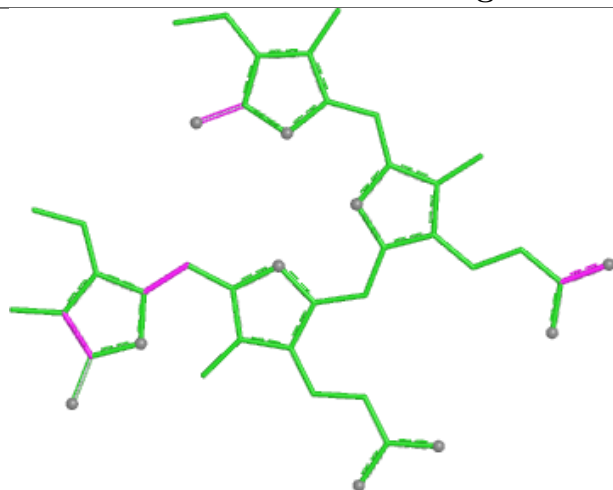
Ligand PEB_OOO_202



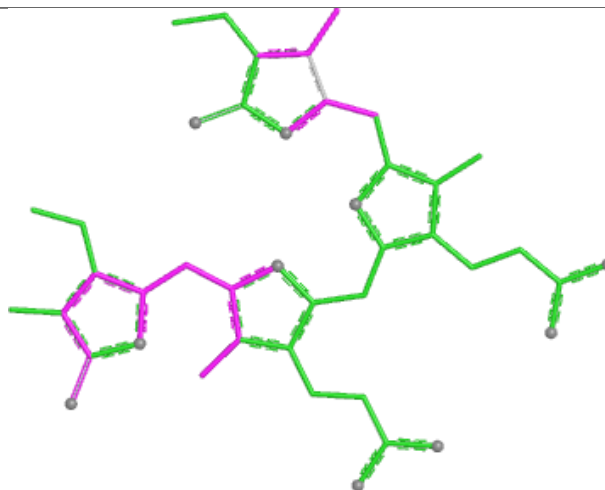
Ligand PEB_OOO_201



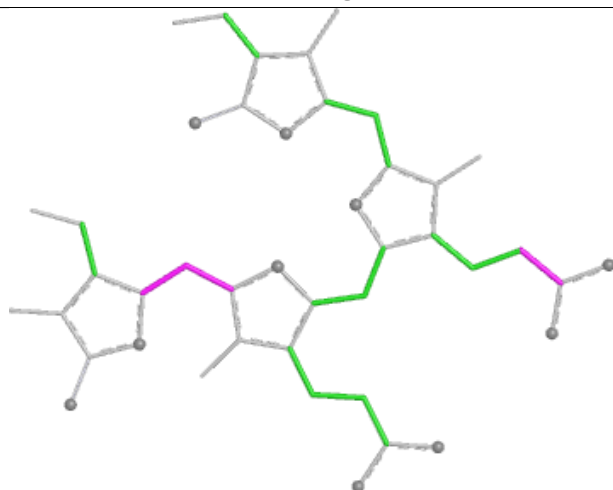
Ligand PEB MMM 201



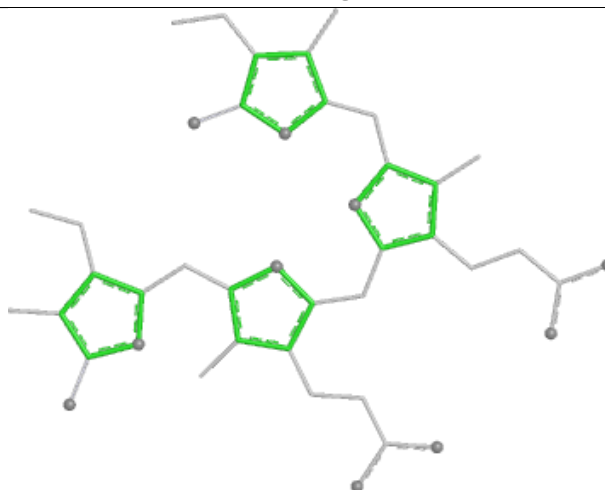
Bond lengths



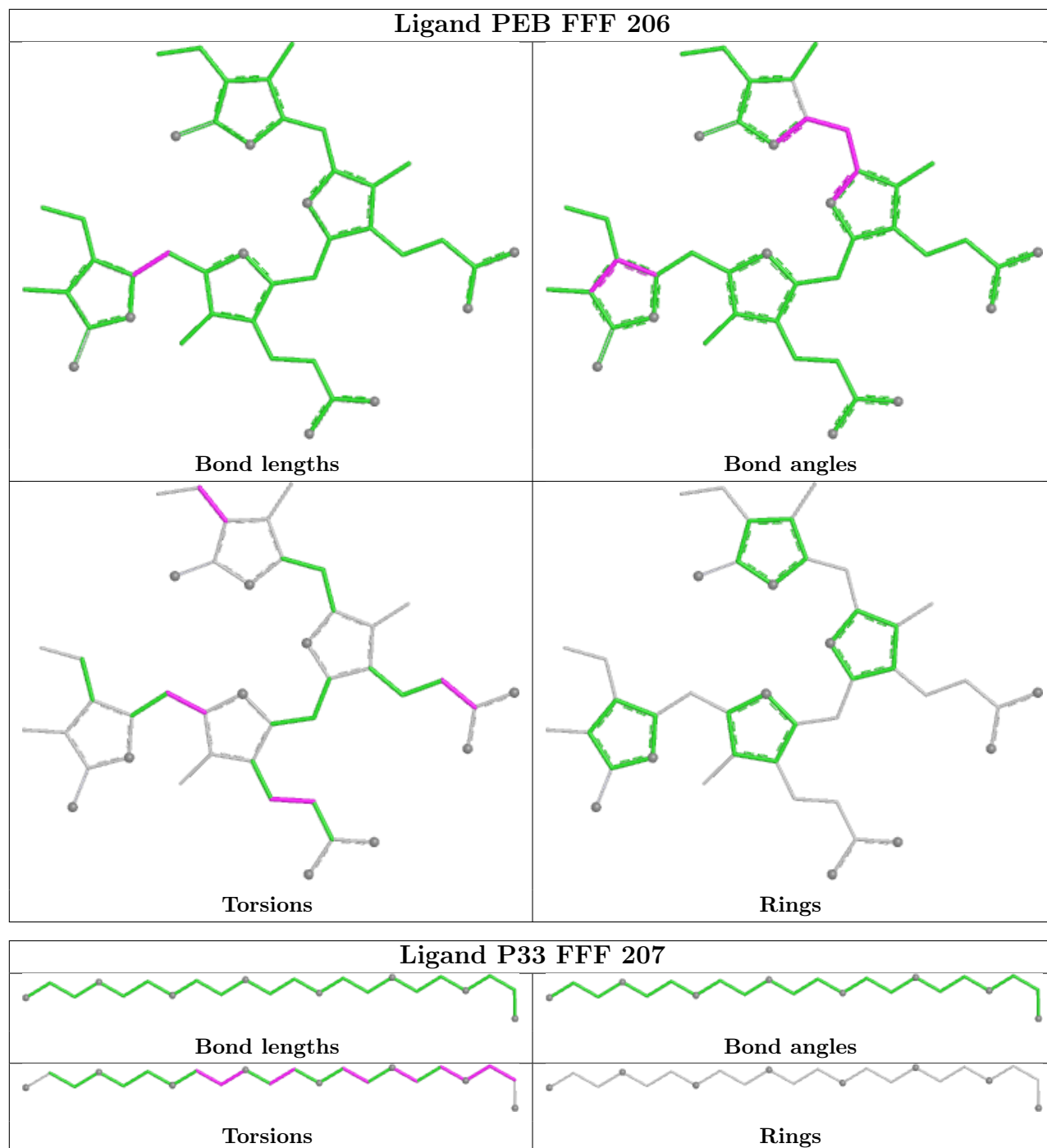
Bond angles



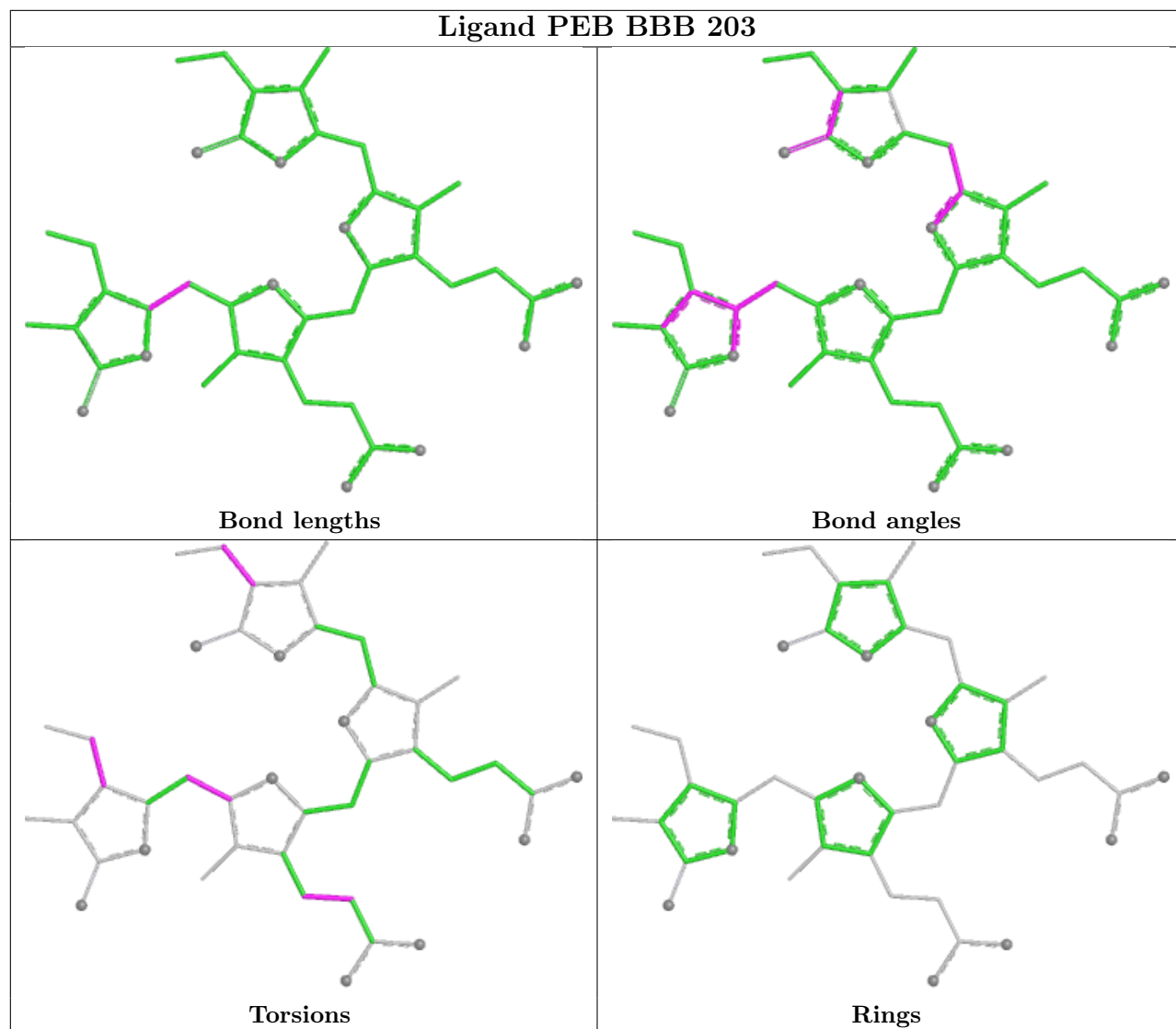
Torsions



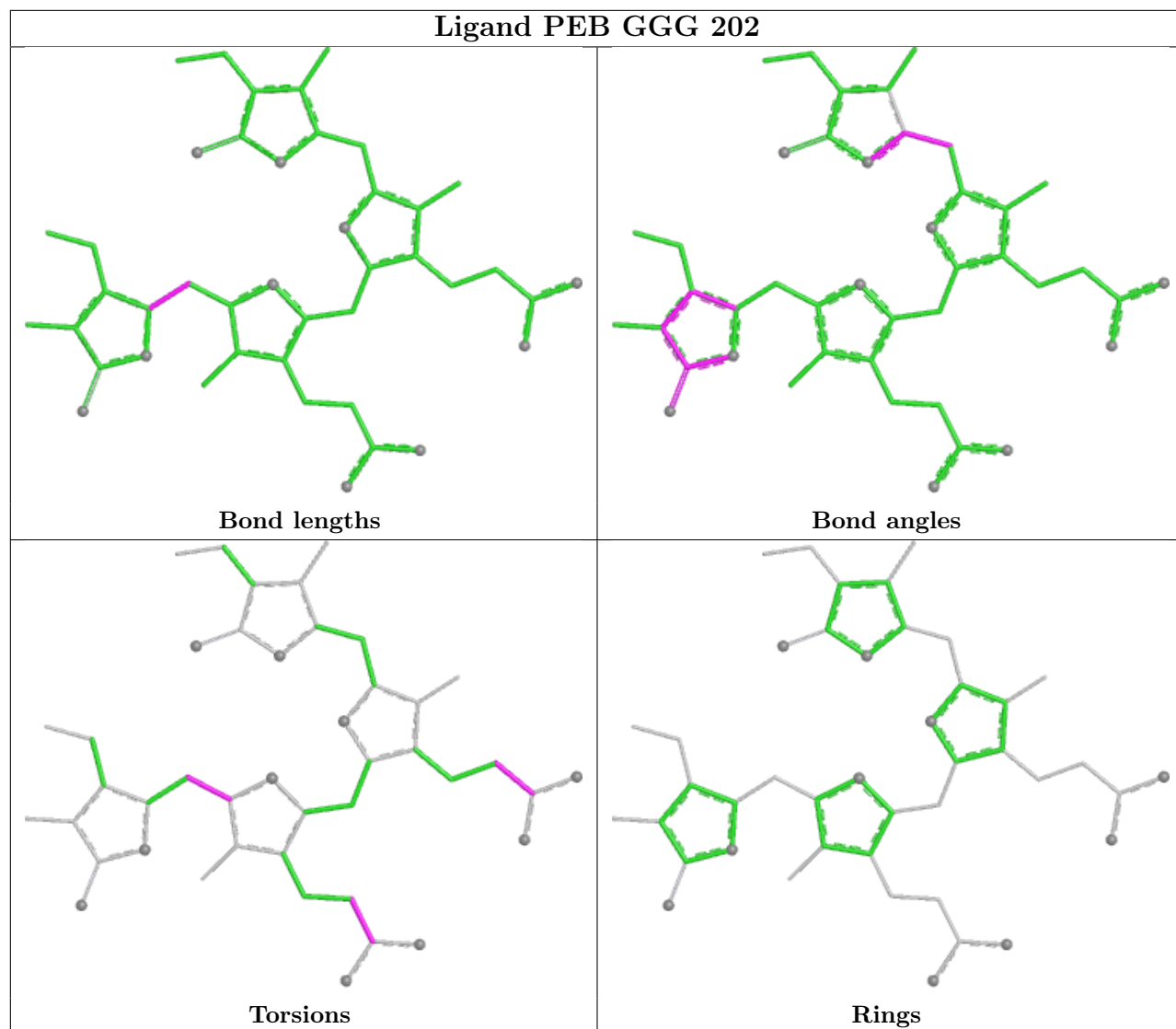
Rings



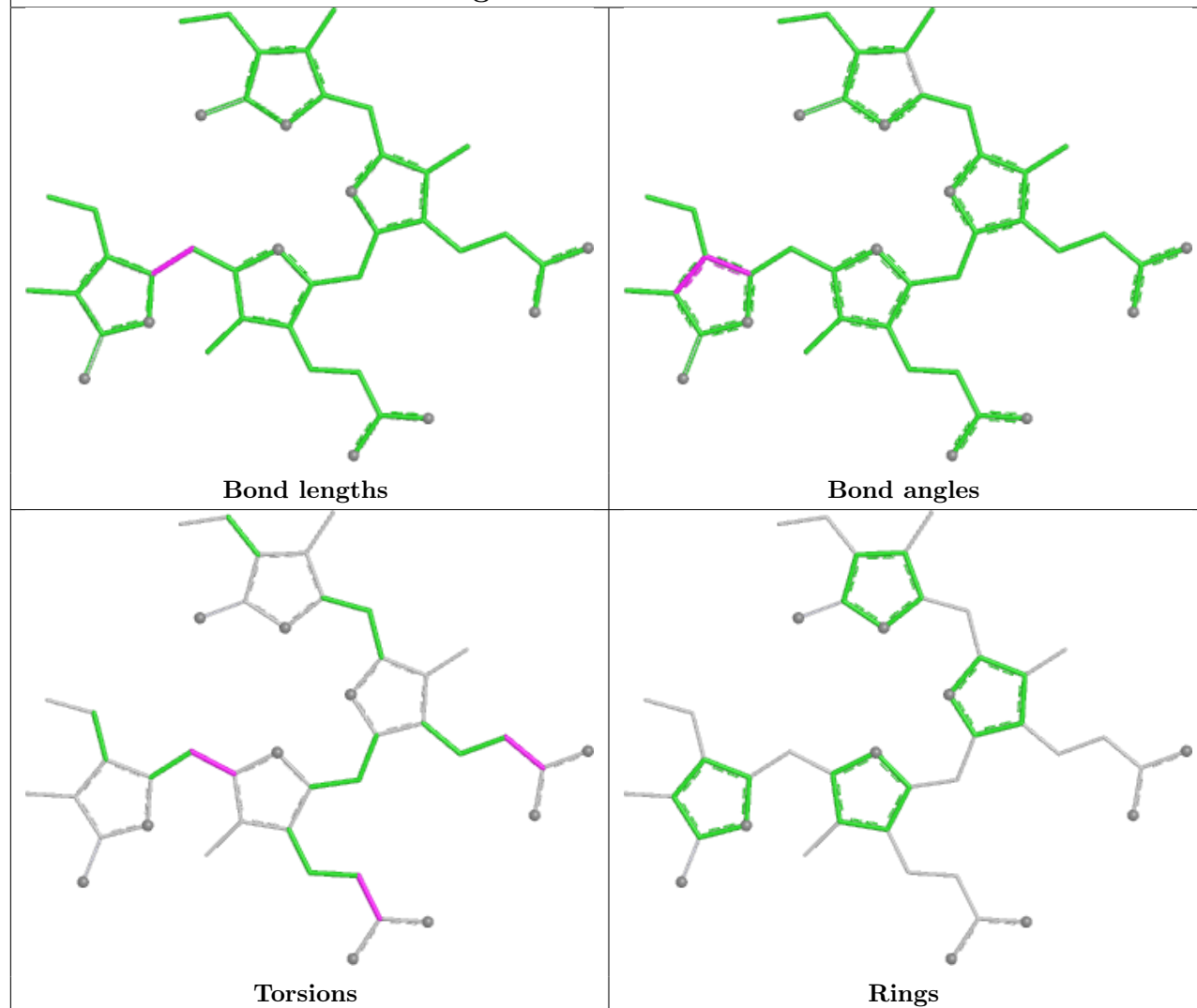
Ligand PEB BBB 203



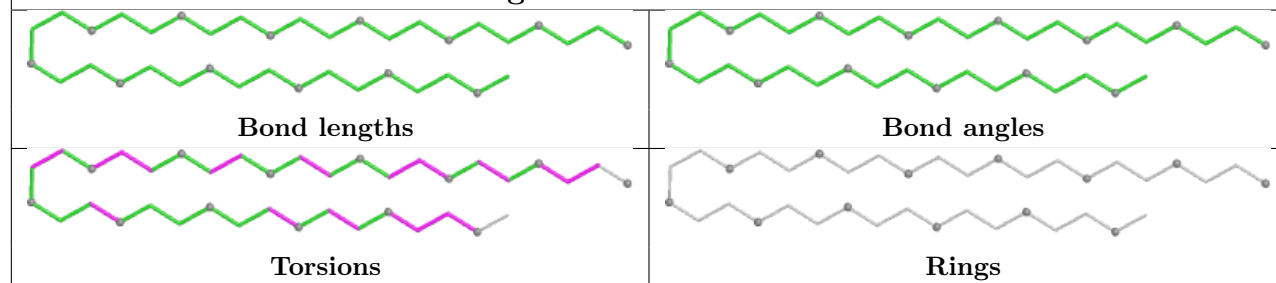
Ligand PEB GGG 202



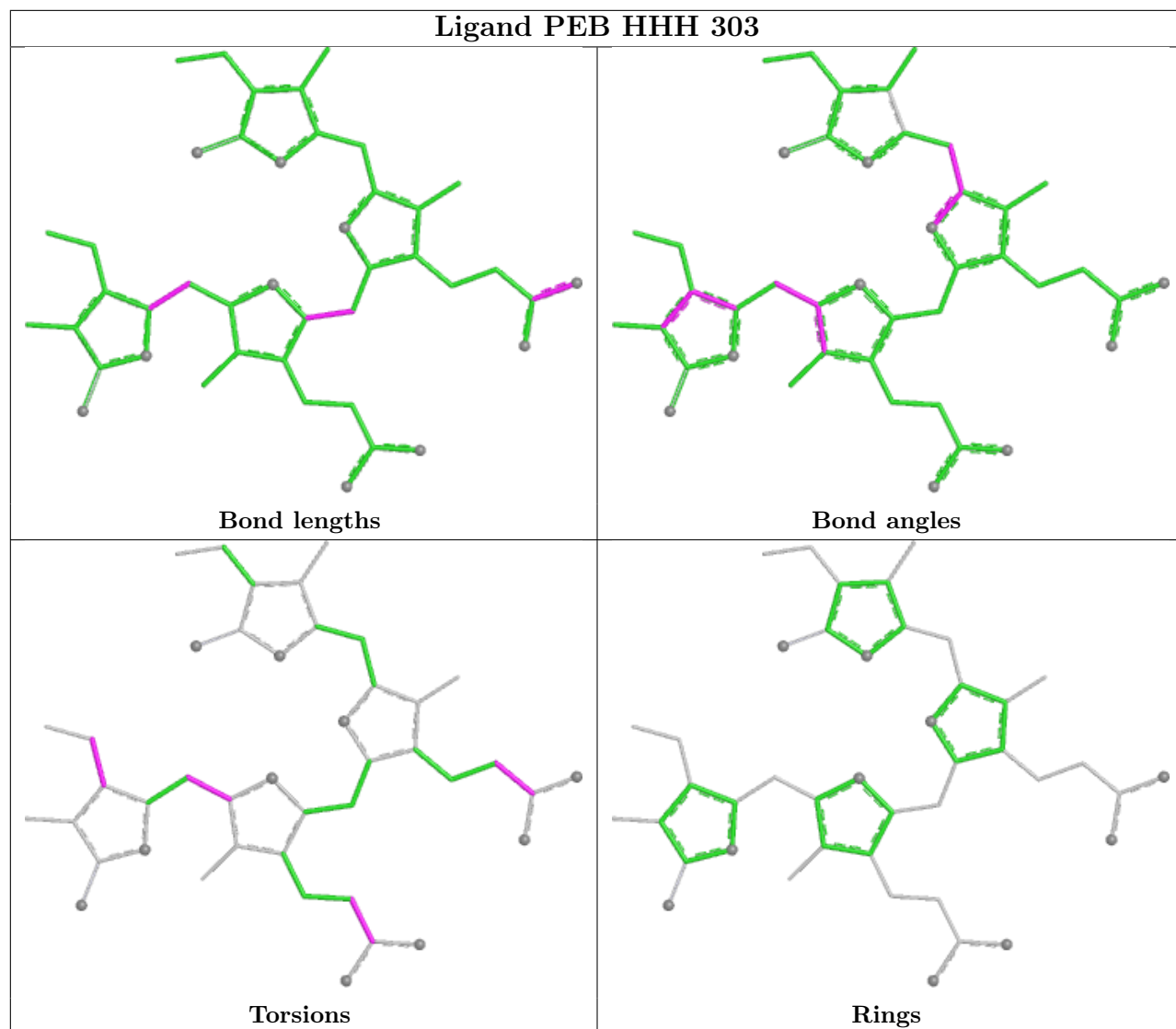
Ligand PEB DDD 202

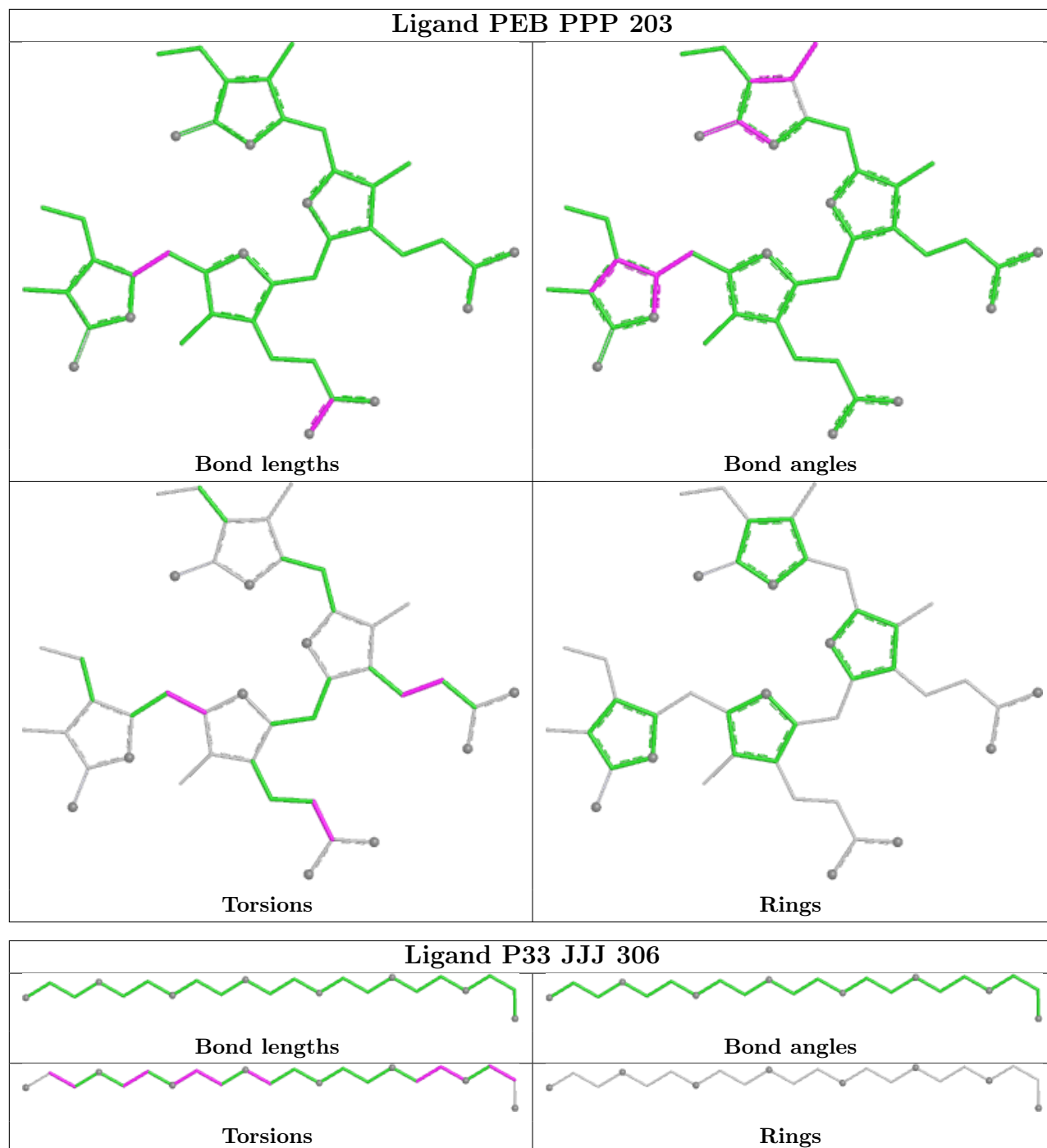


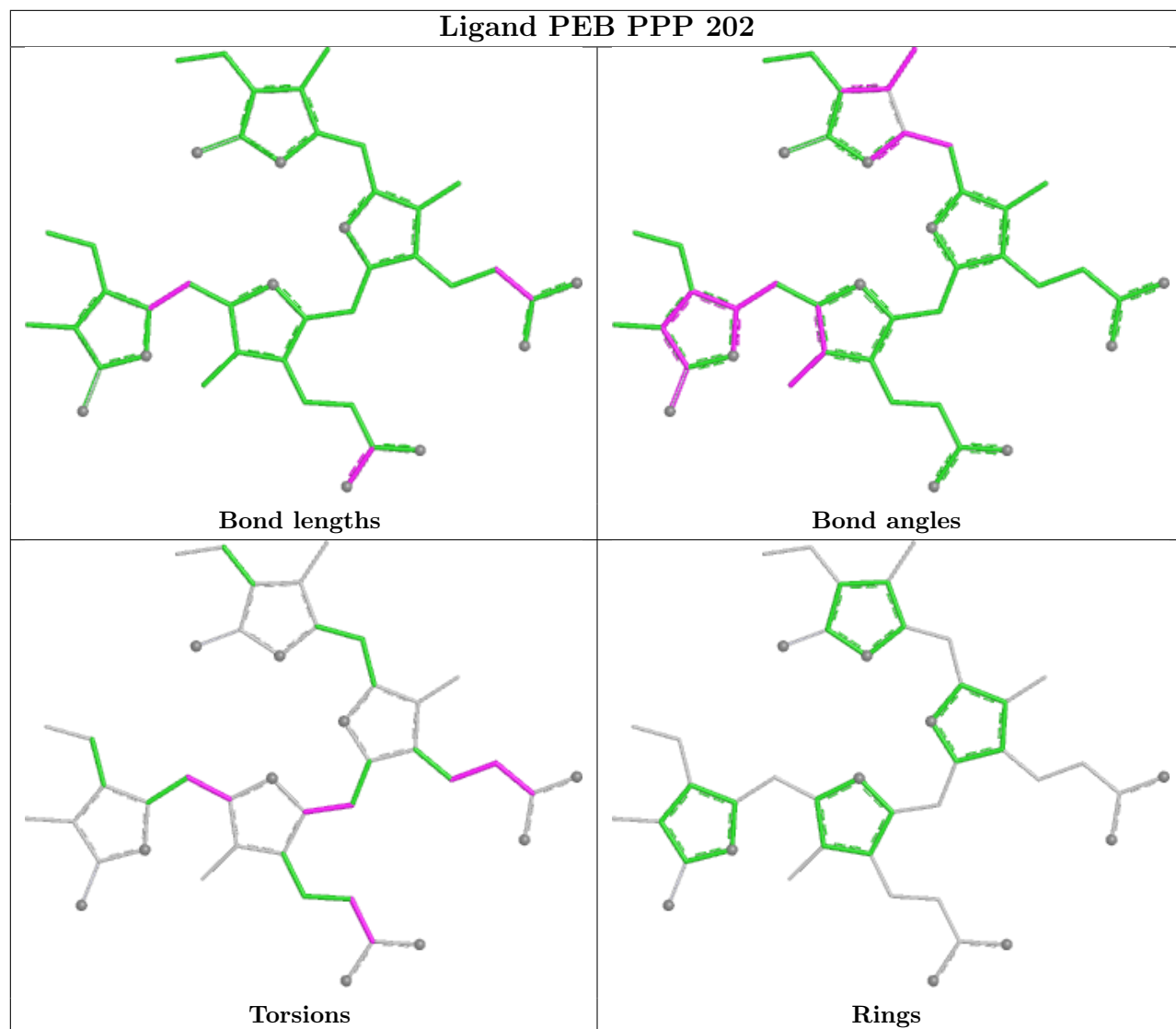
Ligand RWB LLL 204



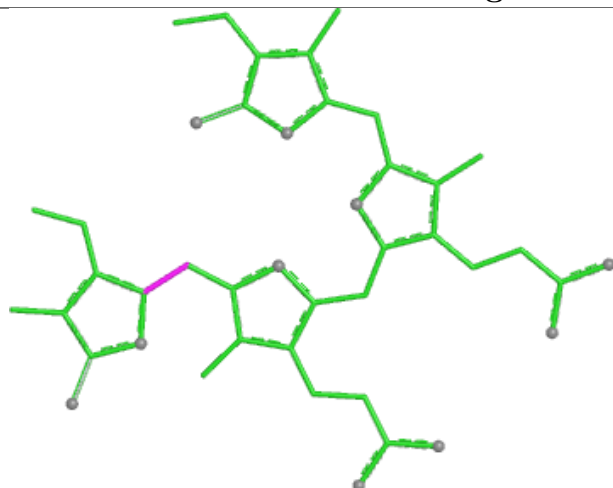
Ligand PEB HHH 303



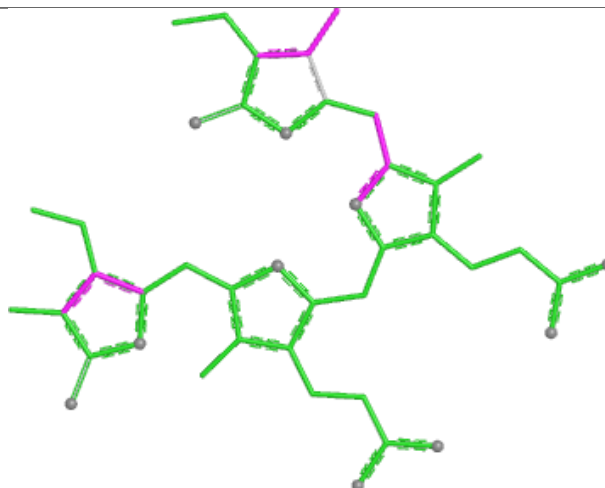




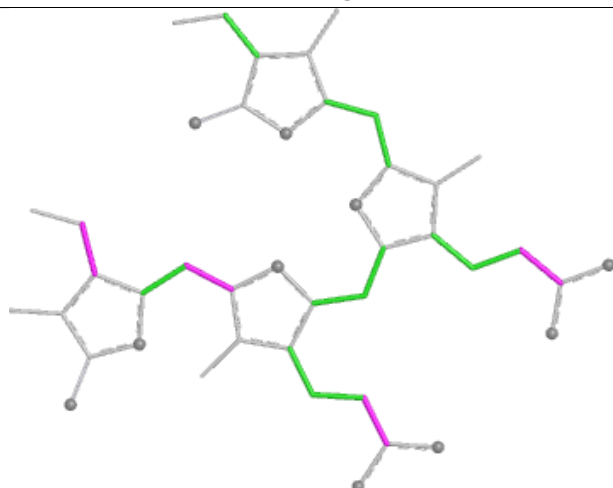
Ligand PEB NNN 204



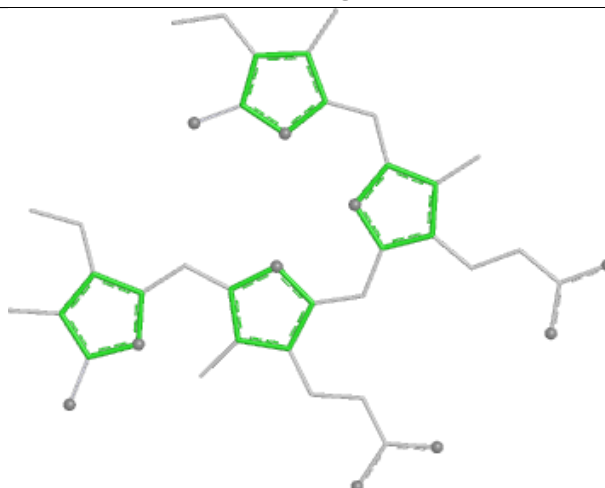
Bond lengths



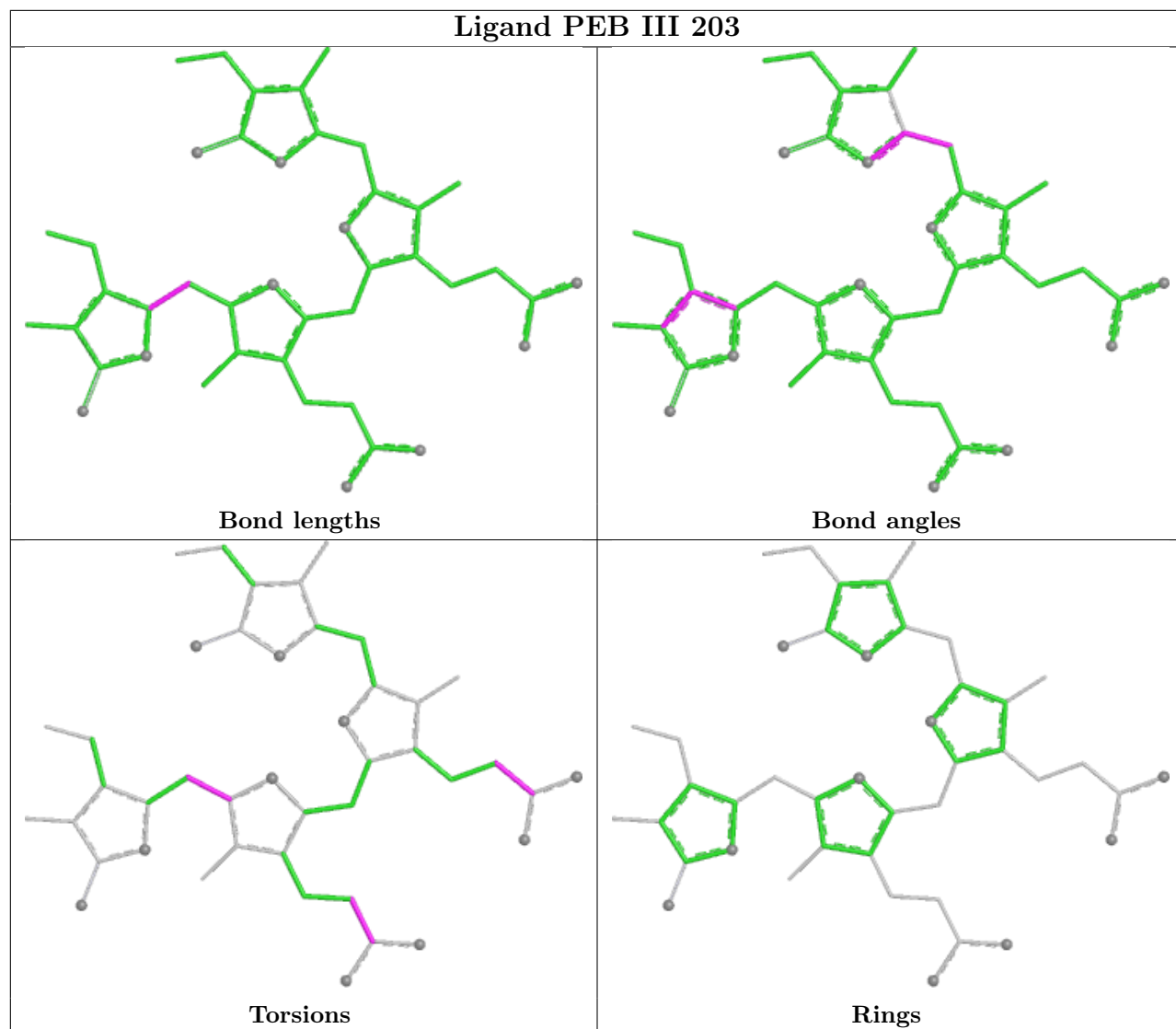
Bond angles



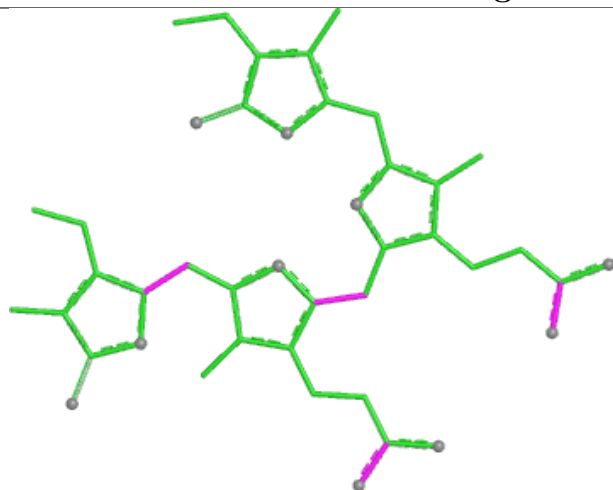
Torsions



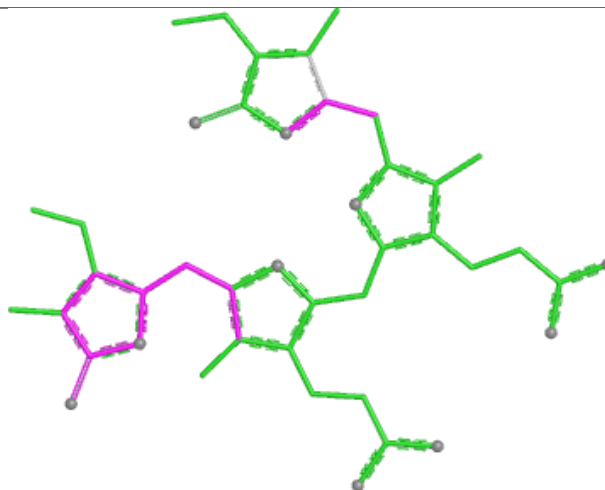
Rings



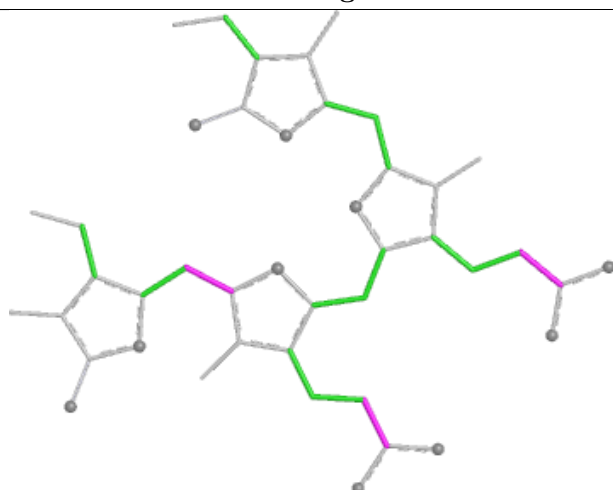
Ligand PEB FFF 204



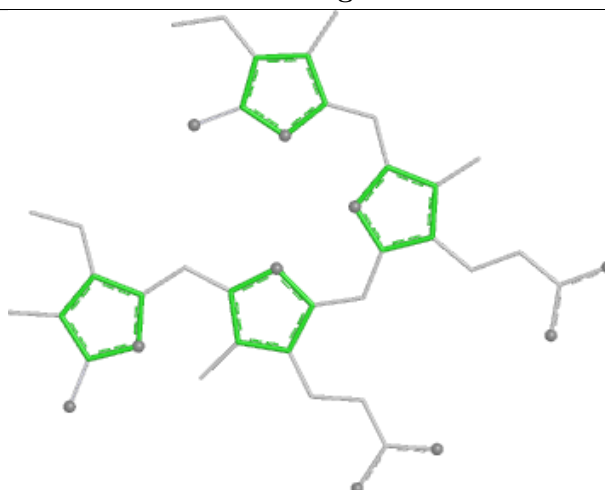
Bond lengths



Bond angles

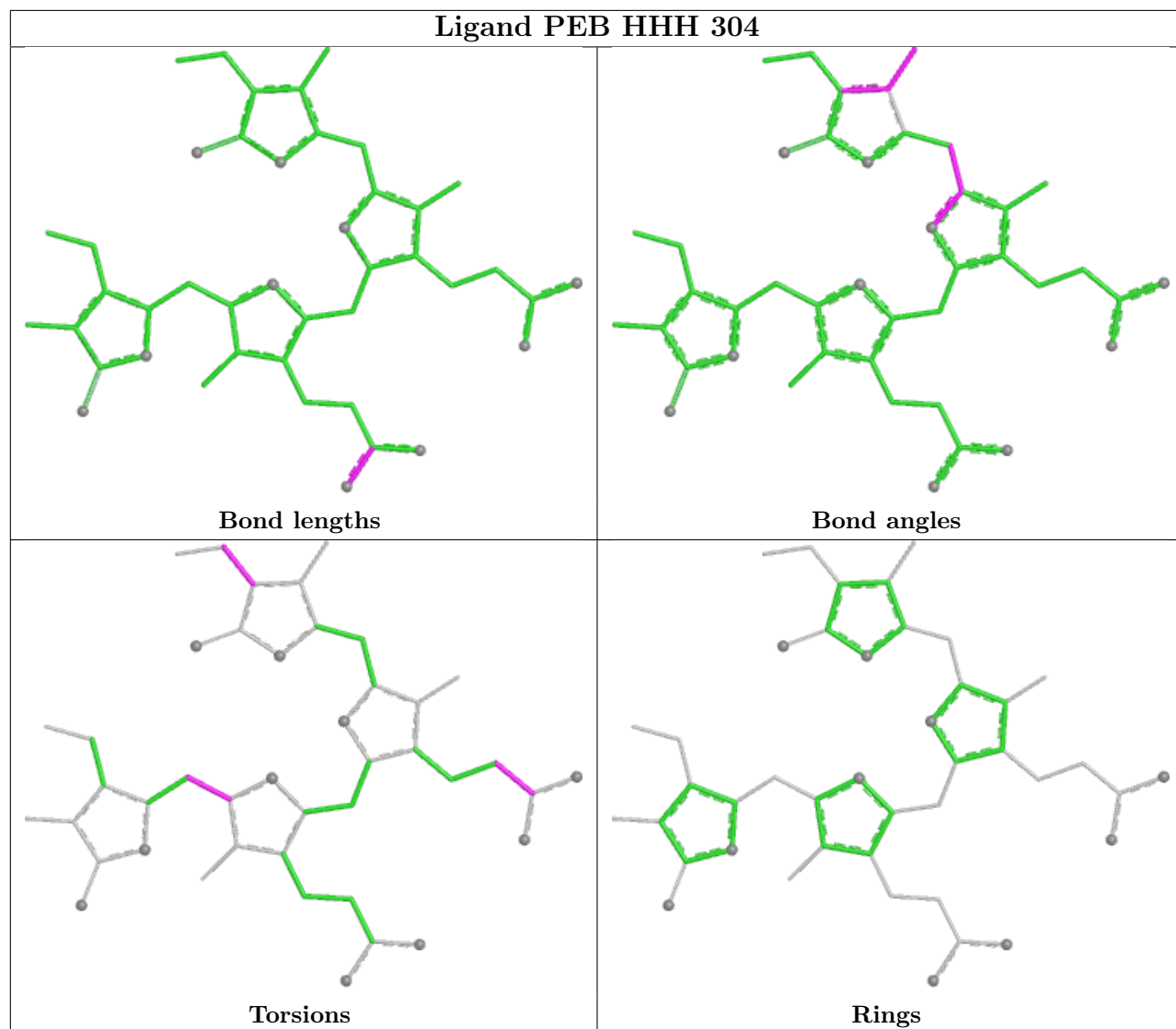


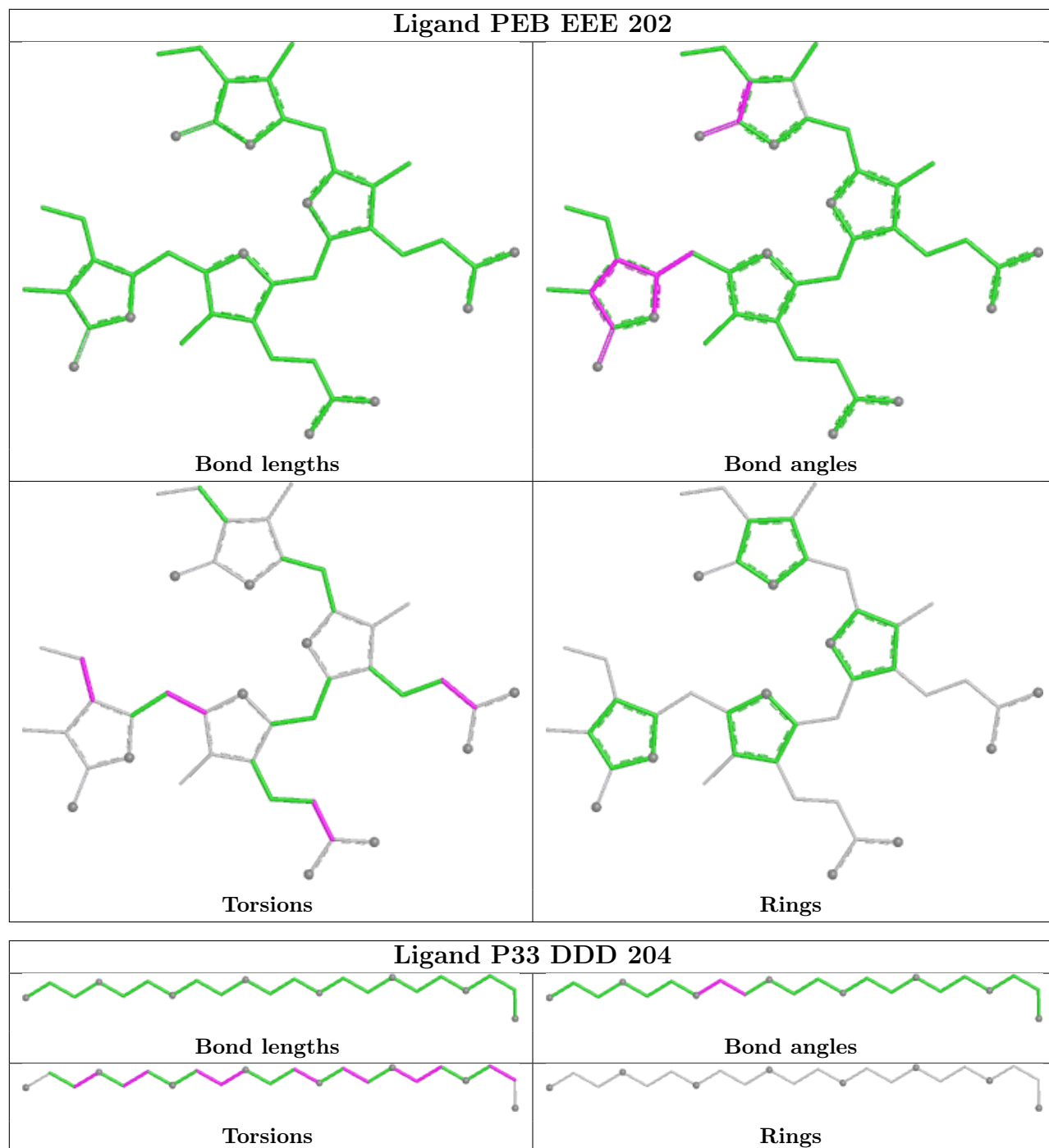
Torsions

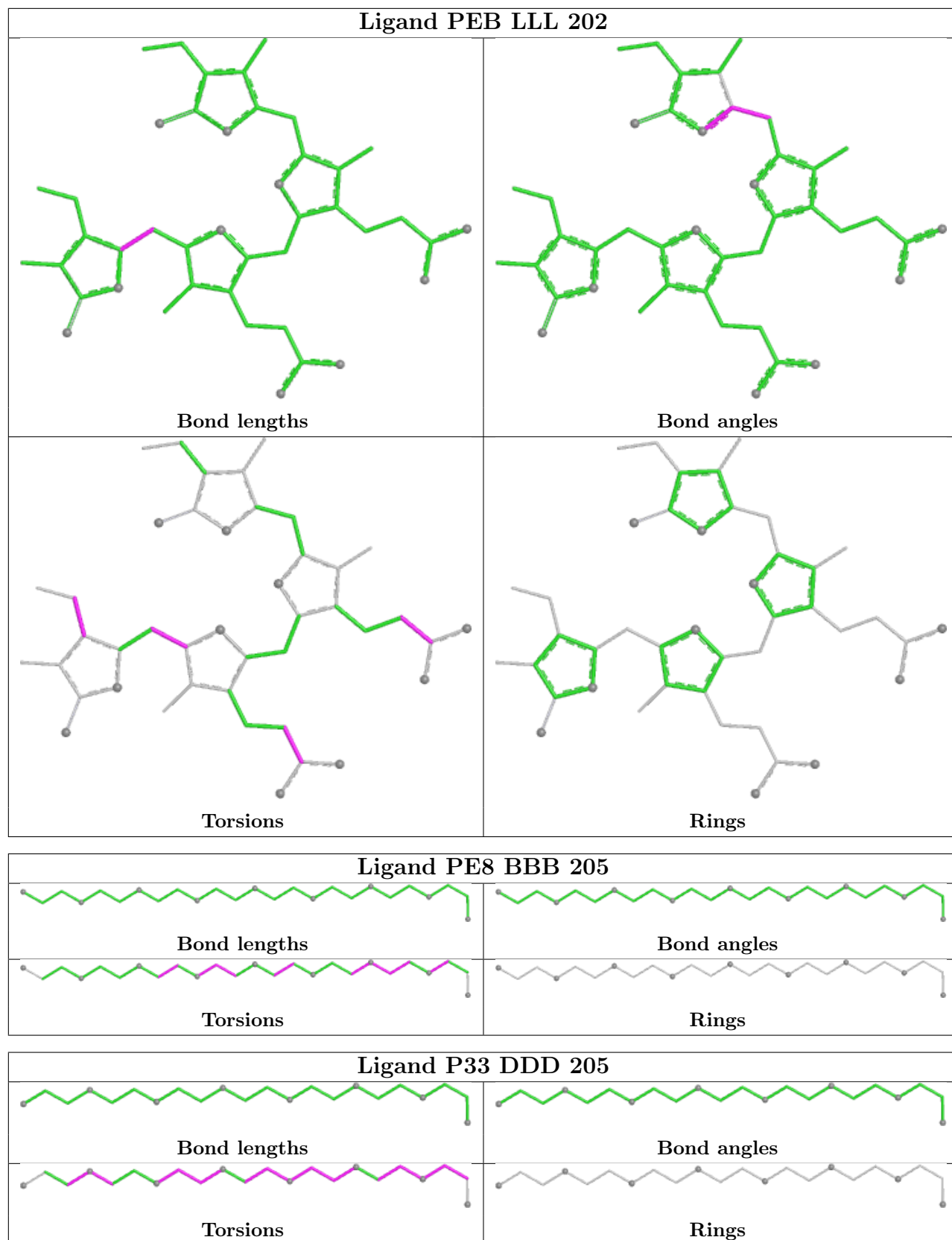


Rings

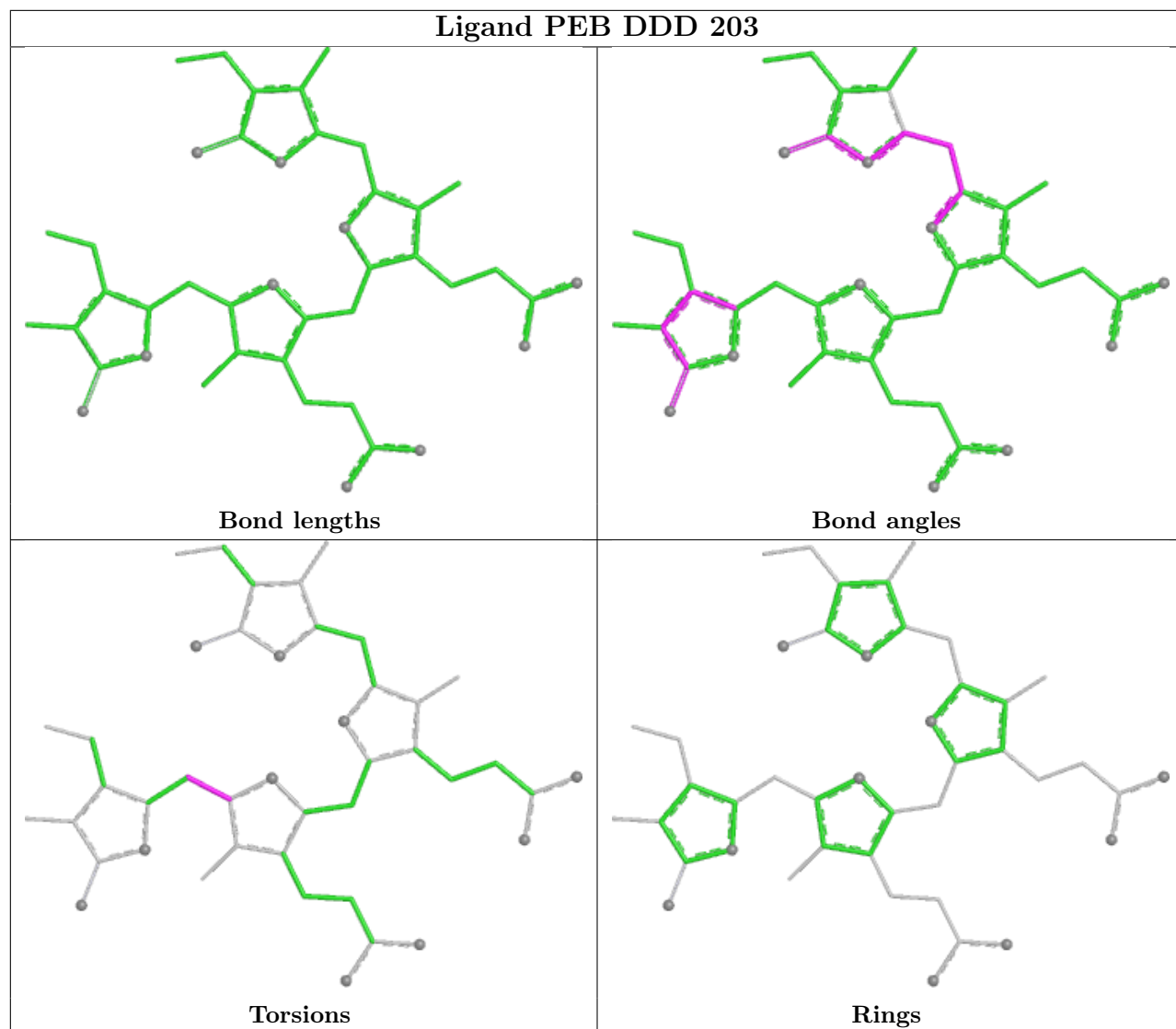
Ligand PEB HHH 304

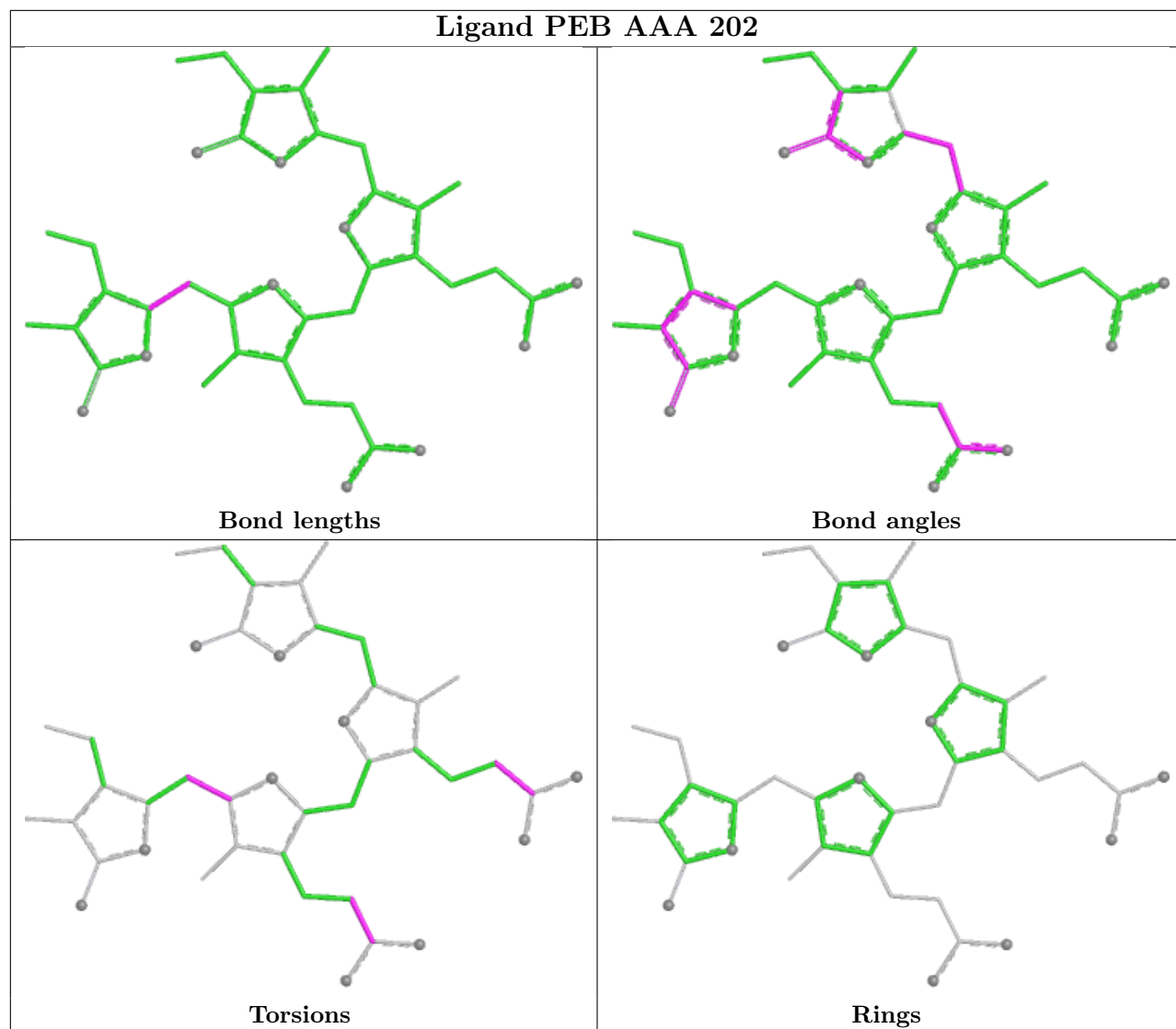




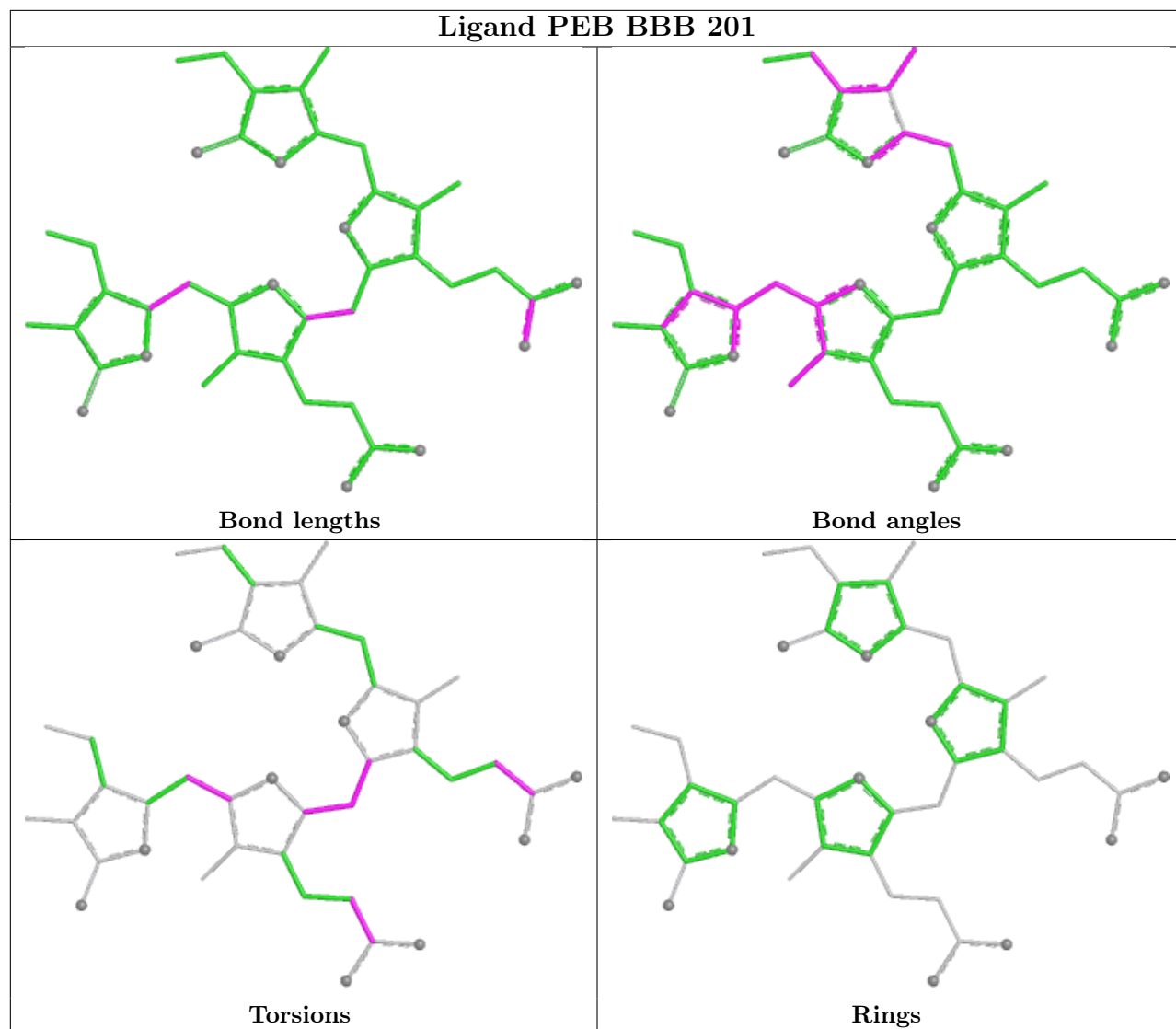


Ligand PEB DDD 203

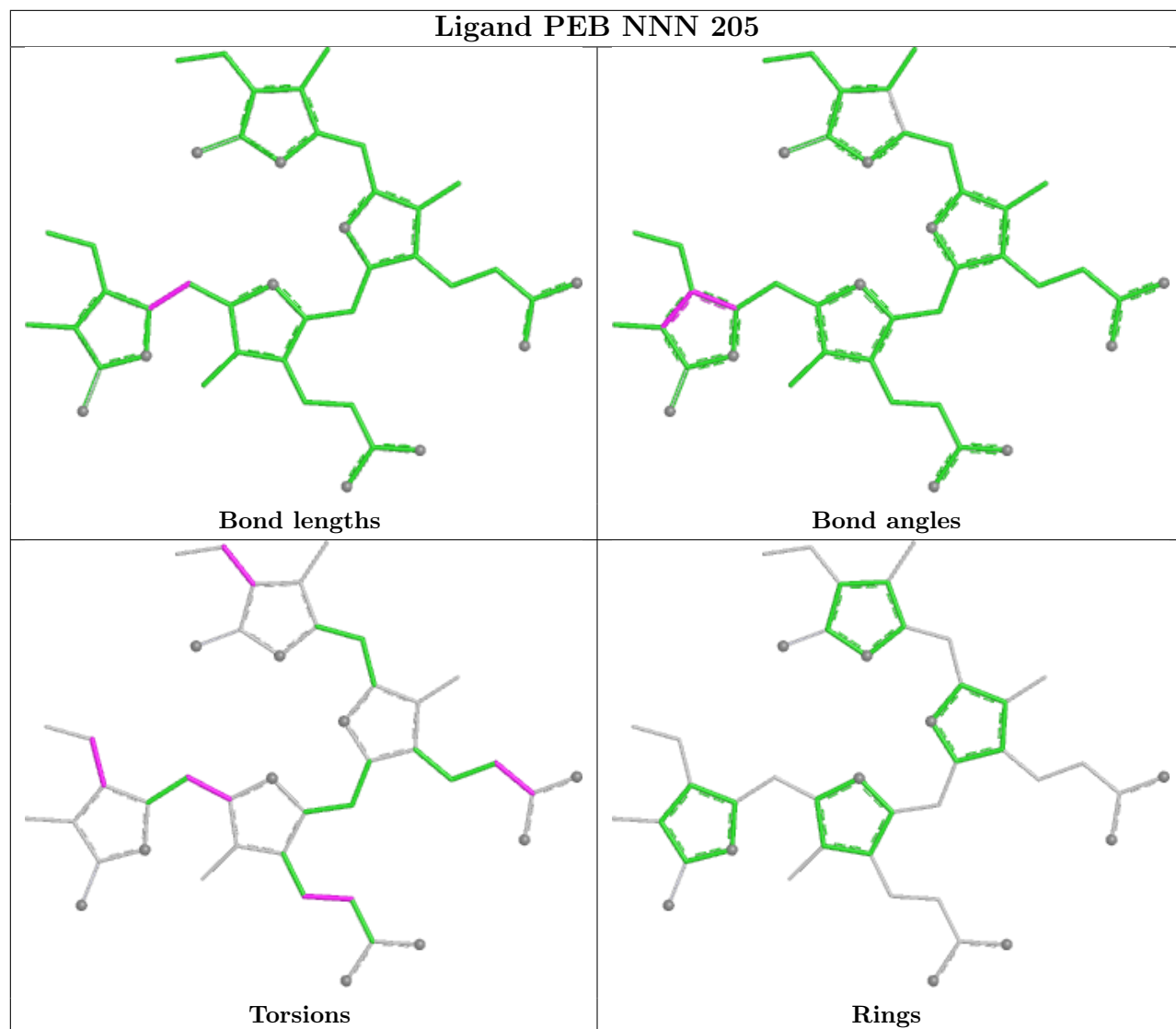




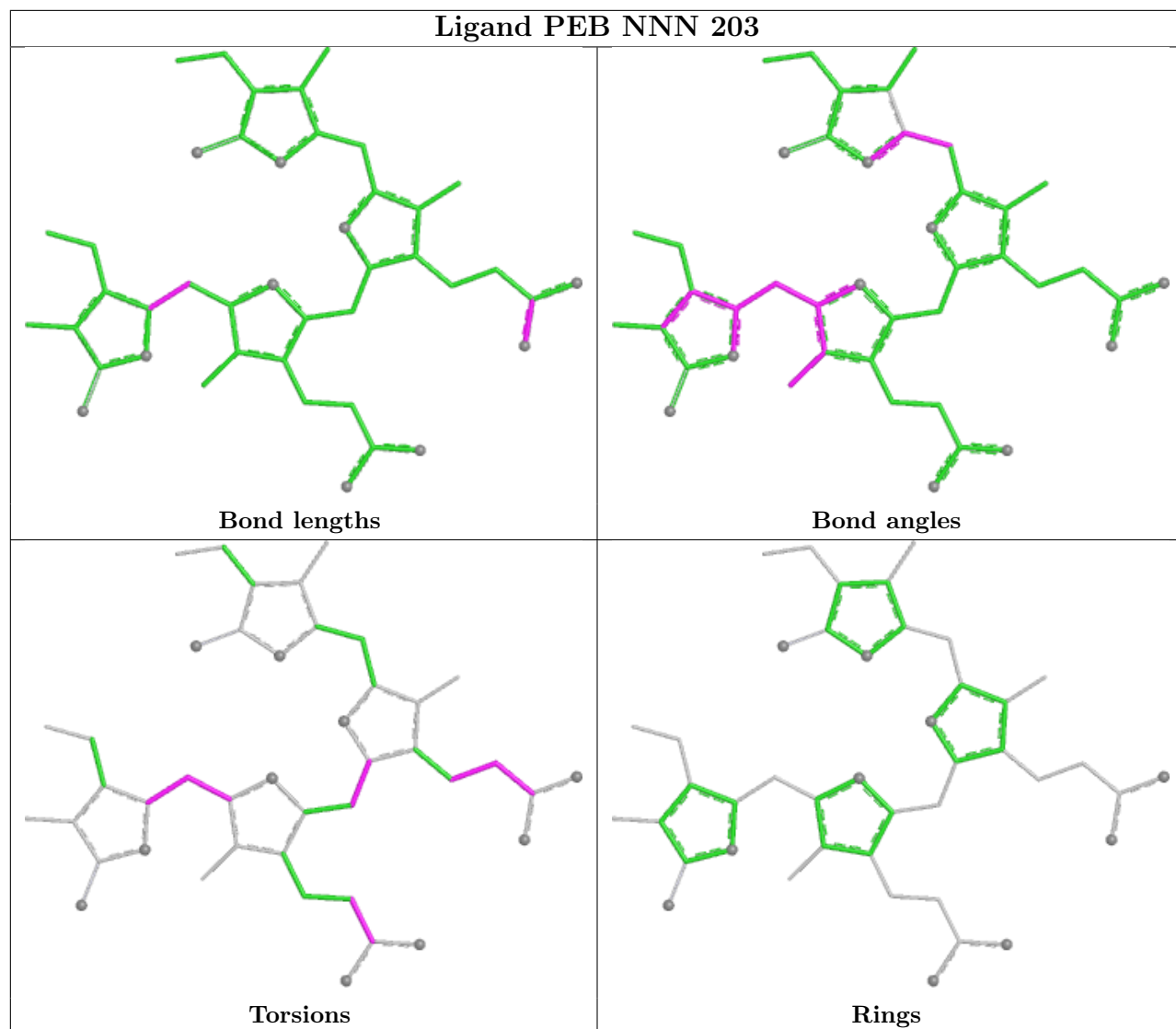
Ligand PEB BBB 201



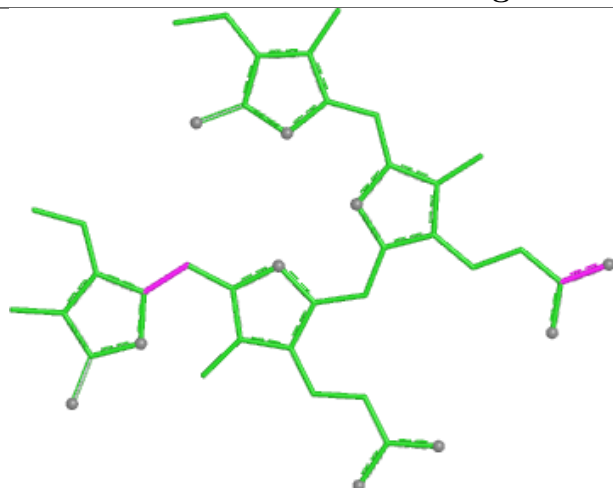
Ligand PEB NNN 205



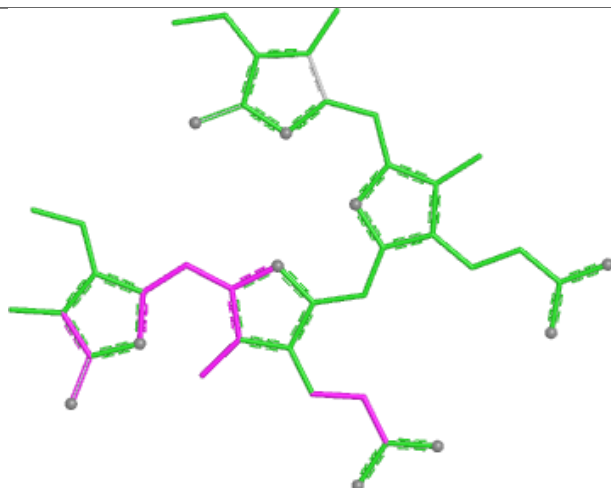
Ligand PEB NNN 203



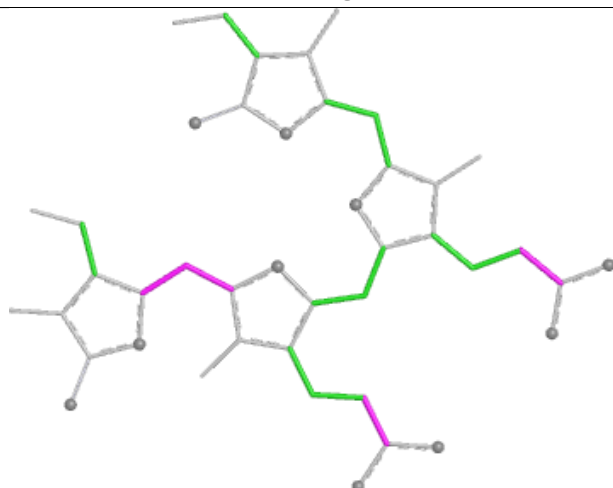
Ligand PEB EEE 201



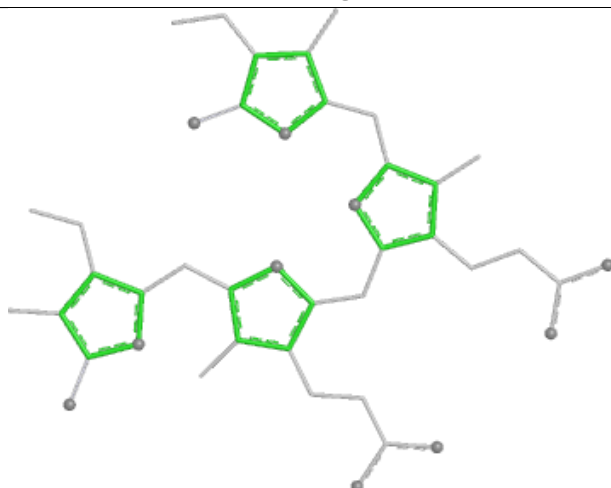
Bond lengths



Bond angles

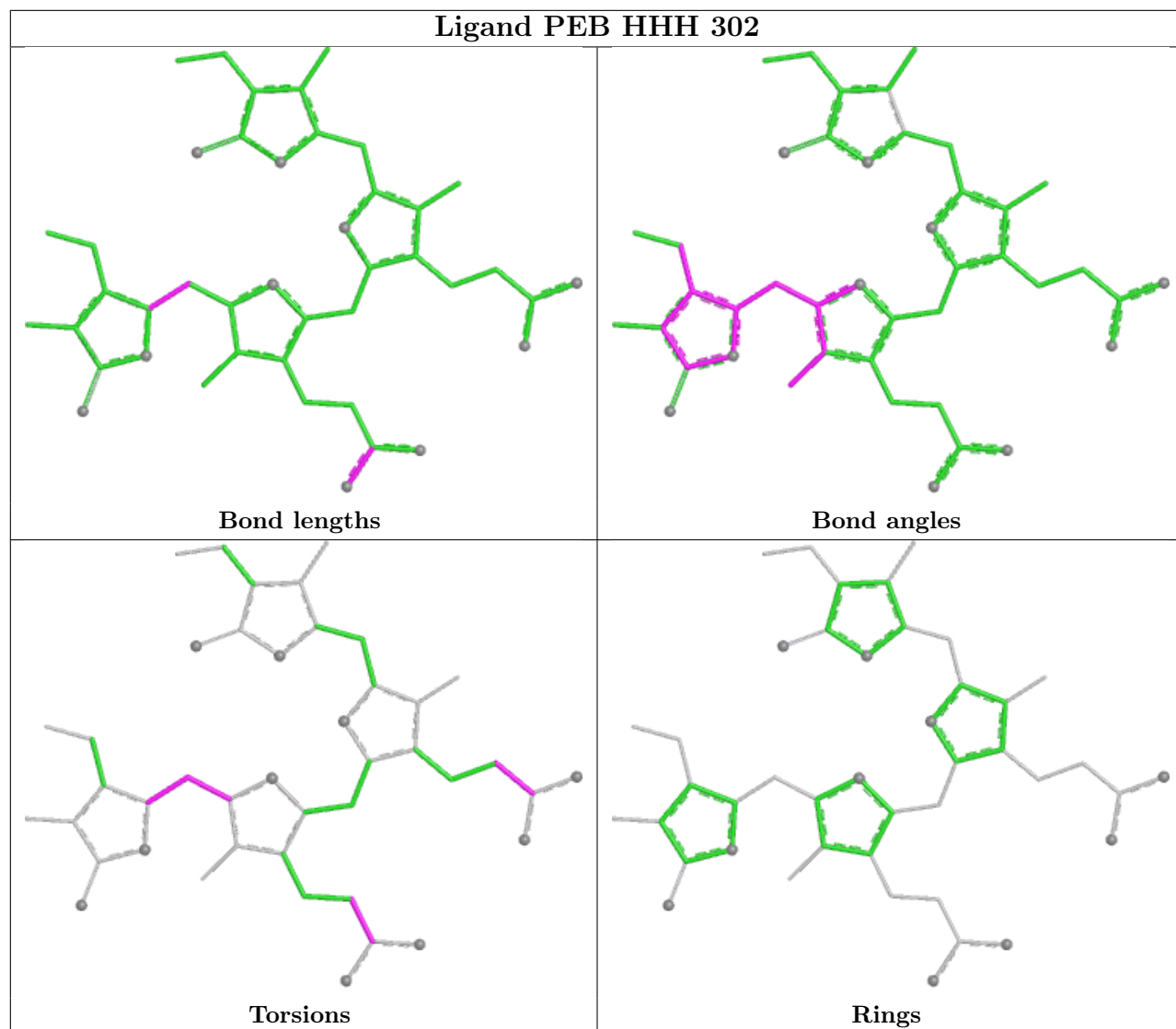


Torsions

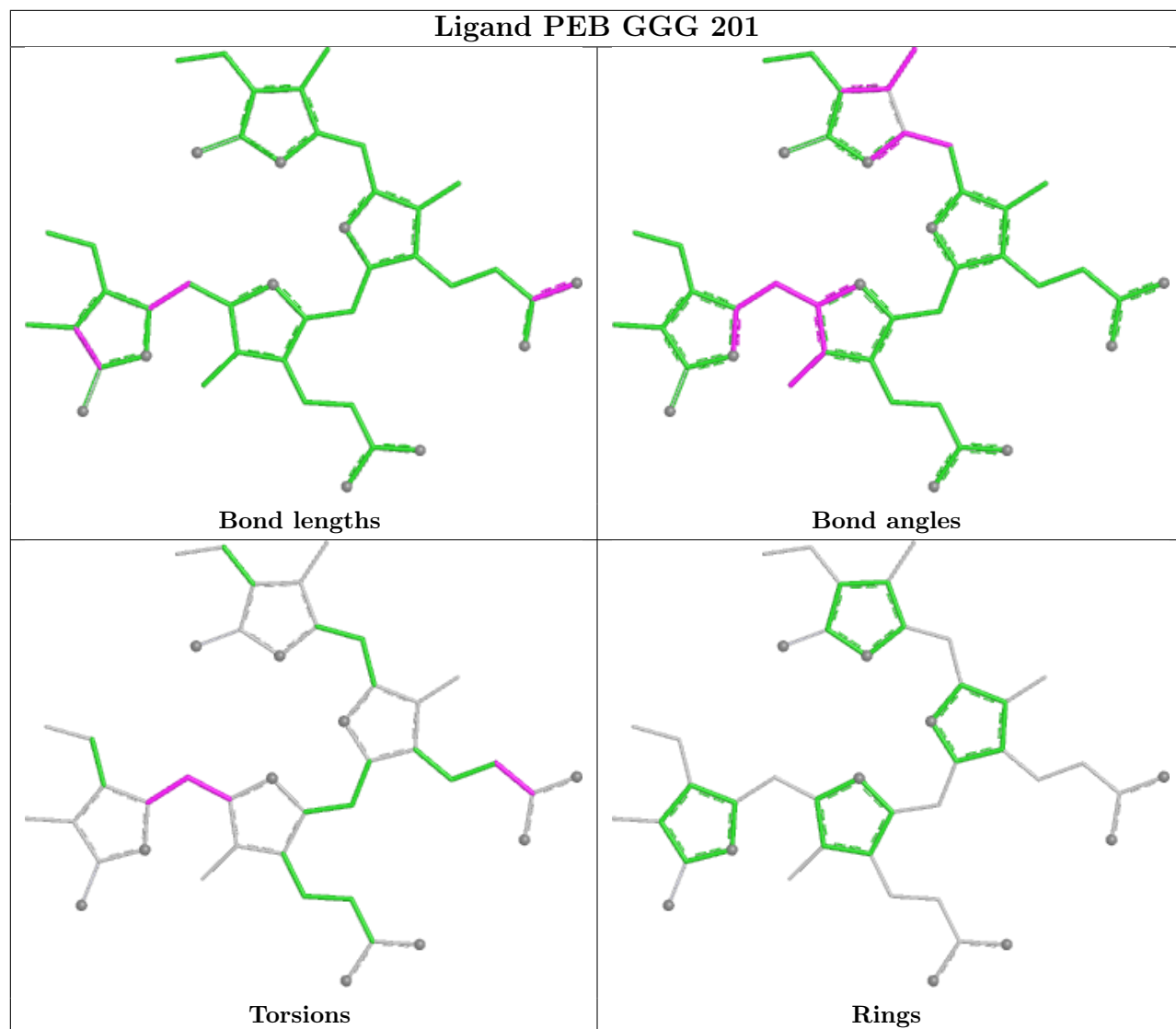


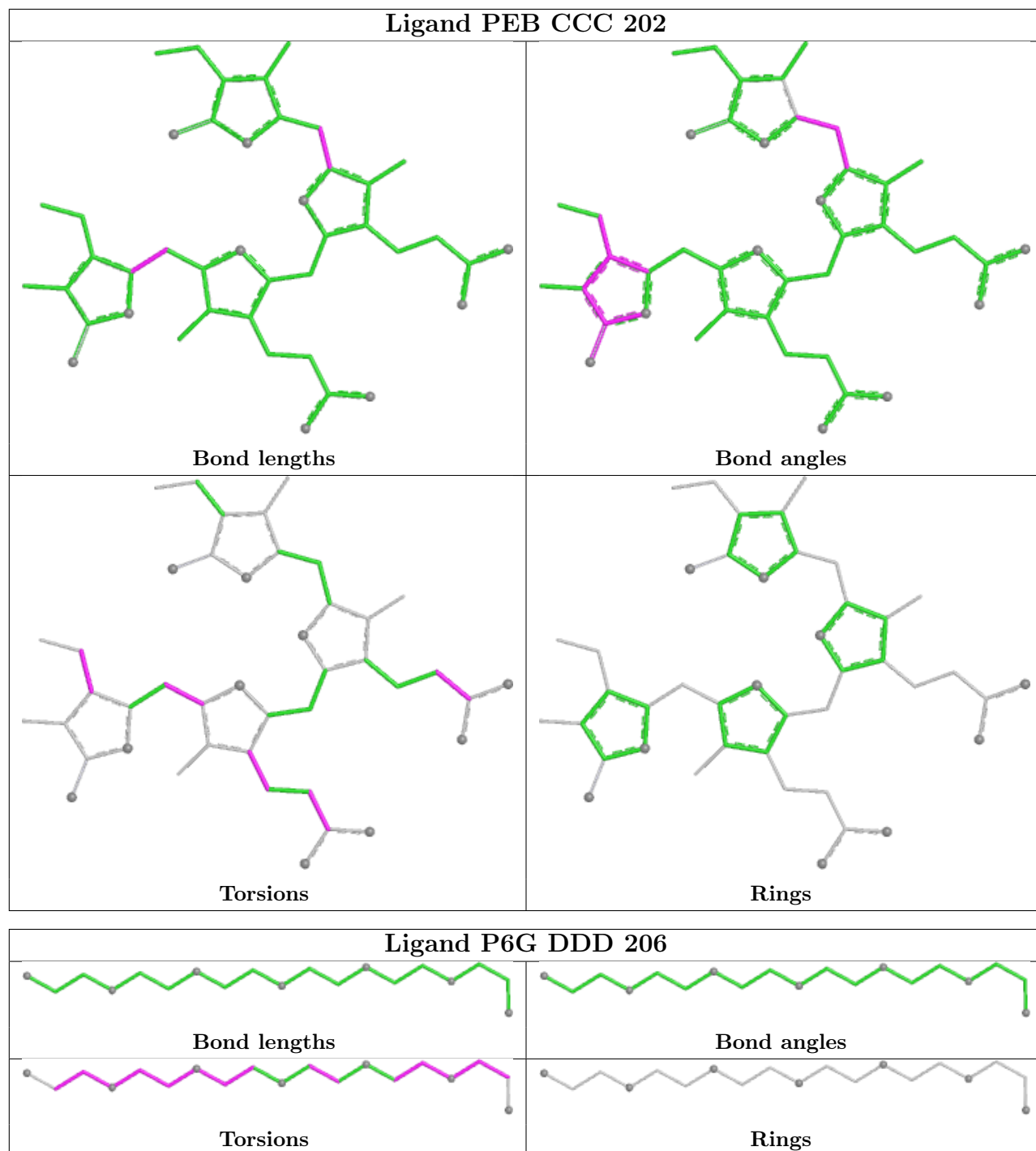
Rings

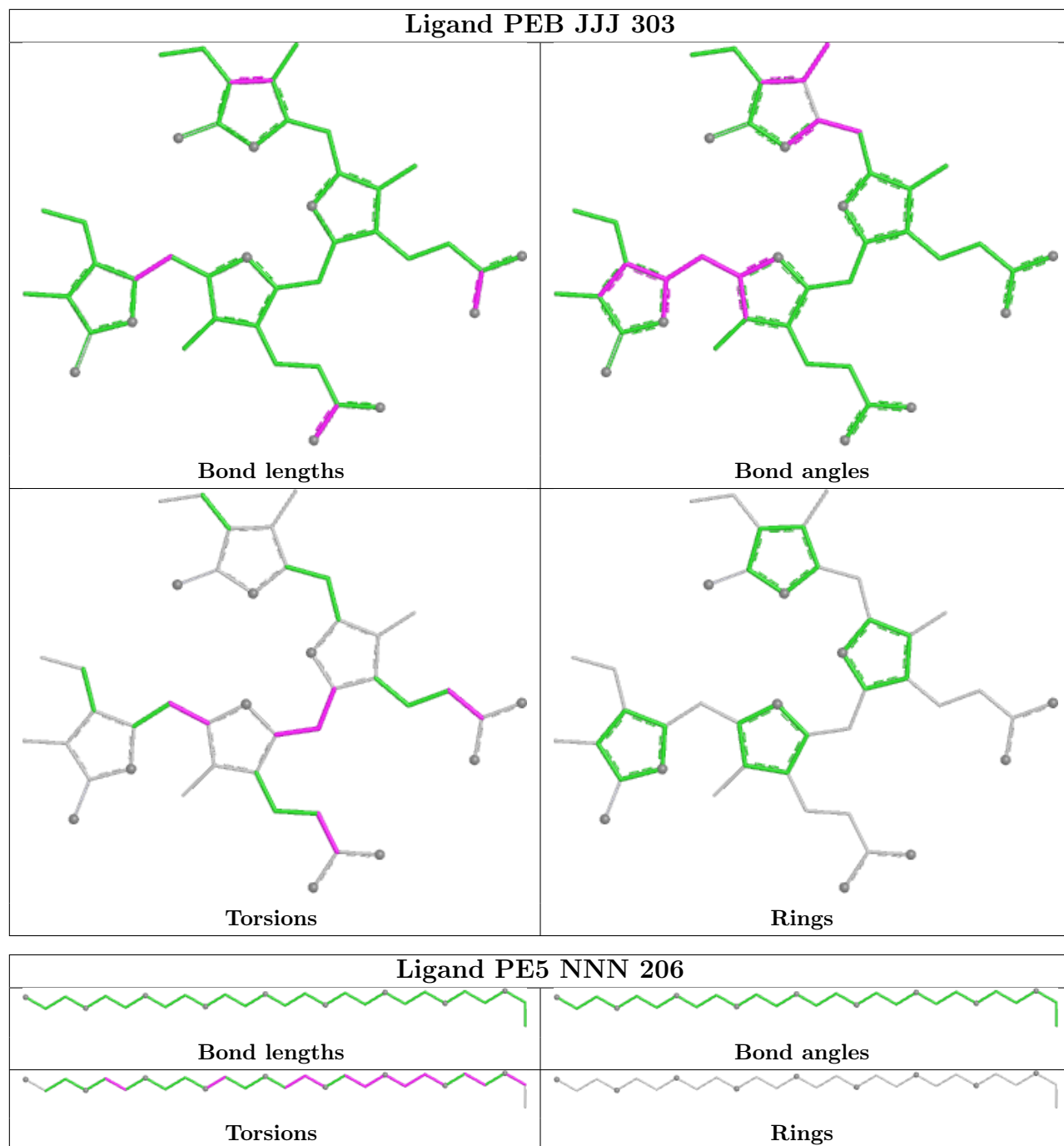
Ligand PEB HHH 302

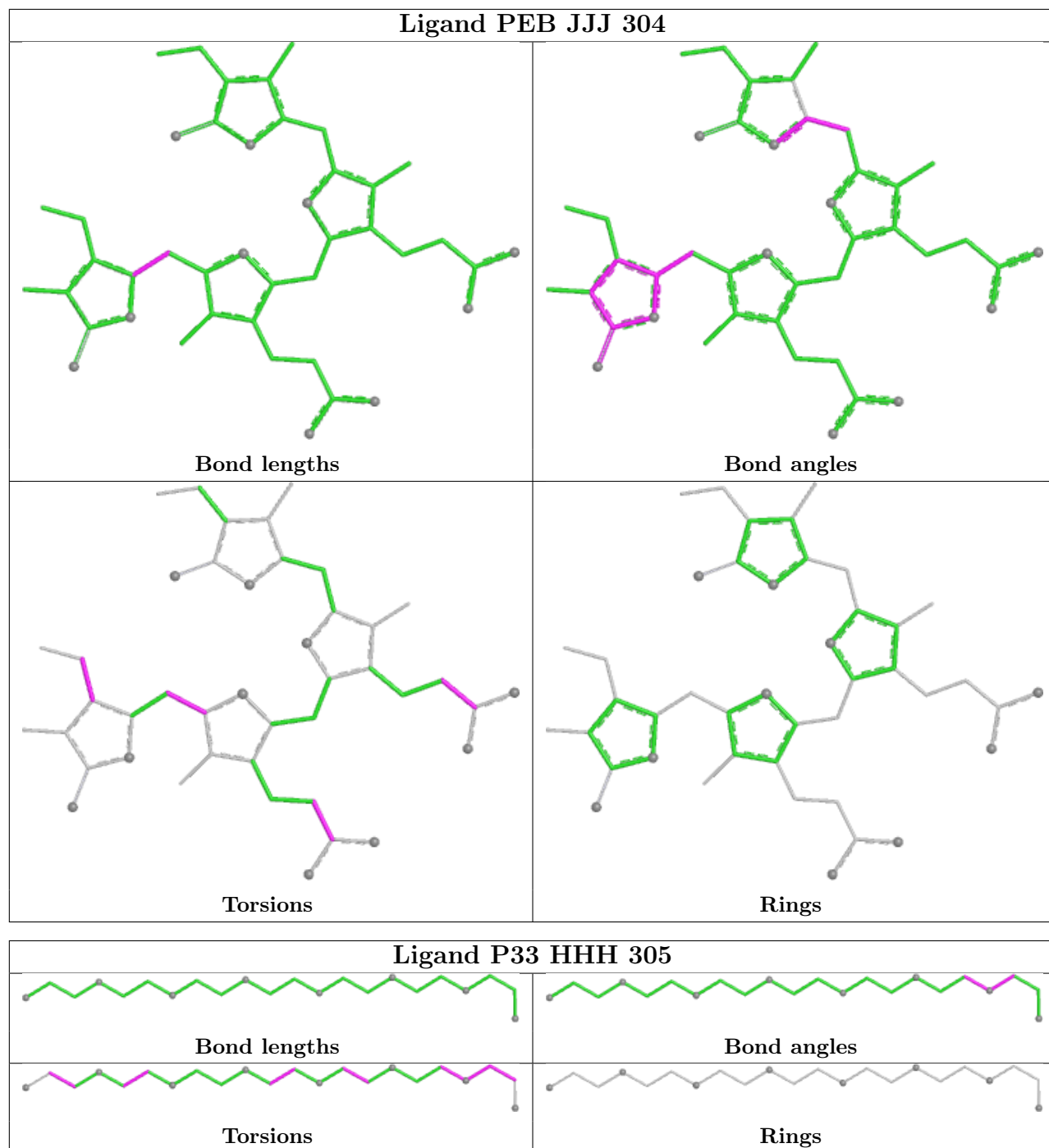


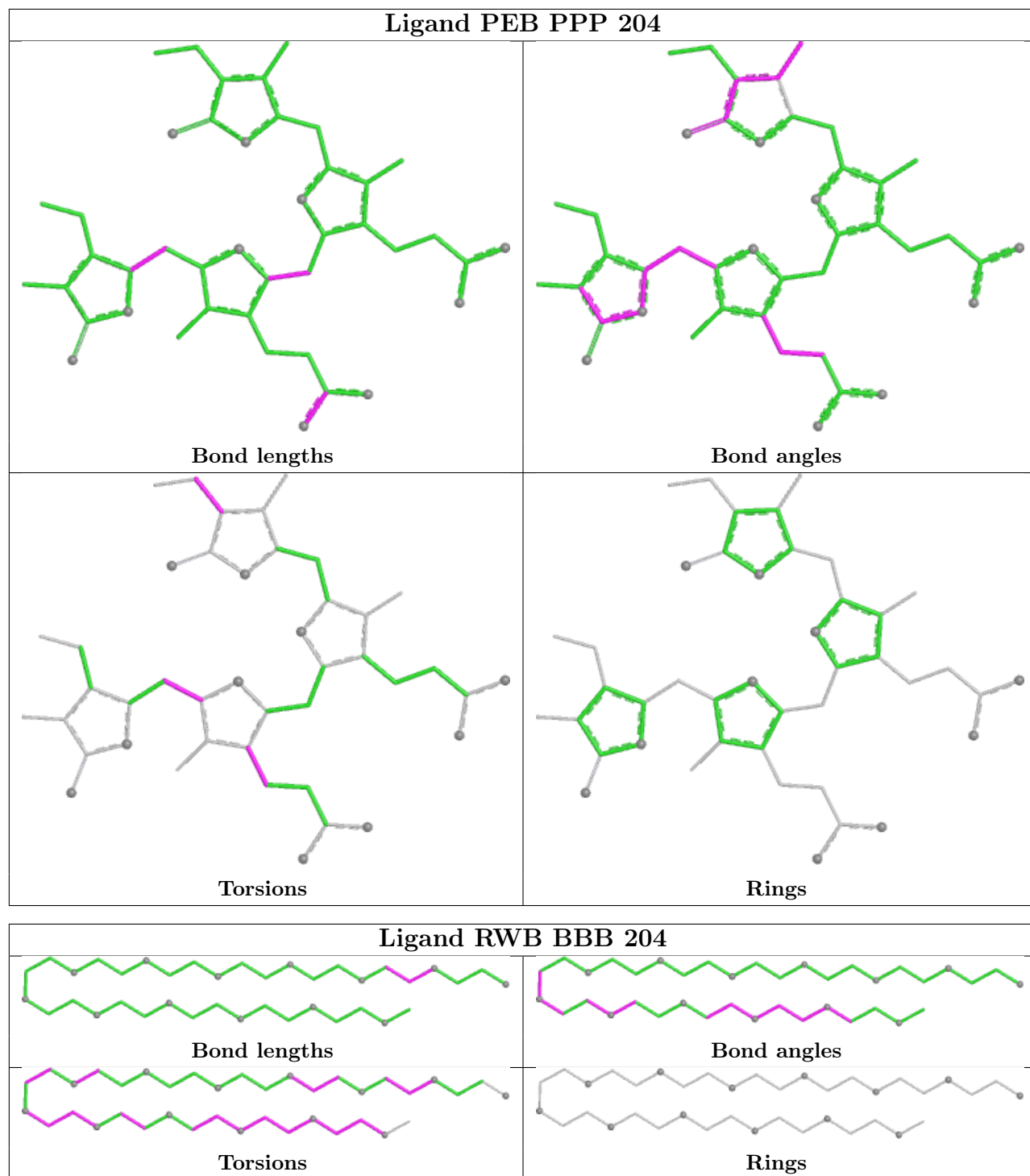
Ligand PEB GGG 201



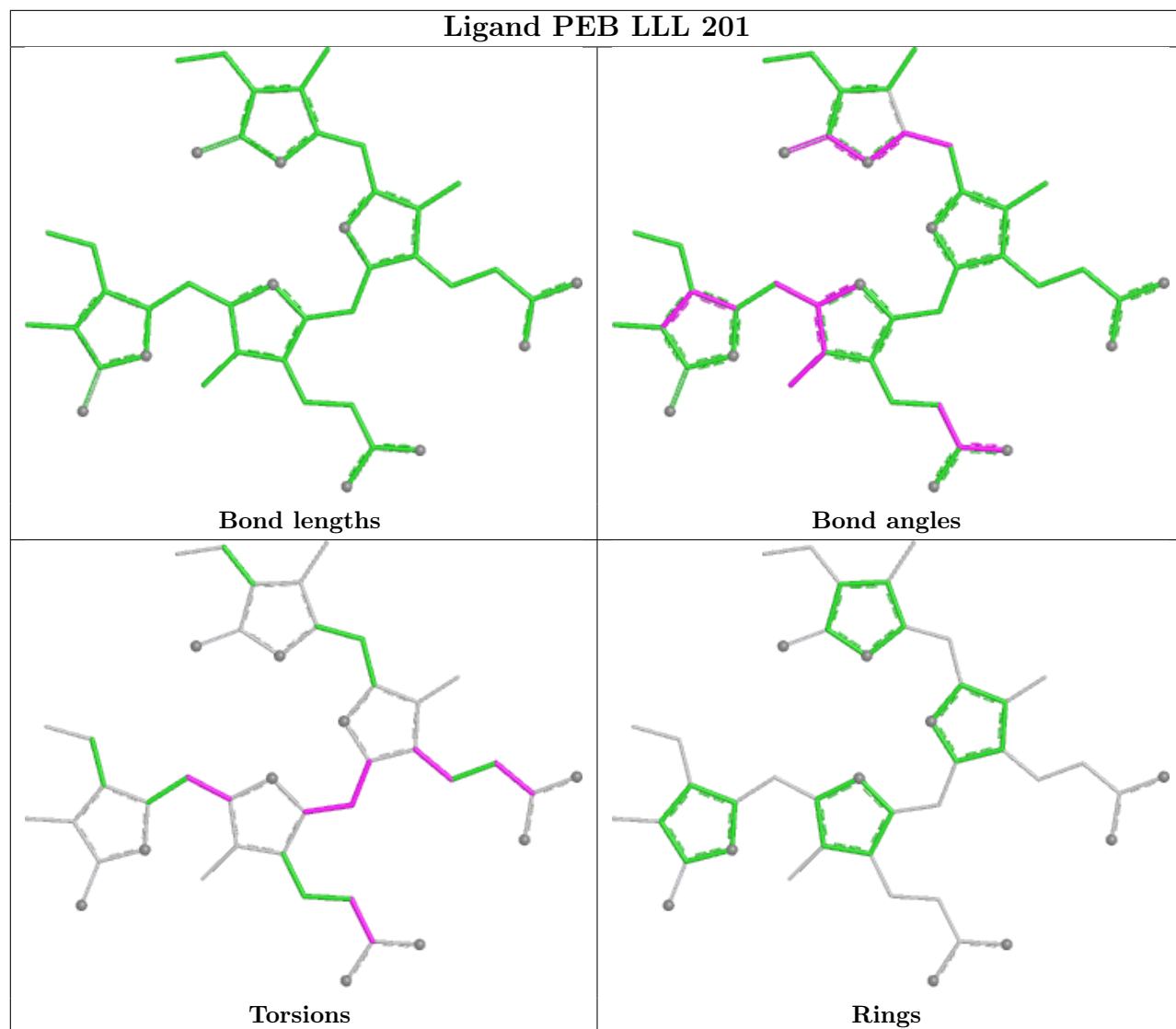




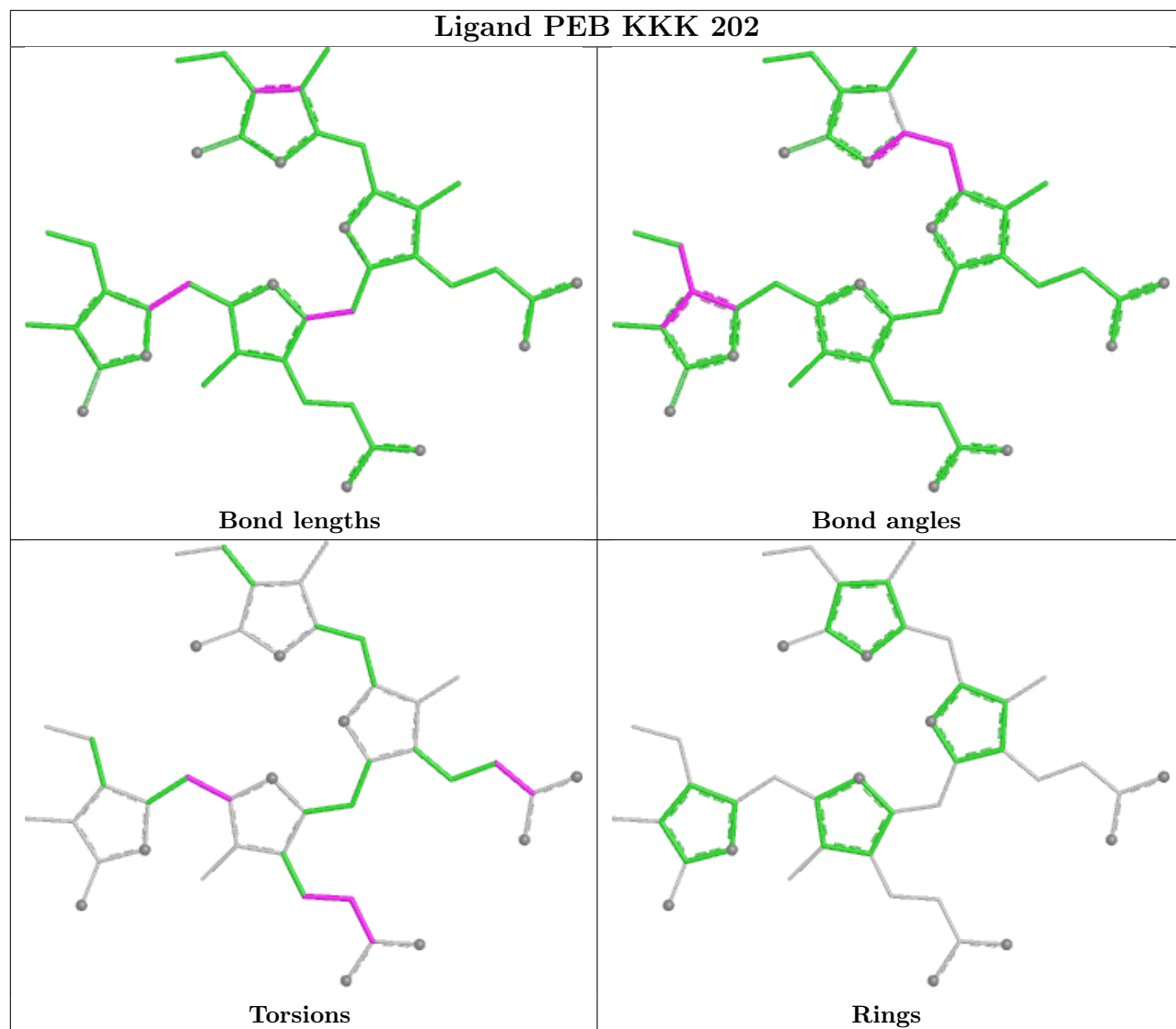




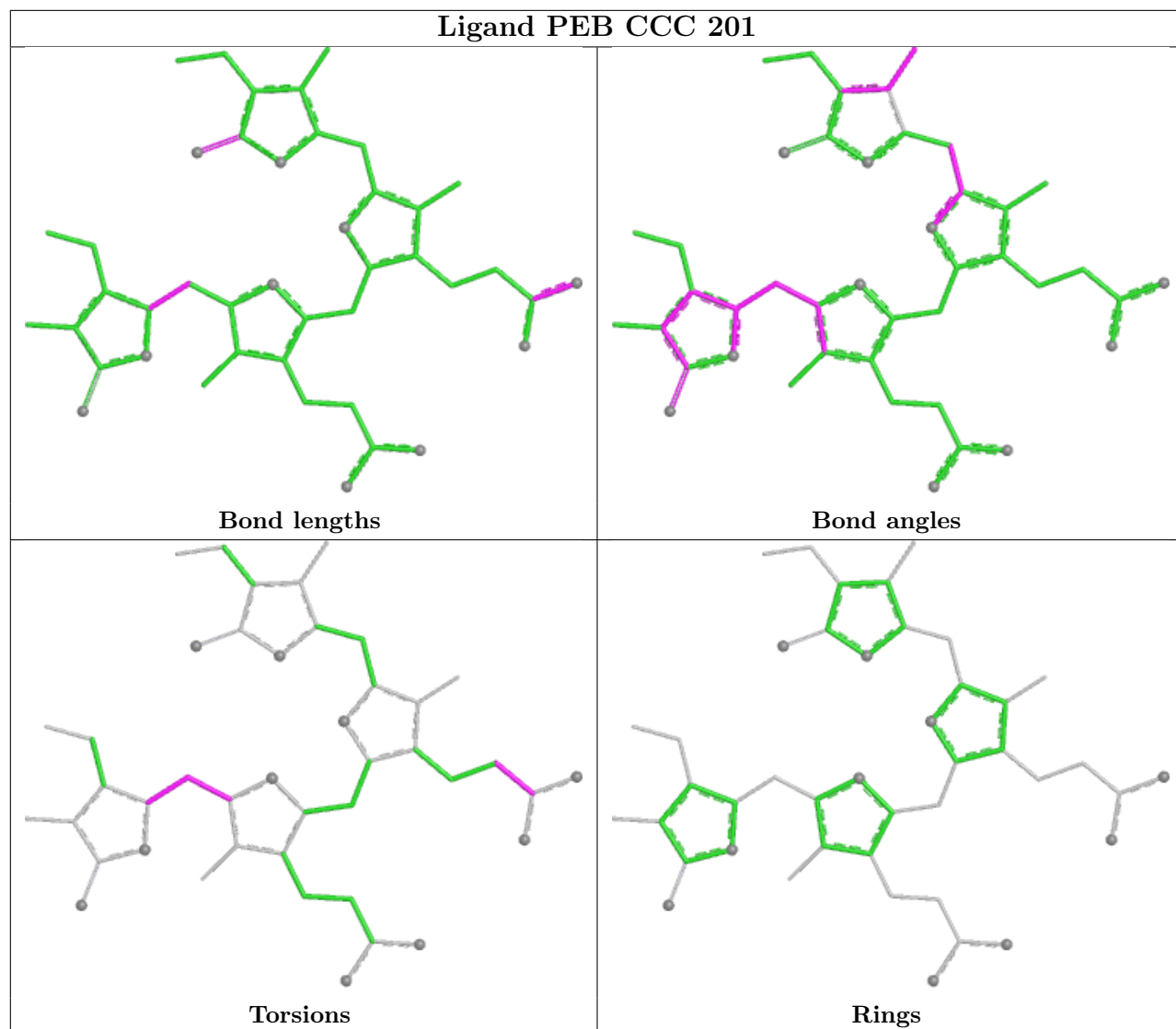
Ligand PEB LLL 201



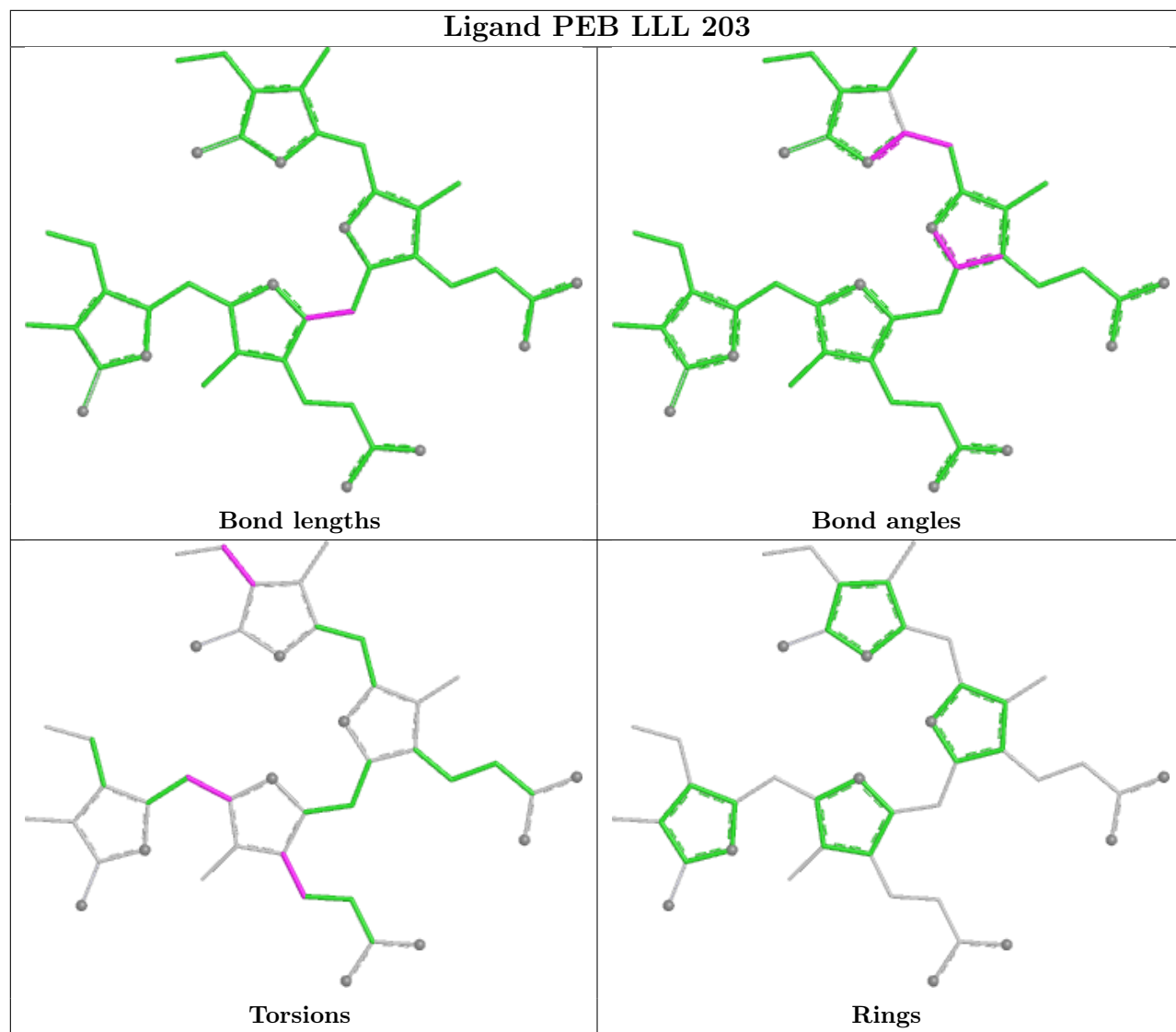
Ligand PEB KKK 202



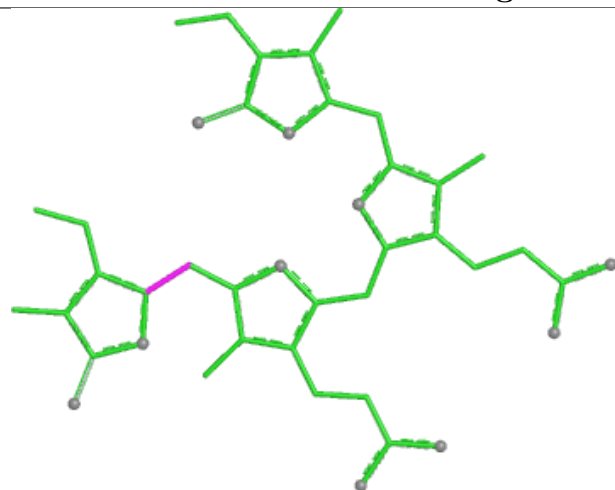
Ligand PEB CCC 201



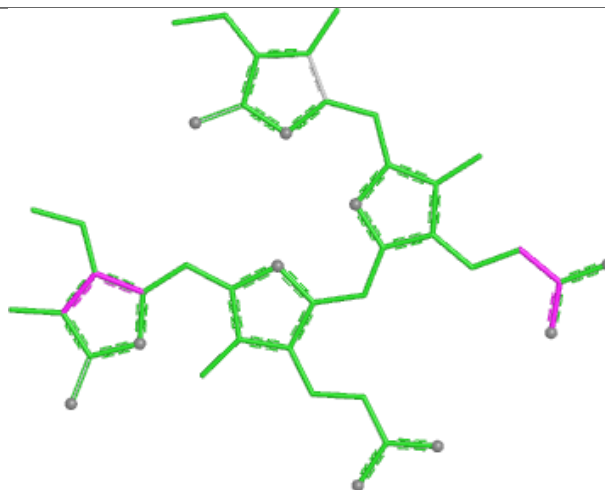
Ligand PEB LLL 203



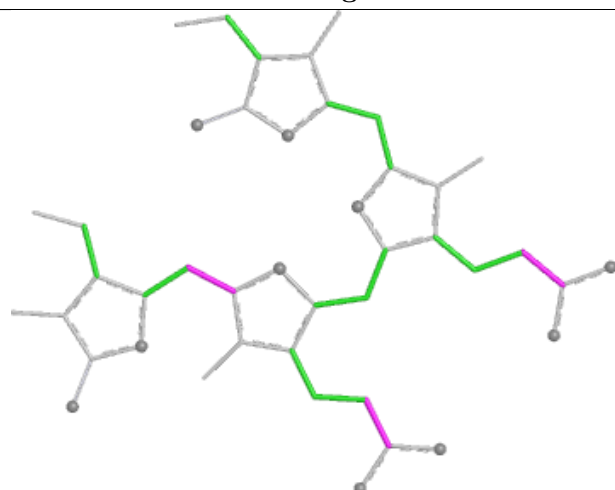
Ligand PEB FFF 205



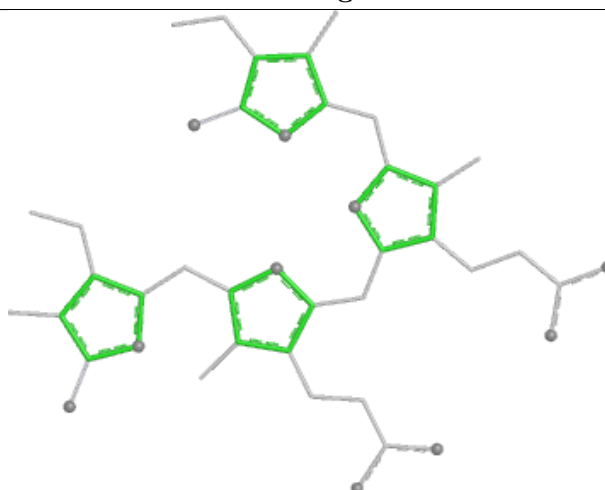
Bond lengths



Bond angles

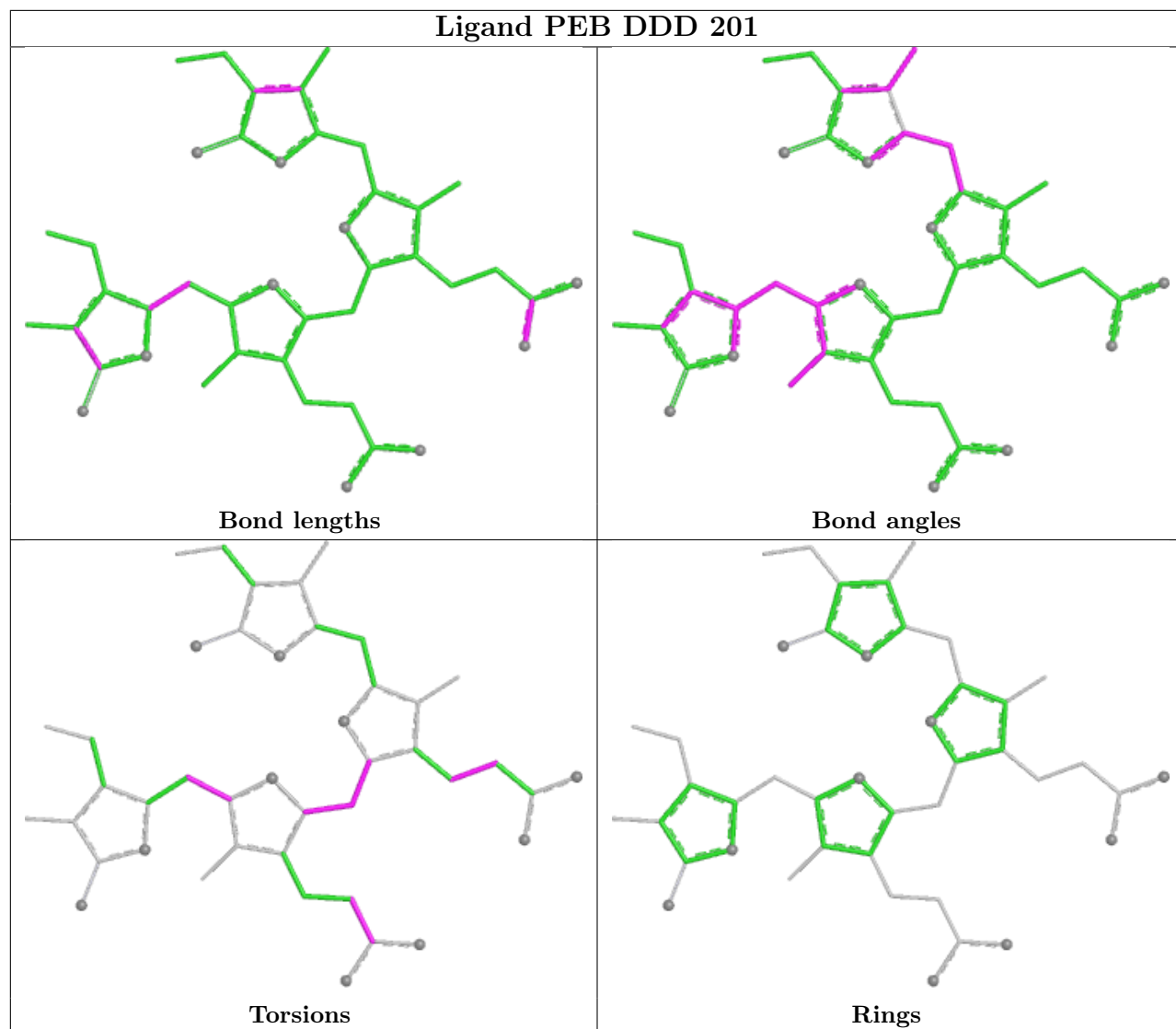


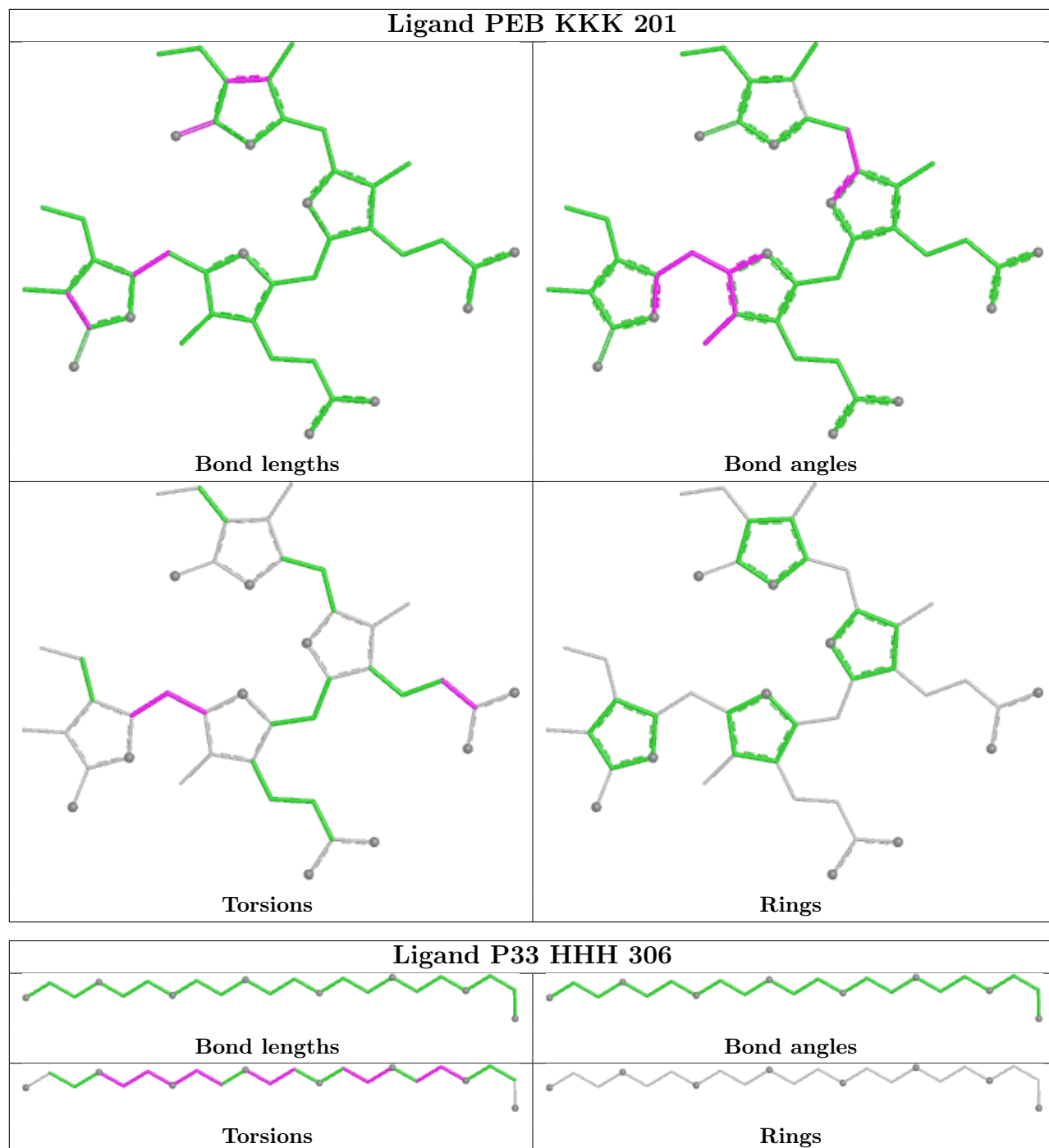
Torsions

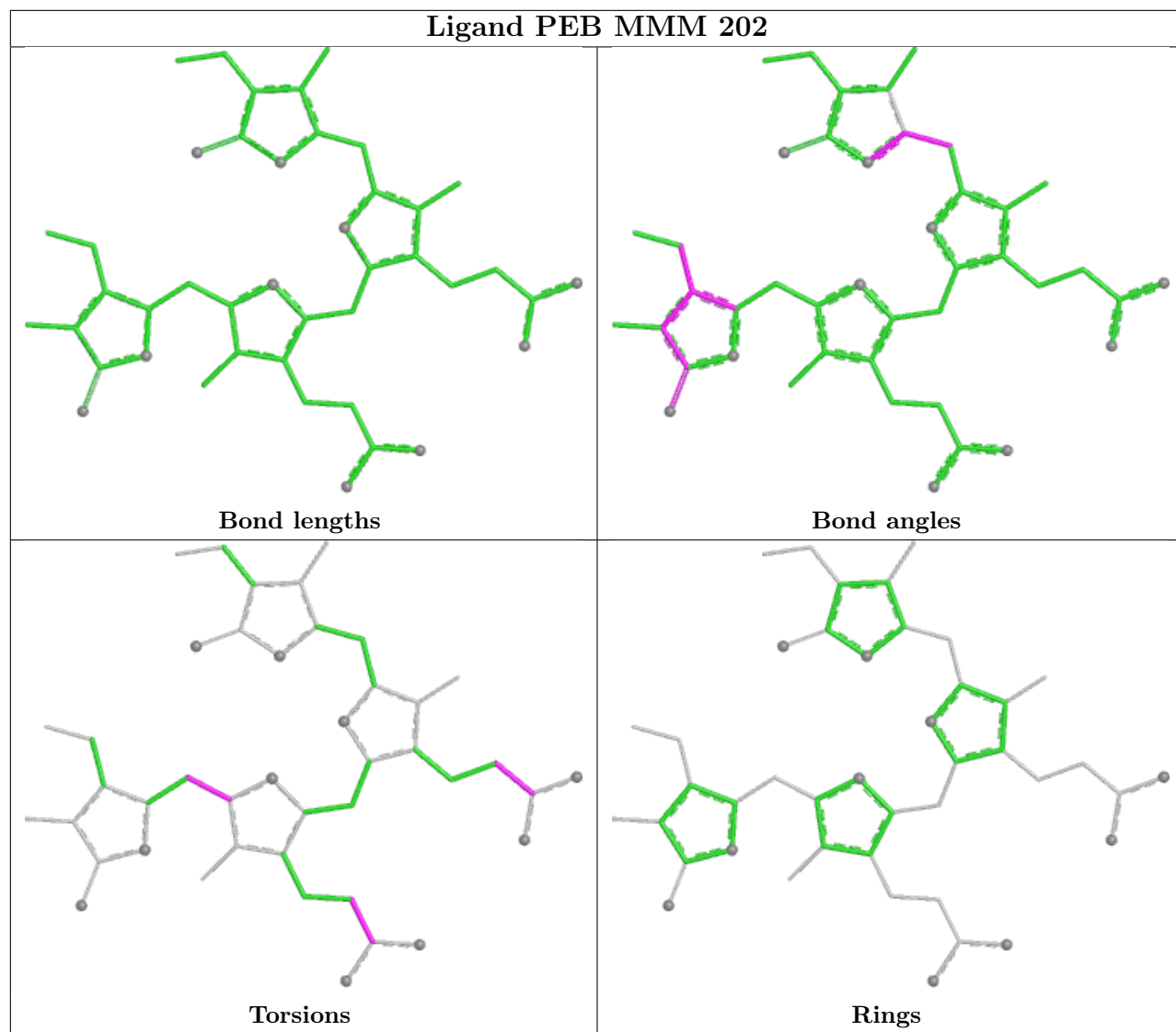


Rings

Ligand PEB DDD 201







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%)

All (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

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Mol	Chain	Res	Type	RSRZ
2	PPP	156	MET	4.4
2	LLL	184	SER	4.3
2	NNN	184	SER	4.2
2	PPP	150	GLY	3.9
2	PPP	184	SER	3.7
1	OOO	31	ILE	3.7
2	PPP	145	SER	3.5
1	OOO	4	VAL	3.5
2	PPP	143	THR	3.4
2	PPP	158	SER	3.4
2	PPP	161	VAL	3.4
2	JJJ	184	SER	3.4
2	PPP	31	SER	3.3
2	PPP	144	PRO	3.3
2	NNN	147	ALA	3.3
1	GGG	164	SER	3.2
2	PPP	157	GLY	3.0
2	PPP	155	LYS	2.8
1	OOO	11	ALA	2.6
2	HHH	28	PHE	2.6
2	PPP	28	PHE	2.6
2	FFF	28	PHE	2.6
2	PPP	148[A]	ARG	2.6
2	PPP	163	ASP	2.6
1	OOO	164	SER	2.5
1	OOO	29	GLY	2.5
2	PPP	160	VAL	2.4
2	JJJ	28	PHE	2.4
1	OOO	37	ARG	2.3
1	OOO	30	SER	2.3
1	OOO	161	ASN	2.3
2	LLL	167	SER	2.3
1	OOO	128	VAL	2.3
1	MMM	69	ALA	2.2
2	NNN	183	LEU	2.2
1	OOO	159	ALA	2.2
1	OOO	24	LEU	2.2
2	PPP	164	ARG	2.2
2	LLL	28	PHE	2.2
1	OOO	70	GLY	2.2
2	FFF	162	GLU	2.1
1	MMM	45	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	PPP	149	ALA	2.1
2	PPP	154	ARG	2.1
1	OOO	163	LEU	2.1
2	FFF	184	SER	2.1
1	OOO	115	GLU	2.1
1	OOO	27	VAL	2.1
1	OOO	119	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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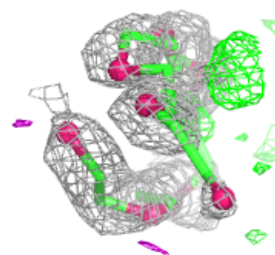
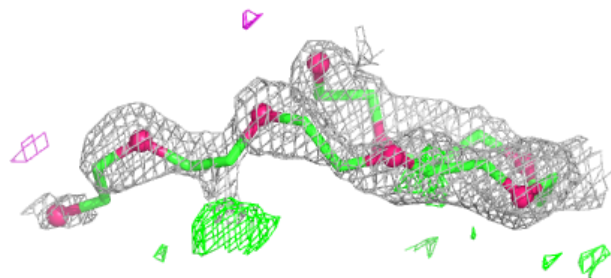
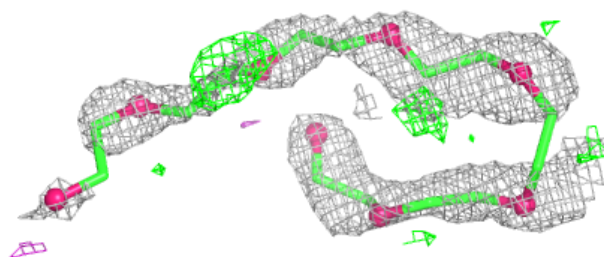
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEB	HHH	302	43/43	0.95	0.07	33,37,44,63	0
3	PEB	HHH	303	43/43	0.95	0.08	37,41,51,58	0
3	PEB	CCC	202	43/43	0.95	0.07	34,41,47,50	0
3	PEB	JJJ	303	43/43	0.95	0.07	34,38,49,75	0
3	PEB	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
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

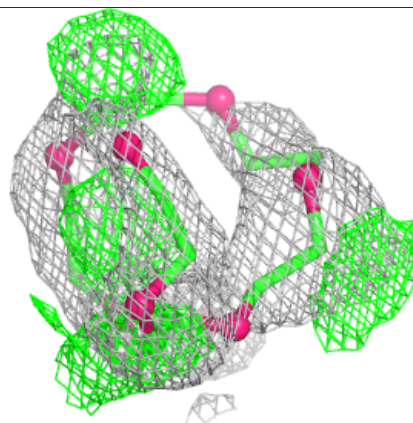
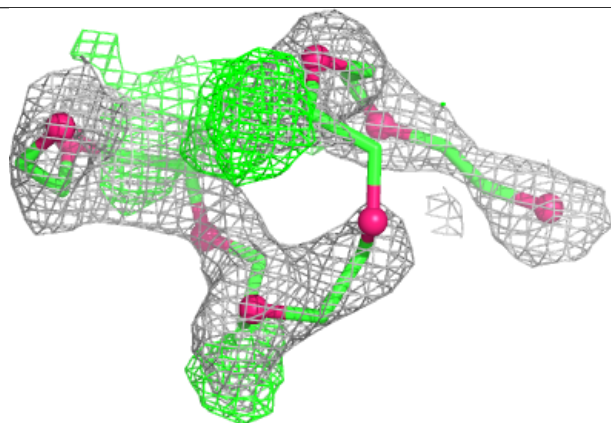
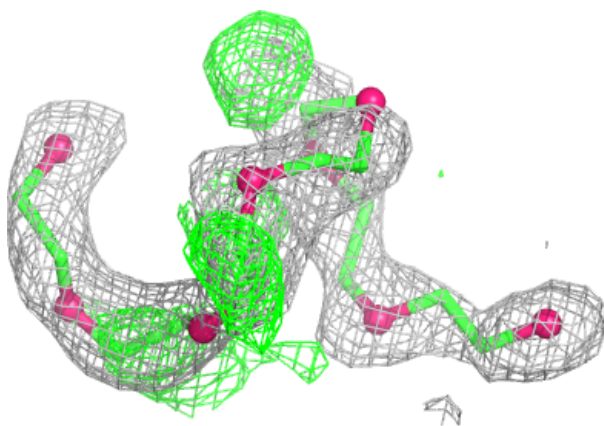
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

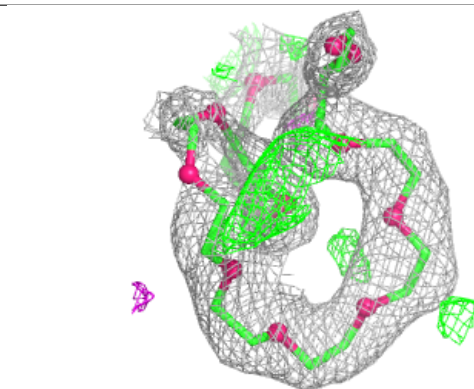
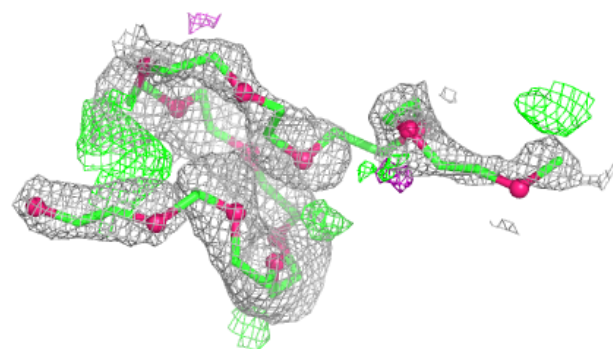
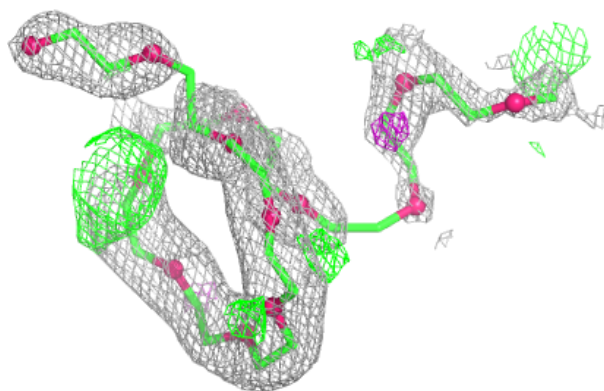
**Electron density around P33 HHH 306:**

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

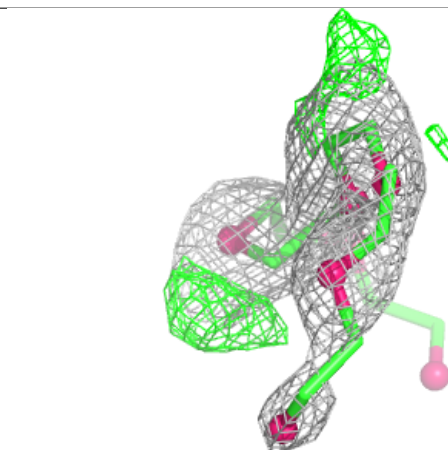
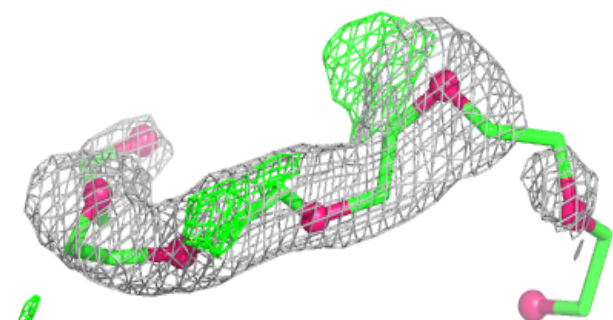
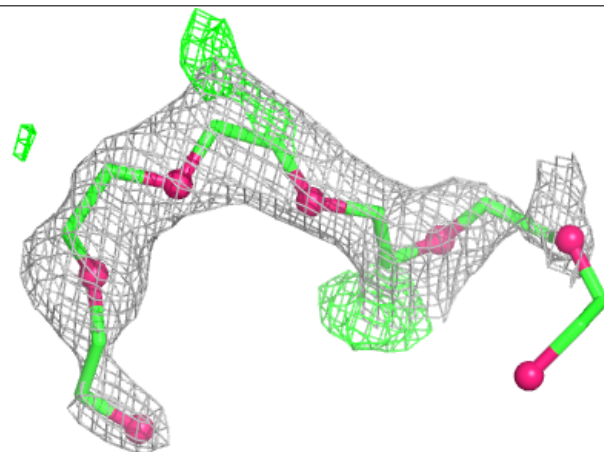


Electron density around RWB BBB 204:

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

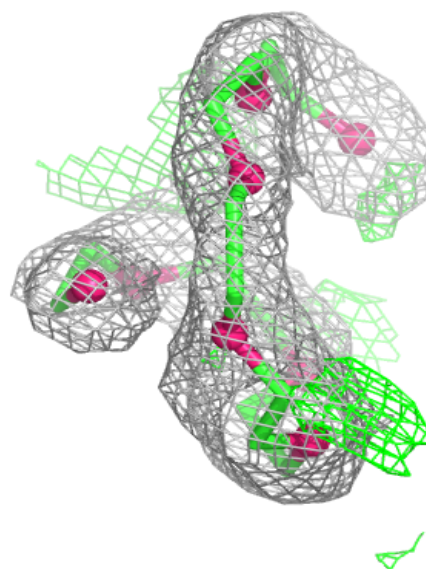
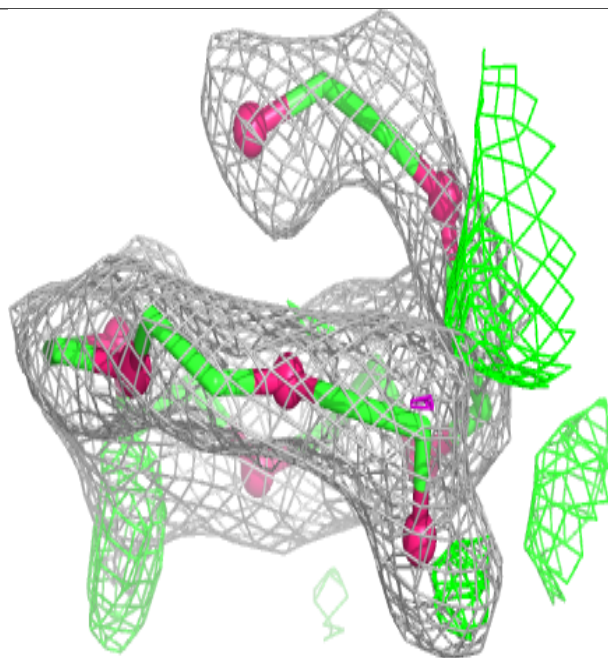
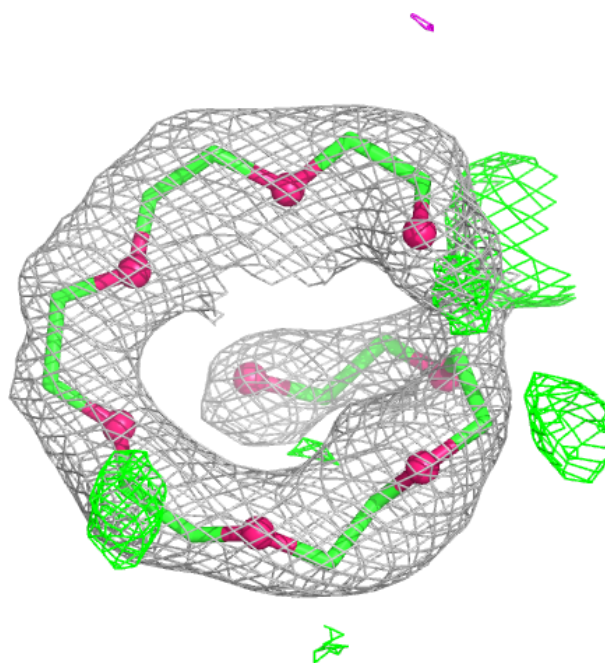
**Electron density around P6G DDD 206:**

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



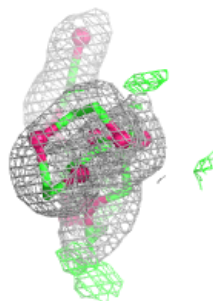
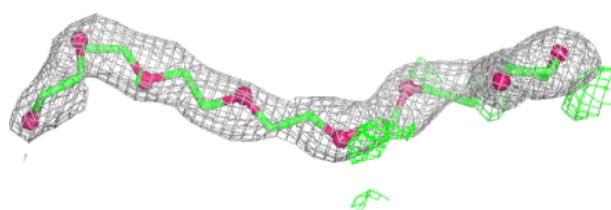
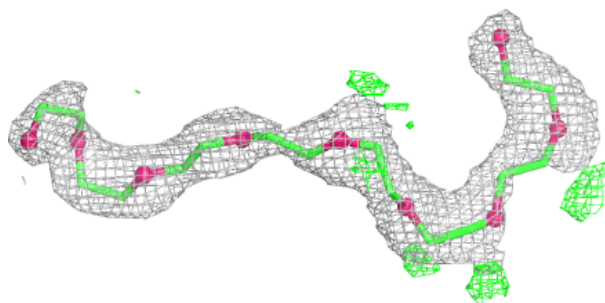
Electron density around P33 FFF 207:

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

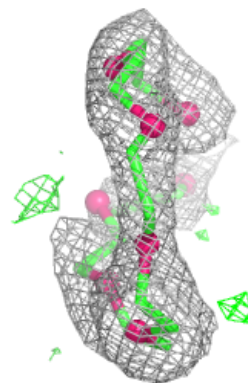
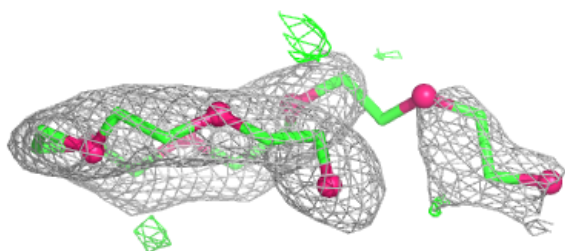
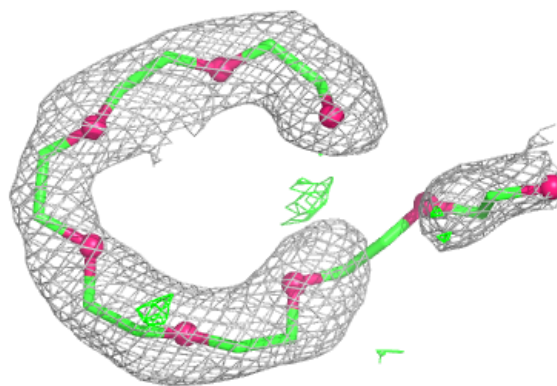


Electron density around PE8 BBB 205:

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

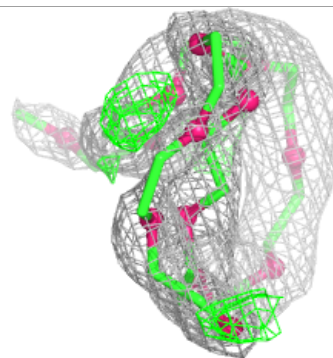
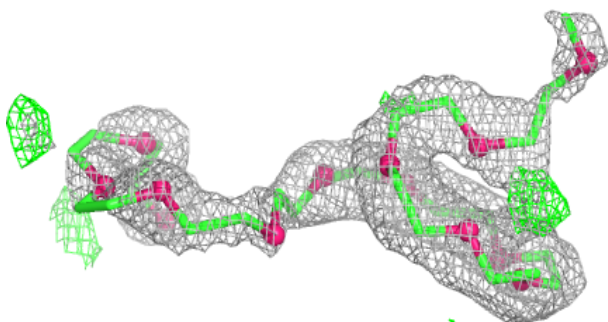
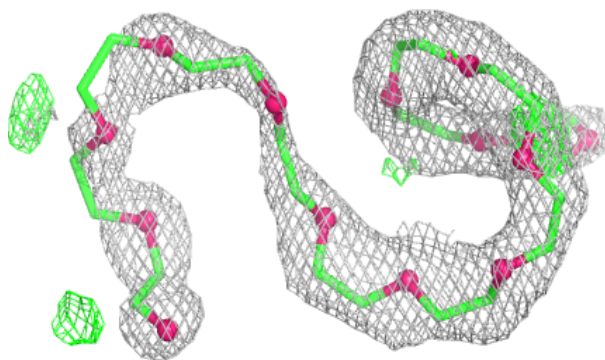
**Electron density around P33 JJJ 306:**

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

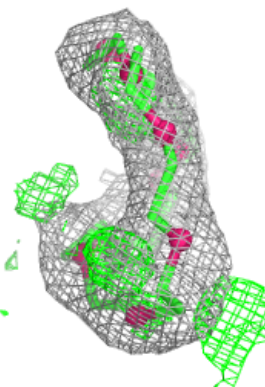
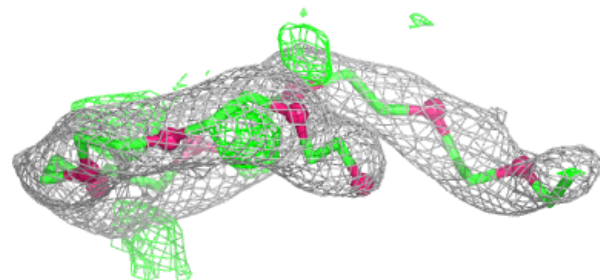
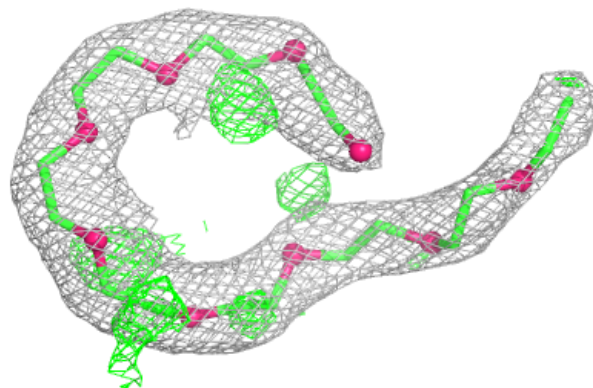


Electron density around RWB LLL 204:

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

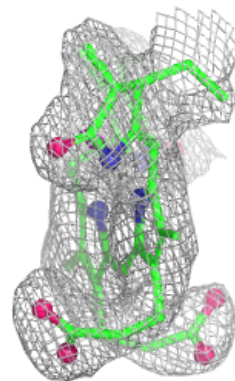
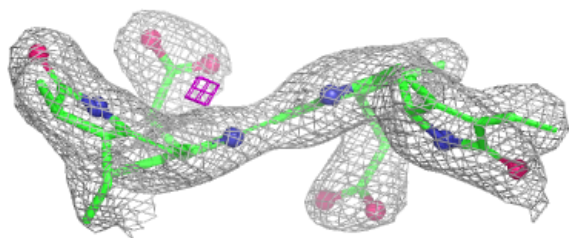
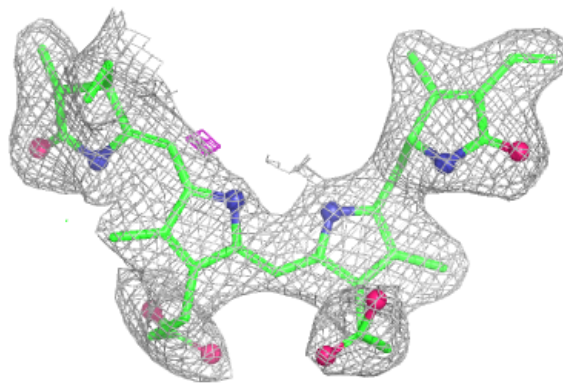
**Electron density around PE5 NNN 206:**

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



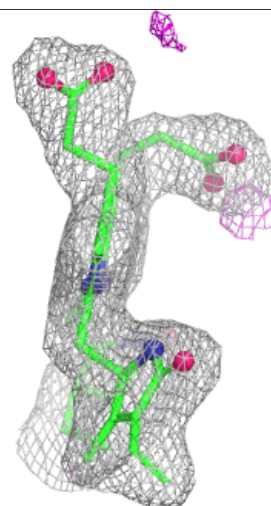
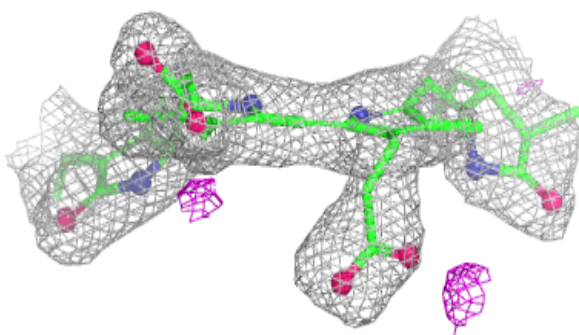
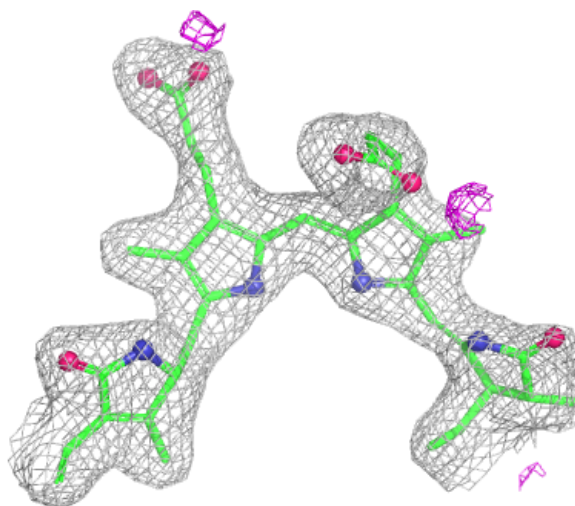
Electron density around PEB OOO 202:

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



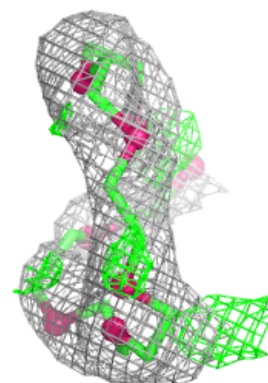
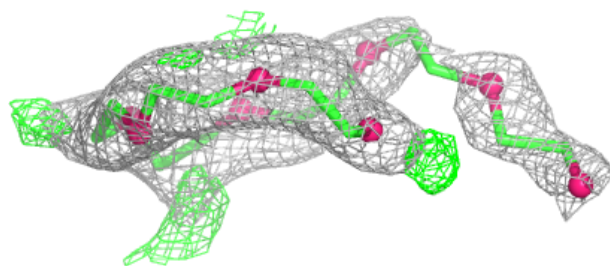
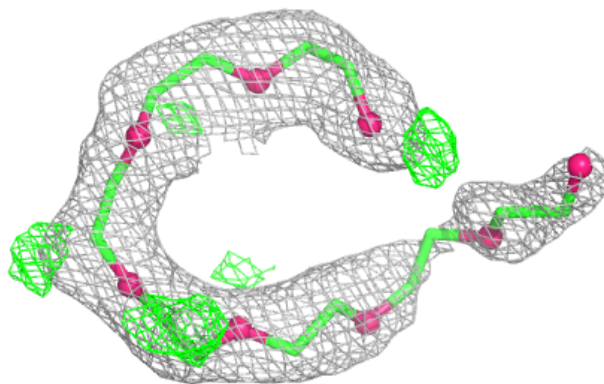
Electron density around PEB PPP 204:

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



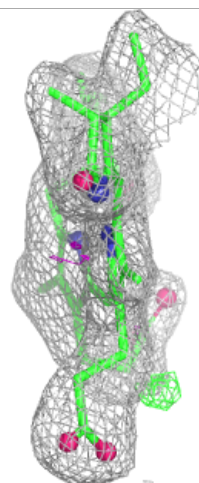
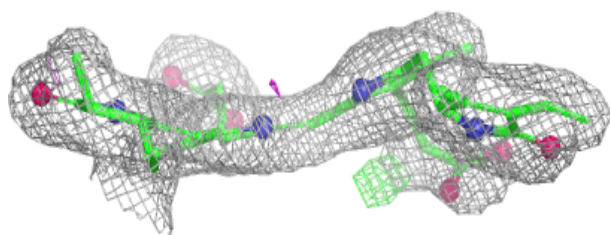
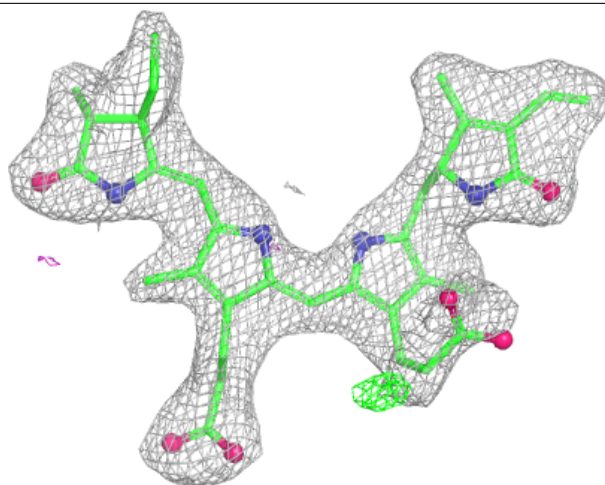
Electron density around P33 DDD 204:

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



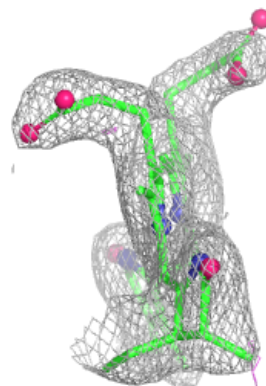
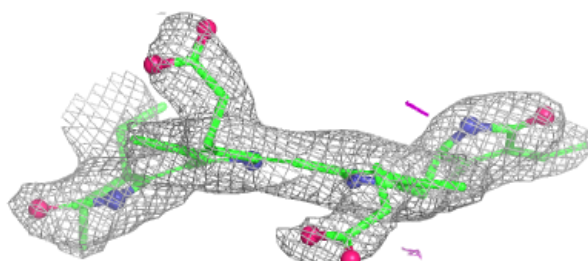
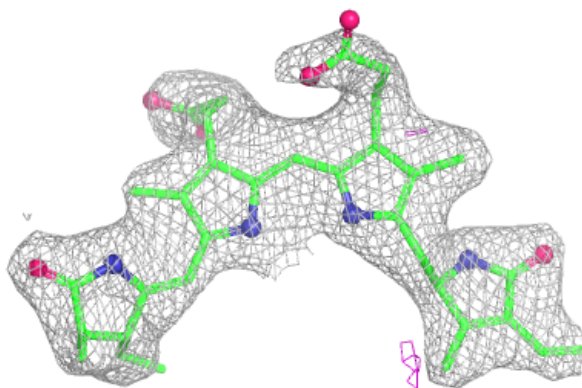
Electron density around PEB PPP 202:

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

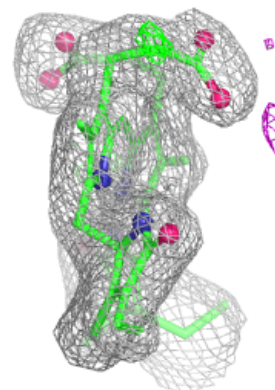
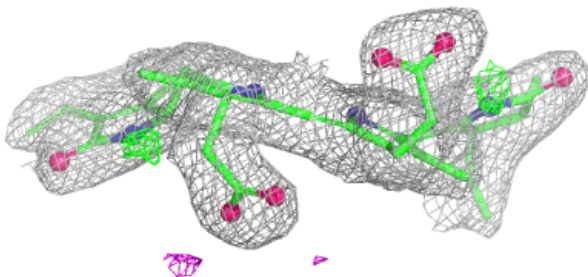
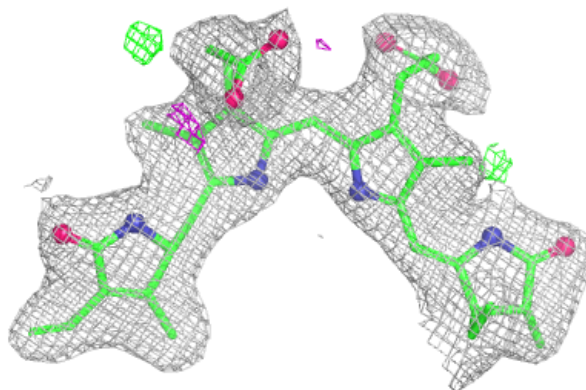


Electron density around PEB PPP 203:

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

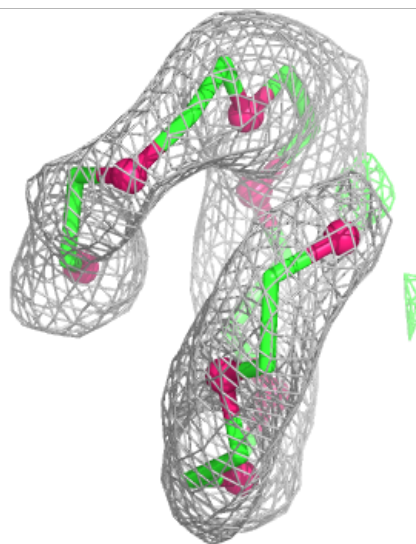
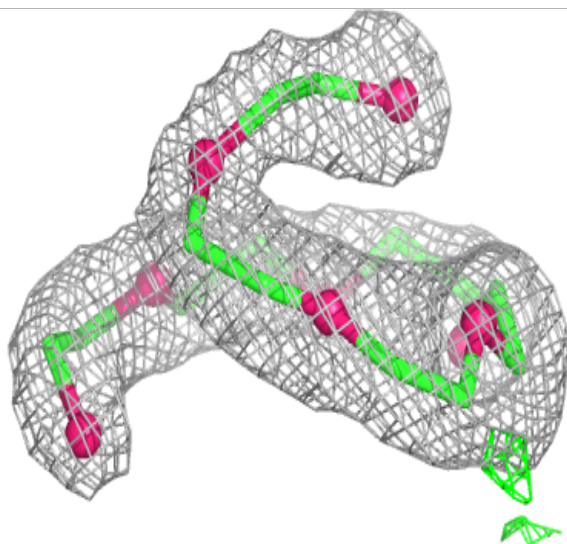
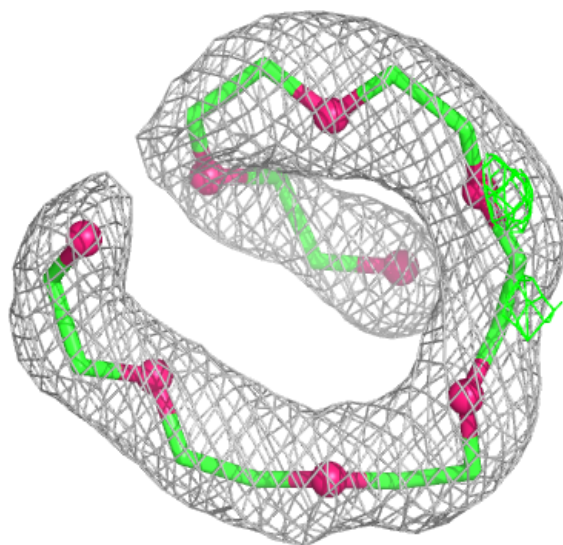
**Electron density around PEB III 203:**

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



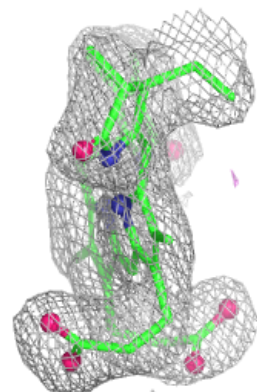
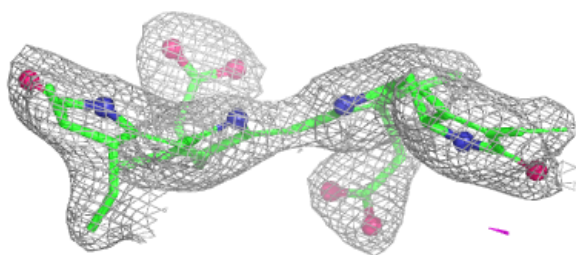
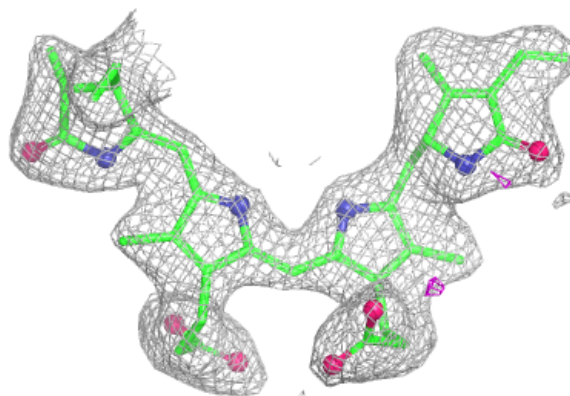
Electron density around P33 HHH 305:

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



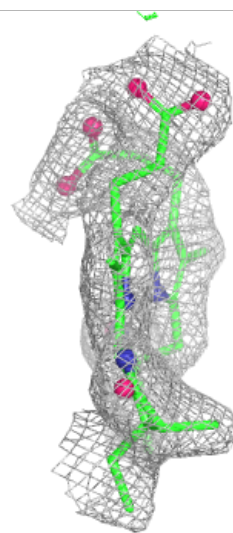
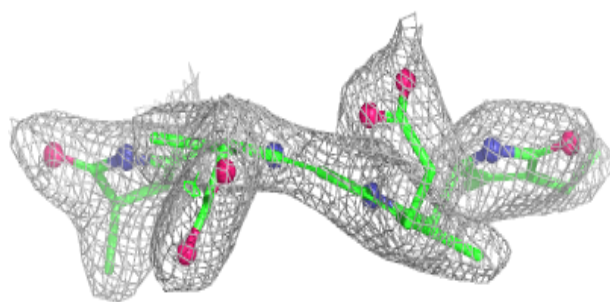
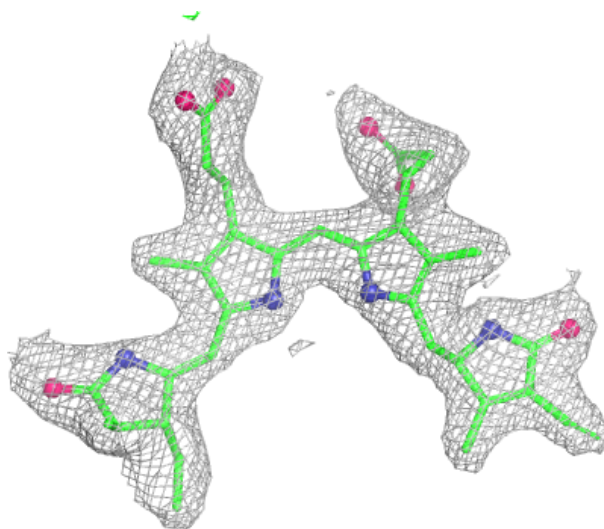
Electron density around PEB KKK 202:

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



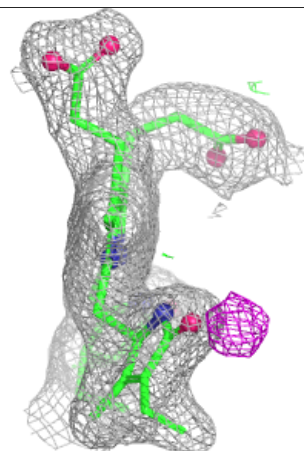
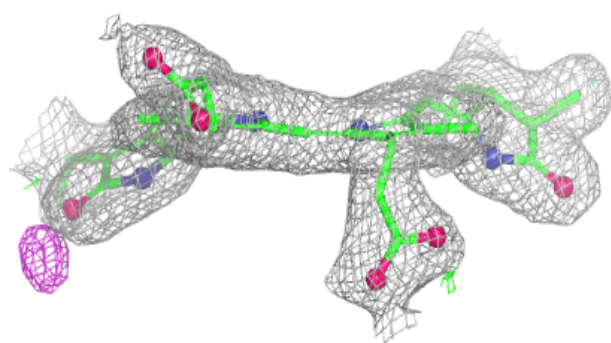
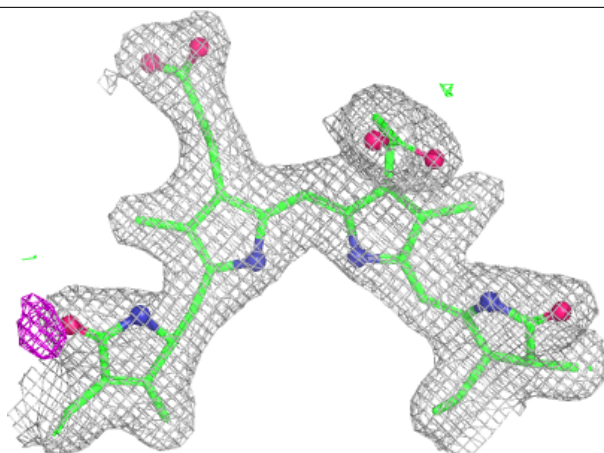
Electron density around PEB OOO 201:

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

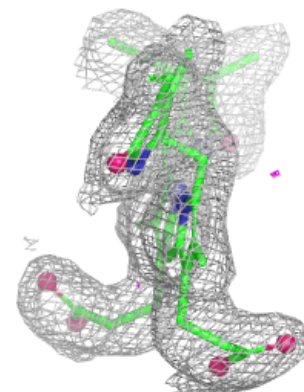
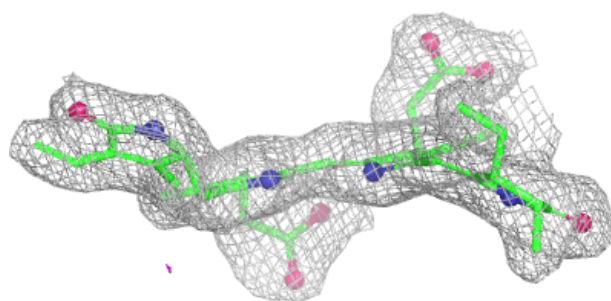
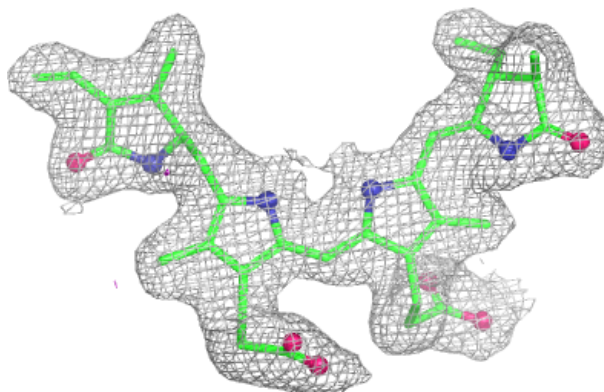


Electron density around PEB FFF 206:

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

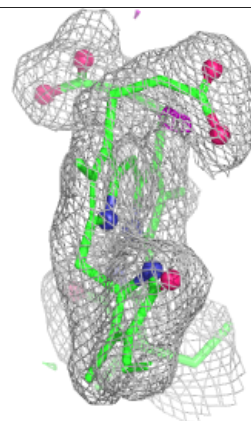
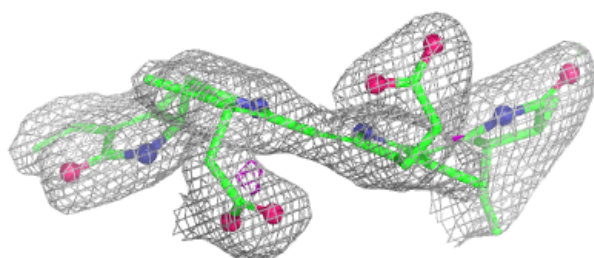
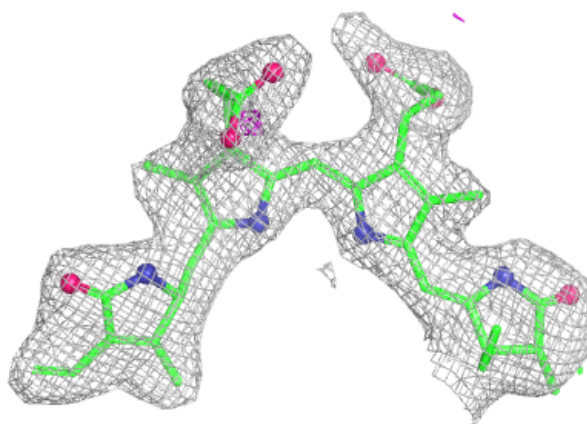
**Electron density around PEB BBB 202:**

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

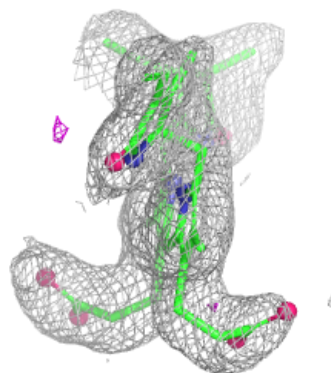
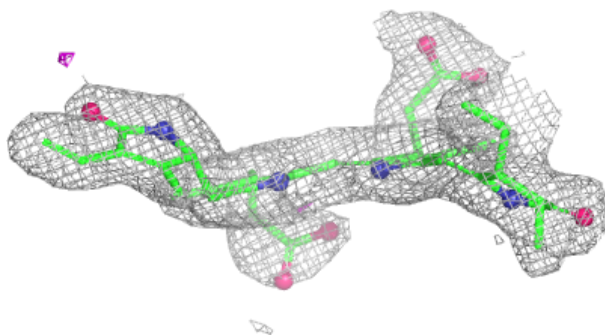
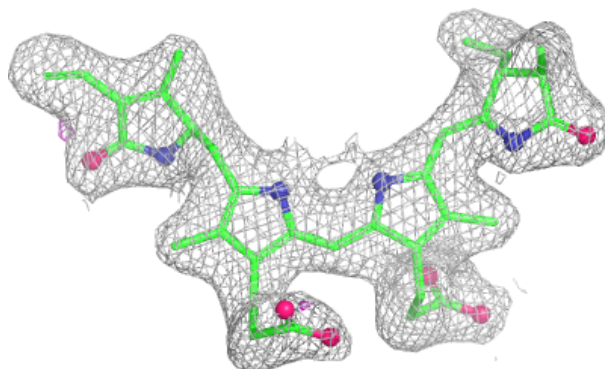


Electron density around PEB EEE 202:

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

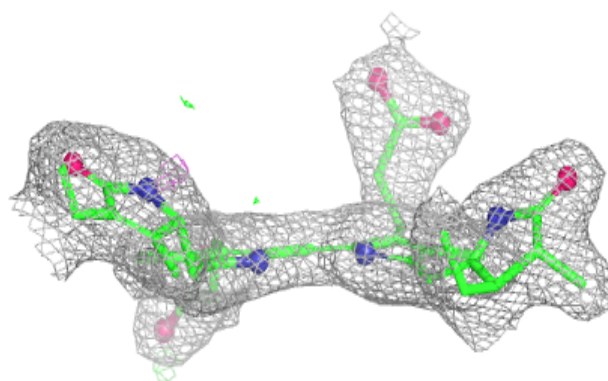
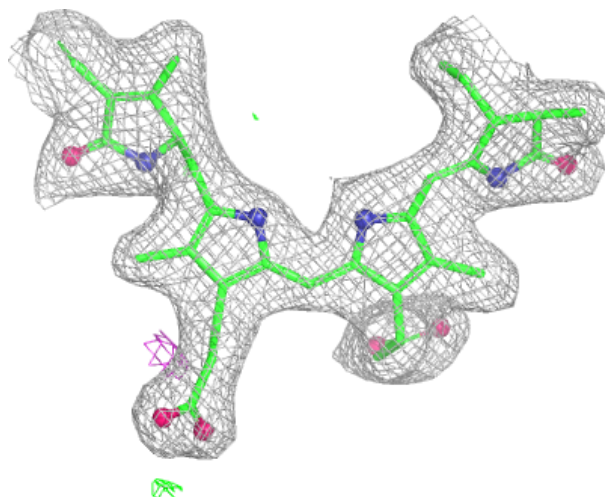
**Electron density around PEB LLL 202:**

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



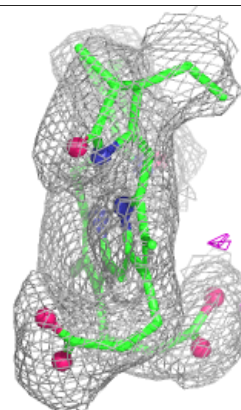
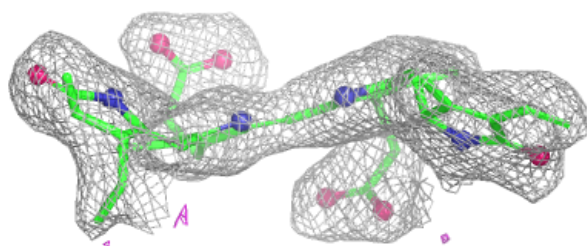
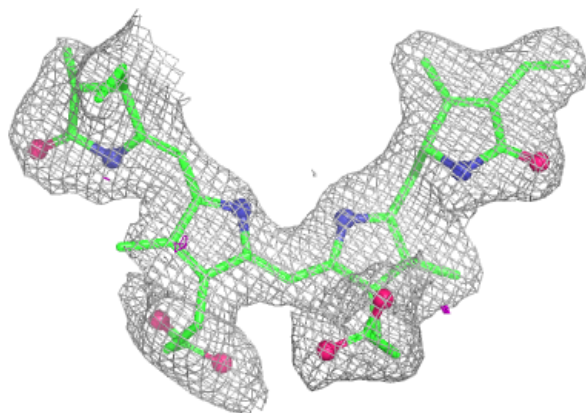
Electron density around PEB LLL 203:

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



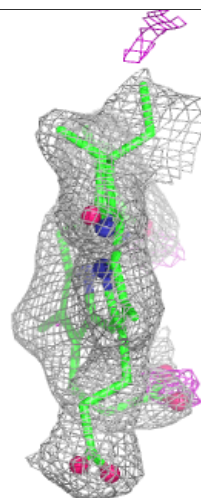
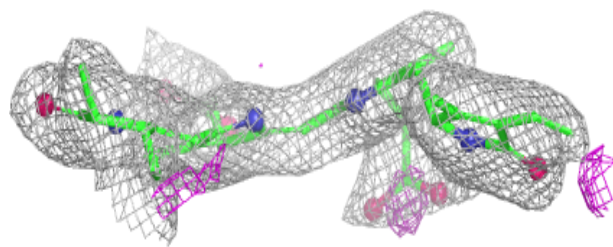
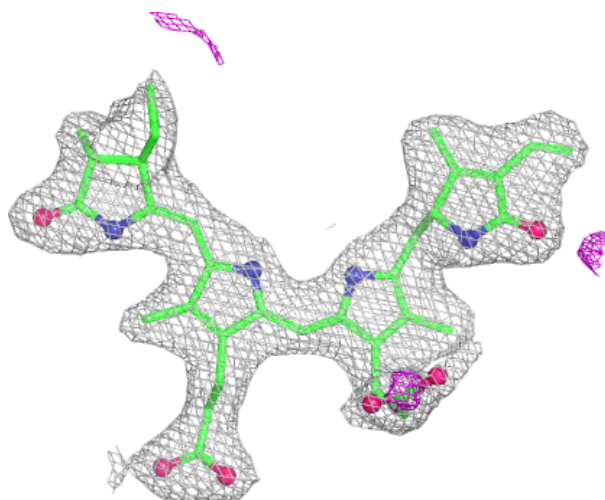
Electron density around PEB MMM 202:

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



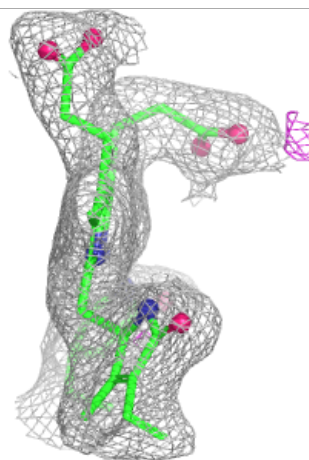
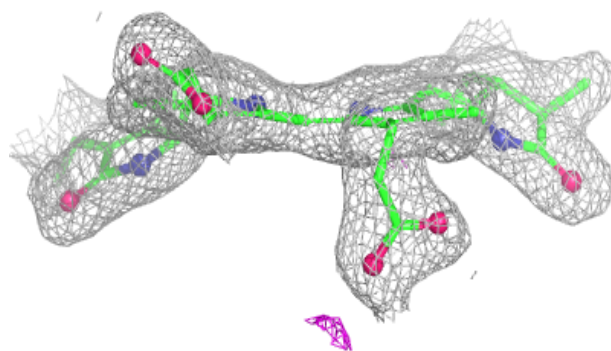
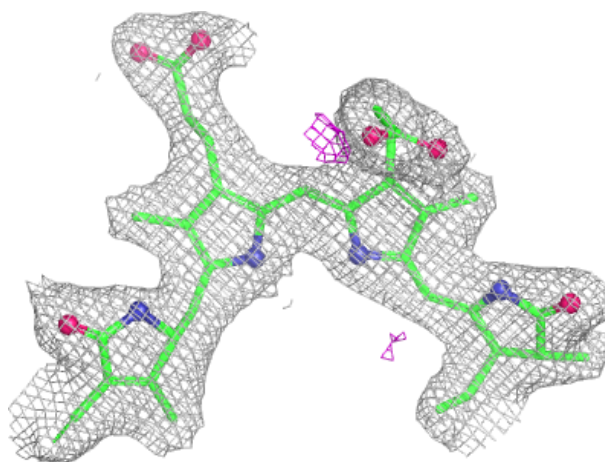
Electron density around PEB NNN 203:

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



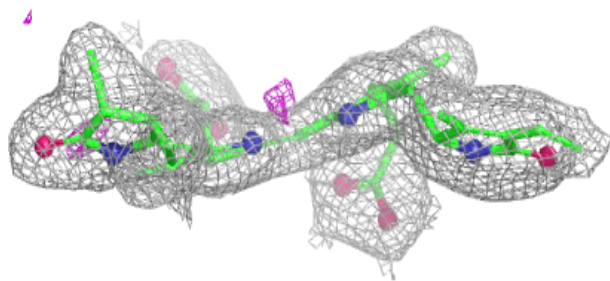
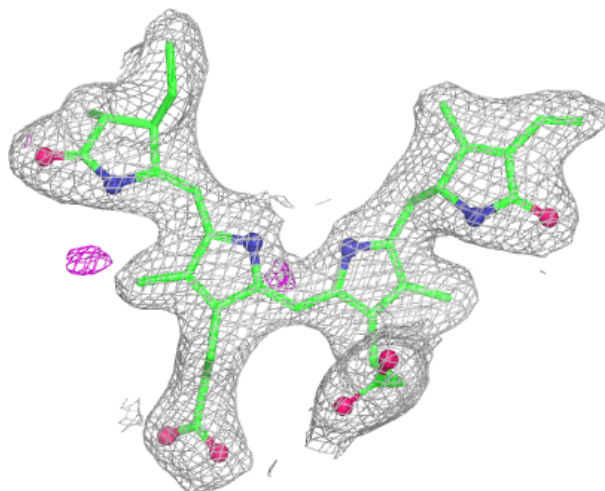
Electron density around PEB NNN 205:

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



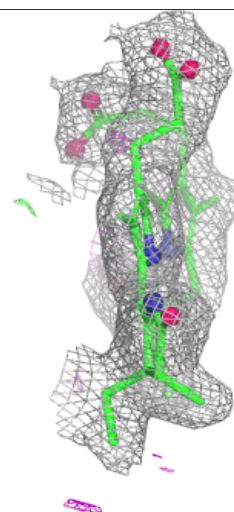
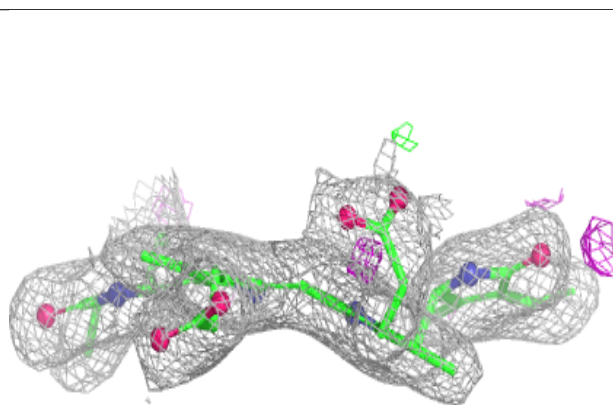
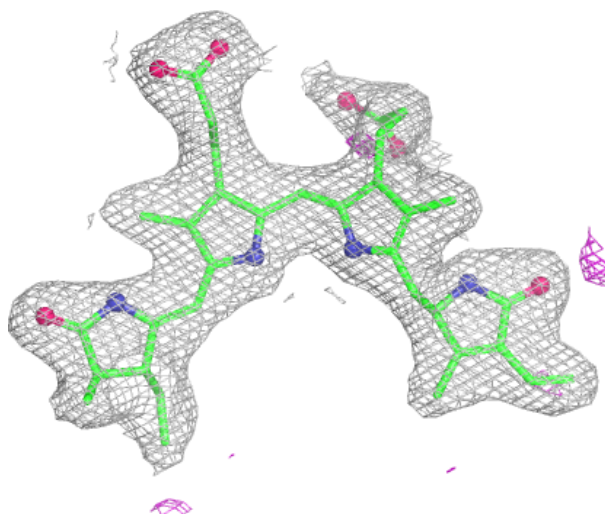
Electron density around PEB EEE 201:

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



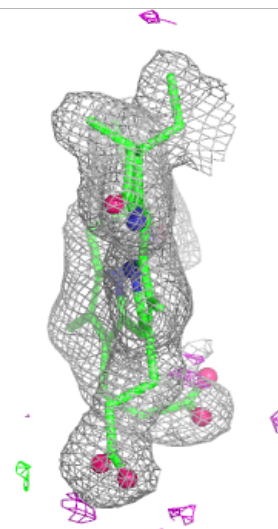
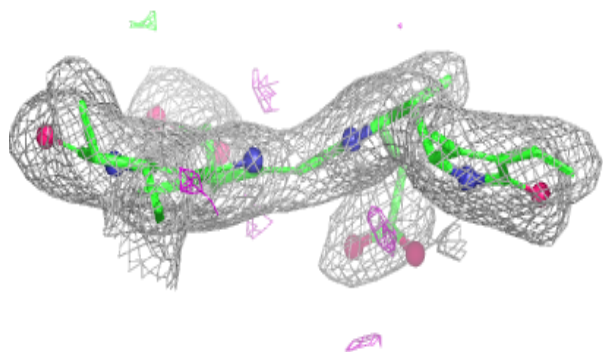
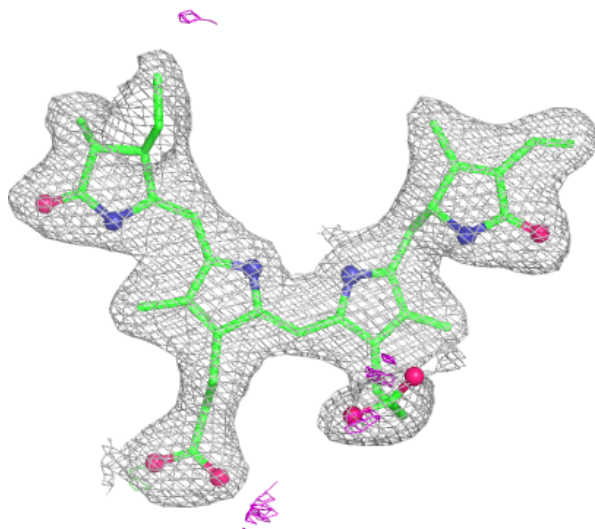
Electron density around PEB BBB 201:

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



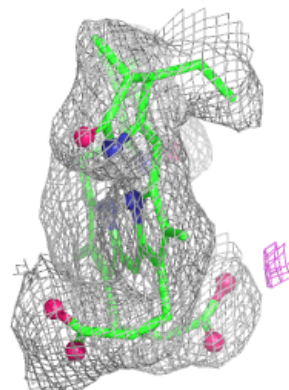
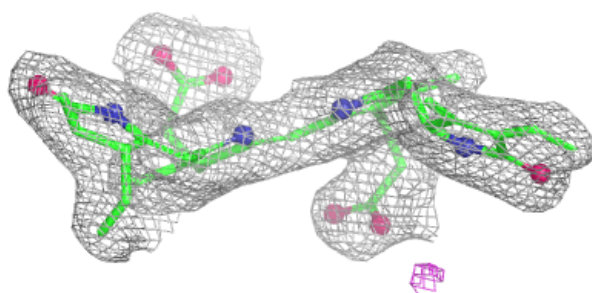
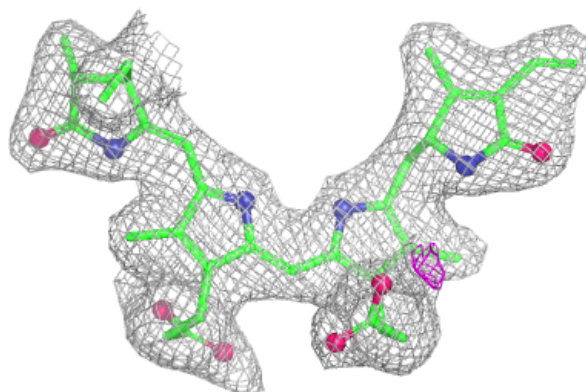
Electron density around PEB FFF 204:

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

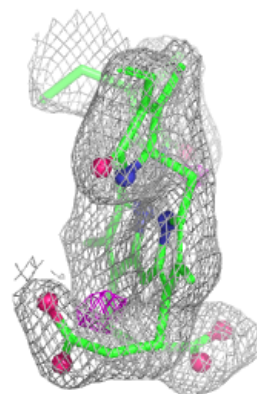
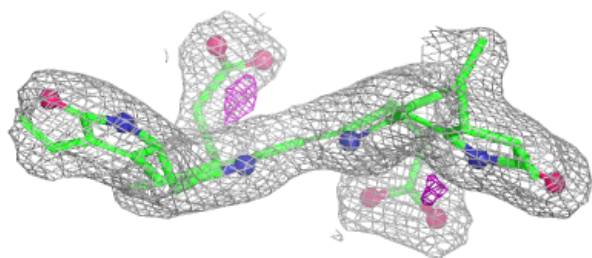
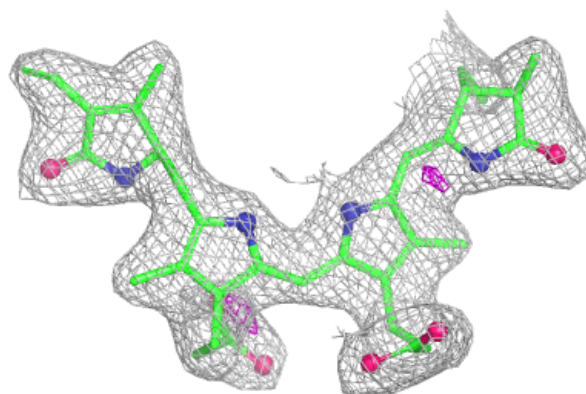


Electron density around PEB AAA 202:

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

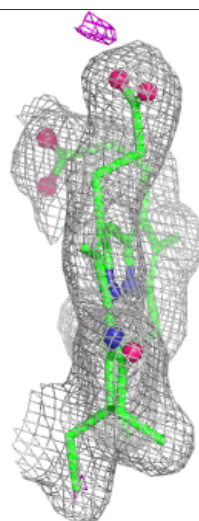
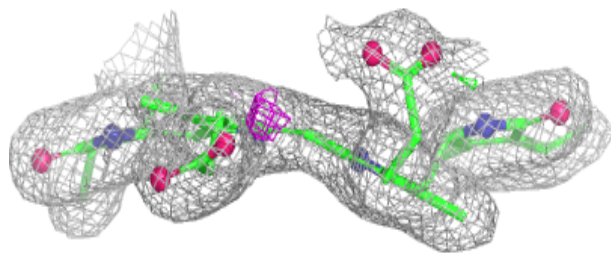
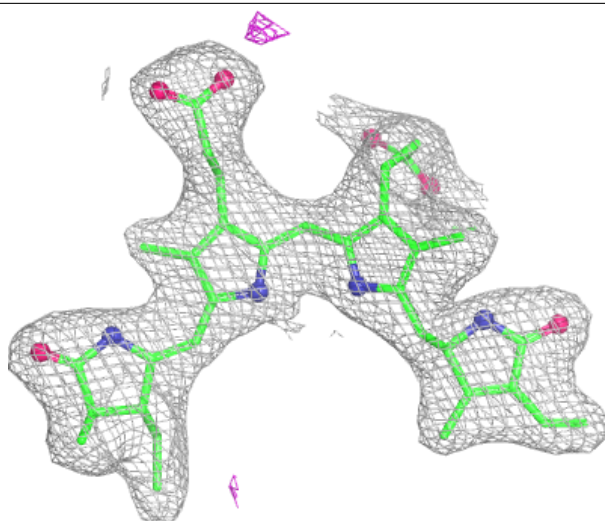
**Electron density around PEB GGG 202:**

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



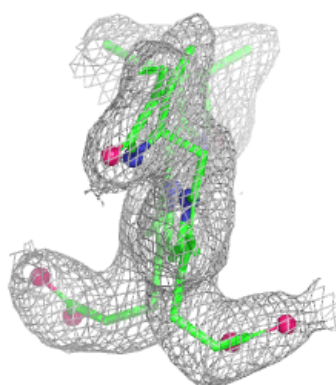
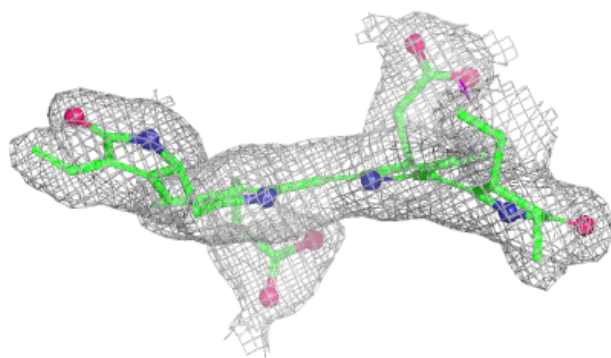
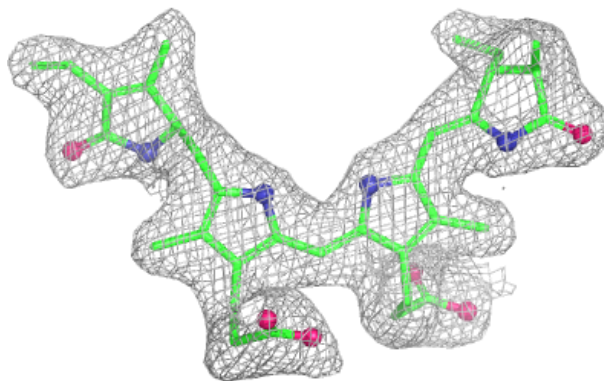
Electron density around PEB HHH 302:

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

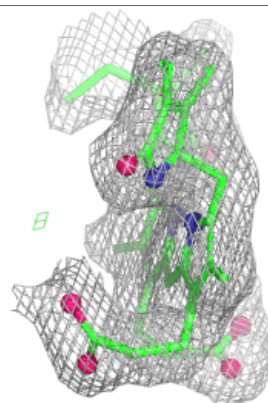
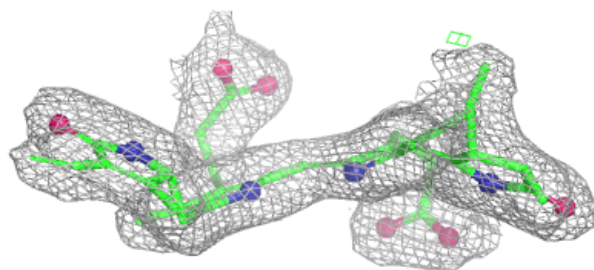
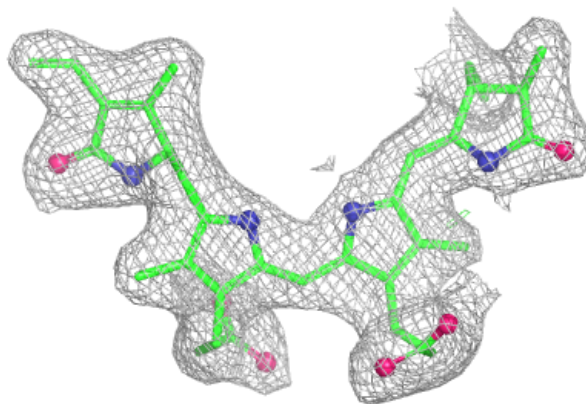


Electron density around PEB HHH 303:

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

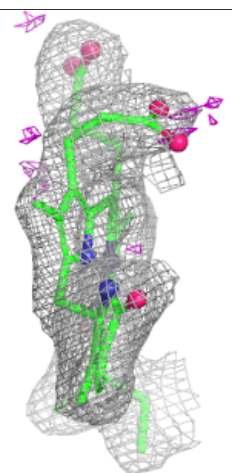
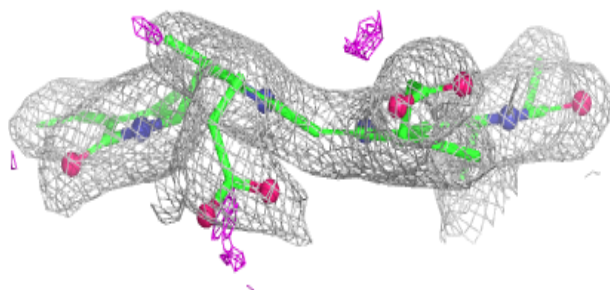
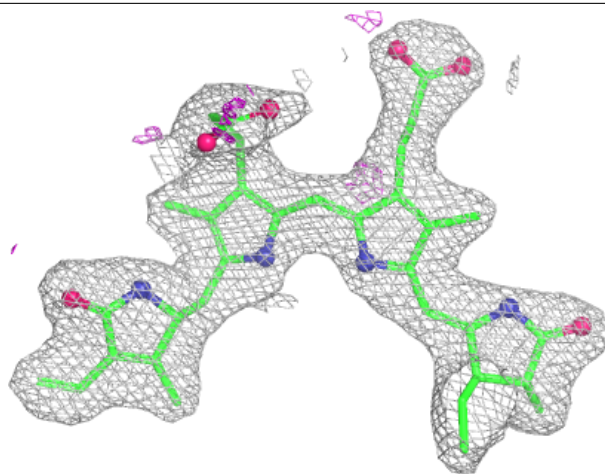
**Electron density around PEB CCC 202:**

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



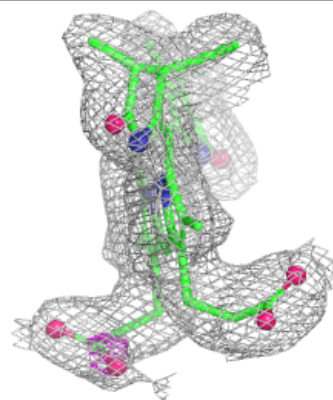
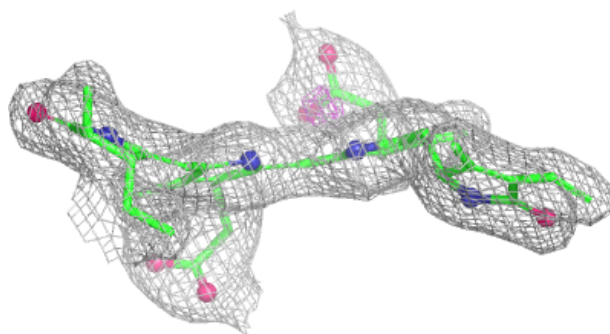
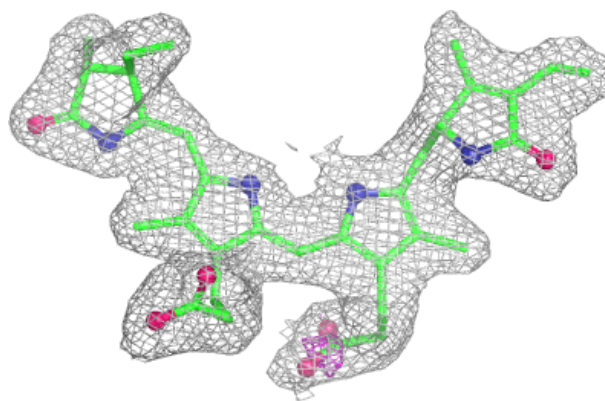
Electron density around PEB JJJ 303:

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



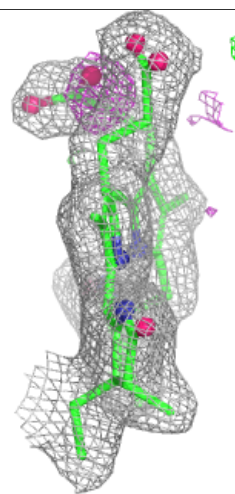
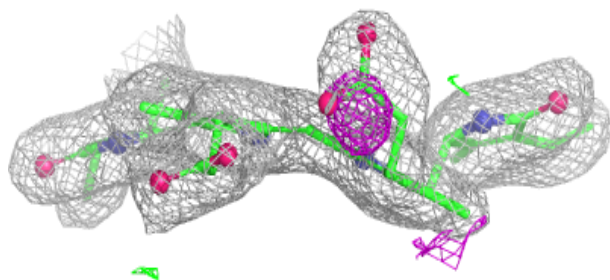
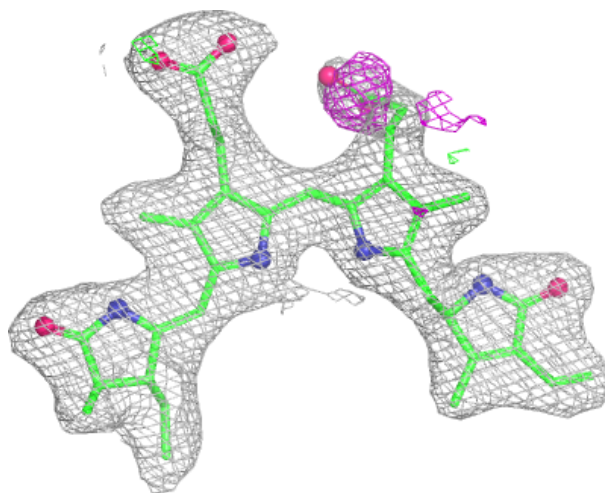
Electron density around PEB JJJ 304:

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



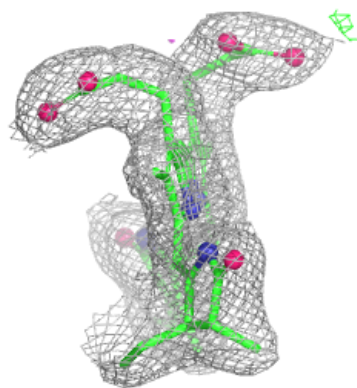
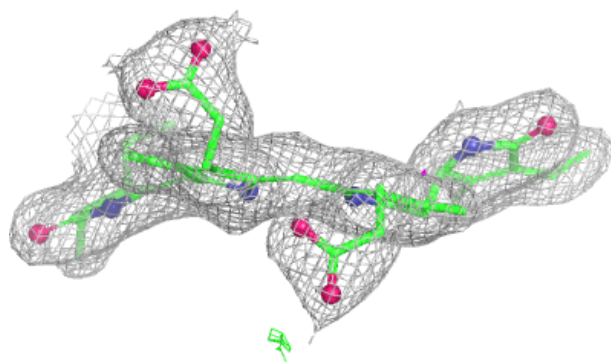
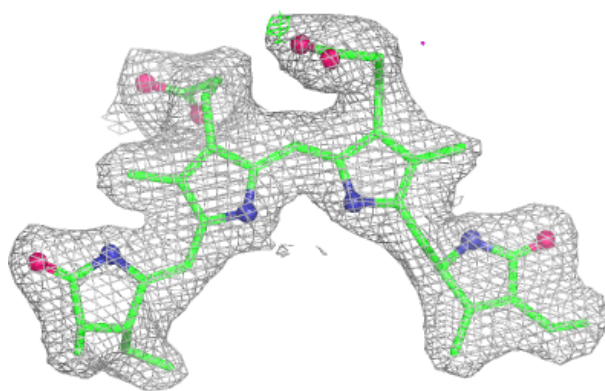
Electron density around PEB DDD 201:

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



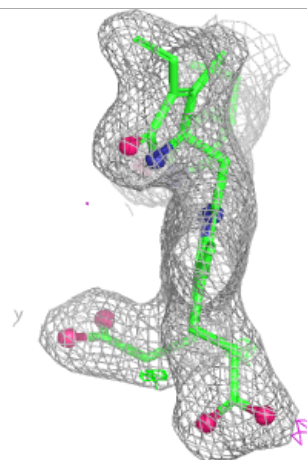
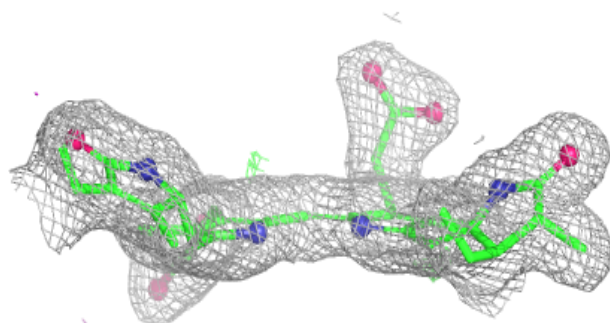
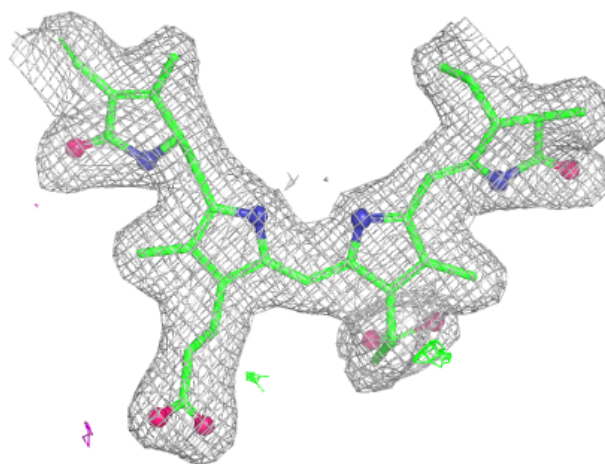
Electron density around PEB NNN 204:

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



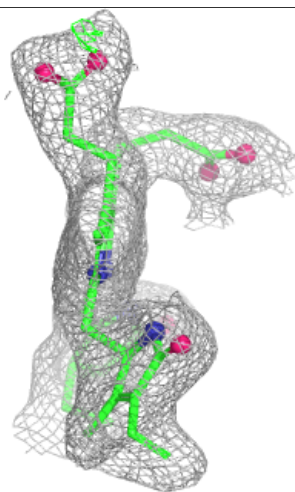
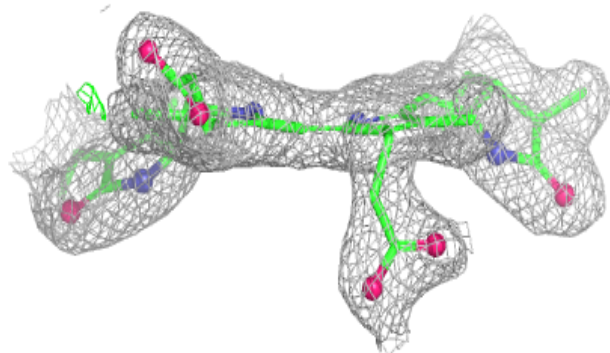
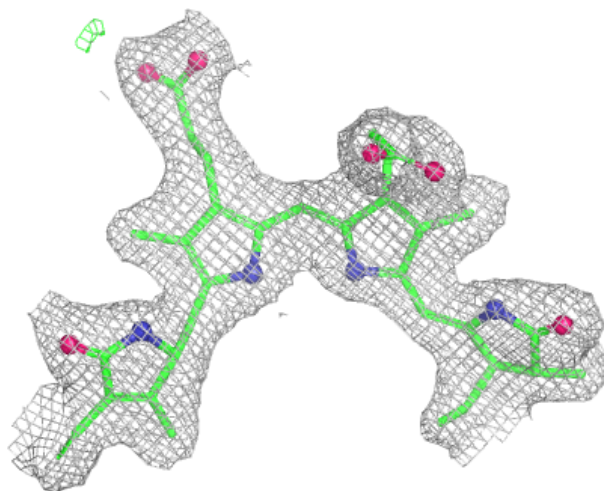
Electron density around PEB BBB 203:

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



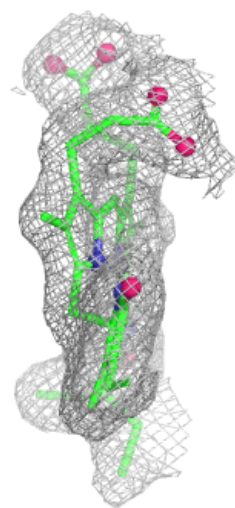
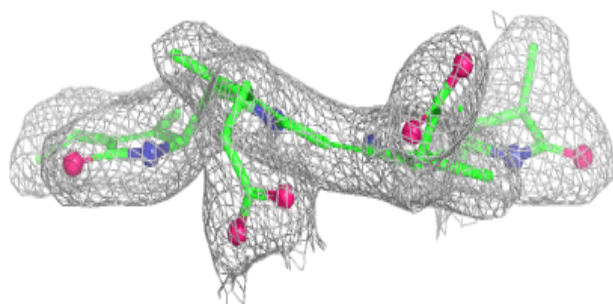
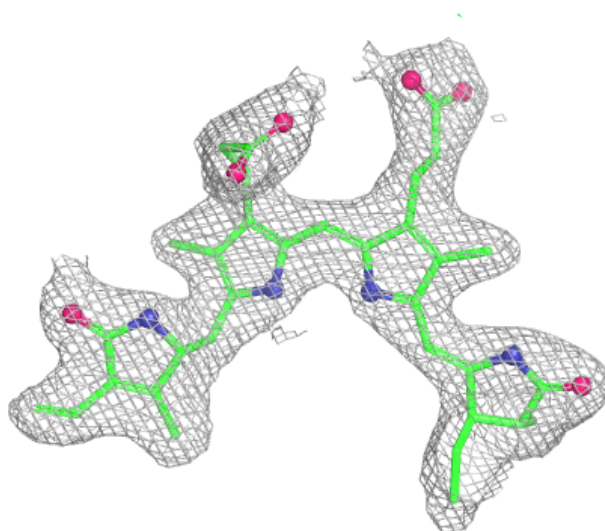
Electron density around PEB JJJ 305:

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



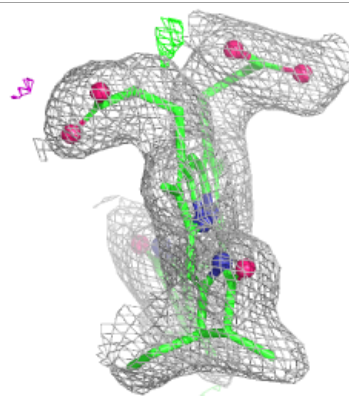
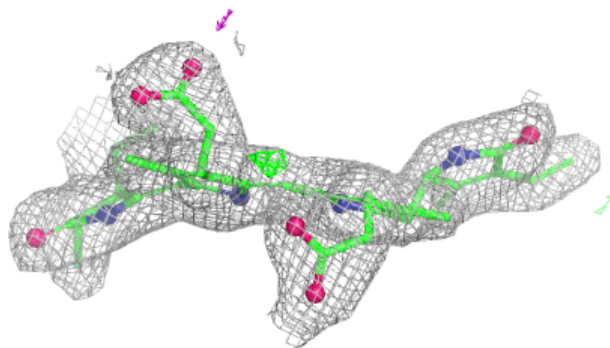
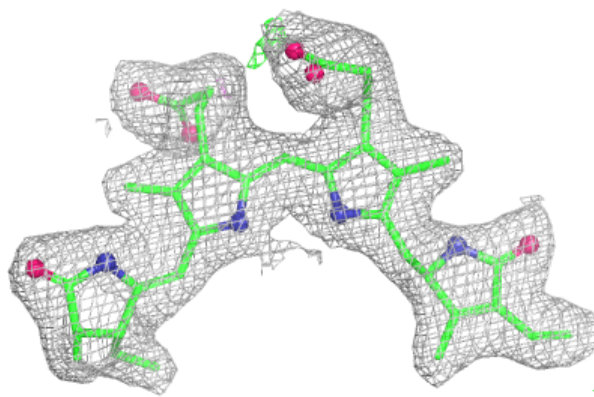
Electron density around PEB KKK 201:

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



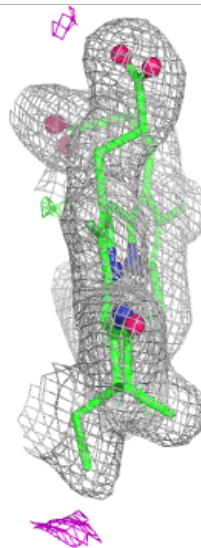
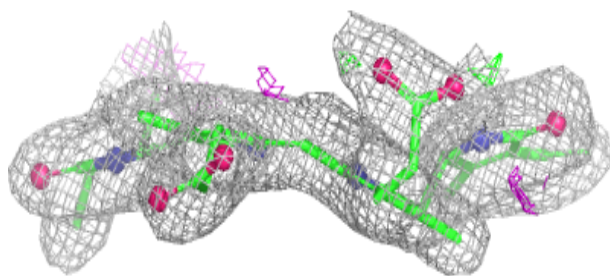
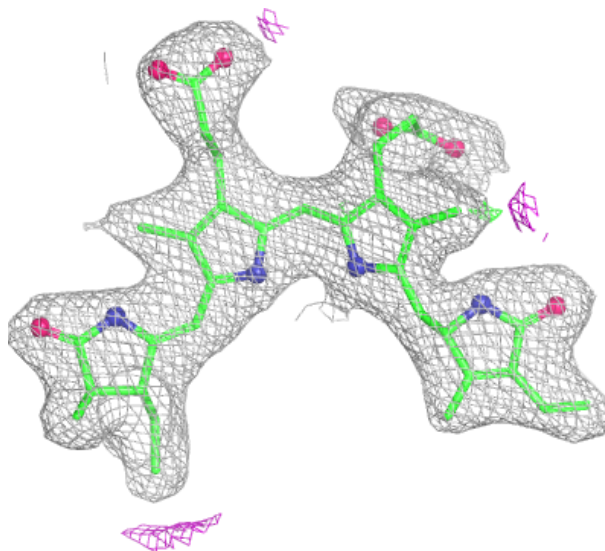
Electron density around PEB DDD 202:

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



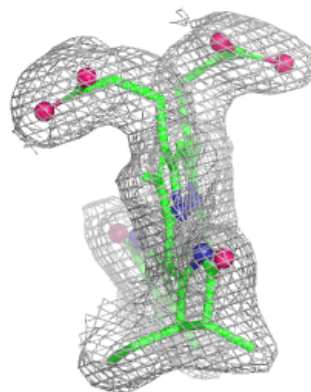
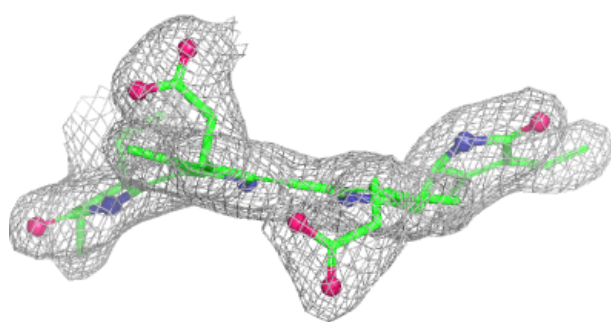
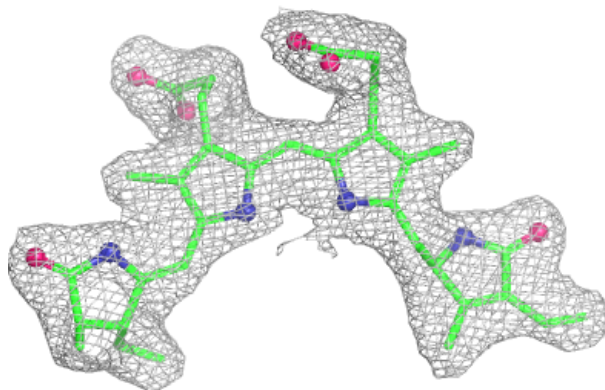
Electron density around PEB LLL 201:

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



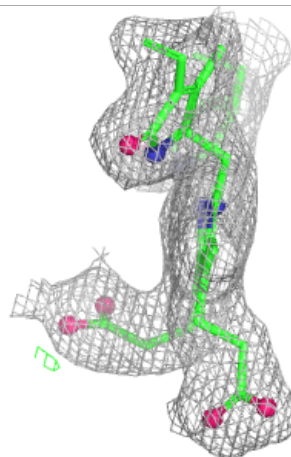
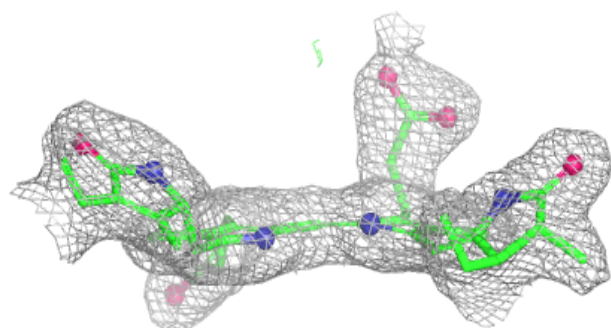
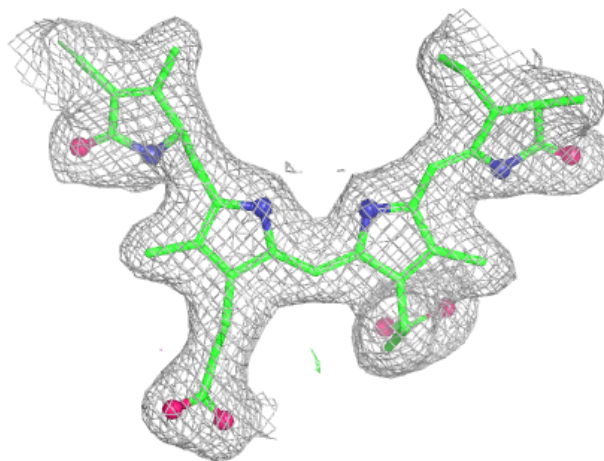
Electron density around PEB FFF 205:

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



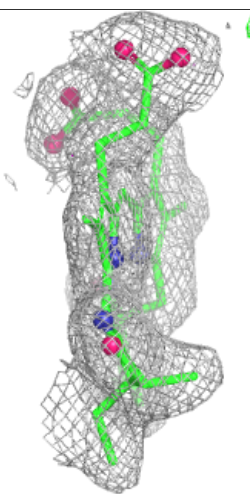
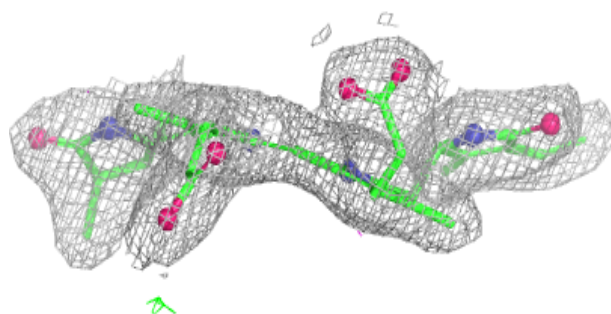
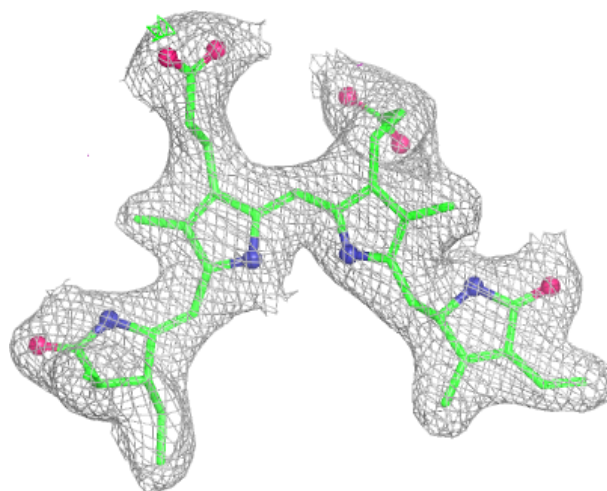
Electron density around PEB HHH 304:

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



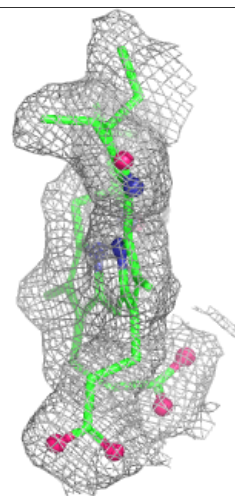
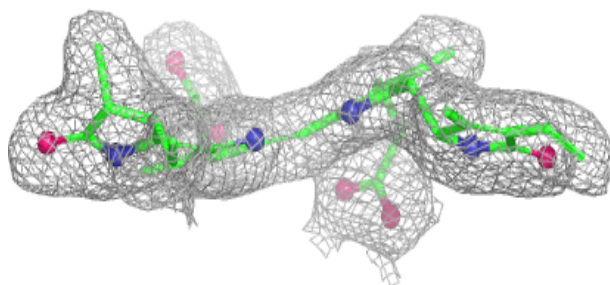
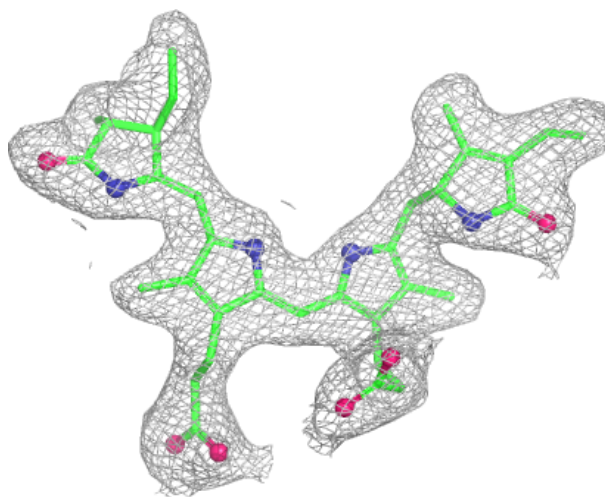
Electron density around PEB MMM 201:

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



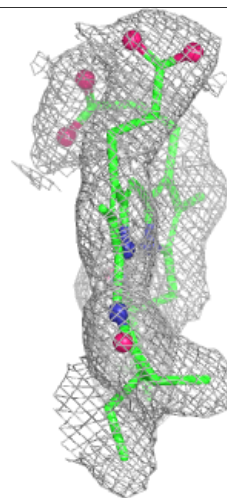
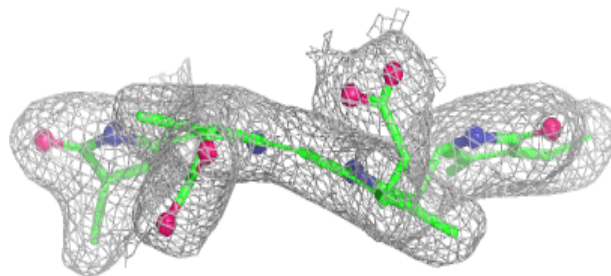
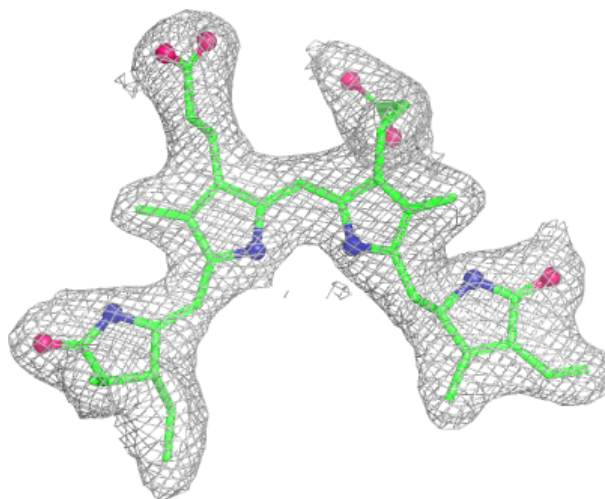
Electron density around PEB AAA 201:

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



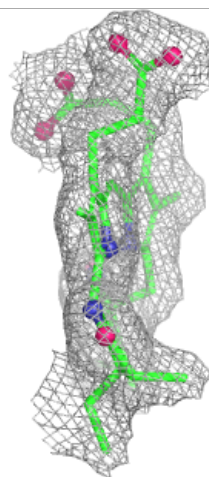
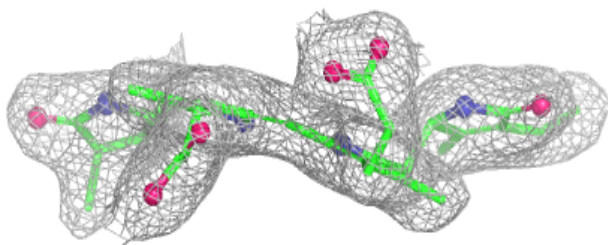
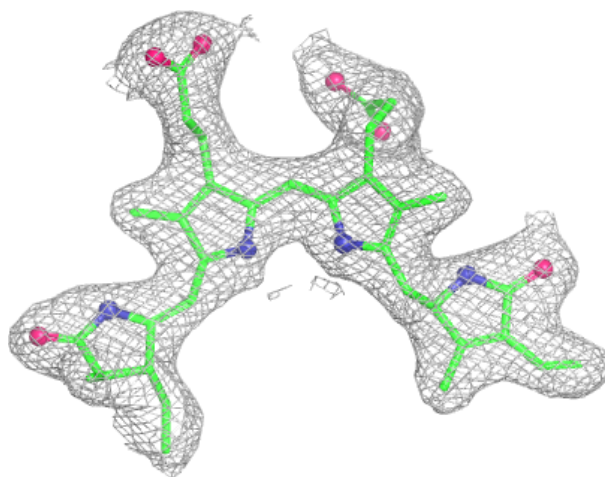
Electron density around PEB GGG 201:

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



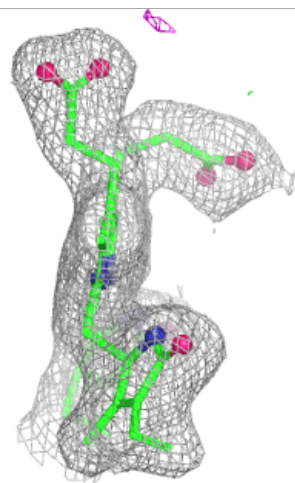
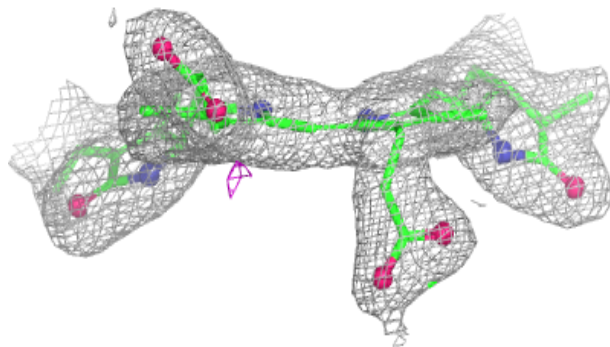
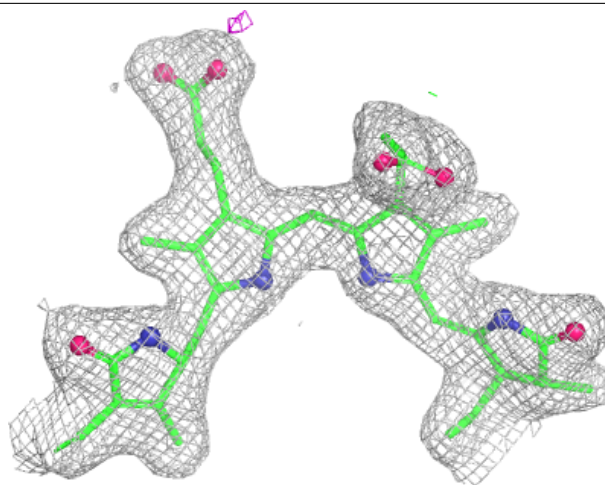
Electron density around PEB CCC 201:

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



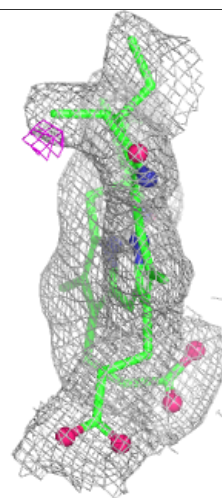
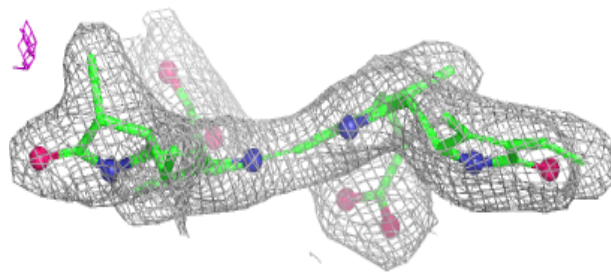
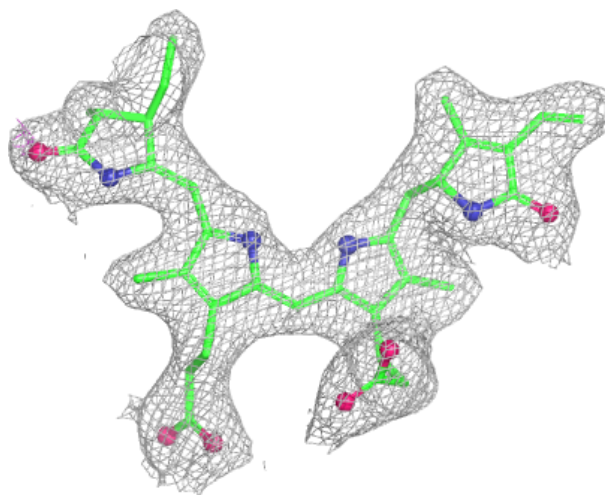
Electron density around PEB DDD 203:

$2mF_o-DF_c$ (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.