



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2022 – 12:55 PM EST

PDB ID : 7TLF  
Title : Structure of the photoacclimated Light Harvesting Complex PE545 from *Proteomonas sulcata*  
Authors : Jeffrey, P.D.; Spangler, L.C.; Scholes, G.D.  
Deposited on : 2022-01-18  
Resolution : 2.80 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](mailto: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.

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

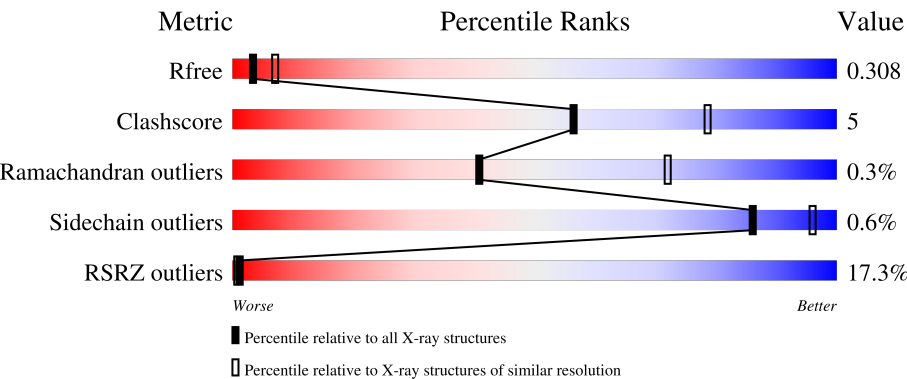
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.26  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

# 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 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	A	76	<div><div>25%</div><div><div></div><div>79%</div><div>16%</div><div>5%</div></div></div>
1	E	76	<div><div>11%</div><div><div></div><div>91%</div><div>7%</div><div>.</div></div></div>
1	I	76	<div><div>21%</div><div><div></div><div>93%</div><div>5%</div><div>.</div></div></div>
1	M	76	<div><div>14%</div><div><div></div><div>93%</div><div>.</div><div>.</div></div></div>
2	B	177	<div><div>25%</div><div><div></div><div>76%</div><div>16%</div><div>8%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	D	177	
2	F	177	
2	H	177	
2	J	177	
2	L	177	
2	N	177	
2	P	177	
3	C	67	
3	G	67	
3	K	67	
3	O	67	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15397 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 Phycoerythrin alpha-subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	72	Total	C	N	O	S	0	0	0
			528	326	91	108	3			
1	E	74	Total	C	N	O	S	0	0	0
			544	337	94	110	3			
1	I	75	Total	C	N	O	S	0	0	0
			553	343	96	111	3			
1	M	74	Total	C	N	O	S	0	0	0
			544	337	94	110	3			

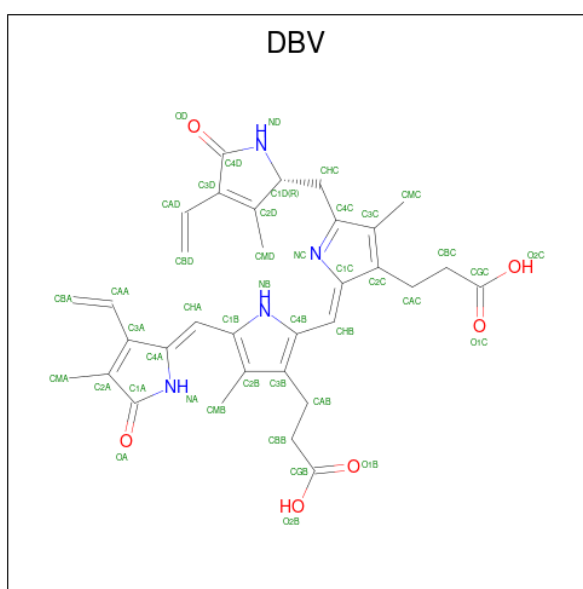
- Molecule 2 is a protein called Phycoerythrin beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	162	Total	C	N	O	S	0	1	0
			1180	728	206	236	10			
2	D	173	Total	C	N	O	S	0	0	0
			1262	776	220	256	10			
2	F	166	Total	C	N	O	S	0	1	0
			1207	743	209	245	10			
2	H	170	Total	C	N	O	S	0	0	0
			1231	759	211	251	10			
2	J	170	Total	C	N	O	S	0	0	0
			1241	765	217	249	10			
2	L	172	Total	C	N	O	S	0	0	0
			1253	771	219	253	10			
2	N	170	Total	C	N	O	S	0	0	0
			1239	765	217	247	10			
2	P	173	Total	C	N	O	S	0	1	0
			1261	777	220	254	10			

- Molecule 3 is a protein called Phycoerythrin alpha-subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	60	Total	C	N	O	S	0	0	0
			445	274	78	89	4			
3	G	67	Total	C	N	O	S	0	0	0
			496	304	87	100	5			
3	K	67	Total	C	N	O	S	0	0	0
			496	304	87	100	5			
3	O	67	Total	C	N	O	S	0	0	0
			496	304	87	100	5			

- Molecule 4 is 15,16-DIHYDROBILIVERDIN (three-letter code: DBV) (formula:  $C_{33}H_{36}N_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



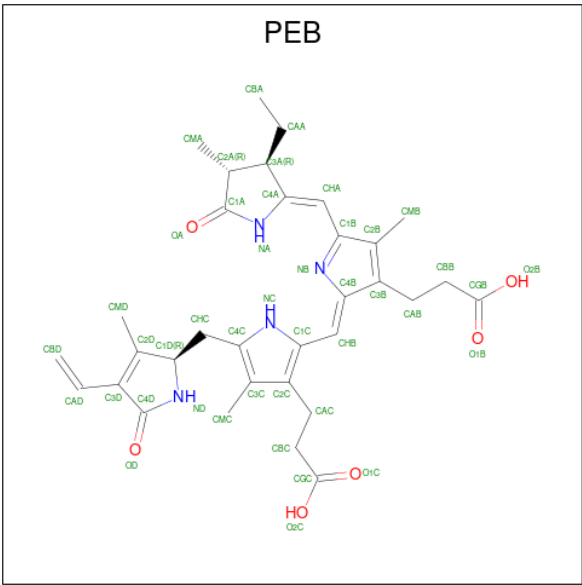
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			43	33	4	6		
4	C	1	Total	C	N	O	0	0
			43	33	4	6		
4	E	1	Total	C	N	O	0	0
			43	33	4	6		
4	G	1	Total	C	N	O	0	0
			43	33	4	6		
4	I	1	Total	C	N	O	0	0
			43	33	4	6		
4	K	1	Total	C	N	O	0	0
			43	33	4	6		
4	M	1	Total	C	N	O	0	0
			43	33	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	O	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 5 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: C<sub>33</sub>H<sub>40</sub>N<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			43	33	4	6		
5	B	1	Total	C	N	O	0	0
			43	33	4	6		
5	B	1	Total	C	N	O	0	0
			43	33	4	6		
5	D	1	Total	C	N	O	0	0
			43	33	4	6		
5	D	1	Total	C	N	O	0	0
			43	33	4	6		
5	D	1	Total	C	N	O	0	0
			43	33	4	6		
5	F	1	Total	C	N	O	0	0
			43	33	4	6		
5	F	1	Total	C	N	O	0	0
			43	33	4	6		
5	F	1	Total	C	N	O	0	0
			43	33	4	6		
5	H	1	Total	C	N	O	0	0
			43	33	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	N	O	0	0
			43	33	4	6		
5	H	1	Total	C	N	O	0	0
			43	33	4	6		
5	J	1	Total	C	N	O	0	0
			43	33	4	6		
5	J	1	Total	C	N	O	0	0
			43	33	4	6		
5	J	1	Total	C	N	O	0	0
			43	33	4	6		
5	L	1	Total	C	N	O	0	0
			43	33	4	6		
5	L	1	Total	C	N	O	0	0
			43	33	4	6		
5	L	1	Total	C	N	O	0	0
			43	33	4	6		
5	N	1	Total	C	N	O	0	0
			43	33	4	6		
5	N	1	Total	C	N	O	0	0
			43	33	4	6		
5	N	1	Total	C	N	O	0	0
			43	33	4	6		
5	P	1	Total	C	N	O	0	0
			43	33	4	6		
5	P	1	Total	C	N	O	0	0
			43	33	4	6		
5	P	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	O	0	0
			2	2		
6	C	2	Total	O	0	0
			2	2		
6	D	4	Total	O	0	0
			4	4		
6	E	4	Total	O	0	0
			4	4		
6	G	2	Total	O	0	0
			2	2		

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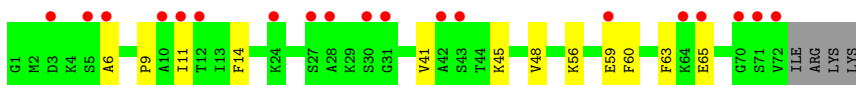
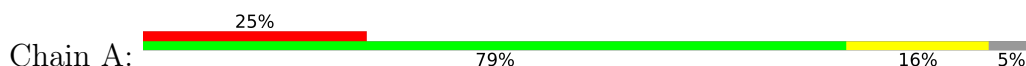
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	5	Total 5	O 5	0	0
6	H	8	Total 8	O 8	0	0
6	I	4	Total 4	O 4	0	0
6	K	2	Total 2	O 2	0	0
6	J	3	Total 3	O 3	0	0
6	L	2	Total 2	O 2	0	0
6	M	2	Total 2	O 2	0	0
6	O	1	Total 1	O 1	0	0
6	N	1	Total 1	O 1	0	0
6	P	3	Total 3	O 3	0	0

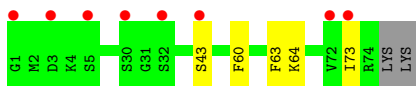
### 3 Residue-property plots [i](#)

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: Phycoerythrin alpha-subunit 1



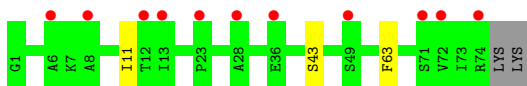
- Molecule 1: Phycoerythrin alpha-subunit 1



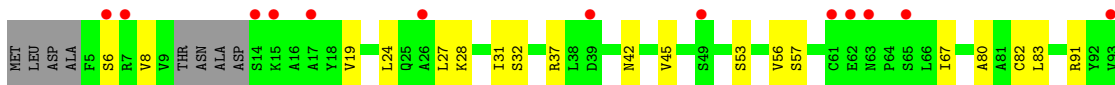
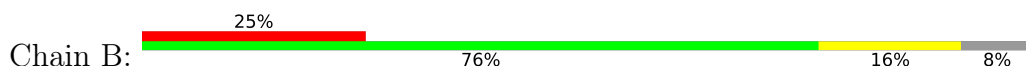
- Molecule 1: Phycoerythrin alpha-subunit 1

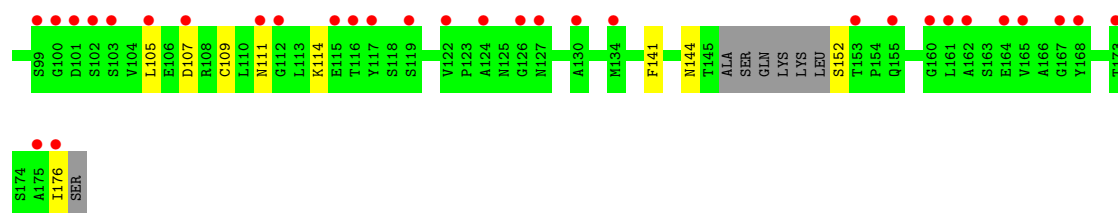


- Molecule 1: Phycoerythrin alpha-subunit 1

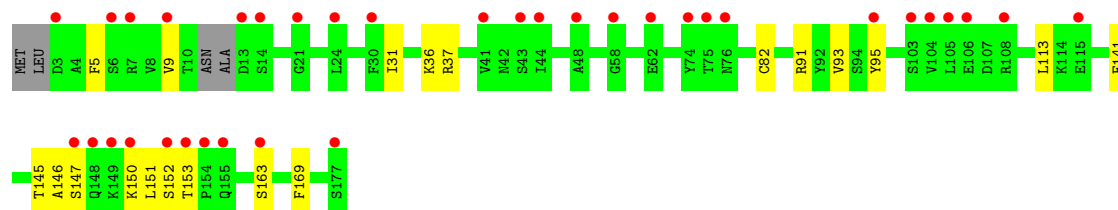
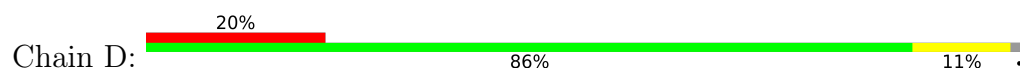


- Molecule 2: Phycoerythrin beta-subunit

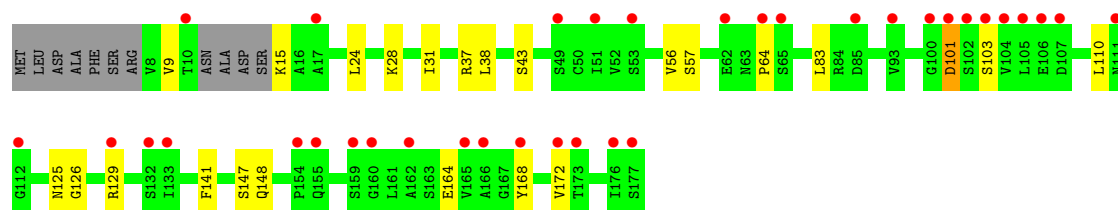
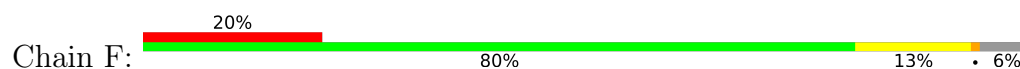




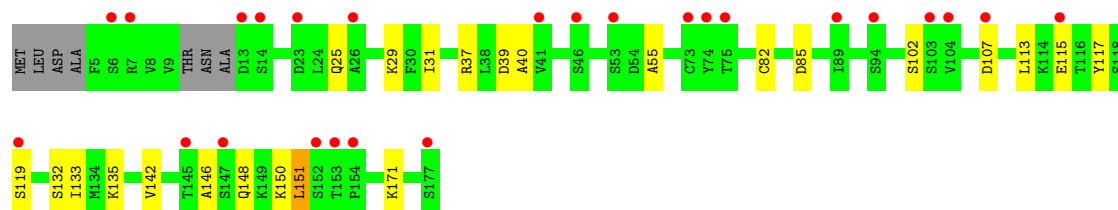
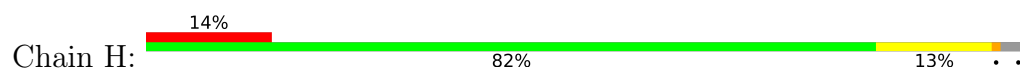
• Molecule 2: Phycoerythrin beta-subunit



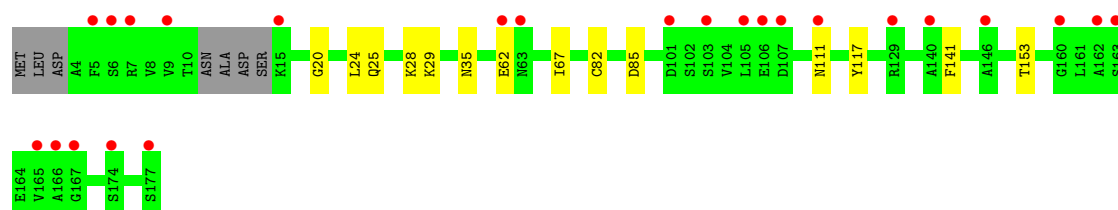
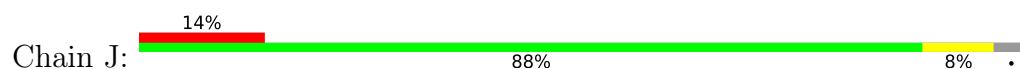
• Molecule 2: Phycoerythrin beta-subunit



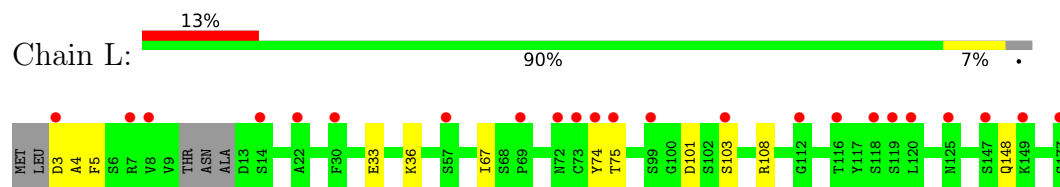
• Molecule 2: Phycoerythrin beta-subunit



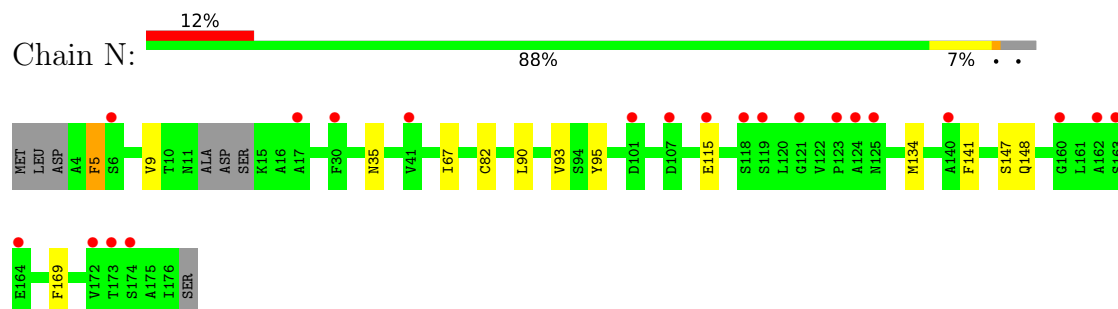
• Molecule 2: Phycoerythrin beta-subunit



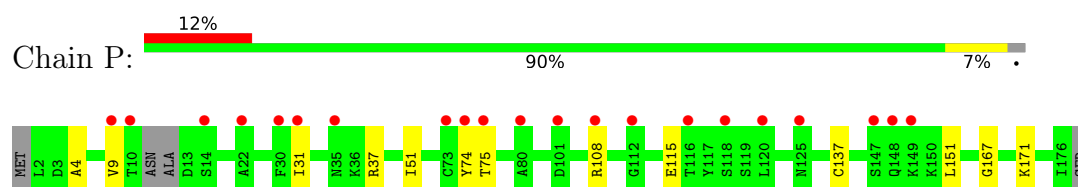
- Molecule 2: Phycoerythrin beta-subunit



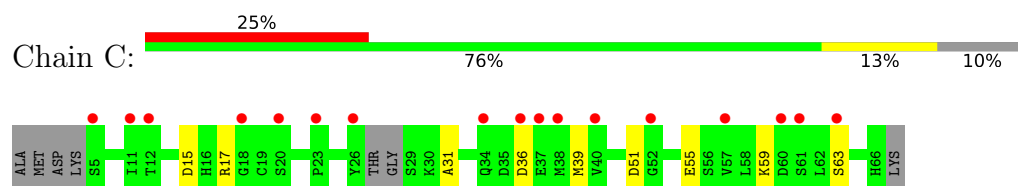
- Molecule 2: Phycoerythrin beta-subunit



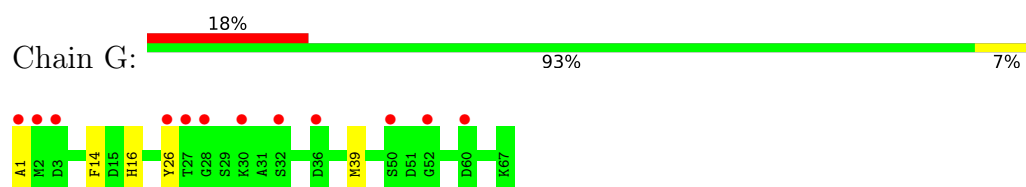
- Molecule 2: Phycoerythrin beta-subunit



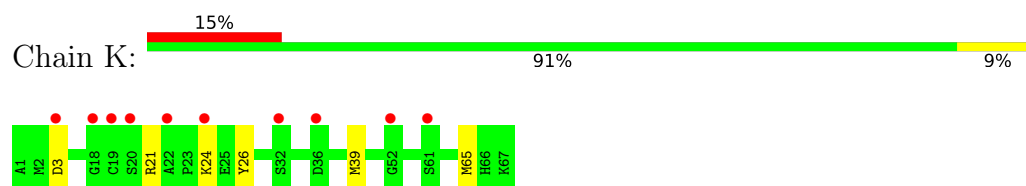
- Molecule 3: Phycoerythrin alpha-subunit 2



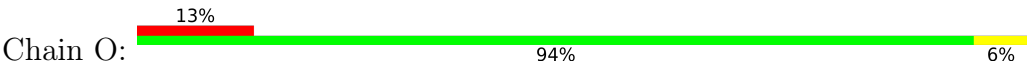
- Molecule 3: Phycoerythrin alpha-subunit 2



- Molecule 3: Phycoerythrin alpha-subunit 2



- Molecule 3: Phycoerythrin alpha-subunit 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.25Å 132.24Å 93.41Å 90.00° 116.92° 90.00°	Depositor
Resolution (Å)	29.35 – 2.80 29.35 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.35-2.80) 97.3 (29.35-2.78)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, $R_{free}$	0.245 , 0.306 0.246 , 0.308	Depositor DCC
$R_{free}$ test set	2457 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 61.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	15397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2086e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PEB, DBV

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.33	0/533	0.62	0/711
1	E	0.31	0/549	0.59	0/732
1	I	0.29	0/558	0.54	0/743
1	M	0.32	0/549	0.52	0/732
2	B	0.31	0/1191	0.48	0/1607
2	D	0.31	0/1274	0.47	0/1720
2	F	0.30	0/1221	0.51	0/1649
2	H	0.34	0/1243	0.53	0/1678
2	J	0.31	0/1253	0.48	0/1690
2	L	0.29	0/1265	0.44	0/1706
2	N	0.31	0/1251	0.47	0/1689
2	P	0.30	0/1276	0.45	0/1723
3	C	0.29	0/449	0.53	0/600
3	G	0.28	0/501	0.53	0/668
3	K	0.28	0/501	0.53	0/668
3	O	0.29	0/501	0.49	0/668
All	All	0.30	0/14115	0.50	0/18984

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	528	0	533	13	0
1	E	544	0	555	6	0
1	I	553	0	568	4	0
1	M	544	0	555	3	0
2	B	1180	0	1171	18	0
2	D	1262	0	1257	16	0
2	F	1207	0	1206	19	0
2	H	1231	0	1219	15	0
2	J	1241	0	1244	13	0
2	L	1253	0	1248	7	0
2	N	1239	0	1241	12	0
2	P	1261	0	1257	7	0
3	C	445	0	447	5	0
3	G	496	0	505	3	0
3	K	496	0	505	5	0
3	O	496	0	505	3	0
4	A	43	0	33	3	0
4	C	43	0	32	2	0
4	E	43	0	33	2	0
4	G	43	0	32	2	0
4	I	43	0	32	2	0
4	K	43	0	32	2	0
4	M	43	0	32	2	0
4	O	43	0	32	2	0
5	B	129	0	110	3	0
5	D	129	0	109	5	0
5	F	129	0	110	3	0
5	H	129	0	110	4	0
5	J	129	0	110	7	0
5	L	129	0	110	2	0
5	N	129	0	109	5	0
5	P	129	0	110	2	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	4	0	0	1	0
6	E	4	0	0	0	0
6	F	5	0	0	1	0
6	G	2	0	0	0	0
6	H	8	0	0	0	0
6	I	4	0	0	0	0
6	J	3	0	0	0	0
6	K	2	0	0	0	0
6	L	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	2	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
6	P	3	0	0	0	0
All	All	15397	0	15152	151	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 (151) 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)
2:D:31:ILE:HD12	2:D:37:ARG:HD2	1.68	0.76
3:G:1:ALA:N	2:H:107:ASP:O	2.21	0.73
2:B:31:ILE:HD12	2:B:37:ARG:HD2	1.72	0.71
4:G:101:DBV:HNA	4:G:101:DBV:HMB3	1.56	0.70
2:H:146:ALA:HB1	2:H:150:LYS:HG3	1.74	0.70
4:A:101:DBV:HMB3	4:A:101:DBV:HNA	1.56	0.69
2:H:31:ILE:HD12	2:H:37:ARG:HD2	1.74	0.68
4:M:101:DBV:HNA	4:M:101:DBV:HMB3	1.57	0.68
2:J:141:PHE:HZ	5:J:201:PEB:HMA3	1.59	0.68
4:C:101:DBV:HNA	4:C:101:DBV:HMB3	1.59	0.68
2:D:36:LYS:HE2	5:D:202:PEB:HMB3	1.76	0.68
2:H:102:SER:OG	2:H:171:LYS:NZ	2.22	0.66
4:E:101:DBV:HNA	4:E:101:DBV:HMB3	1.60	0.65
2:H:25:GLN:HG2	2:H:29:LYS:HE3	1.80	0.64
2:D:146:ALA:HB1	2:D:150:LYS:HG3	1.80	0.63
2:B:32:SER:HB3	2:B:37:ARG:HH21	1.62	0.63
1:E:64:LYS:NZ	2:H:39:ASP:OD1	2.28	0.62
4:O:101:DBV:HNA	4:O:101:DBV:HMB3	1.64	0.62
2:F:31:ILE:HD12	2:F:37:ARG:HD2	1.80	0.61
4:I:101:DBV:HNA	4:I:101:DBV:HMB3	1.66	0.61
2:D:141:PHE:HZ	5:D:201:PEB:HMA3	1.65	0.60
2:N:141:PHE:HZ	5:N:201:PEB:HMA3	1.67	0.59
5:P:203:PEB:HMB2	5:P:203:PEB:HNA	1.68	0.58
5:F:203:PEB:HNA	5:F:203:PEB:HMB2	1.69	0.58
1:I:73:ILE:HD12	2:J:62:GLU:HB2	1.86	0.57
5:L:203:PEB:HMB2	5:L:203:PEB:HNA	1.68	0.57
4:K:101:DBV:HNA	4:K:101:DBV:HMB3	1.69	0.57
2:F:56:VAL:HG21	2:F:83:LEU:HD23	1.86	0.57
2:D:147:SER:HB3	2:D:150:LYS:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:203:PEB:HNA	5:B:203:PEB:HMB2	1.71	0.56
2:N:115:GLU:N	2:N:115:GLU:OE1	2.38	0.56
1:A:56:LYS:HE2	2:B:53:SER:HB2	1.87	0.55
2:B:141:PHE:HZ	5:B:201:PEB:HMA3	1.72	0.55
2:F:101:ASP:OD2	2:F:103:SER:OG	2.25	0.54
2:N:147:SER:OG	2:N:148:GLN:OE1	2.24	0.54
2:L:148:GLN:O	2:L:148:GLN:NE2	2.41	0.54
5:N:203:PEB:HMB2	5:N:203:PEB:HNA	1.73	0.53
1:A:14:PHE:HB2	4:A:101:DBV:HMD3	1.89	0.53
3:K:21:ARG:NH2	3:K:24:LYS:HE2	2.24	0.53
2:H:115:GLU:OE1	2:H:115:GLU:N	2.37	0.52
1:E:73:ILE:HG21	2:F:129:ARG:HH21	1.74	0.52
3:C:39:MET:HE2	4:C:101:DBV:HHC2	1.91	0.52
1:I:1:GLY:HA2	2:J:111:ASN:HB3	1.90	0.52
1:I:63:PHE:CZ	2:J:67:ILE:HD11	2.45	0.52
2:F:147:SER:OG	2:F:148:GLN:OE1	2.24	0.52
2:L:3:ASP:O	2:L:5:PHE:N	2.44	0.51
1:E:43:SER:HB2	2:F:9:VAL:HA	1.92	0.51
2:P:31:ILE:HD12	2:P:37:ARG:HD2	1.92	0.51
3:C:15:ASP:OD1	3:C:17:ARG:HG3	2.11	0.50
1:A:11:ILE:O	2:B:45:VAL:HG11	2.12	0.50
2:J:141:PHE:CZ	5:J:201:PEB:HMA3	2.44	0.50
2:P:115:GLU:N	2:P:115:GLU:OE1	2.40	0.50
2:B:42:ASN:OD1	3:C:63:SER:HB2	2.12	0.50
1:A:63:PHE:CZ	2:B:67:ILE:HD11	2.46	0.49
2:N:93:VAL:HG11	2:N:169:PHE:CE2	2.48	0.49
2:B:56:VAL:HG21	2:B:83:LEU:HD23	1.95	0.49
2:D:91:ARG:NH2	6:D:302:HOH:O	2.45	0.49
2:B:107:ASP:O	2:B:111:ASN:HB3	2.13	0.49
5:D:203:PEB:HMB2	5:D:203:PEB:HNA	1.78	0.48
2:J:35:ASN:HB3	5:J:202:PEB:C1C	2.43	0.48
5:J:203:PEB:HNA	5:J:203:PEB:HMB2	1.79	0.48
1:E:63:PHE:CZ	2:F:64:PRO:HB3	2.49	0.48
5:H:203:PEB:HMB2	5:H:203:PEB:HNA	1.79	0.48
2:F:141:PHE:HZ	5:F:201:PEB:HMA3	1.79	0.48
4:M:101:DBV:HMB3	4:M:101:DBV:NA	2.27	0.48
2:B:114:LYS:HB2	2:B:176:ILE:HA	1.96	0.47
3:C:51:ASP:O	3:C:55:GLU:HG3	2.13	0.47
2:D:82:CYS:HA	5:D:203:PEB:HAA1	1.76	0.47
1:E:60:PHE:CE1	2:F:57:SER:HB2	2.49	0.47
5:D:202:PEB:HMB2	5:D:202:PEB:HNA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:O	2:B:91:ARG:HB3	2.14	0.47
2:D:151:LEU:HD23	2:D:153:THR:O	2.14	0.47
1:E:73:ILE:HG21	2:F:129:ARG:NH2	2.29	0.47
2:N:90:LEU:HB2	2:N:134:MET:CE	2.44	0.47
2:J:25:GLN:HG2	2:J:29:LYS:HE3	1.97	0.47
2:H:132:SER:O	2:H:135:LYS:HB3	2.14	0.47
2:F:164:GLU:HG2	2:F:168:TYR:CE2	2.51	0.46
1:M:43:SER:HB2	2:N:9:VAL:HA	1.97	0.46
2:H:85:ASP:OD2	2:H:117:TYR:OH	2.27	0.46
1:A:41:VAL:HG12	2:B:8:VAL:HG11	1.98	0.46
2:F:101:ASP:OD1	2:F:103:SER:HB3	2.16	0.46
2:L:74:TYR:O	2:L:75:THR:OG1	2.30	0.46
2:B:19:VAL:HG11	2:B:27:LEU:HD22	1.97	0.46
1:A:65:GLU:CD	2:D:152:SER:HG	2.20	0.45
1:I:14:PHE:HB2	4:I:101:DBV:HMD3	1.98	0.45
2:J:24:LEU:HG	2:J:28:LYS:HE2	1.98	0.45
2:J:25:GLN:O	2:J:29:LYS:HG3	2.16	0.45
2:J:153:THR:HG21	5:J:202:PEB:HMA3	1.98	0.45
2:J:85:ASP:OD2	2:J:117:TYR:OH	2.26	0.45
2:D:146:ALA:HB3	2:D:151:LEU:HD12	1.99	0.45
1:A:60:PHE:CE1	2:B:57:SER:HB2	2.52	0.45
1:A:11:ILE:HG12	1:A:41:VAL:HG22	1.98	0.45
1:A:48:VAL:O	2:B:80:ALA:HB1	2.17	0.45
2:P:9:VAL:O	2:P:108:ARG:NH1	2.50	0.45
2:B:24:LEU:HG	2:B:28:LYS:HE2	1.98	0.44
1:A:56:LYS:NZ	1:A:59:GLU:OE1	2.37	0.44
2:F:110:LEU:HD21	2:F:172:VAL:HG22	1.99	0.44
2:H:113:LEU:HD11	5:H:203:PEB:HMD3	1.99	0.44
2:H:40:ALA:HB1	2:H:142:VAL:HG22	2.00	0.44
2:N:35:ASN:HB3	5:N:202:PEB:C1C	2.48	0.44
2:P:74:TYR:O	2:P:75:THR:OG1	2.31	0.44
2:D:93:VAL:HG11	2:D:169:PHE:CE2	2.53	0.43
2:D:5:PHE:HB3	2:D:95:TYR:OH	2.18	0.43
3:G:14:PHE:HD2	3:G:16:HIS:CE1	2.36	0.43
2:F:101:ASP:CG	2:F:103:SER:H	2.22	0.43
2:L:101:ASP:OD1	2:L:103:SER:N	2.32	0.43
3:O:65:MET:HB3	3:O:65:MET:HE2	1.88	0.43
2:P:167:GLY:O	2:P:171:LYS:HG3	2.19	0.43
2:H:148:GLN:HA	2:H:151:LEU:HB2	2.01	0.43
2:D:147:SER:O	2:D:151:LEU:N	2.52	0.42
2:F:24:LEU:HG	2:F:28:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:202:PEB:HHB1	5:F:202:PEB:HAB1	1.85	0.42
2:L:33:GLU:OE2	2:L:36:LYS:NZ	2.38	0.42
2:N:5:PHE:HD1	2:N:5:PHE:HA	1.70	0.42
5:L:201:PEB:HNA	5:L:201:PEB:HMB3	1.84	0.42
1:A:6:ALA:HB3	1:A:45:LYS:HG3	2.02	0.42
4:G:101:DBV:HMB3	4:G:101:DBV:NA	2.28	0.42
2:H:82:CYS:HA	5:H:203:PEB:HAA1	1.79	0.42
5:H:202:PEB:HMB2	5:H:202:PEB:HNA	1.84	0.42
2:H:25:GLN:O	2:H:29:LYS:HG3	2.19	0.42
3:G:26:TYR:HB2	3:G:39:MET:CE	2.49	0.42
2:J:82:CYS:HA	5:J:203:PEB:HAA1	1.85	0.42
2:F:101:ASP:OD1	2:F:103:SER:CB	2.68	0.42
4:A:101:DBV:HNA	4:A:101:DBV:CMB	2.29	0.41
5:J:202:PEB:HNA	5:J:202:PEB:HMB2	1.86	0.41
1:A:65:GLU:OE1	2:D:152:SER:OG	2.32	0.41
1:M:63:PHE:CZ	2:N:67:ILE:HD11	2.55	0.41
2:P:51:ILE:HG12	2:P:137:CYS:HB3	2.01	0.41
3:K:26:TYR:HB2	3:K:39:MET:HE2	2.02	0.41
1:M:11:ILE:HD11	2:N:95:TYR:HA	2.03	0.41
2:F:15:LYS:N	6:F:301:HOH:O	2.52	0.41
2:B:82:CYS:HA	5:B:203:PEB:HAA1	1.90	0.41
3:K:3:ASP:OD2	2:L:108:ARG:NH2	2.53	0.41
3:K:65:MET:HE1	2:L:67:ILE:HD11	2.03	0.41
2:N:82:CYS:HA	5:N:203:PEB:HAA1	1.87	0.41
2:N:90:LEU:HB2	2:N:134:MET:HE2	2.02	0.41
4:E:101:DBV:HMB3	4:E:101:DBV:NA	2.31	0.41
3:O:26:TYR:HB3	4:O:101:DBV:HBD1	2.02	0.41
2:B:105:LEU:O	2:B:109:CYS:HB3	2.20	0.41
2:F:38:LEU:HA	2:F:38:LEU:HD23	1.84	0.41
3:O:30:LYS:HA	3:O:30:LYS:HD3	1.94	0.41
5:N:201:PEB:HMB3	5:N:201:PEB:HNA	1.86	0.41
2:P:151:LEU:HD12	2:P:151:LEU:HA	1.88	0.41
5:P:201:PEB:HNA	5:P:201:PEB:HMB3	1.86	0.41
2:D:113:LEU:HD12	2:D:113:LEU:HA	1.92	0.40
2:H:55:ALA:HA	2:H:133:ILE:HG21	2.04	0.40
3:C:31:ALA:N	3:C:36:ASP:OD1	2.48	0.40
3:K:26:TYR:HB3	4:K:101:DBV:HBD1	2.03	0.40
2:D:146:ALA:HB1	2:D:150:LYS:HE3	2.02	0.40
2:F:125:ASN:OD1	2:F:126:GLY:N	2.52	0.40
2:J:20:GLY:HA2	2:J:24:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	70/76 (92%)	65 (93%)	5 (7%)	0	100	100
1	E	72/76 (95%)	69 (96%)	3 (4%)	0	100	100
1	I	73/76 (96%)	69 (94%)	4 (6%)	0	100	100
1	M	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
2	B	156/177 (88%)	152 (97%)	2 (1%)	2 (1%)	12	36
2	D	169/177 (96%)	163 (96%)	5 (3%)	1 (1%)	25	56
2	F	163/177 (92%)	161 (99%)	2 (1%)	0	100	100
2	H	166/177 (94%)	164 (99%)	2 (1%)	0	100	100
2	J	166/177 (94%)	163 (98%)	3 (2%)	0	100	100
2	L	168/177 (95%)	163 (97%)	4 (2%)	1 (1%)	25	56
2	N	166/177 (94%)	163 (98%)	3 (2%)	0	100	100
2	P	170/177 (96%)	165 (97%)	4 (2%)	1 (1%)	25	56
3	C	56/67 (84%)	54 (96%)	2 (4%)	0	100	100
3	G	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
3	K	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
3	O	65/67 (97%)	63 (97%)	1 (2%)	1 (2%)	10	33
All	All	1862/1988 (94%)	1810 (97%)	46 (2%)	6 (0%)	41	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	4	ALA
2	B	6	SER
2	B	144	ASN
2	D	9	VAL
3	O	24	LYS
2	P	4	ALA

### 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	A	57/62 (92%)	57 (100%)	0	100	100
1	E	59/62 (95%)	59 (100%)	0	100	100
1	I	60/62 (97%)	60 (100%)	0	100	100
1	M	59/62 (95%)	59 (100%)	0	100	100
2	B	130/143 (91%)	129 (99%)	1 (1%)	81	94
2	D	140/143 (98%)	138 (99%)	2 (1%)	67	90
2	F	134/143 (94%)	132 (98%)	2 (2%)	65	89
2	H	136/143 (95%)	134 (98%)	2 (2%)	65	89
2	J	137/143 (96%)	137 (100%)	0	100	100
2	L	138/143 (96%)	138 (100%)	0	100	100
2	N	136/143 (95%)	135 (99%)	1 (1%)	84	95
2	P	139/143 (97%)	139 (100%)	0	100	100
3	C	50/55 (91%)	49 (98%)	1 (2%)	55	84
3	G	55/55 (100%)	55 (100%)	0	100	100
3	K	55/55 (100%)	55 (100%)	0	100	100
3	O	55/55 (100%)	55 (100%)	0	100	100
All	All	1540/1612 (96%)	1531 (99%)	9 (1%)	86	96

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	152	SER
3	C	59	LYS
2	D	145	THR
2	D	163	SER
2	F	43	SER
2	F	101	ASP
2	H	119	SER
2	H	151	LEU

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Mol	Chain	Res	Type
2	N	5	PHE

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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

32 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	PEB	F	203	2	37,46,46	1.11	3 (8%)	39,67,67	1.64	10 (25%)
4	DBV	M	101	1	36,46,46	1.38	4 (11%)	36,67,67	1.81	12 (33%)
5	PEB	D	202	2	37,46,46	1.21	5 (13%)	39,67,67	1.44	7 (17%)
5	PEB	J	203	2	37,46,46	1.29	4 (10%)	39,67,67	1.64	8 (20%)
4	DBV	C	101	3	36,46,46	1.40	6 (16%)	36,67,67	1.87	11 (30%)
4	DBV	I	101	1	36,46,46	1.45	6 (16%)	36,67,67	1.89	13 (36%)
5	PEB	B	202	2	37,46,46	1.13	3 (8%)	39,67,67	1.45	8 (20%)
5	PEB	H	202	2	37,46,46	1.27	3 (8%)	39,67,67	1.66	7 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEB	B	203	2	37,46,46	1.17	3 (8%)	39,67,67	1.59	9 (23%)
5	PEB	F	202	2	37,46,46	1.20	3 (8%)	39,67,67	1.51	7 (17%)
4	DBV	K	101	3	36,46,46	1.35	6 (16%)	36,67,67	1.88	12 (33%)
5	PEB	J	202	2	37,46,46	1.17	4 (10%)	39,67,67	1.41	5 (12%)
5	PEB	N	201	2	37,46,46	1.14	3 (8%)	39,67,67	1.39	6 (15%)
5	PEB	P	203	2	37,46,46	1.13	2 (5%)	39,67,67	1.65	10 (25%)
5	PEB	D	203	2	37,46,46	1.18	3 (8%)	39,67,67	1.58	9 (23%)
5	PEB	L	201	2	37,46,46	1.15	1 (2%)	39,67,67	1.74	10 (25%)
4	DBV	G	101	3	36,46,46	1.45	5 (13%)	36,67,67	1.82	11 (30%)
5	PEB	H	201	2	37,46,46	1.07	3 (8%)	39,67,67	1.47	6 (15%)
5	PEB	J	201	2	37,46,46	1.18	3 (8%)	39,67,67	1.53	8 (20%)
5	PEB	L	202	2	37,46,46	1.25	4 (10%)	39,67,67	1.47	6 (15%)
5	PEB	P	202	2	37,46,46	1.32	7 (18%)	39,67,67	1.54	7 (17%)
5	PEB	B	201	2	37,46,46	1.15	3 (8%)	39,67,67	1.38	7 (17%)
4	DBV	O	101	3	36,46,46	1.37	5 (13%)	36,67,67	1.94	13 (36%)
5	PEB	H	203	2	37,46,46	1.14	4 (10%)	39,67,67	1.60	9 (23%)
5	PEB	L	203	2	37,46,46	1.22	4 (10%)	39,67,67	1.51	9 (23%)
5	PEB	P	201	2	37,46,46	1.07	2 (5%)	39,67,67	1.72	10 (25%)
5	PEB	N	202	2	37,46,46	1.30	5 (13%)	39,67,67	1.40	7 (17%)
5	PEB	D	201	2	37,46,46	1.12	2 (5%)	39,67,67	1.77	11 (28%)
5	PEB	N	203	2	37,46,46	1.14	2 (5%)	39,67,67	1.53	8 (20%)
4	DBV	A	101	1	36,46,46	1.51	7 (19%)	36,67,67	1.90	10 (27%)
5	PEB	F	201	2	37,46,46	1.24	4 (10%)	39,67,67	1.57	10 (25%)
4	DBV	E	101	1	36,46,46	1.39	6 (16%)	36,67,67	1.91	11 (30%)

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	PEB	F	203	2	-	2/20/74/74	0/4/4/4
4	DBV	M	101	1	-	7/22/74/74	0/4/4/4
5	PEB	D	202	2	-	6/20/74/74	0/4/4/4
5	PEB	J	203	2	-	2/20/74/74	0/4/4/4
4	DBV	C	101	3	-	11/22/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DBV	I	101	1	-	6/22/74/74	0/4/4/4
5	PEB	B	202	2	-	6/20/74/74	0/4/4/4
5	PEB	H	202	2	-	5/20/74/74	0/4/4/4
5	PEB	B	203	2	-	2/20/74/74	0/4/4/4
5	PEB	F	202	2	-	4/20/74/74	0/4/4/4
4	DBV	K	101	3	-	5/22/74/74	0/4/4/4
5	PEB	J	202	2	-	4/20/74/74	0/4/4/4
5	PEB	N	201	2	-	4/20/74/74	0/4/4/4
5	PEB	P	203	2	-	2/20/74/74	0/4/4/4
5	PEB	D	203	2	-	2/20/74/74	0/4/4/4
5	PEB	L	201	2	-	4/20/74/74	0/4/4/4
4	DBV	G	101	3	-	5/22/74/74	0/4/4/4
5	PEB	H	201	2	-	5/20/74/74	0/4/4/4
5	PEB	J	201	2	-	4/20/74/74	0/4/4/4
5	PEB	L	202	2	-	7/20/74/74	0/4/4/4
5	PEB	P	202	2	-	5/20/74/74	0/4/4/4
5	PEB	B	201	2	-	6/20/74/74	0/4/4/4
4	DBV	O	101	3	-	4/22/74/74	0/4/4/4
5	PEB	H	203	2	-	3/20/74/74	0/4/4/4
5	PEB	L	203	2	-	2/20/74/74	0/4/4/4
5	PEB	P	201	2	-	4/20/74/74	0/4/4/4
5	PEB	N	202	2	-	4/20/74/74	0/4/4/4
5	PEB	D	201	2	-	5/20/74/74	0/4/4/4
5	PEB	N	203	2	-	2/20/74/74	0/4/4/4
4	DBV	A	101	1	-	5/22/74/74	0/4/4/4
5	PEB	F	201	2	-	4/20/74/74	0/4/4/4
4	DBV	E	101	1	-	5/22/74/74	0/4/4/4

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	101	DBV	C1B-CHA	3.50	1.54	1.41
4	G	101	DBV	CAB-C3B	-3.43	1.47	1.52
4	A	101	DBV	CHB-C1C	3.34	1.37	1.35
4	I	101	DBV	C1B-CHA	3.30	1.54	1.41
4	O	101	DBV	C1B-CHA	3.30	1.53	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	101	DBV	C1B-CHA	3.27	1.53	1.41
4	M	101	DBV	C4B-CHB	3.23	1.53	1.41
5	P	202	PEB	CAC-C2C	-3.23	1.47	1.52
4	I	101	DBV	C4B-CHB	3.19	1.53	1.41
4	K	101	DBV	C1B-CHA	3.14	1.53	1.41
4	A	101	DBV	C4B-CHB	3.13	1.53	1.41
4	O	101	DBV	C4B-CHB	3.09	1.53	1.41
5	F	201	PEB	CAC-C2C	-3.06	1.47	1.52
4	C	101	DBV	C4B-CHB	3.06	1.53	1.41
4	A	101	DBV	C3A-C2A	3.05	1.43	1.37
4	E	101	DBV	C1B-CHA	3.04	1.52	1.41
4	O	101	DBV	C1C-NC	-2.99	1.32	1.38
5	J	201	PEB	CAC-C2C	-2.96	1.47	1.52
4	E	101	DBV	C4B-CHB	2.94	1.52	1.41
4	C	101	DBV	C3A-C2A	2.93	1.43	1.37
4	G	101	DBV	C3A-C2A	2.93	1.43	1.37
4	A	101	DBV	C1B-CHA	2.93	1.52	1.41
4	A	101	DBV	CAB-C3B	-2.87	1.47	1.52
4	K	101	DBV	C4B-CHB	2.87	1.52	1.41
5	H	202	PEB	CHC-C1D	-2.87	1.46	1.54
4	M	101	DBV	C3A-C2A	2.85	1.43	1.37
5	D	203	PEB	CHB-C4B	2.83	1.37	1.35
5	H	202	PEB	CMD-C2D	-2.82	1.45	1.50
4	E	101	DBV	CAB-C3B	-2.81	1.47	1.52
4	M	101	DBV	C1B-CHA	2.80	1.52	1.41
5	N	202	PEB	CAC-C2C	-2.80	1.47	1.52
4	E	101	DBV	C3A-C2A	2.73	1.42	1.37
5	J	203	PEB	CHC-C1D	-2.68	1.47	1.54
4	I	101	DBV	C3A-C2A	2.68	1.42	1.37
4	I	101	DBV	C1C-NC	-2.67	1.32	1.38
5	B	203	PEB	CMC-C3C	-2.66	1.46	1.51
4	G	101	DBV	C4B-CHB	2.62	1.51	1.41
5	J	201	PEB	CHB-C4B	2.60	1.37	1.35
5	H	203	PEB	CAC-C2C	-2.58	1.48	1.52
5	N	201	PEB	CAC-C2C	-2.56	1.48	1.52
5	D	203	PEB	CMD-C2D	-2.53	1.46	1.50
5	P	202	PEB	CHB-C4B	2.53	1.37	1.35
5	N	202	PEB	CMD-C2D	-2.53	1.46	1.50
5	F	202	PEB	C4B-NB	-2.51	1.33	1.38
5	P	203	PEB	CMD-C2D	-2.49	1.46	1.50
5	P	203	PEB	CHB-C4B	2.48	1.37	1.35
5	J	203	PEB	CMC-C3C	-2.47	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	101	DBV	C1C-NC	-2.46	1.33	1.38
4	K	101	DBV	C1C-NC	-2.45	1.33	1.38
5	P	202	PEB	C4B-NB	-2.43	1.33	1.38
5	D	202	PEB	CMD-C2D	-2.43	1.46	1.50
5	J	202	PEB	C4B-C3B	-2.43	1.41	1.45
5	N	202	PEB	C4B-C3B	-2.41	1.41	1.45
5	L	203	PEB	C3C-C4C	2.41	1.45	1.42
5	F	201	PEB	CHB-C4B	2.40	1.37	1.35
4	I	101	DBV	CAB-C3B	-2.40	1.48	1.52
5	L	203	PEB	CHC-C1D	-2.39	1.48	1.54
4	C	101	DBV	C1C-NC	-2.38	1.33	1.38
5	F	203	PEB	CAC-C2C	-2.37	1.48	1.52
5	L	202	PEB	CMD-C2D	-2.37	1.46	1.50
4	K	101	DBV	C3A-C2A	2.37	1.42	1.37
5	L	202	PEB	CAC-C2C	-2.36	1.48	1.52
5	F	203	PEB	C4B-NB	-2.34	1.33	1.38
5	H	203	PEB	CHB-C4B	2.33	1.37	1.35
5	F	202	PEB	CHC-C1D	-2.32	1.48	1.54
5	N	203	PEB	CMC-C3C	-2.32	1.46	1.51
5	J	201	PEB	CMC-C3C	-2.32	1.46	1.51
5	N	201	PEB	C4B-NB	-2.32	1.33	1.38
5	L	203	PEB	C2D-C3D	2.31	1.37	1.34
5	B	202	PEB	C4B-NB	-2.31	1.33	1.38
5	B	203	PEB	C4B-NB	-2.30	1.33	1.38
5	N	202	PEB	CHA-C4A	-2.27	1.32	1.36
5	D	202	PEB	CHC-C1D	-2.27	1.48	1.54
4	C	101	DBV	CAB-C3B	-2.27	1.48	1.52
5	P	201	PEB	C4B-NB	-2.26	1.33	1.38
5	D	202	PEB	CHA-C1B	2.25	1.45	1.40
5	F	203	PEB	CMC-C3C	-2.23	1.47	1.51
5	B	202	PEB	C3C-C4C	2.23	1.45	1.42
5	J	202	PEB	CMD-C2D	-2.22	1.46	1.50
4	E	101	DBV	C1C-NC	-2.22	1.33	1.38
5	H	201	PEB	C4B-C3B	-2.20	1.42	1.45
5	F	202	PEB	CMD-C2D	-2.20	1.46	1.50
5	B	202	PEB	CAC-C2C	-2.20	1.48	1.52
5	H	203	PEB	CMC-C3C	-2.20	1.47	1.51
5	J	203	PEB	CHB-C4B	2.19	1.36	1.35
5	L	202	PEB	C4B-NB	-2.19	1.33	1.38
5	L	201	PEB	CHB-C4B	2.18	1.36	1.35
4	O	101	DBV	C3A-C2A	2.17	1.41	1.37
5	H	201	PEB	C3C-C4C	2.16	1.45	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	201	PEB	C4B-NB	-2.16	1.33	1.38
5	B	201	PEB	CAC-C2C	-2.16	1.48	1.52
5	D	203	PEB	CMC-C3C	-2.15	1.47	1.51
5	J	202	PEB	CMC-C3C	-2.15	1.47	1.51
5	F	201	PEB	C1C-CHB	2.15	1.49	1.41
4	A	101	DBV	CHC-C4C	2.15	1.52	1.50
5	B	201	PEB	C3C-C4C	2.13	1.45	1.42
5	H	202	PEB	C4B-NB	-2.12	1.34	1.38
5	J	203	PEB	CAC-C2C	-2.12	1.48	1.52
4	I	101	DBV	CMB-C2B	-2.11	1.47	1.51
5	N	201	PEB	CMC-C3C	-2.11	1.47	1.51
4	K	101	DBV	CMB-C2B	-2.11	1.47	1.51
5	P	202	PEB	CHC-C1D	-2.10	1.48	1.54
5	L	202	PEB	C3C-C4C	2.10	1.45	1.42
5	P	202	PEB	C1C-CHB	2.10	1.49	1.41
4	K	101	DBV	CAB-C3B	-2.10	1.49	1.52
5	B	203	PEB	CMD-C2D	-2.10	1.47	1.50
5	F	201	PEB	C4B-NB	-2.09	1.34	1.38
4	C	101	DBV	CMB-C2B	-2.09	1.47	1.51
4	O	101	DBV	CAD-C3D	2.09	1.53	1.47
4	A	101	DBV	C1C-NC	-2.08	1.34	1.38
4	E	101	DBV	CMB-C2B	-2.07	1.47	1.51
5	P	202	PEB	C3C-C4C	2.07	1.45	1.42
5	D	202	PEB	C4B-C3B	-2.07	1.42	1.45
5	H	201	PEB	C4B-NB	-2.07	1.34	1.38
5	N	202	PEB	CMC-C3C	-2.07	1.47	1.51
5	D	201	PEB	CAC-C2C	-2.06	1.49	1.52
5	D	202	PEB	C4B-NB	-2.06	1.34	1.38
4	G	101	DBV	C1C-NC	-2.06	1.34	1.38
5	N	203	PEB	CHC-C1D	-2.05	1.48	1.54
5	L	203	PEB	C4B-NB	-2.04	1.34	1.38
5	D	201	PEB	C4B-C3B	-2.04	1.42	1.45
5	P	201	PEB	C1C-CHB	2.04	1.49	1.41
5	P	202	PEB	CMD-C2D	-2.03	1.47	1.50
5	H	203	PEB	CAA-C3A	-2.02	1.50	1.54
5	J	202	PEB	C3C-C4C	2.00	1.45	1.42

All (287) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	101	DBV	C1D-CHC-C4C	4.93	124.09	113.37
5	P	202	PEB	C1C-CHB-C4B	4.86	134.61	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	202	PEB	C1C-CHB-C4B	4.70	134.42	128.81
5	F	202	PEB	C1C-CHB-C4B	4.54	134.23	128.81
4	A	101	DBV	C1D-CHC-C4C	4.24	122.59	113.37
5	H	202	PEB	CBC-CAC-C2C	4.20	120.24	112.49
5	J	202	PEB	C1C-CHB-C4B	4.17	133.78	128.81
5	L	201	PEB	C2A-C3A-C4A	4.15	107.55	101.34
4	K	101	DBV	C1D-CHC-C4C	4.10	122.28	113.37
4	K	101	DBV	C4A-NA-C1A	-4.04	105.53	110.67
4	I	101	DBV	C4A-NA-C1A	-4.04	105.53	110.67
5	P	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
5	L	202	PEB	C1C-CHB-C4B	4.00	133.58	128.81
4	O	101	DBV	C4A-NA-C1A	-3.94	105.65	110.67
4	A	101	DBV	CAB-CBB-CGB	3.91	119.23	112.67
4	M	101	DBV	C4A-NA-C1A	-3.91	105.69	110.67
5	L	201	PEB	C2A-C1A-NA	3.90	111.63	108.27
5	D	201	PEB	C2A-C1A-NA	3.88	111.62	108.27
4	E	101	DBV	C4A-NA-C1A	-3.85	105.76	110.67
5	F	203	PEB	C2A-C1A-NA	3.84	111.58	108.27
5	P	201	PEB	C2A-C3A-C4A	3.78	107.00	101.34
5	J	203	PEB	C2A-C1A-NA	3.76	111.52	108.27
5	D	201	PEB	C2A-C3A-C4A	3.76	106.97	101.34
4	C	101	DBV	CAC-CBC-CGC	3.76	118.98	112.67
5	H	203	PEB	CHA-C4A-NA	3.72	129.63	125.20
5	H	203	PEB	C2A-C3A-C4A	3.69	106.86	101.34
5	D	201	PEB	CHC-C1D-ND	-3.65	109.71	113.95
5	D	203	PEB	C2A-C3A-C4A	3.64	106.79	101.34
5	H	203	PEB	C1C-CHB-C4B	3.64	133.15	128.81
4	C	101	DBV	C4A-NA-C1A	-3.62	106.06	110.67
5	P	203	PEB	C2A-C1A-NA	3.60	111.38	108.27
4	G	101	DBV	C1D-CHC-C4C	3.59	121.18	113.37
5	L	203	PEB	C2A-C3A-C4A	3.59	106.71	101.34
4	A	101	DBV	C4A-NA-C1A	-3.57	106.12	110.67
5	L	201	PEB	OA-C1A-C2A	-3.56	123.34	126.17
5	N	201	PEB	C2A-C1A-NA	3.56	111.34	108.27
5	L	201	PEB	C1C-CHB-C4B	3.53	133.03	128.81
5	J	203	PEB	C2A-C3A-C4A	3.50	106.59	101.34
5	P	203	PEB	C2A-C3A-C4A	3.48	106.56	101.34
5	P	201	PEB	C2A-C1A-NA	3.48	111.27	108.27
5	B	201	PEB	C2A-C1A-NA	3.46	111.26	108.27
5	H	201	PEB	C2A-C1A-NA	3.45	111.25	108.27
5	B	203	PEB	C2A-C1A-NA	3.43	111.23	108.27
5	J	203	PEB	C1C-CHB-C4B	3.43	132.90	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	101	DBV	C1C-C2C-C3C	-3.42	103.00	106.78
4	G	101	DBV	C4A-NA-C1A	-3.40	106.33	110.67
4	E	101	DBV	CAC-CBC-CGC	3.40	118.37	112.67
4	I	101	DBV	CAC-CBC-CGC	3.38	118.34	112.67
5	L	203	PEB	C2A-C1A-NA	3.38	111.18	108.27
5	D	203	PEB	CHA-C4A-NA	3.37	129.21	125.20
5	F	201	PEB	C1C-CHB-C4B	3.36	132.82	128.81
5	H	201	PEB	C2A-C3A-C4A	3.35	106.35	101.34
4	C	101	DBV	C1D-CHC-C4C	3.34	120.64	113.37
4	O	101	DBV	C3D-C4D-ND	3.27	113.68	107.26
4	I	101	DBV	CMD-C2D-C3D	-3.26	125.47	130.06
5	D	203	PEB	C1C-CHB-C4B	3.25	132.70	128.81
4	M	101	DBV	C1D-CHC-C4C	3.24	120.42	113.37
5	F	201	PEB	C2A-C3A-C4A	3.22	106.17	101.34
5	B	202	PEB	CHA-C1B-C2B	3.20	133.12	124.90
5	F	203	PEB	C2A-C3A-C4A	3.18	106.09	101.34
4	E	101	DBV	C1D-CHC-C4C	3.16	120.25	113.37
5	N	203	PEB	C2A-C1A-NA	3.16	111.00	108.27
4	M	101	DBV	CAC-CBC-CGC	3.15	117.96	112.67
4	E	101	DBV	CHA-C4A-NA	-3.15	119.82	130.40
5	D	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
5	N	202	PEB	CBC-CAC-C2C	3.14	118.28	112.49
5	J	201	PEB	C2A-C1A-NA	3.14	110.98	108.27
4	G	101	DBV	CHA-C4A-NA	-3.13	119.88	130.40
4	C	101	DBV	C3D-C4D-ND	3.12	113.38	107.26
5	P	201	PEB	CMC-C3C-C2C	3.09	130.77	124.94
5	P	203	PEB	C1C-CHB-C4B	3.08	132.48	128.81
5	N	203	PEB	C2A-C3A-C4A	3.07	105.94	101.34
5	D	201	PEB	CHA-C4A-NA	3.06	128.84	125.20
4	K	101	DBV	C3D-C4D-ND	3.05	113.25	107.26
5	N	201	PEB	CHB-C4B-NB	-3.05	124.60	128.83
4	K	101	DBV	CMD-C2D-C3D	-3.03	125.79	130.06
4	M	101	DBV	CHA-C4A-NA	-3.02	120.26	130.40
5	N	202	PEB	CHC-C1D-ND	-3.02	110.44	113.95
4	E	101	DBV	C1C-C2C-C3C	-3.00	103.46	106.78
4	M	101	DBV	C3D-C4D-ND	3.00	113.14	107.26
4	E	101	DBV	CMD-C2D-C3D	-2.99	125.84	130.06
5	D	202	PEB	CHA-C1B-C2B	2.99	132.60	124.90
5	J	201	PEB	C2A-C3A-C4A	2.99	105.82	101.34
4	I	101	DBV	C1C-C2C-C3C	-2.98	103.48	106.78
5	N	202	PEB	C1C-CHB-C4B	2.98	132.37	128.81
5	H	202	PEB	CAC-CBC-CGC	2.96	117.64	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	203	PEB	CHA-C4A-NA	2.96	128.73	125.20
4	A	101	DBV	CHA-C4A-NA	-2.96	120.45	130.40
5	B	203	PEB	CHB-C4B-NB	-2.96	124.72	128.83
4	A	101	DBV	C3D-C4D-ND	2.95	113.06	107.26
5	B	203	PEB	CHA-C1B-C2B	2.95	132.49	124.90
4	I	101	DBV	C3D-C4D-ND	2.95	113.05	107.26
4	I	101	DBV	C1D-CHC-C4C	2.95	119.78	113.37
5	F	201	PEB	C2A-C1A-NA	2.94	110.81	108.27
4	O	101	DBV	CHA-C4A-NA	-2.93	120.56	130.40
5	F	203	PEB	CHA-C1B-C2B	2.93	132.43	124.90
5	B	202	PEB	CHB-C4B-NB	-2.93	124.77	128.83
4	C	101	DBV	OD-C4D-C3D	-2.92	122.84	129.46
4	A	101	DBV	C1C-C2C-C3C	-2.92	103.55	106.78
5	P	201	PEB	CHA-C1B-C2B	2.92	132.41	124.90
5	P	202	PEB	C2A-C3A-C4A	2.91	105.70	101.34
4	M	101	DBV	C1C-C2C-C3C	-2.90	103.58	106.78
4	E	101	DBV	C3D-C4D-ND	2.89	112.93	107.26
5	J	201	PEB	CHC-C1D-ND	-2.89	110.59	113.95
5	F	203	PEB	CHB-C4B-NB	-2.88	124.83	128.83
4	K	101	DBV	C1C-C2C-C3C	-2.88	103.60	106.78
5	J	201	PEB	CHB-C4B-NB	-2.87	124.84	128.83
5	F	203	PEB	C1C-CHB-C4B	2.87	132.24	128.81
5	B	203	PEB	C2A-C3A-C4A	2.87	105.64	101.34
5	H	203	PEB	C2A-C1A-NA	2.86	110.74	108.27
5	B	202	PEB	C1C-CHB-C4B	2.86	132.23	128.81
5	F	202	PEB	CHA-C1B-C2B	2.85	132.22	124.90
5	L	203	PEB	CHA-C1B-C2B	2.84	132.21	124.90
5	P	203	PEB	CMC-C3C-C2C	2.84	130.30	124.94
4	G	101	DBV	C4B-CHB-C1C	-2.84	125.41	128.81
5	H	202	PEB	C2A-C1A-NA	2.83	110.71	108.27
5	J	202	PEB	CBC-CAC-C2C	2.82	117.68	112.49
5	D	202	PEB	C2A-C3A-C4A	2.81	105.56	101.34
4	O	101	DBV	C1C-C2C-C3C	-2.81	103.67	106.78
5	D	202	PEB	CMC-C3C-C2C	2.81	130.24	124.94
5	P	203	PEB	CHA-C1B-C2B	2.80	132.10	124.90
4	K	101	DBV	CHA-C4A-NA	-2.80	120.99	130.40
5	F	202	PEB	C2A-C3A-C4A	2.80	105.53	101.34
4	C	101	DBV	CHA-C4A-NA	-2.79	121.02	130.40
4	G	101	DBV	C3D-C4D-ND	2.79	112.74	107.26
5	L	202	PEB	CHA-C1B-C2B	2.79	132.08	124.90
5	F	201	PEB	CHB-C4B-NB	-2.79	124.96	128.83
4	G	101	DBV	C1C-C2C-C3C	-2.77	103.71	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	101	DBV	OD-C4D-C3D	-2.77	123.18	129.46
5	D	203	PEB	C2A-C1A-NA	2.77	110.66	108.27
5	L	201	PEB	OD-C4D-C3D	-2.76	123.20	129.46
4	O	101	DBV	CHC-C1D-ND	2.76	117.22	113.72
5	J	203	PEB	OA-C1A-C2A	-2.75	123.98	126.17
5	N	201	PEB	C2A-C3A-C4A	2.71	105.39	101.34
5	H	203	PEB	CHA-C1B-C2B	2.70	131.84	124.90
4	C	101	DBV	CMD-C2D-C3D	-2.67	126.29	130.06
4	O	101	DBV	OD-C4D-C3D	-2.67	123.42	129.46
5	J	203	PEB	CHA-C1B-C2B	2.66	131.74	124.90
5	H	202	PEB	C2A-C3A-C4A	2.66	105.32	101.34
4	E	101	DBV	C2A-C1A-NA	2.66	113.56	106.45
5	P	202	PEB	CHA-C1B-C2B	2.65	131.72	124.90
5	D	201	PEB	CHB-C4B-NB	-2.65	125.15	128.83
5	J	201	PEB	OD-C4D-C3D	-2.65	123.47	129.46
5	N	203	PEB	CHA-C1B-C2B	2.63	131.65	124.90
5	B	201	PEB	C2A-C3A-C4A	2.63	105.27	101.34
5	H	201	PEB	CHA-C1B-C2B	2.62	131.64	124.90
4	M	101	DBV	C2A-C1A-NA	2.62	113.45	106.45
5	L	203	PEB	CMC-C3C-C2C	2.62	129.88	124.94
5	D	203	PEB	CBC-CAC-C2C	2.61	117.31	112.49
5	B	202	PEB	CHA-C1B-NB	-2.61	119.47	124.93
5	H	201	PEB	CHB-C4B-NB	-2.61	125.20	128.83
5	N	203	PEB	CHB-C4B-NB	-2.61	125.20	128.83
4	K	101	DBV	OD-C4D-C3D	-2.61	123.55	129.46
4	O	101	DBV	CAC-CBC-CGC	2.61	117.05	112.67
5	F	201	PEB	CHA-C4A-NA	2.60	128.29	125.20
5	H	203	PEB	CMC-C3C-C2C	2.59	129.82	124.94
4	K	101	DBV	C2A-C1A-NA	2.58	113.36	106.45
4	I	101	DBV	CHA-C4A-NA	-2.58	121.75	130.40
4	G	101	DBV	C2A-C1A-NA	2.57	113.33	106.45
5	P	201	PEB	CHC-C1D-ND	-2.56	110.97	113.95
4	O	101	DBV	C2A-C1A-NA	2.56	113.30	106.45
5	D	202	PEB	CHB-C4B-NB	-2.56	125.28	128.83
5	B	202	PEB	CBC-CAC-C2C	2.55	117.19	112.49
5	L	202	PEB	C2A-C3A-C4A	2.55	105.16	101.34
5	B	202	PEB	C2A-C1A-NA	2.55	110.47	108.27
5	P	202	PEB	OA-C1A-C2A	-2.55	124.15	126.17
5	L	201	PEB	CMC-C3C-C2C	2.54	129.73	124.94
5	D	203	PEB	CHA-C1B-C2B	2.54	131.43	124.90
5	D	202	PEB	C2A-C1A-NA	2.54	110.46	108.27
5	P	202	PEB	CHB-C4B-NB	-2.53	125.32	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	101	DBV	CMD-C2D-C3D	-2.53	126.50	130.06
5	N	203	PEB	CMC-C3C-C2C	2.53	129.71	124.94
4	A	101	DBV	OD-C4D-C3D	-2.51	123.77	129.46
4	I	101	DBV	C2A-C1A-NA	2.50	113.14	106.45
5	N	203	PEB	C1C-CHB-C4B	2.49	131.79	128.81
5	D	201	PEB	CHA-C1B-C2B	2.49	131.30	124.90
4	I	101	DBV	OD-C4D-ND	-2.49	122.25	125.93
5	B	201	PEB	OD-C4D-C3D	-2.48	123.85	129.46
5	L	201	PEB	CHA-C1B-C2B	2.47	131.26	124.90
4	C	101	DBV	C2A-C1A-NA	2.47	113.06	106.45
5	H	202	PEB	CHA-C1B-C2B	2.47	131.26	124.90
4	G	101	DBV	OD-C4D-ND	-2.47	122.27	125.93
5	H	201	PEB	CMC-C3C-C2C	2.46	129.59	124.94
4	M	101	DBV	OD-C4D-ND	-2.46	122.28	125.93
5	F	202	PEB	CMC-C3C-C2C	2.46	129.58	124.94
5	N	203	PEB	CHC-C1D-ND	2.46	116.80	113.95
5	D	203	PEB	CMC-C3C-C2C	2.46	129.58	124.94
4	M	101	DBV	C3A-C4A-NA	2.46	110.64	106.80
5	J	202	PEB	CMC-C3C-C2C	2.45	129.56	124.94
5	B	202	PEB	C2A-C3A-C4A	2.43	104.98	101.34
4	A	101	DBV	C2A-C1A-NA	2.43	112.94	106.45
5	P	203	PEB	CHB-C4B-NB	-2.42	125.47	128.83
5	N	202	PEB	CMC-C3C-C2C	2.42	129.50	124.94
5	N	201	PEB	OD-C4D-C3D	-2.42	123.98	129.46
4	G	101	DBV	CMD-C2D-C3D	-2.42	126.65	130.06
5	H	203	PEB	CHB-C4B-NB	-2.42	125.47	128.83
4	E	101	DBV	C3A-C4A-NA	2.41	110.57	106.80
5	D	201	PEB	OD-C4D-C3D	-2.41	124.01	129.46
5	B	201	PEB	CHB-C4B-NB	-2.40	125.50	128.83
5	L	201	PEB	CHA-C4A-NA	2.39	128.05	125.20
5	L	202	PEB	CMC-C3C-C2C	2.39	129.45	124.94
4	O	101	DBV	CBA-CAA-C3A	-2.38	115.76	127.62
5	L	203	PEB	C1C-CHB-C4B	2.38	131.65	128.81
5	F	201	PEB	CMC-C3C-C2C	2.36	129.39	124.94
4	A	101	DBV	C3A-C4A-NA	2.35	110.47	106.80
5	P	203	PEB	CHA-C4A-NA	2.35	128.00	125.20
5	P	201	PEB	CHB-C4B-NB	-2.34	125.58	128.83
5	B	203	PEB	CBC-CAC-C2C	2.32	116.77	112.49
5	F	202	PEB	C2A-C1A-NA	2.32	110.27	108.27
5	H	201	PEB	OD-C4D-C3D	-2.31	124.22	129.46
5	D	203	PEB	CHC-C1D-ND	-2.31	111.27	113.95
5	L	203	PEB	CHA-C4A-NA	2.31	127.95	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	202	PEB	CHA-C1B-C2B	2.30	130.81	124.90
5	P	202	PEB	C2A-C1A-NA	2.30	110.25	108.27
5	B	203	PEB	CMC-C3C-C2C	2.29	129.27	124.94
5	L	202	PEB	C2A-C1A-NA	2.29	110.25	108.27
5	F	203	PEB	CMC-C3C-C2C	2.29	129.25	124.94
5	J	203	PEB	CMC-C3C-C2C	2.29	129.25	124.94
5	F	201	PEB	OD-C4D-C3D	-2.28	124.29	129.46
4	K	101	DBV	CAC-CBC-CGC	2.28	116.50	112.67
5	L	202	PEB	CHB-C4B-NB	-2.28	125.66	128.83
5	P	203	PEB	CAB-CBB-CGB	2.27	116.49	112.67
5	F	203	PEB	CHA-C4A-NA	2.27	127.90	125.20
5	B	201	PEB	CHA-C1B-C2B	2.25	130.68	124.90
4	G	101	DBV	CBA-CAA-C3A	-2.25	116.45	127.62
5	F	203	PEB	CBC-CAC-C2C	2.24	116.62	112.49
4	I	101	DBV	C3A-C4A-NA	2.24	110.30	106.80
5	L	203	PEB	CHB-C4B-NB	-2.24	125.72	128.83
5	F	202	PEB	CHB-C4B-NB	-2.24	125.73	128.83
5	B	203	PEB	CMB-C2B-C1B	2.24	128.51	125.06
5	J	201	PEB	CMA-C2A-C1A	2.23	117.22	112.40
5	J	201	PEB	CAA-C3A-C4A	2.23	118.39	112.67
5	B	203	PEB	CHC-C1D-ND	2.22	116.53	113.95
5	N	202	PEB	CHA-C1B-C2B	2.21	130.58	124.90
5	F	201	PEB	CHA-C1B-C2B	2.20	130.56	124.90
5	H	202	PEB	CMC-C3C-C2C	2.20	129.09	124.94
4	C	101	DBV	C3A-C4A-NA	2.20	110.23	106.80
4	E	101	DBV	CBA-CAA-C3A	-2.19	116.72	127.62
5	D	203	PEB	OA-C1A-C2A	-2.19	124.43	126.17
4	K	101	DBV	CBA-CAA-C3A	-2.18	116.77	127.62
5	P	203	PEB	CAC-CBC-CGC	2.18	116.33	112.67
5	P	201	PEB	CHA-C1B-NB	-2.18	120.38	124.93
4	I	101	DBV	C4B-CHB-C1C	-2.17	126.21	128.81
5	B	203	PEB	CHA-C1B-NB	-2.17	120.39	124.93
4	M	101	DBV	CBA-CAA-C3A	-2.17	116.84	127.62
5	N	201	PEB	CMC-C3C-C2C	2.16	129.02	124.94
4	G	101	DBV	CBB-CAB-C3B	-2.16	108.50	112.49
5	H	203	PEB	OA-C1A-C2A	-2.16	124.46	126.17
4	M	101	DBV	OD-C4D-C3D	-2.16	124.57	129.46
5	P	201	PEB	OD-C4D-C3D	-2.15	124.58	129.46
5	B	201	PEB	CMC-C3C-C2C	2.15	129.00	124.94
5	N	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
5	D	202	PEB	C1C-CHB-C4B	2.14	131.37	128.81
5	J	201	PEB	CHA-C1B-C2B	2.14	130.39	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	201	PEB	OA-C1A-C2A	-2.13	124.48	126.17
5	P	203	PEB	CHA-C1B-NB	-2.13	120.47	124.93
5	J	202	PEB	C2A-C3A-C4A	2.13	104.53	101.34
5	P	201	PEB	C3D-C4D-ND	2.13	111.44	107.26
5	L	201	PEB	C3D-C4D-ND	2.13	111.43	107.26
5	L	203	PEB	CBC-CAC-C2C	2.12	116.40	112.49
5	P	202	PEB	CMC-C3C-C2C	2.10	128.91	124.94
4	C	101	DBV	CBA-CAA-C3A	-2.10	117.16	127.62
4	M	101	DBV	CMD-C2D-C3D	-2.10	127.10	130.06
4	O	101	DBV	CMD-C2D-C3D	-2.10	127.10	130.06
4	I	101	DBV	OD-C4D-C3D	-2.10	124.70	129.46
4	O	101	DBV	C3A-C4A-NA	2.10	110.08	106.80
5	J	203	PEB	CBC-CAC-C2C	2.09	116.34	112.49
5	F	203	PEB	OA-C1A-C2A	-2.08	124.52	126.17
5	L	203	PEB	CHA-C1B-NB	-2.07	120.60	124.93
5	N	202	PEB	C2A-C3A-C4A	2.07	104.44	101.34
5	L	201	PEB	CHB-C4B-NB	-2.07	125.96	128.83
5	H	203	PEB	CHA-C1B-NB	-2.07	120.61	124.93
4	K	101	DBV	CAC-C2C-C3C	2.07	131.72	127.88
5	D	201	PEB	C1C-CHB-C4B	2.07	131.28	128.81
5	N	203	PEB	CHA-C4A-NA	2.06	127.66	125.20
5	F	201	PEB	C3D-C4D-ND	2.06	111.30	107.26
4	I	101	DBV	CBA-CAA-C3A	-2.06	117.39	127.62
4	O	101	DBV	OD-C4D-ND	-2.04	122.90	125.93
5	N	201	PEB	CHA-C1B-C2B	2.04	130.13	124.90
4	K	101	DBV	C3A-C4A-NA	2.03	109.98	106.80
5	F	203	PEB	CHA-C1B-NB	-2.03	120.69	124.93
5	D	201	PEB	CAA-C3A-C4A	2.03	117.87	112.67
5	B	201	PEB	C3D-C4D-ND	2.01	111.21	107.26
5	D	202	PEB	C2B-C1B-NB	-2.01	106.23	110.53
5	F	202	PEB	CAA-C3A-C4A	2.01	117.83	112.67
5	B	202	PEB	CMC-C3C-C2C	2.00	128.72	124.94
5	D	201	PEB	CMC-C3C-C2C	2.00	128.72	124.94

There are no chirality outliers.

All (142) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	101	DBV	C2A-C3A-CAA-CBA
4	A	101	DBV	C4A-C3A-CAA-CBA
4	A	101	DBV	NB-C1B-CHA-C4A
4	A	101	DBV	C2B-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
4	C	101	DBV	C2A-C3A-CAA-CBA
4	C	101	DBV	C4A-C3A-CAA-CBA
4	C	101	DBV	NB-C1B-CHA-C4A
4	C	101	DBV	C2B-C1B-CHA-C4A
4	C	101	DBV	NB-C4B-CHB-C1C
4	C	101	DBV	C3B-C4B-CHB-C1C
4	C	101	DBV	NC-C4C-CHC-C1D
4	E	101	DBV	C2A-C3A-CAA-CBA
4	E	101	DBV	C4A-C3A-CAA-CBA
4	E	101	DBV	NB-C1B-CHA-C4A
4	E	101	DBV	NB-C4B-CHB-C1C
4	E	101	DBV	C3B-C4B-CHB-C1C
4	G	101	DBV	C4A-C3A-CAA-CBA
4	G	101	DBV	NB-C1B-CHA-C4A
4	G	101	DBV	NB-C4B-CHB-C1C
4	G	101	DBV	C3B-C4B-CHB-C1C
4	I	101	DBV	C2A-C3A-CAA-CBA
4	I	101	DBV	C4A-C3A-CAA-CBA
4	I	101	DBV	NB-C1B-CHA-C4A
4	I	101	DBV	NB-C4B-CHB-C1C
4	I	101	DBV	C3B-C4B-CHB-C1C
4	K	101	DBV	C2A-C3A-CAA-CBA
4	K	101	DBV	C4A-C3A-CAA-CBA
4	K	101	DBV	NB-C1B-CHA-C4A
4	K	101	DBV	NB-C4B-CHB-C1C
4	K	101	DBV	C3B-C4B-CHB-C1C
4	M	101	DBV	C2A-C3A-CAA-CBA
4	M	101	DBV	C4A-C3A-CAA-CBA
4	M	101	DBV	NB-C1B-CHA-C4A
4	M	101	DBV	C2B-C1B-CHA-C4A
4	M	101	DBV	NB-C4B-CHB-C1C
4	M	101	DBV	C3B-C4B-CHB-C1C
4	O	101	DBV	C2A-C3A-CAA-CBA
4	O	101	DBV	C4A-C3A-CAA-CBA
4	O	101	DBV	NB-C1B-CHA-C4A
4	O	101	DBV	C3B-C4B-CHB-C1C
5	B	201	PEB	C2D-C3D-CAD-CBD
5	B	201	PEB	C4D-C3D-CAD-CBD
5	B	201	PEB	NB-C1B-CHA-C4A
5	B	201	PEB	C2B-C1B-CHA-C4A
5	B	202	PEB	C2A-C3A-CAA-CBA
5	B	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
5	B	202	PEB	C3A-C4A-CHA-C1B
5	B	203	PEB	NB-C1B-CHA-C4A
5	B	203	PEB	C2B-C1B-CHA-C4A
5	D	201	PEB	C2D-C3D-CAD-CBD
5	D	201	PEB	C4D-C3D-CAD-CBD
5	D	201	PEB	NB-C1B-CHA-C4A
5	D	201	PEB	C2B-C1B-CHA-C4A
5	D	202	PEB	C2A-C3A-CAA-CBA
5	D	202	PEB	C4A-C3A-CAA-CBA
5	D	202	PEB	NB-C1B-CHA-C4A
5	D	202	PEB	C2B-C1B-CHA-C4A
5	D	203	PEB	NB-C1B-CHA-C4A
5	D	203	PEB	C2B-C1B-CHA-C4A
5	F	201	PEB	C2D-C3D-CAD-CBD
5	F	201	PEB	C4D-C3D-CAD-CBD
5	F	201	PEB	NB-C1B-CHA-C4A
5	F	201	PEB	C2B-C1B-CHA-C4A
5	F	202	PEB	C2A-C3A-CAA-CBA
5	F	202	PEB	NB-C1B-CHA-C4A
5	F	202	PEB	C2B-C1B-CHA-C4A
5	F	203	PEB	NB-C1B-CHA-C4A
5	H	201	PEB	NB-C1B-CHA-C4A
5	H	201	PEB	C2B-C1B-CHA-C4A
5	H	202	PEB	C2A-C3A-CAA-CBA
5	H	202	PEB	C4A-C3A-CAA-CBA
5	H	202	PEB	NB-C1B-CHA-C4A
5	H	202	PEB	C2B-C1B-CHA-C4A
5	H	203	PEB	NB-C1B-CHA-C4A
5	H	203	PEB	C2B-C1B-CHA-C4A
5	J	201	PEB	C2D-C3D-CAD-CBD
5	J	201	PEB	C4D-C3D-CAD-CBD
5	J	201	PEB	NB-C1B-CHA-C4A
5	J	201	PEB	C2B-C1B-CHA-C4A
5	J	202	PEB	NB-C1B-CHA-C4A
5	J	202	PEB	C2B-C1B-CHA-C4A
5	J	203	PEB	NB-C1B-CHA-C4A
5	L	201	PEB	C2D-C3D-CAD-CBD
5	L	201	PEB	C4D-C3D-CAD-CBD
5	L	201	PEB	NB-C1B-CHA-C4A
5	L	201	PEB	C2B-C1B-CHA-C4A
5	L	202	PEB	C2A-C3A-CAA-CBA
5	L	202	PEB	C3A-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
5	L	202	PEB	NB-C1B-CHA-C4A
5	L	203	PEB	NB-C1B-CHA-C4A
5	N	201	PEB	C2D-C3D-CAD-CBD
5	N	201	PEB	C4D-C3D-CAD-CBD
5	N	201	PEB	NB-C1B-CHA-C4A
5	N	201	PEB	C2B-C1B-CHA-C4A
5	N	202	PEB	C2A-C3A-CAA-CBA
5	N	202	PEB	NB-C1B-CHA-C4A
5	N	202	PEB	C2B-C1B-CHA-C4A
5	N	203	PEB	NB-C1B-CHA-C4A
5	N	203	PEB	C2B-C1B-CHA-C4A
5	P	201	PEB	C2D-C3D-CAD-CBD
5	P	201	PEB	C4D-C3D-CAD-CBD
5	P	201	PEB	NB-C1B-CHA-C4A
5	P	201	PEB	C2B-C1B-CHA-C4A
5	P	202	PEB	C2A-C3A-CAA-CBA
5	P	202	PEB	C3A-C4A-CHA-C1B
5	P	202	PEB	NB-C1B-CHA-C4A
5	P	203	PEB	NB-C1B-CHA-C4A
5	P	203	PEB	C2B-C1B-CHA-C4A
5	F	203	PEB	C2B-C1B-CHA-C4A
5	J	203	PEB	C2B-C1B-CHA-C4A
5	L	202	PEB	C2B-C1B-CHA-C4A
5	L	203	PEB	C2B-C1B-CHA-C4A
5	P	202	PEB	C2B-C1B-CHA-C4A
5	B	201	PEB	C3B-CAB-CBB-CGB
5	D	201	PEB	C3B-CAB-CBB-CGB
5	B	202	PEB	NB-C1B-CHA-C4A
5	B	202	PEB	C2B-C1B-CHA-C4A
5	B	202	PEB	NA-C4A-CHA-C1B
5	L	202	PEB	C3B-CAB-CBB-CGB
5	H	201	PEB	C4D-C3D-CAD-CBD
4	C	101	DBV	C2D-C3D-CAD-CBD
4	G	101	DBV	C2A-C3A-CAA-CBA
5	H	201	PEB	C2D-C3D-CAD-CBD
4	C	101	DBV	C4D-C3D-CAD-CBD
5	B	201	PEB	C4A-C3A-CAA-CBA
5	F	202	PEB	C4A-C3A-CAA-CBA
5	H	203	PEB	C4A-C3A-CAA-CBA
5	L	202	PEB	C4A-C3A-CAA-CBA
5	N	202	PEB	C4A-C3A-CAA-CBA
5	P	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
4	I	101	DBV	NC-C1C-CHB-C4B
5	L	202	PEB	NA-C4A-CHA-C1B
5	D	202	PEB	C2B-C3B-CAB-CBB
5	D	202	PEB	C4B-C3B-CAB-CBB
4	C	101	DBV	C2C-CAC-CBC-CGC
5	J	202	PEB	C2A-C3A-CAA-CBA
5	H	201	PEB	C4A-C3A-CAA-CBA
5	J	202	PEB	C4A-C3A-CAA-CBA
4	C	101	DBV	C3B-CAB-CBB-CGB
4	M	101	DBV	C3B-CAB-CBB-CGB
5	H	202	PEB	C2C-CAC-CBC-CGC
4	A	101	DBV	NC-C1C-CHB-C4B

There are no ring outliers.

28 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	203	PEB	1	0
4	M	101	DBV	2	0
5	D	202	PEB	2	0
5	J	203	PEB	2	0
4	C	101	DBV	2	0
4	I	101	DBV	2	0
5	H	202	PEB	1	0
5	B	203	PEB	2	0
5	F	202	PEB	1	0
4	K	101	DBV	2	0
5	J	202	PEB	3	0
5	N	201	PEB	2	0
5	P	203	PEB	1	0
5	D	203	PEB	2	0
5	L	201	PEB	1	0
4	G	101	DBV	2	0
5	J	201	PEB	2	0
5	B	201	PEB	1	0
4	O	101	DBV	2	0
5	H	203	PEB	3	0
5	L	203	PEB	1	0
5	P	201	PEB	1	0
5	N	202	PEB	1	0
5	D	201	PEB	1	0
5	N	203	PEB	2	0

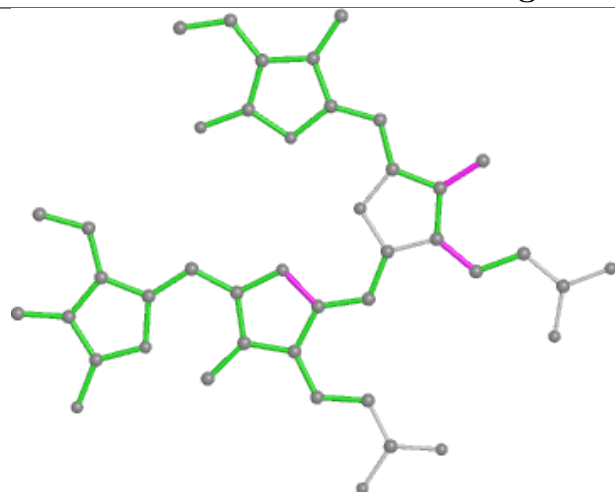
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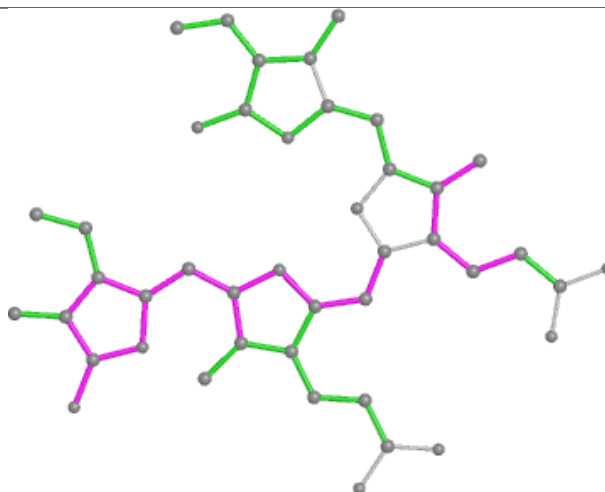
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	101	DBV	3	0
5	F	201	PEB	1	0
4	E	101	DBV	2	0

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

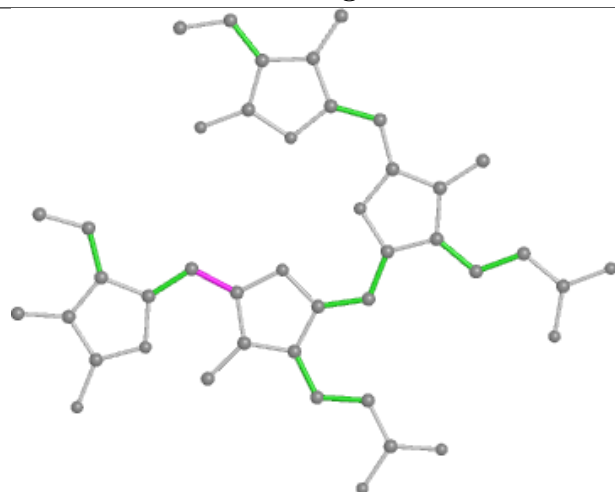
## Ligand PEB F 203



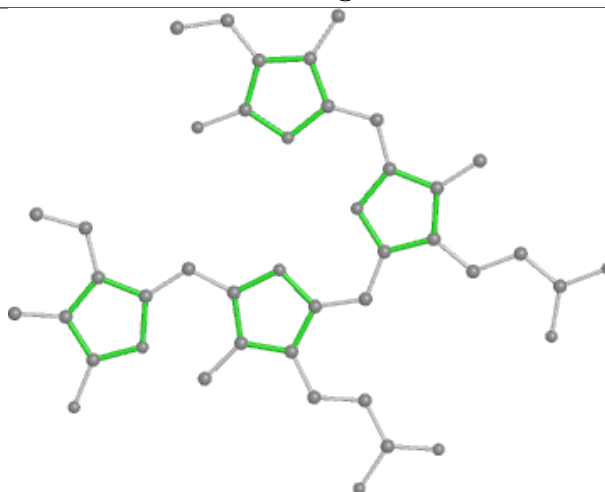
Bond lengths



Bond angles

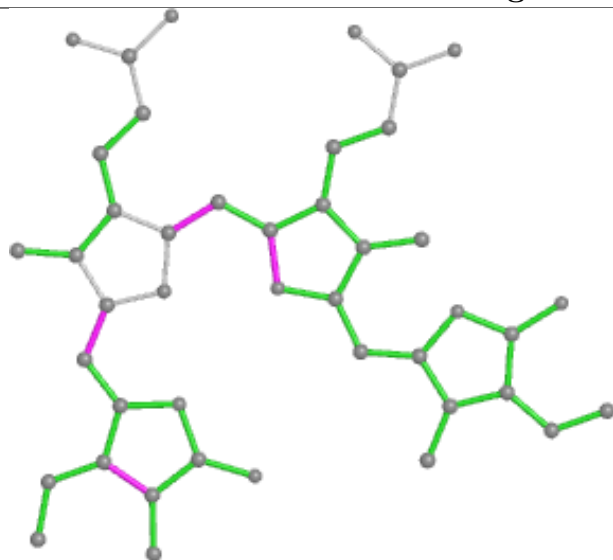


Torsions

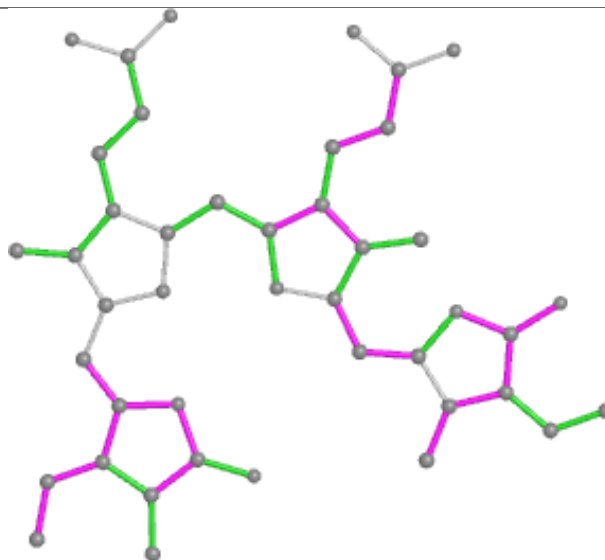


Rings

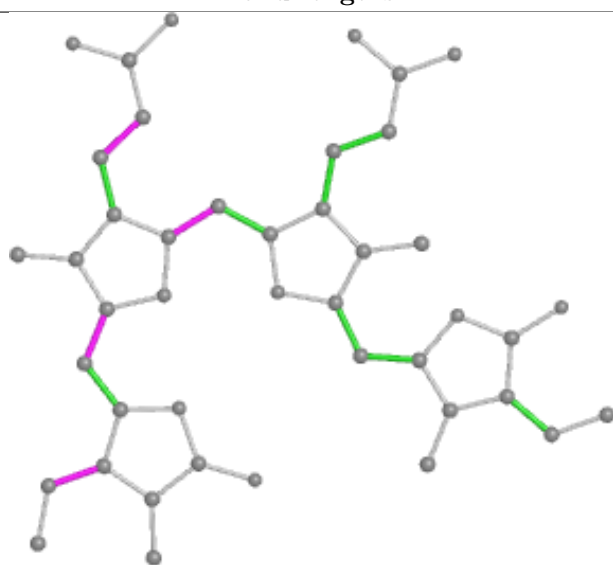
## Ligand DBV M 101



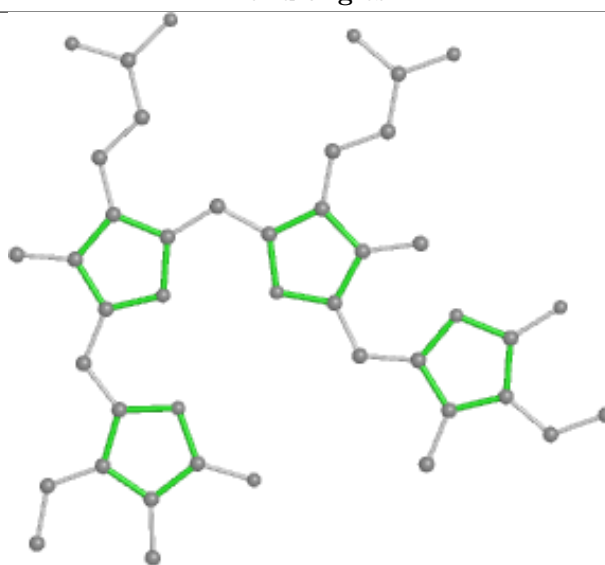
Bond lengths



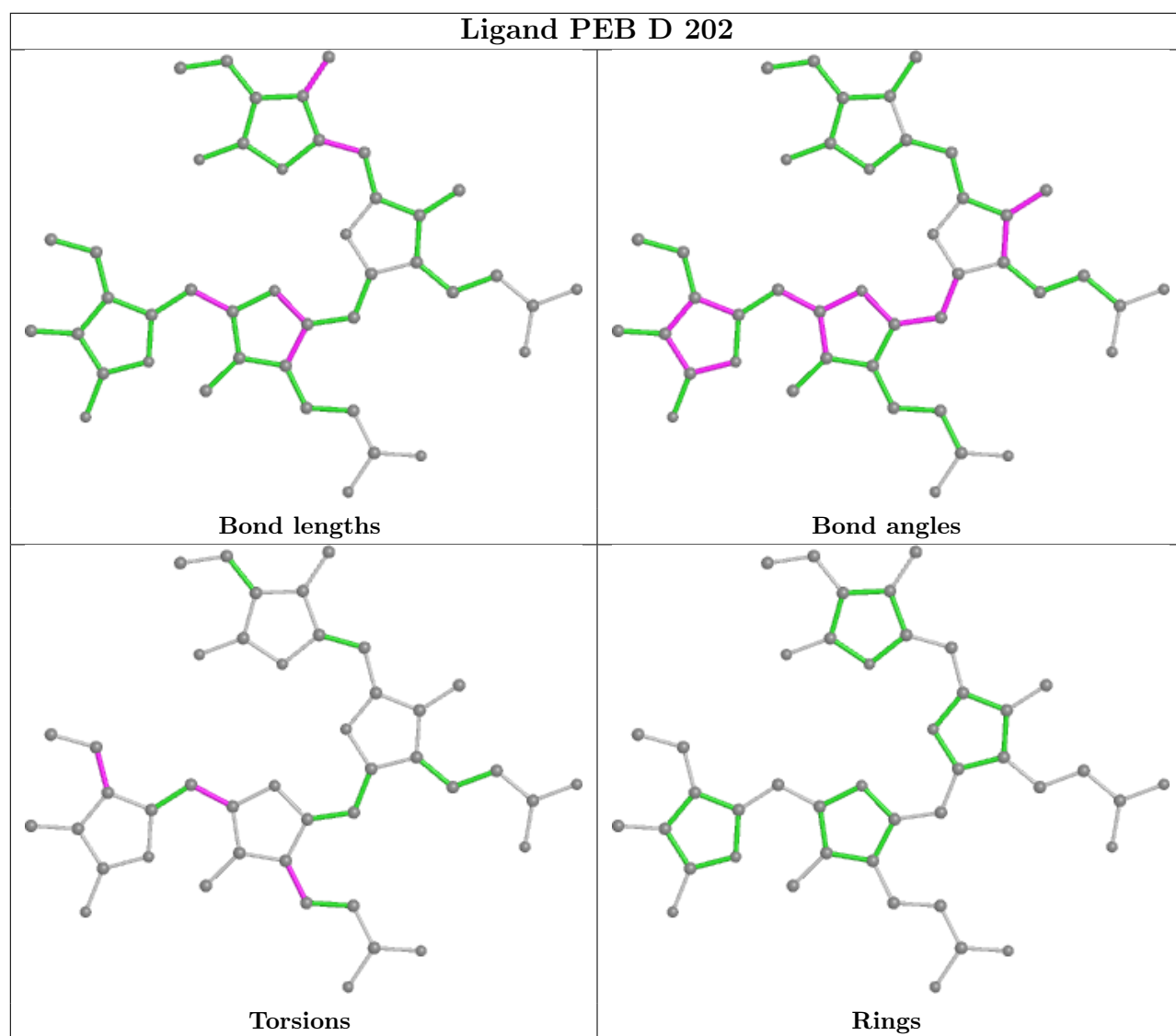
Bond angles



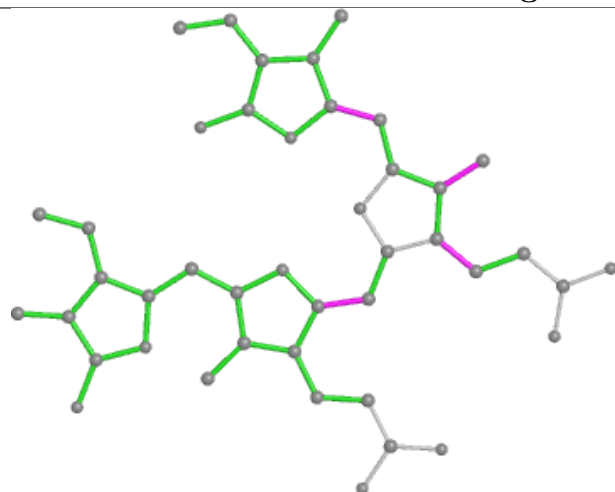
Torsions



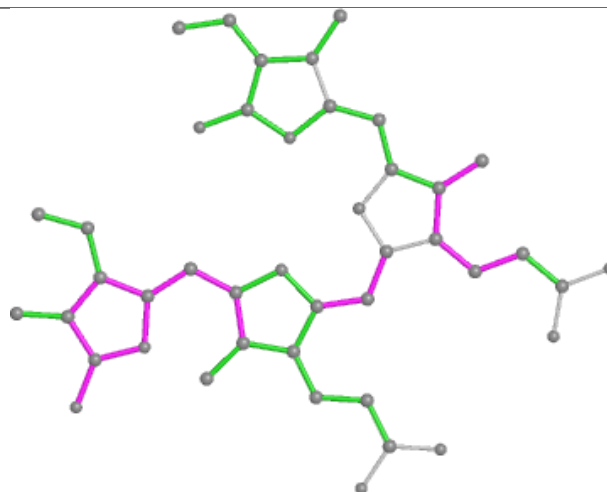
Rings



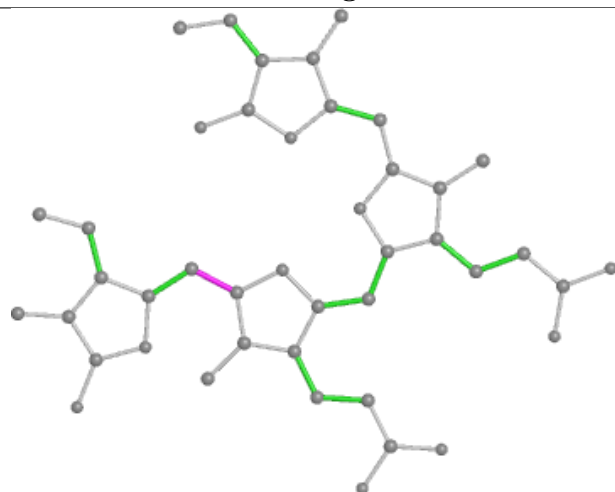
## Ligand PEB J 203



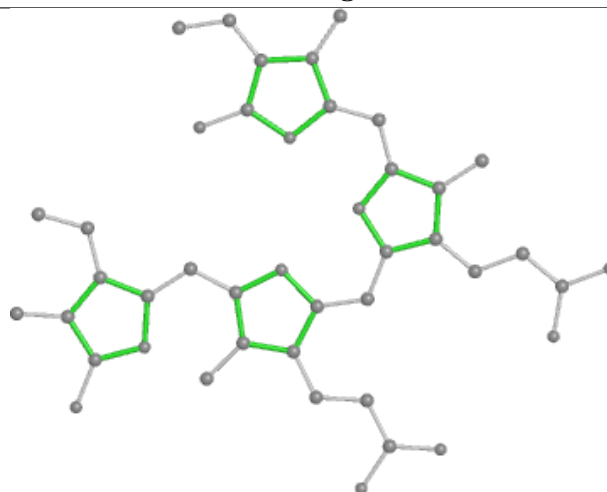
Bond lengths



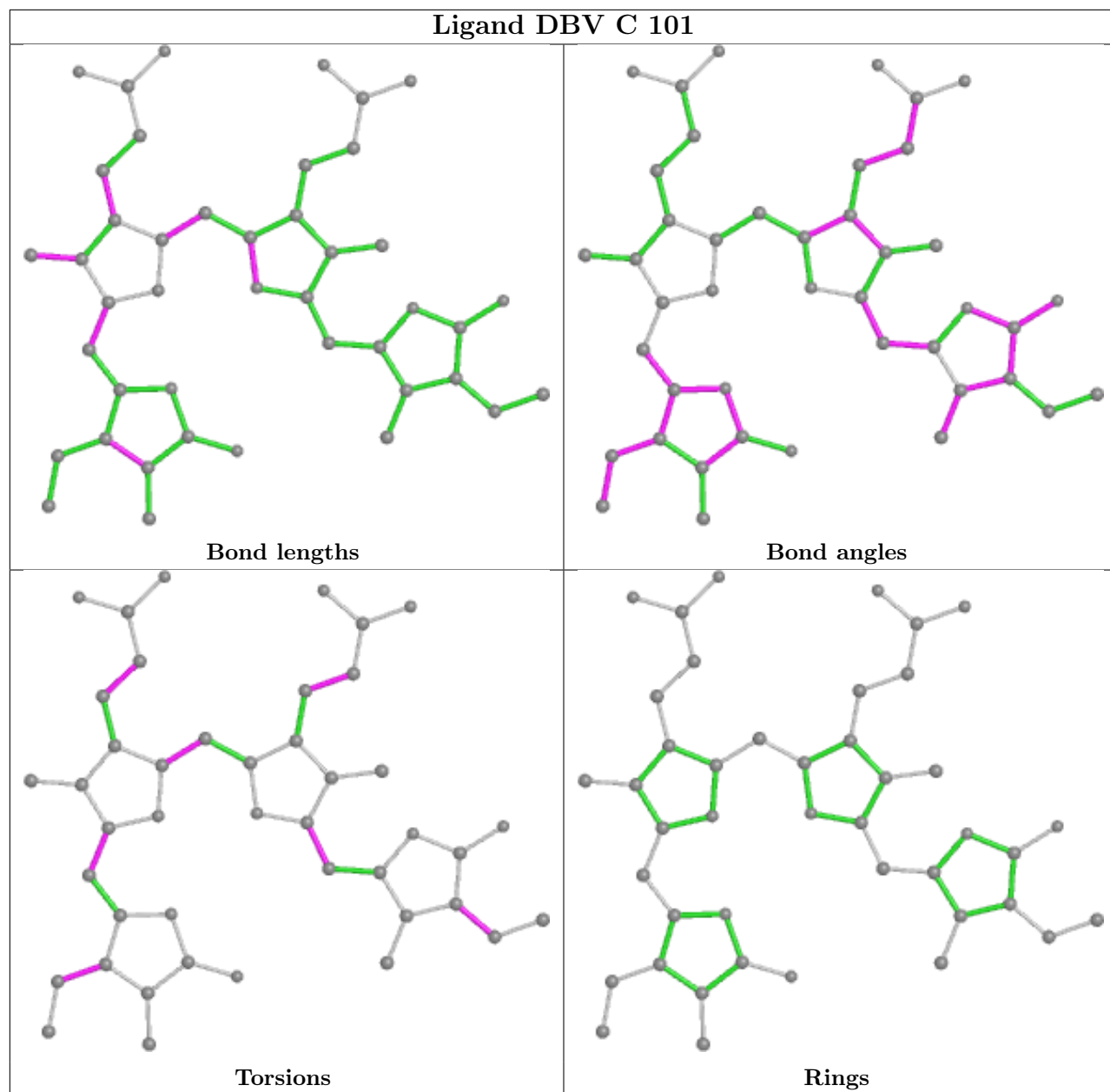
Bond angles



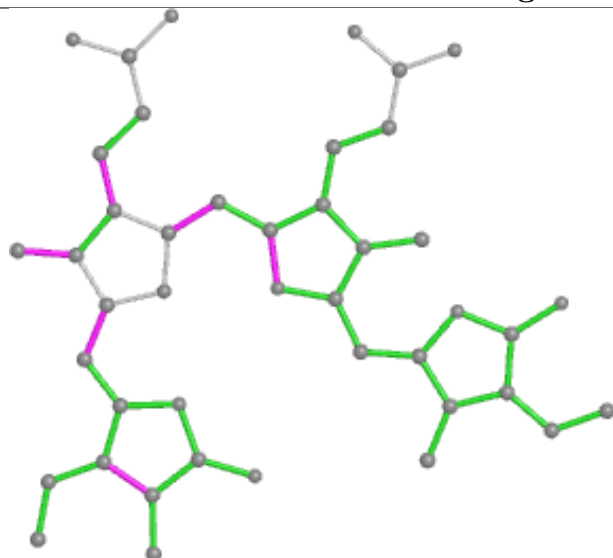
Torsions



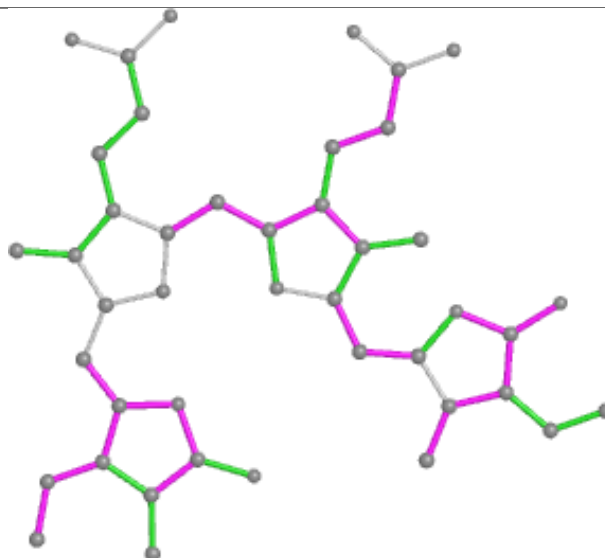
Rings



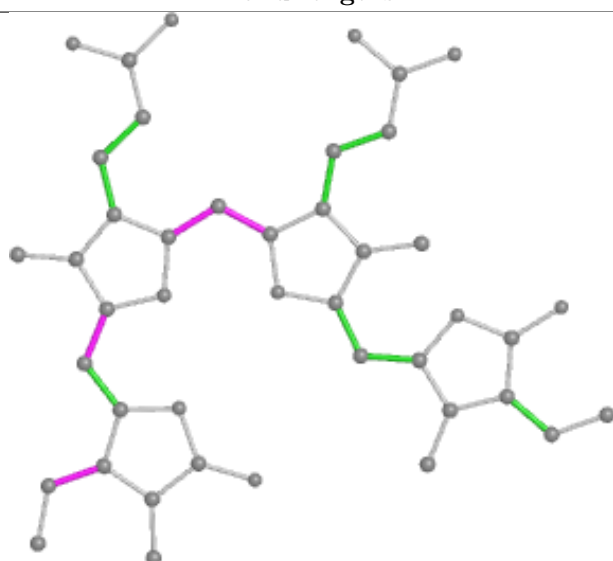
## Ligand DBV I 101



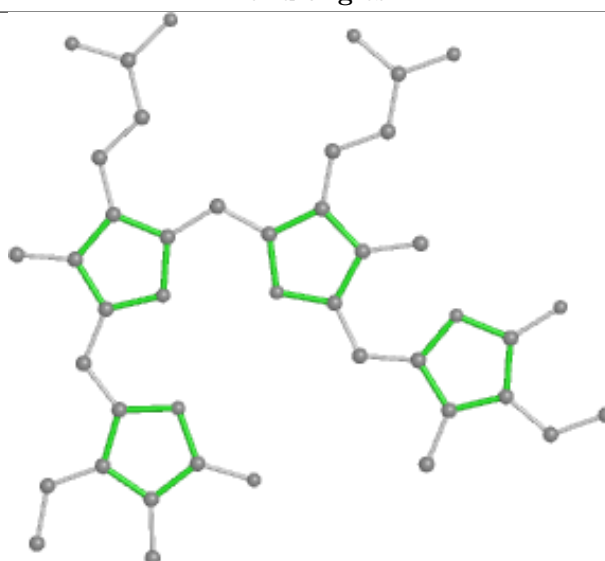
Bond lengths



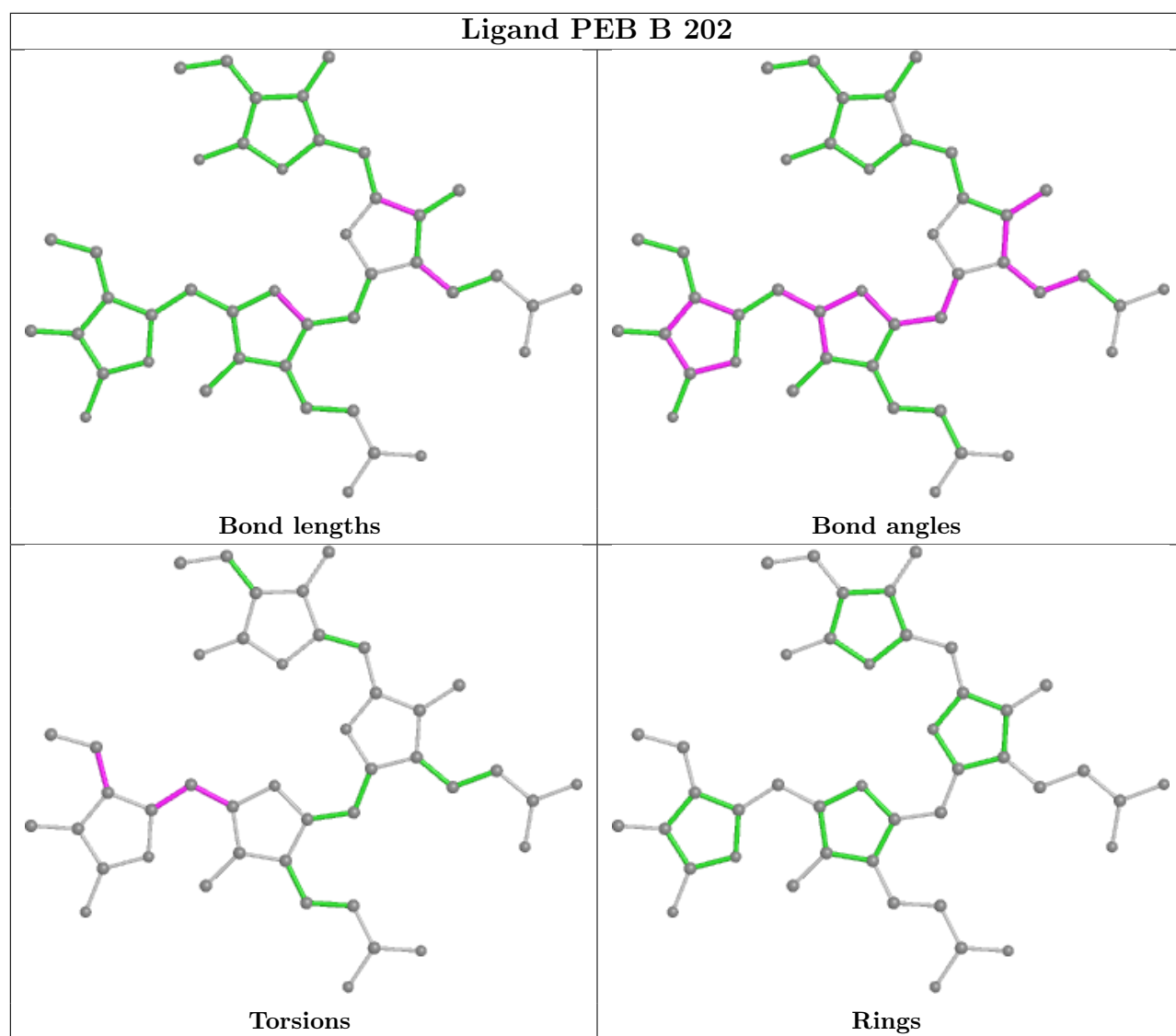
Bond angles

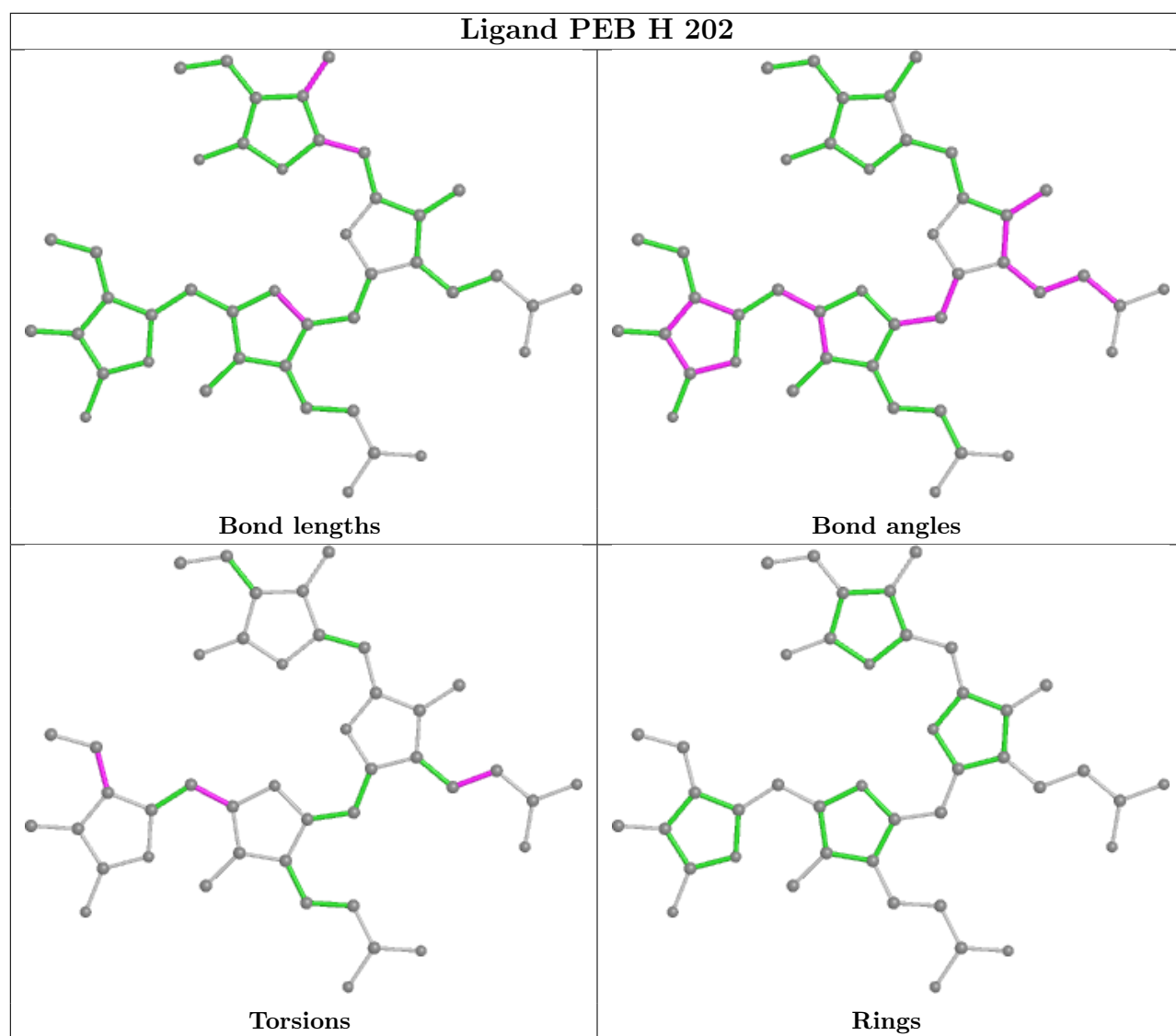


Torsions

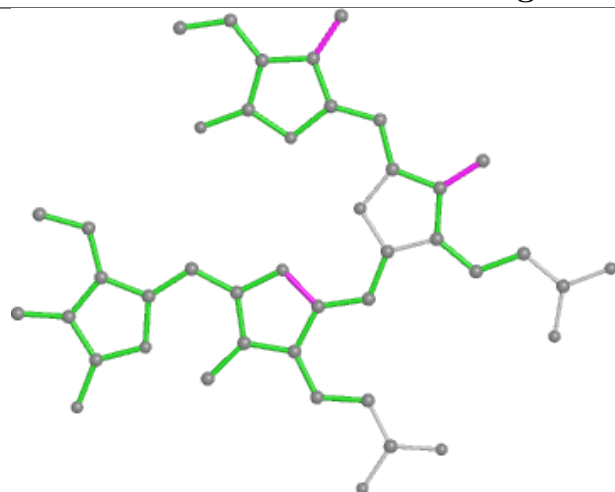


Rings

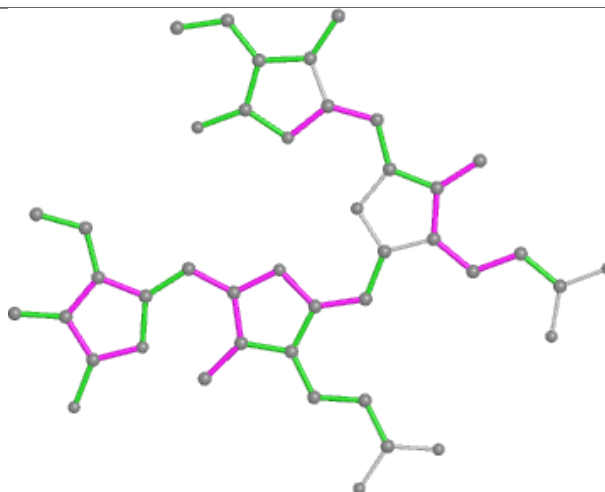




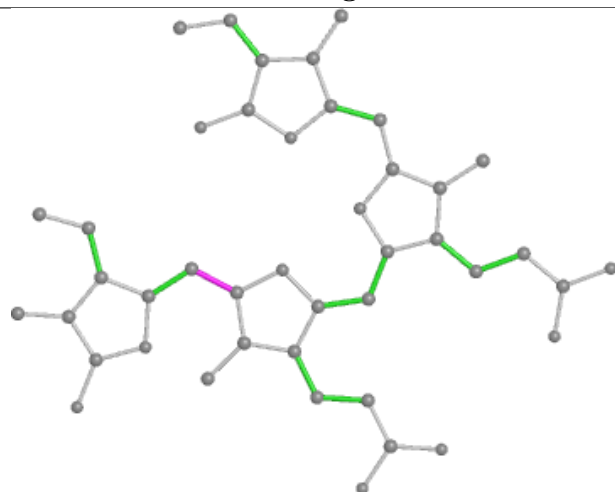
## Ligand PEB B 203



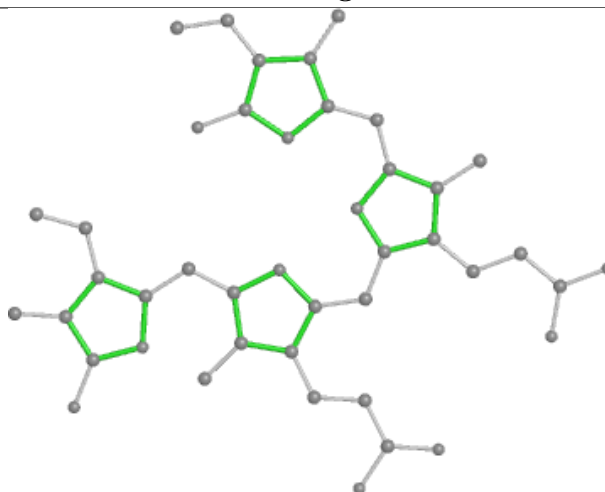
Bond lengths



Bond angles

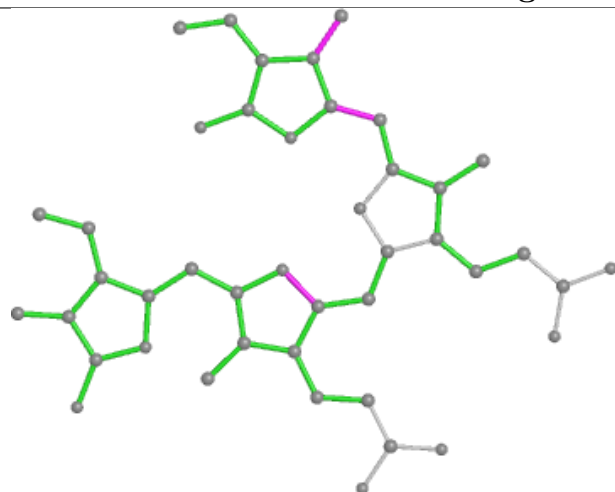


Torsions

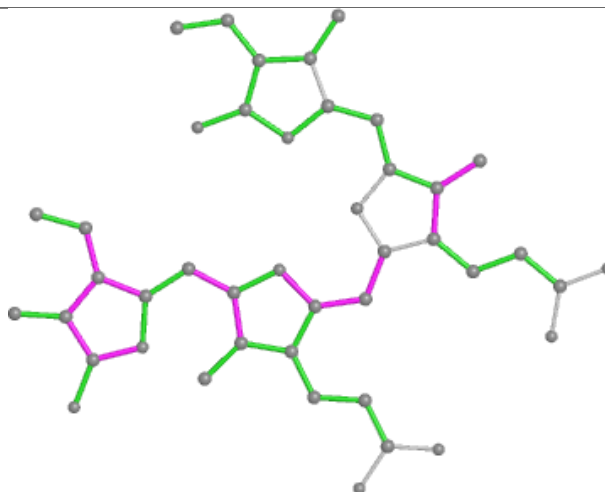


Rings

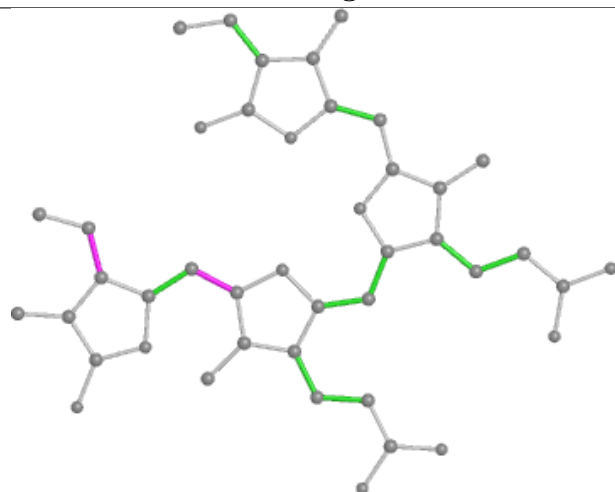
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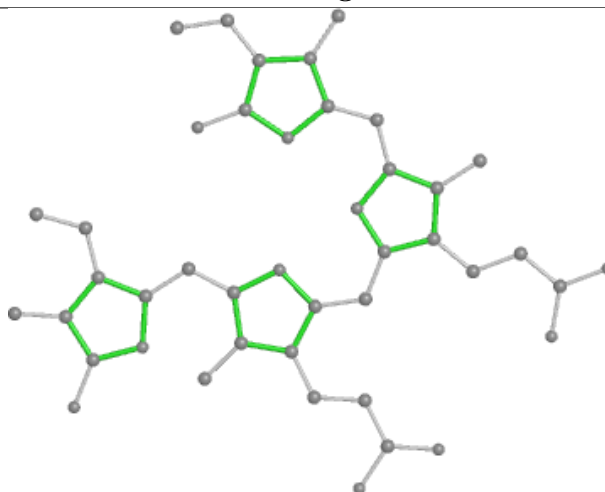
Bond lengths



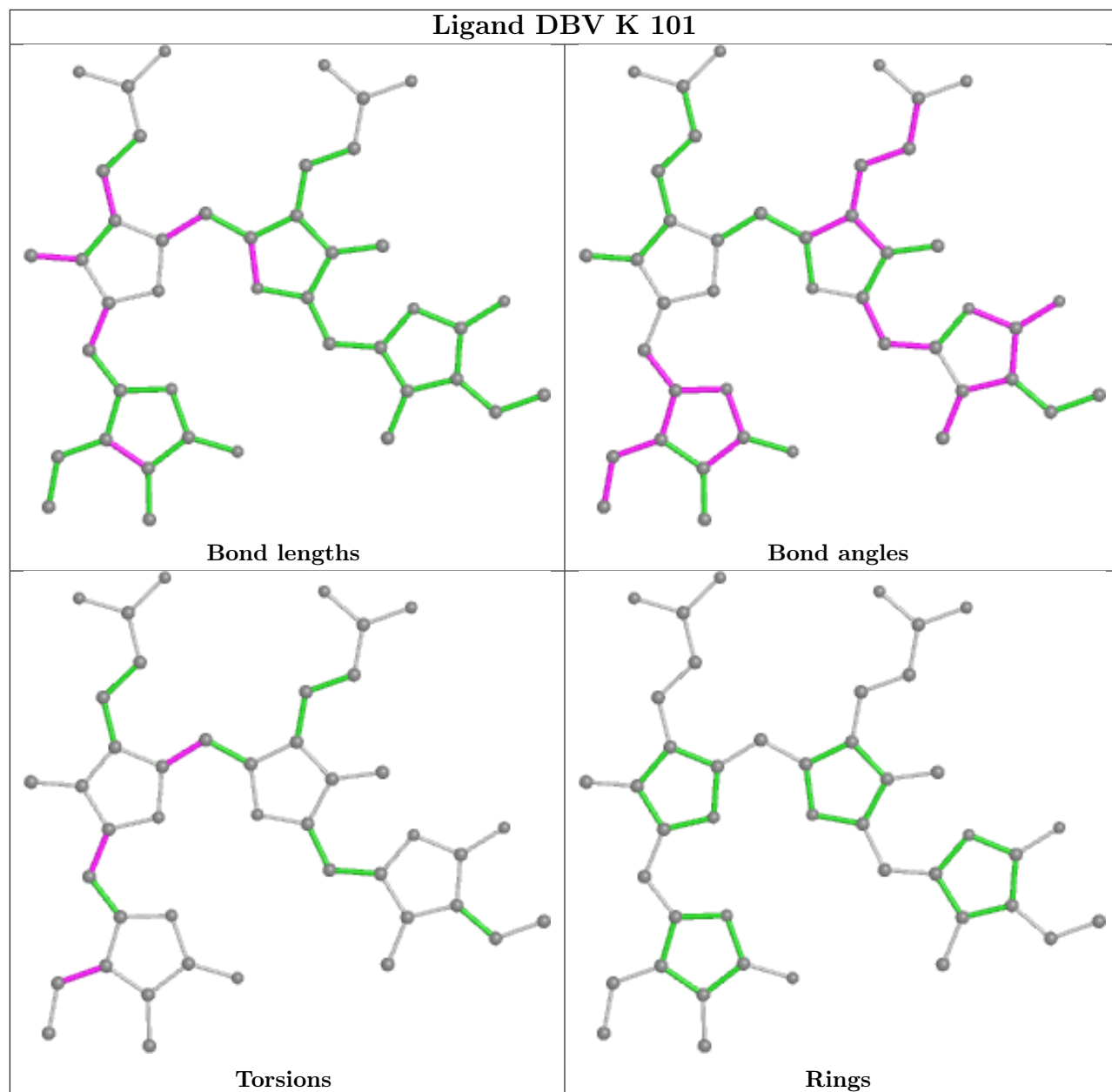
Bond angles



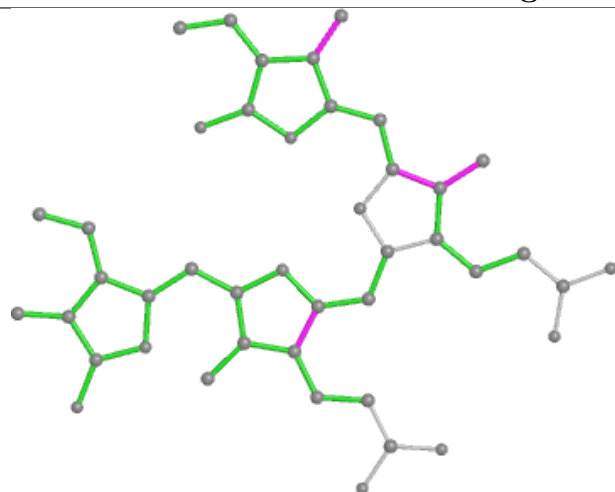
Torsions



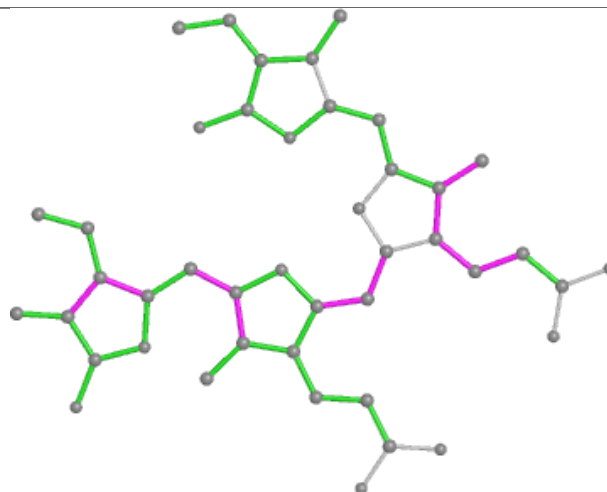
Rings



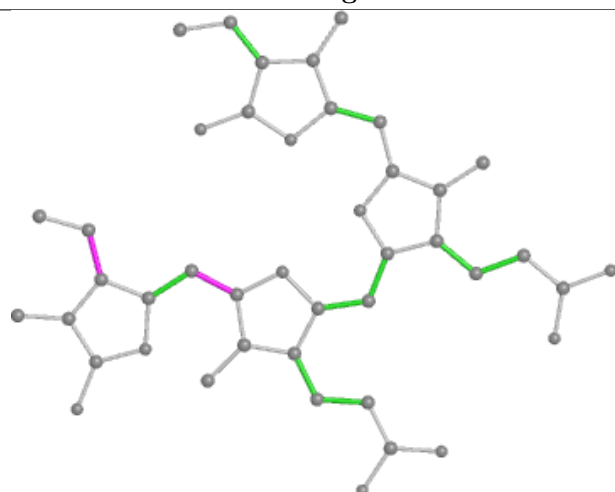
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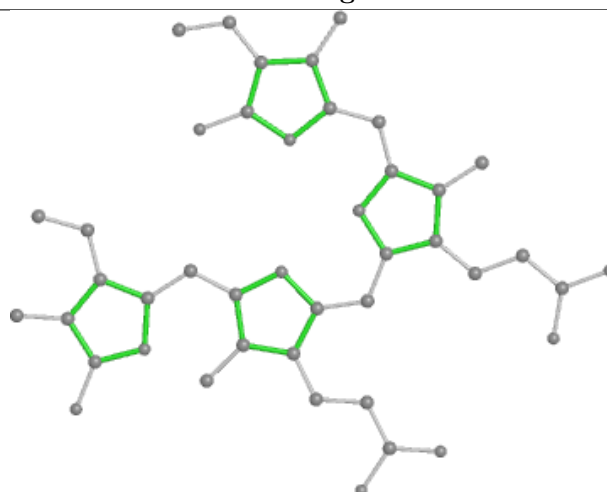
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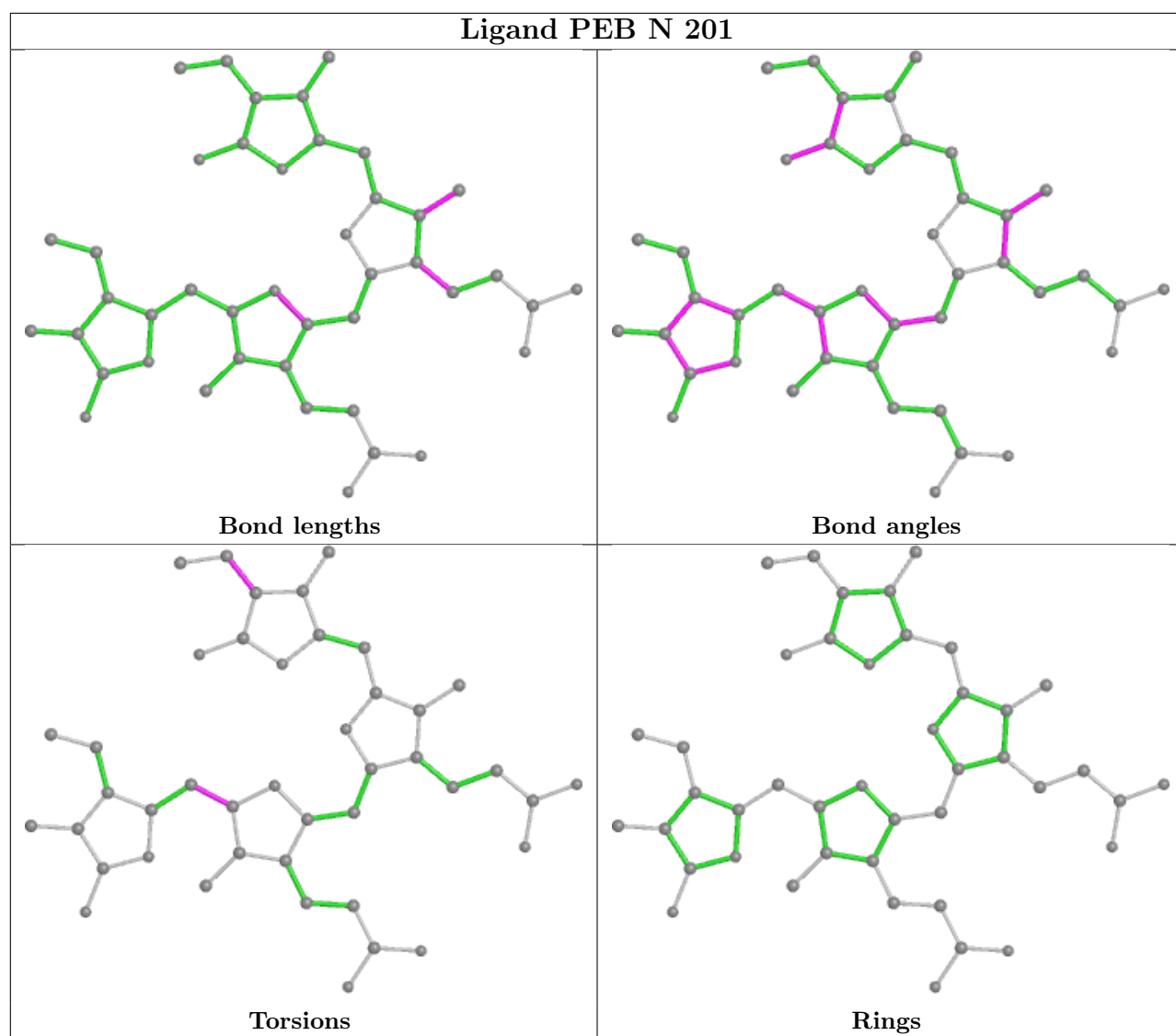
Bond angles

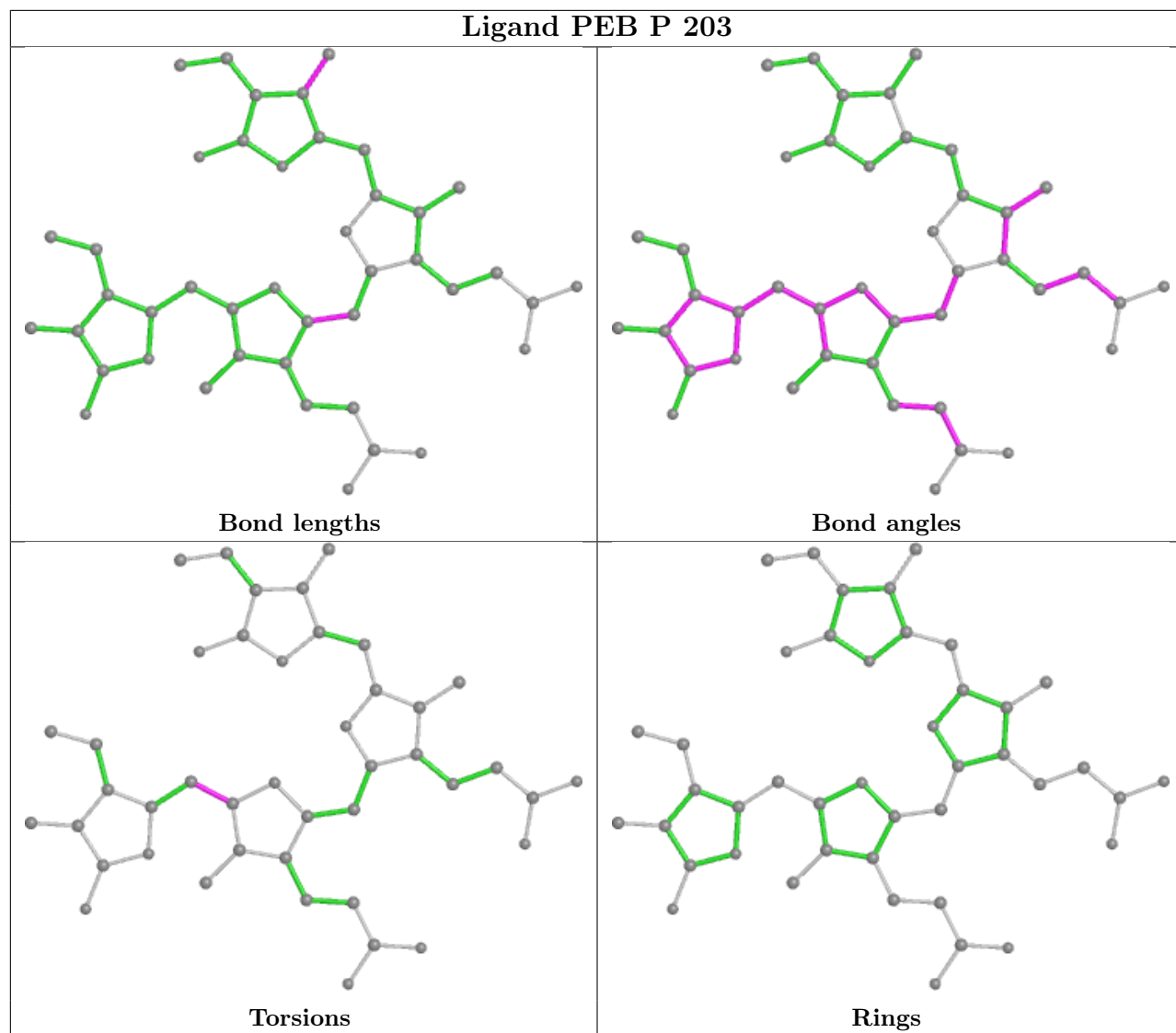


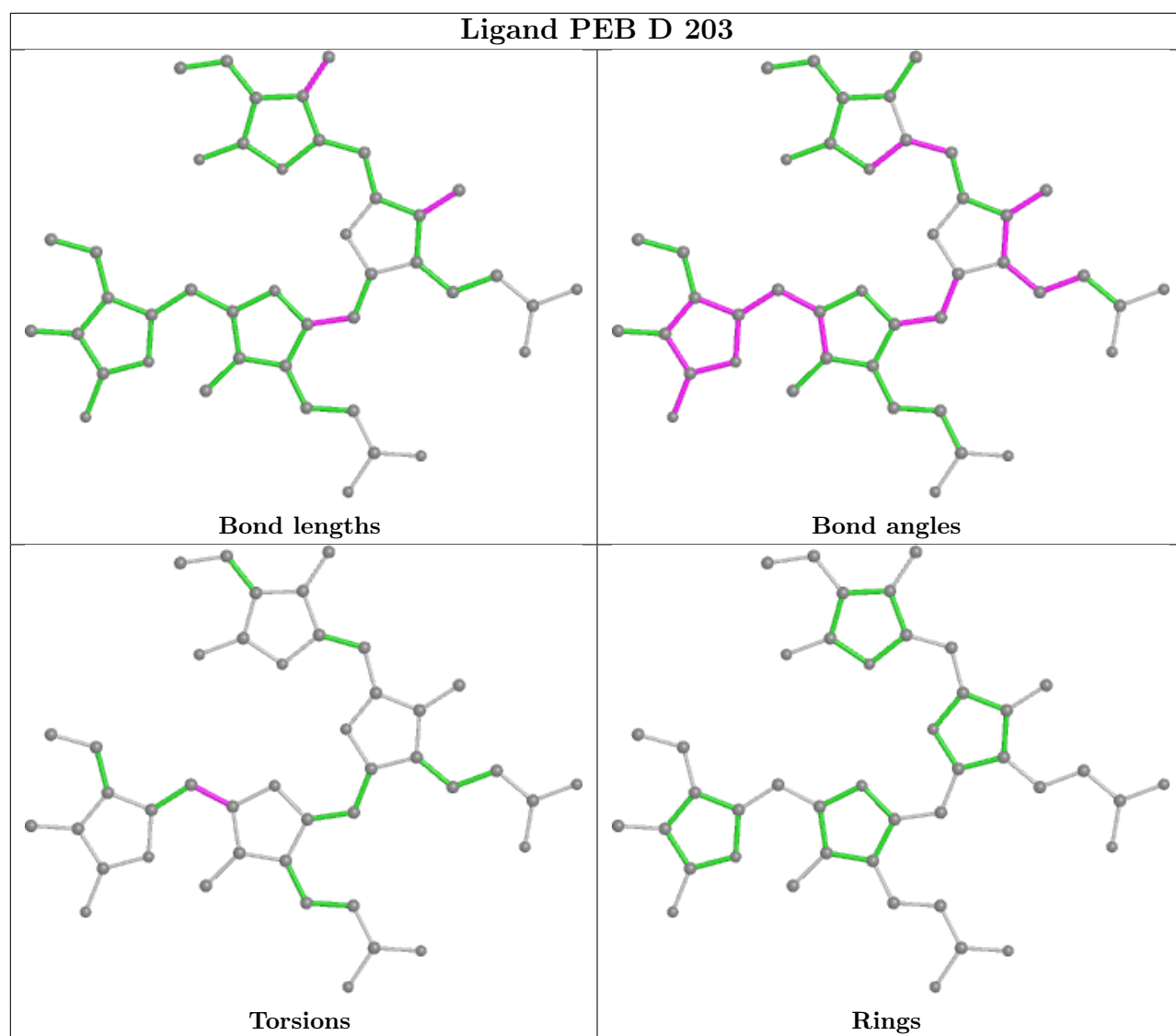
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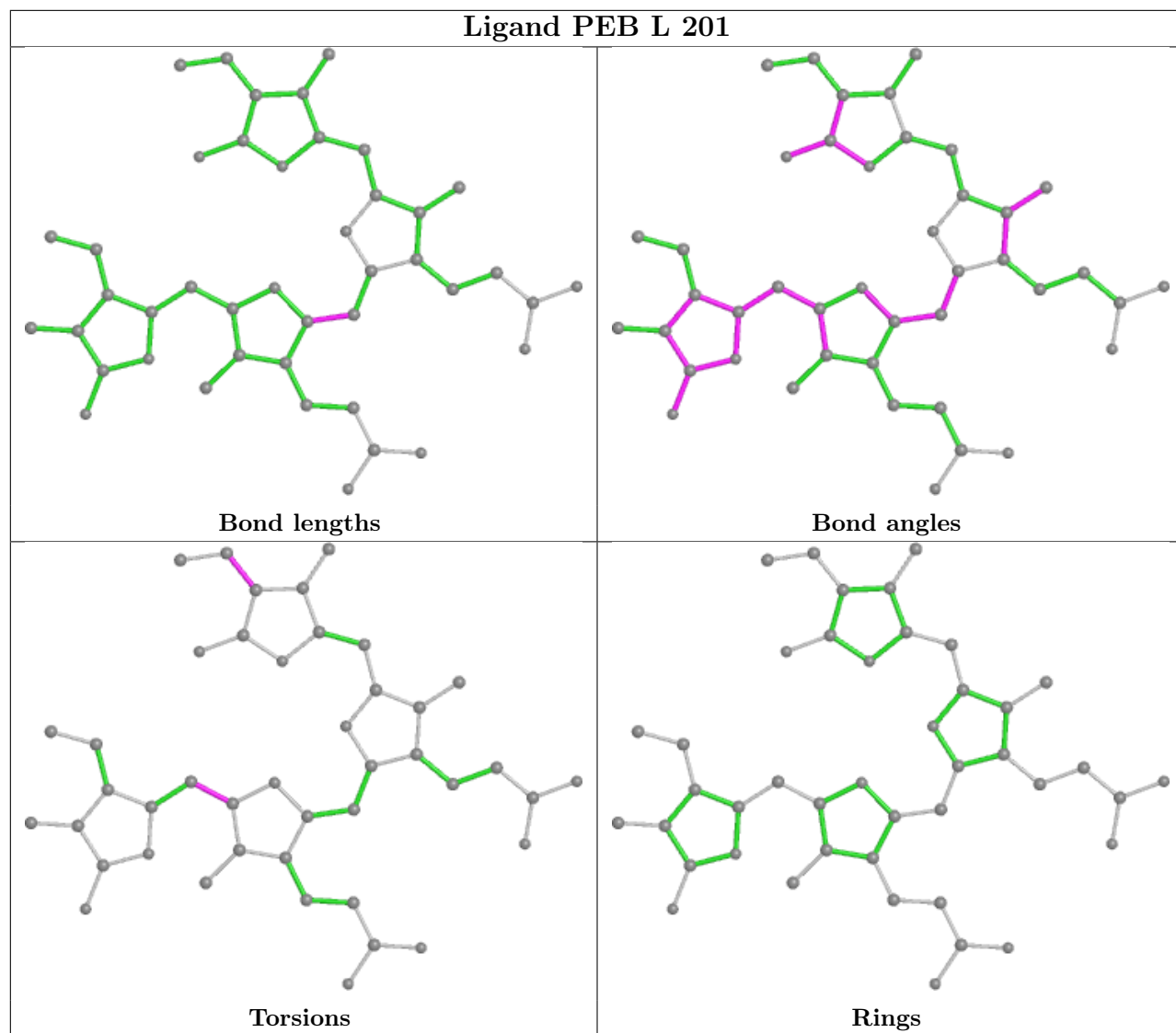
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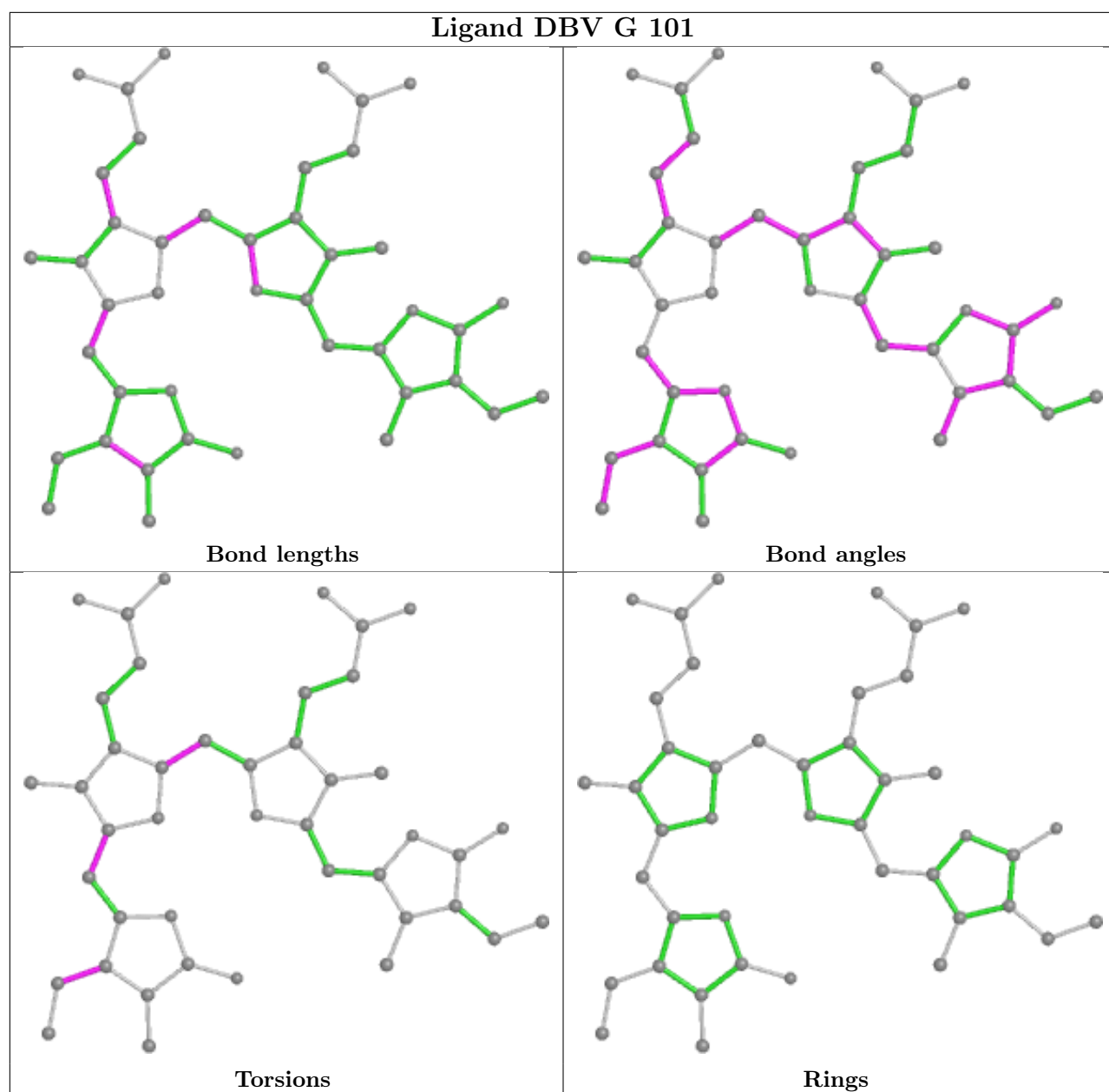




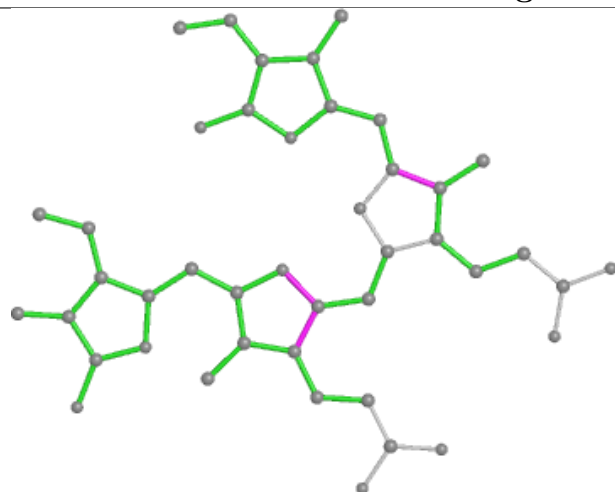


## Ligand PEB L 201

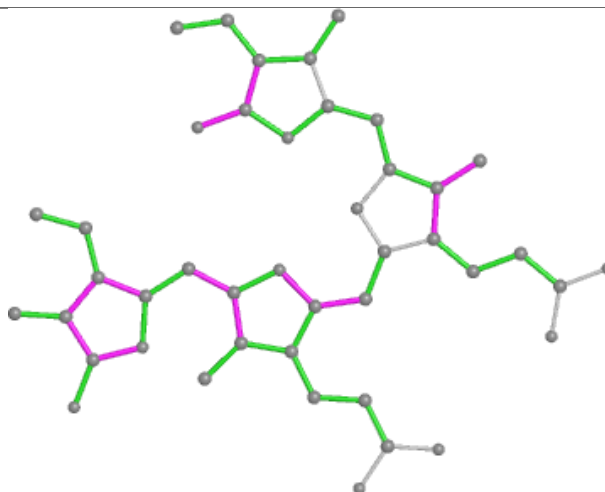




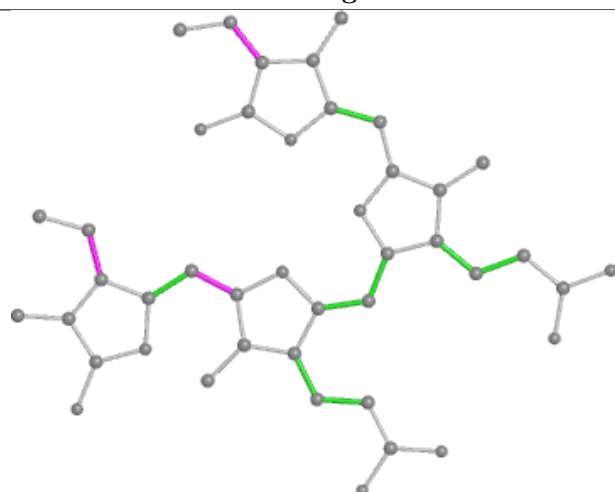
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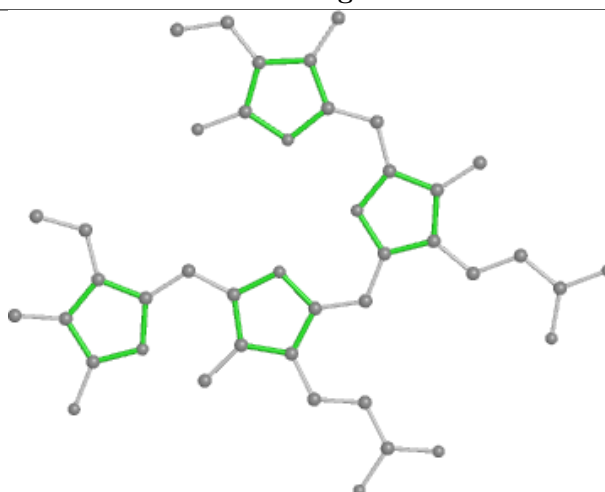
Bond lengths



Bond angles

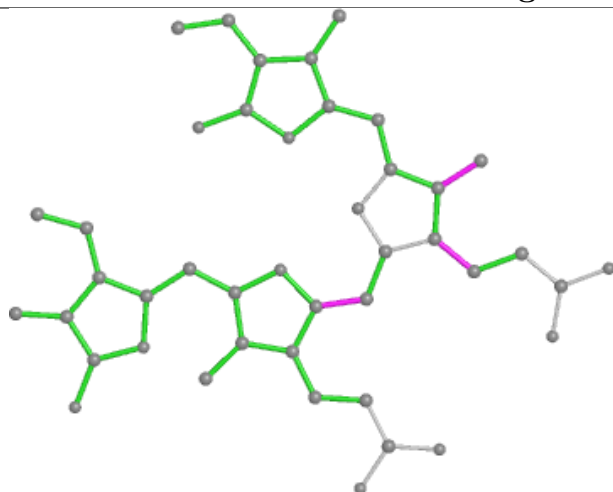


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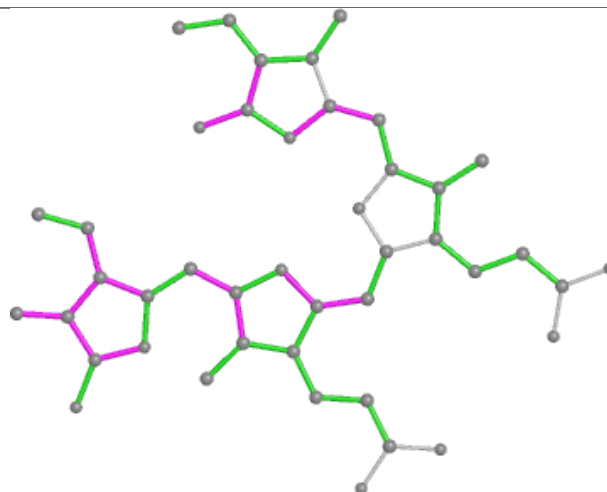


Rings

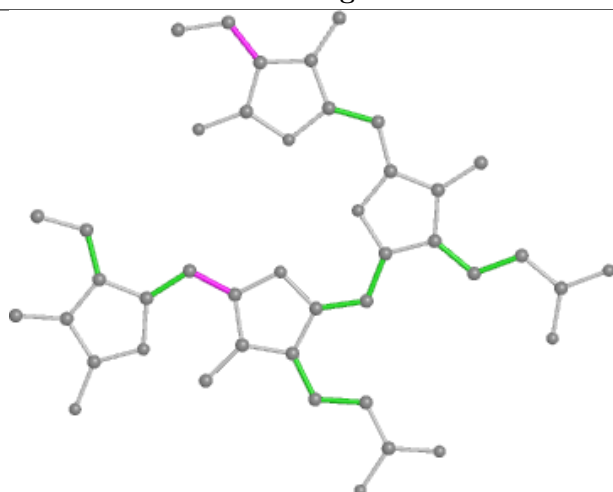
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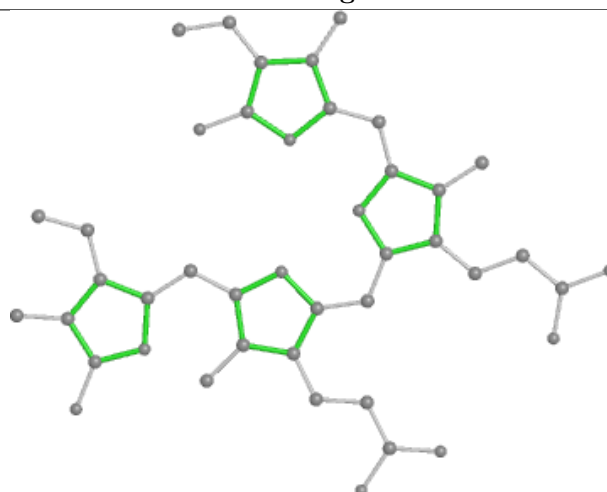
Bond lengths



Bond angles

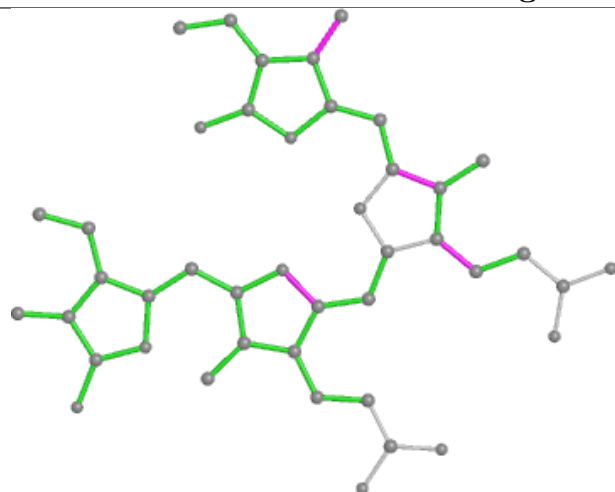


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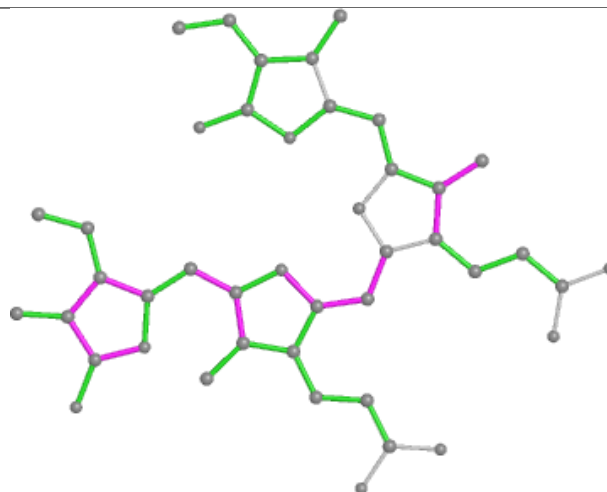


Rings

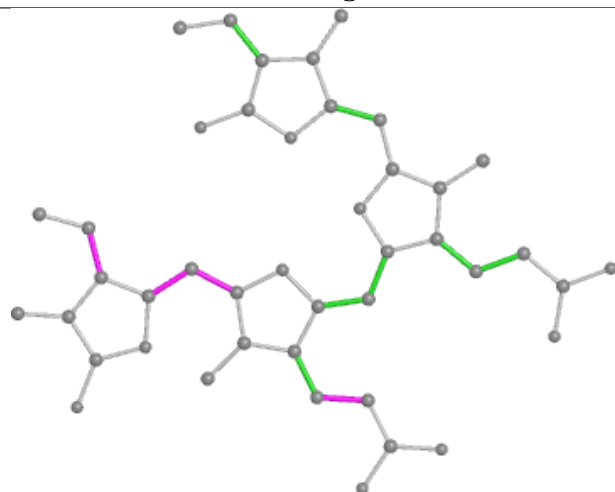
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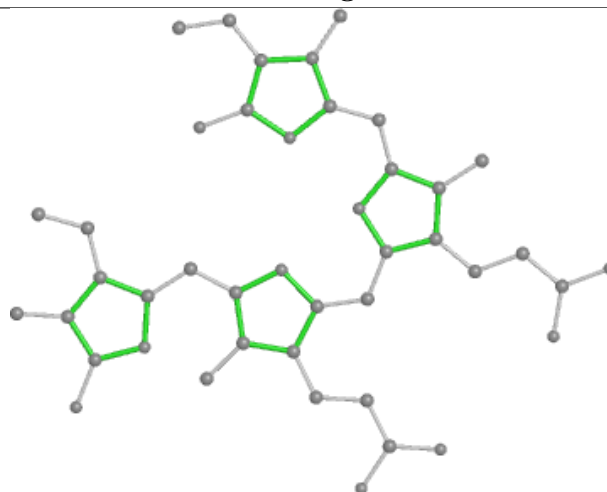
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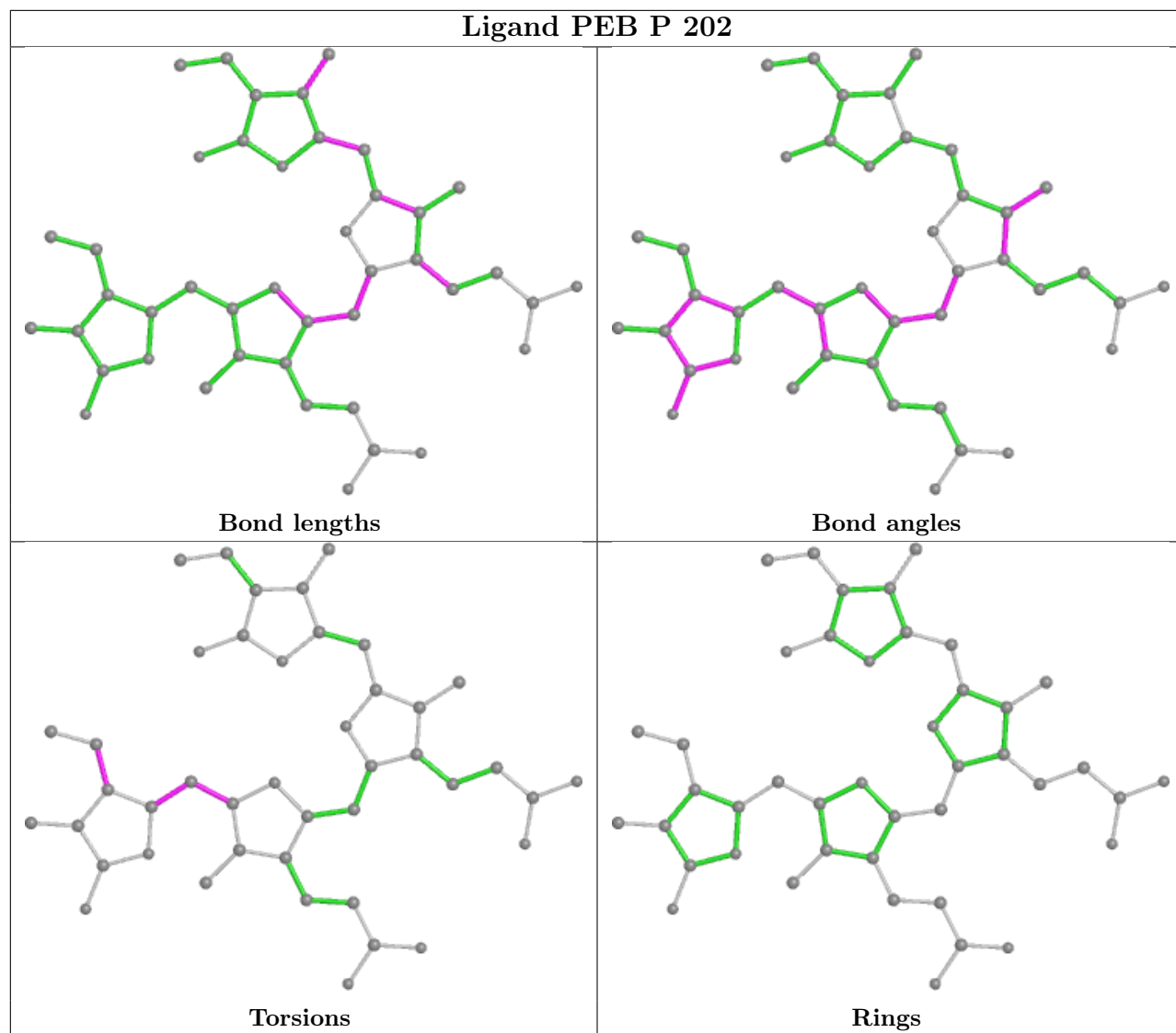
Bond angles

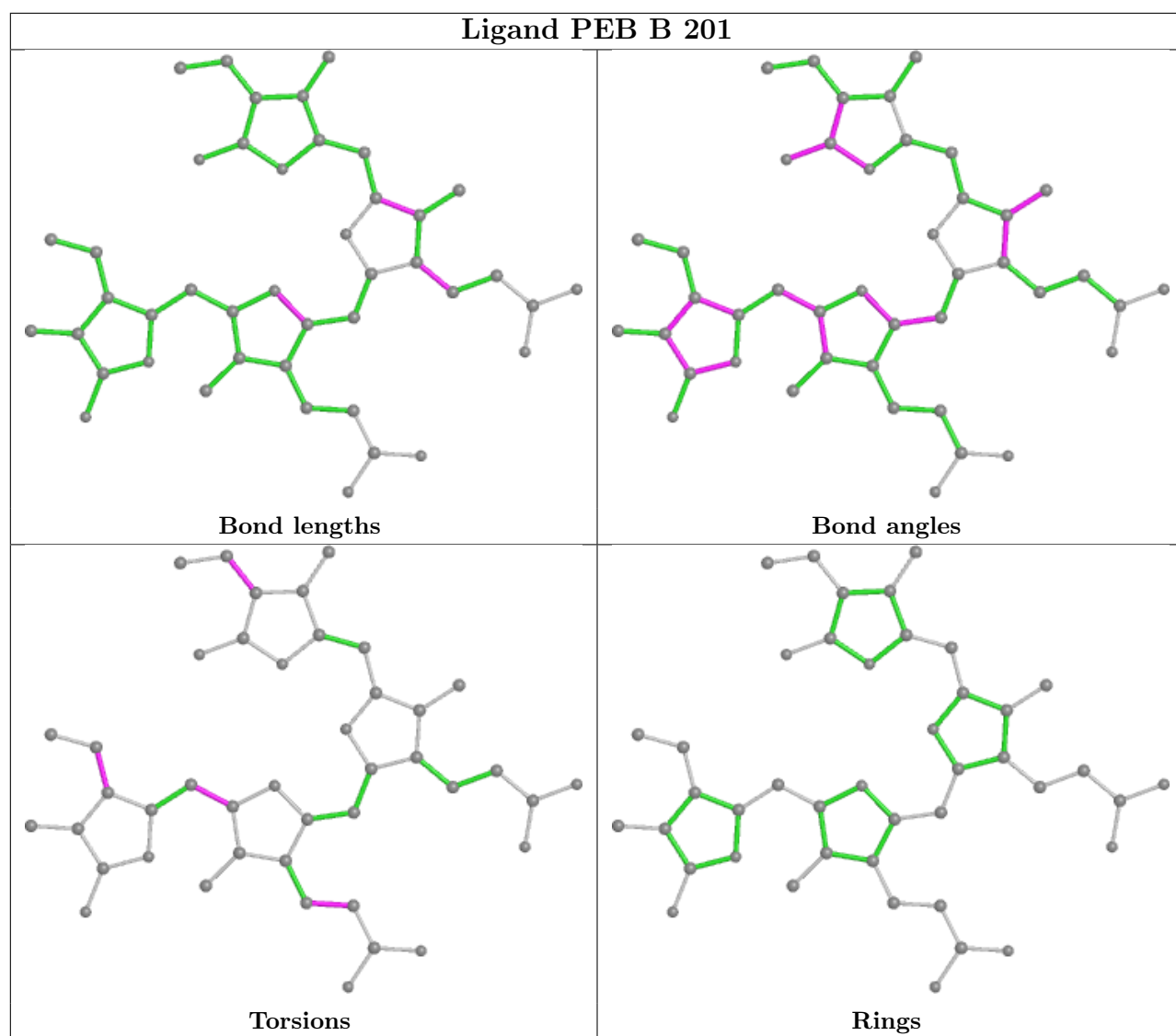


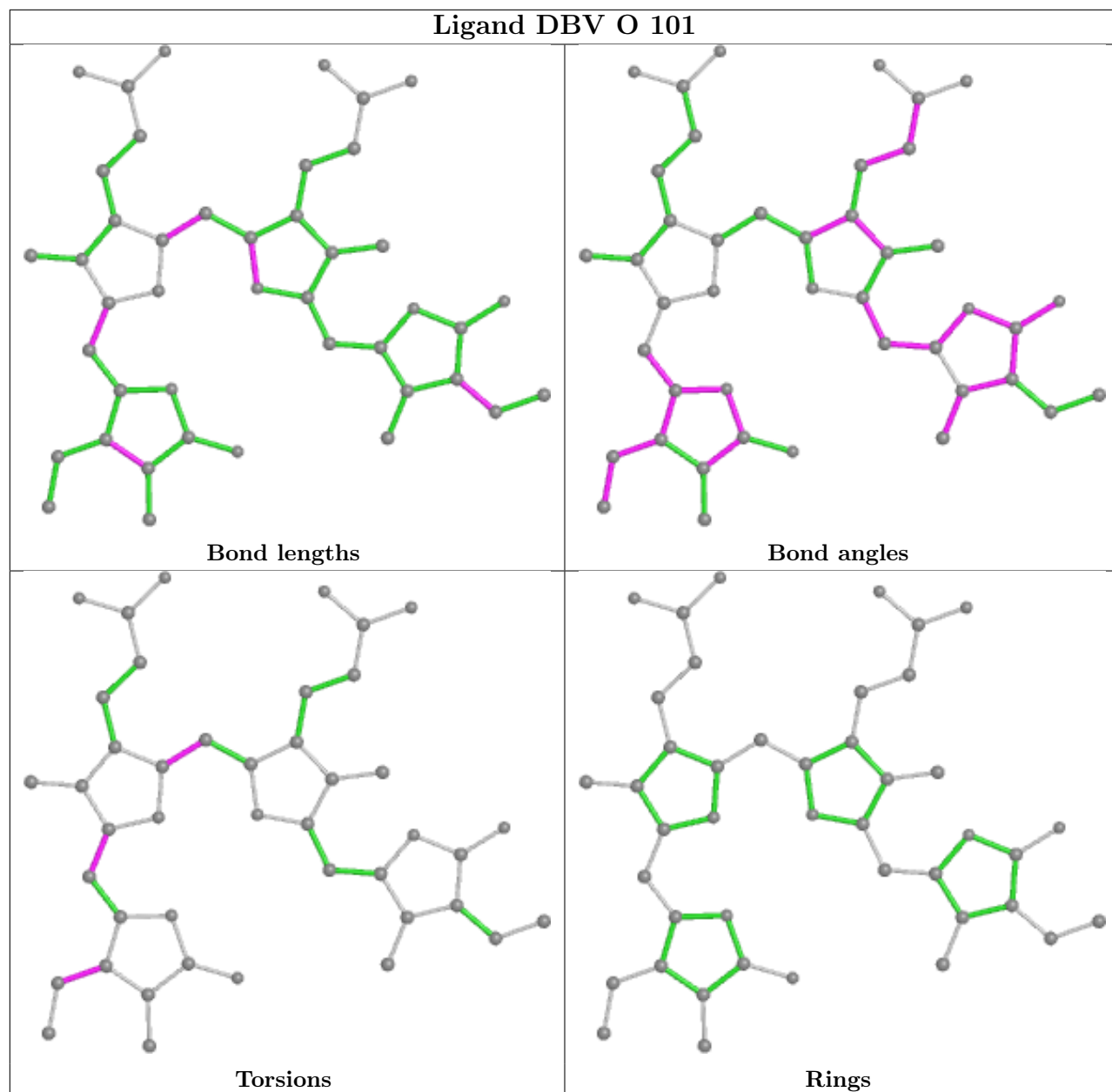
Torsions



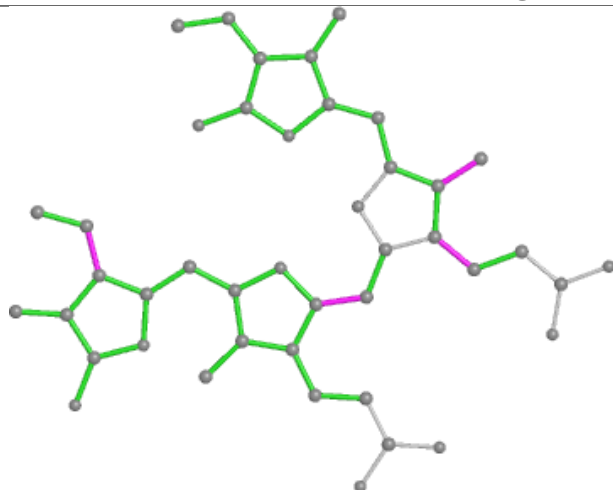
Rings



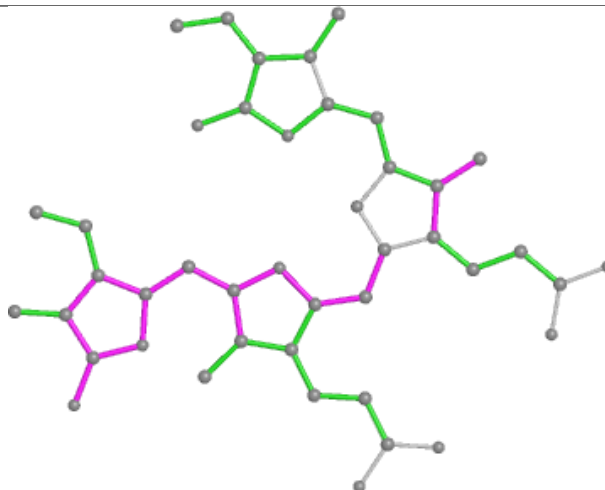




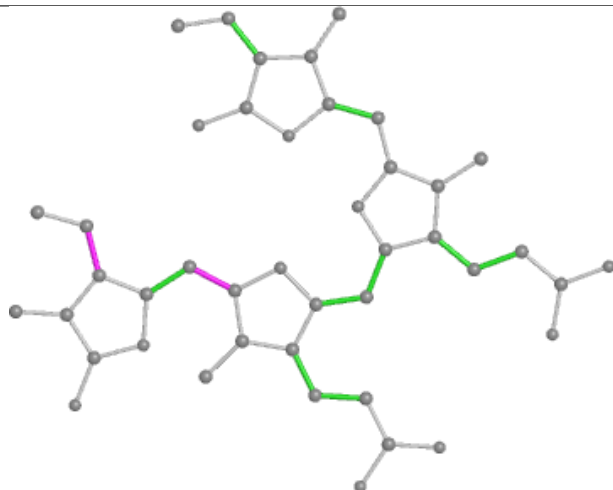
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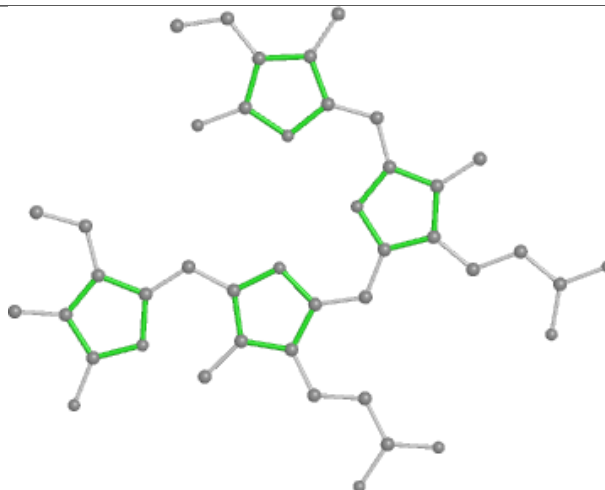
Bond lengths



Bond angles

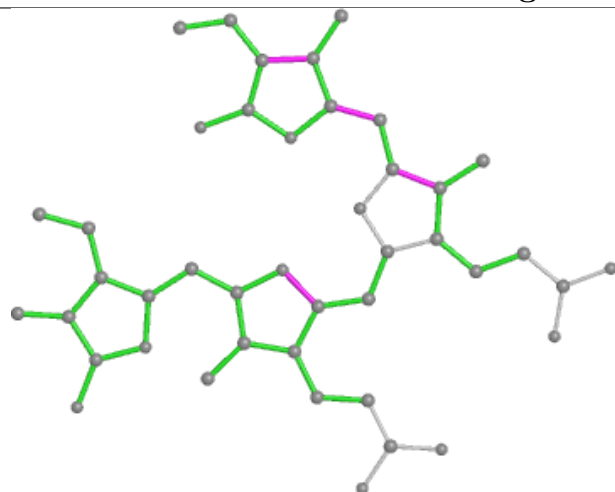


Torsions

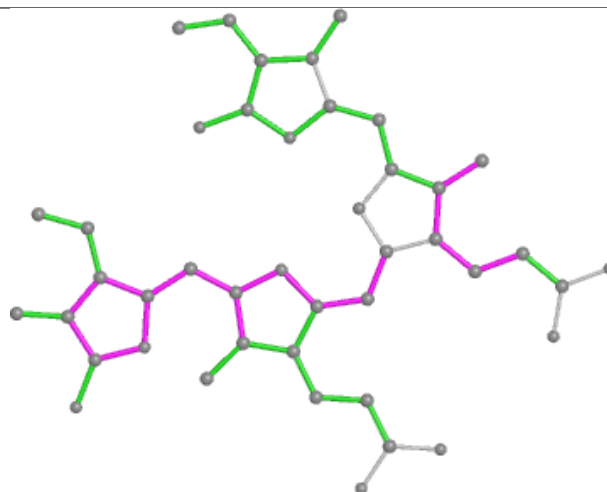


Rings

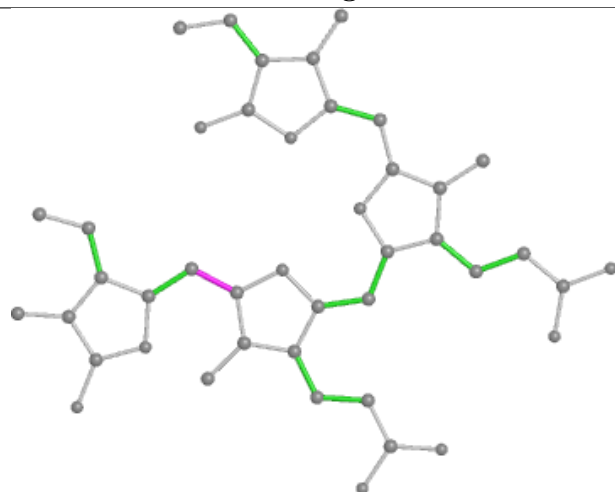
## Ligand PEB L 203



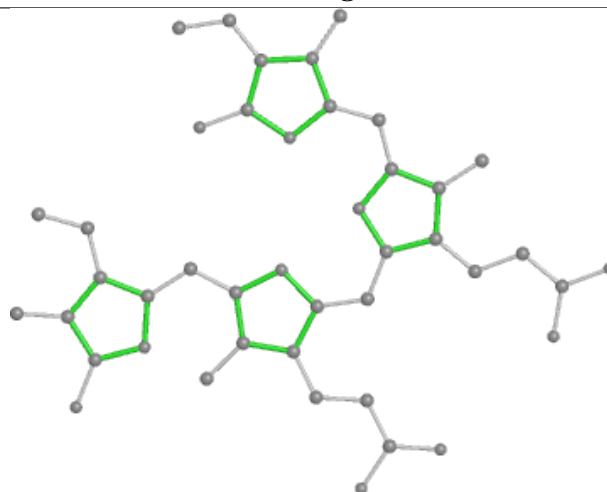
Bond lengths



Bond angles

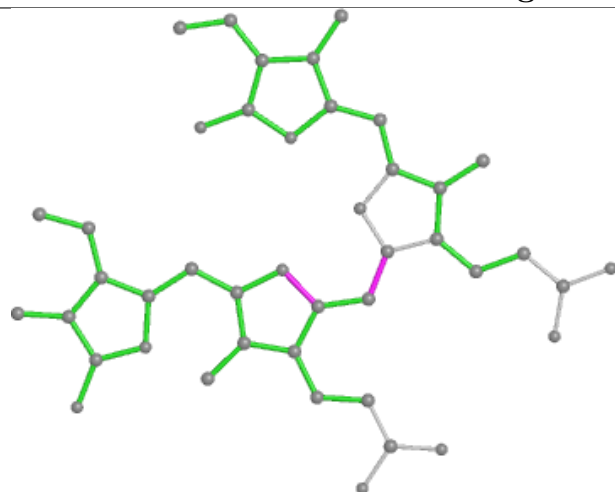


Torsions

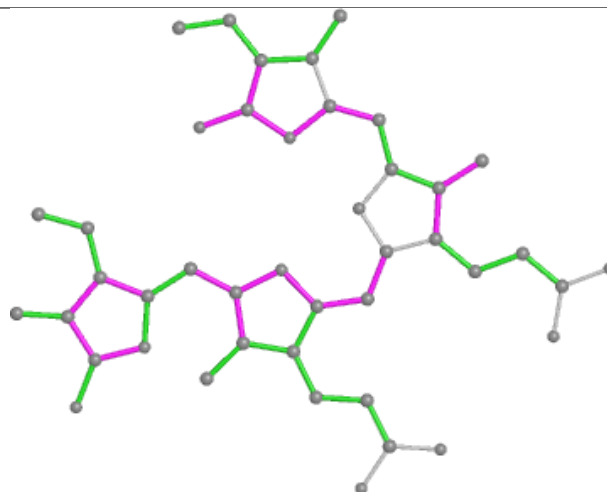


Rings

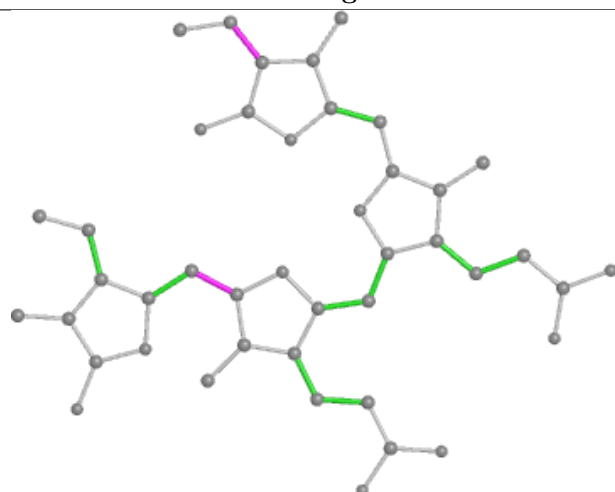
## Ligand PEB P 201



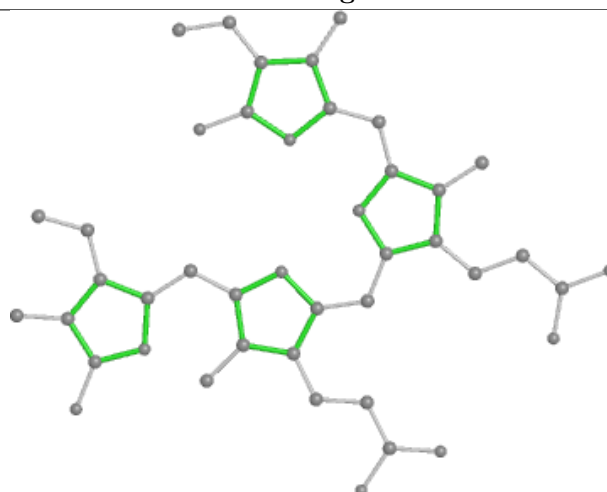
Bond lengths



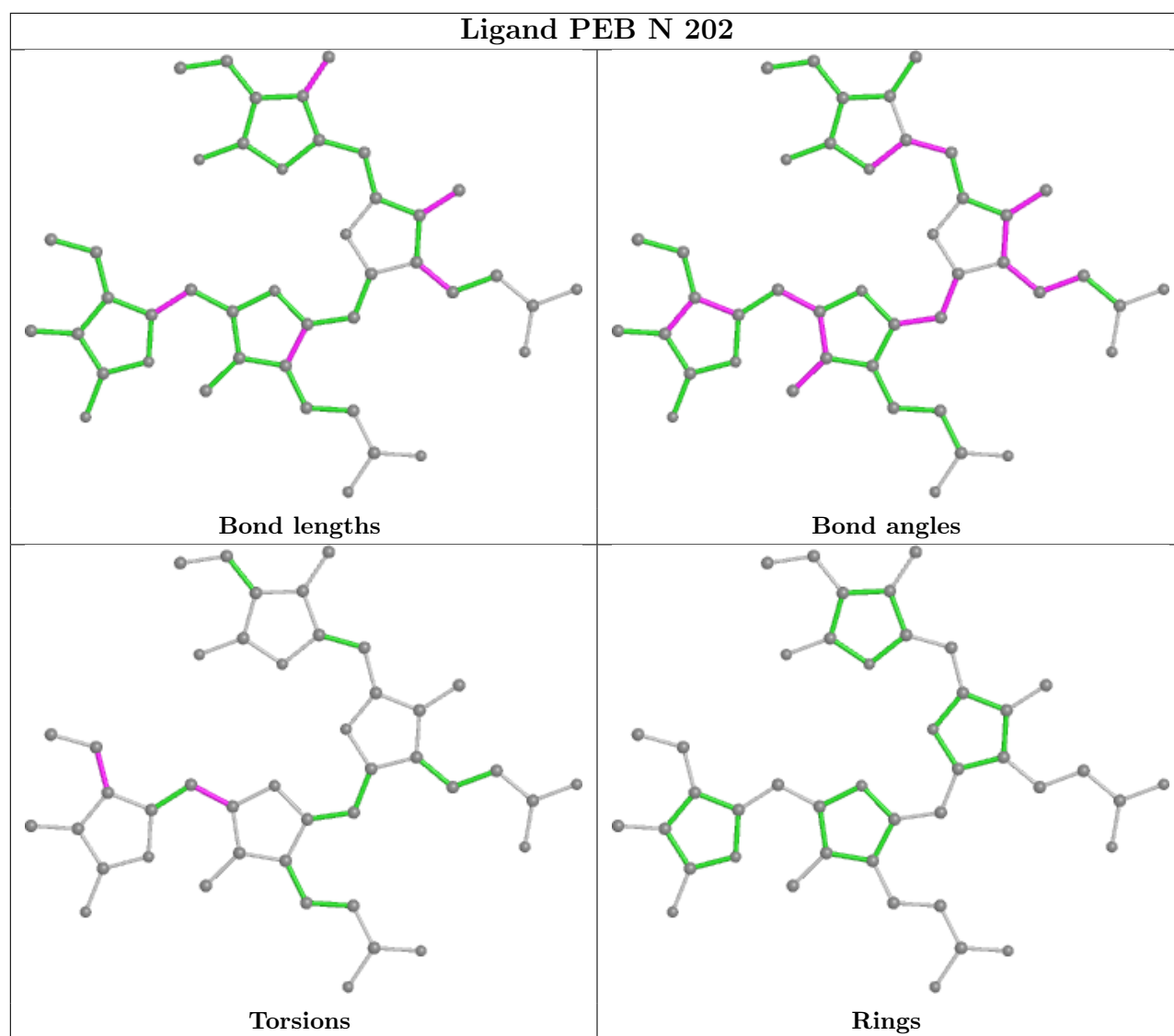
Bond angles

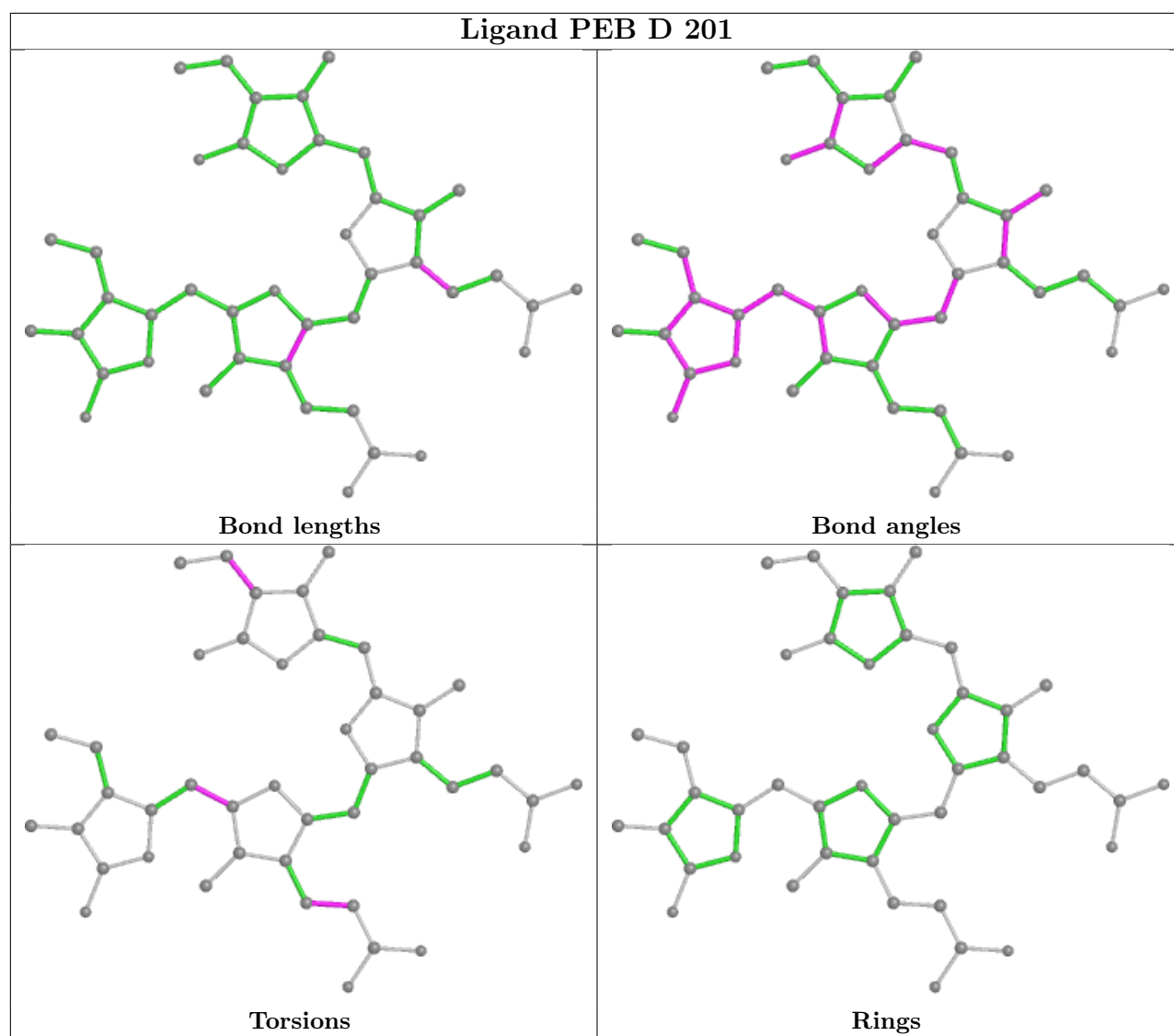


Torsions

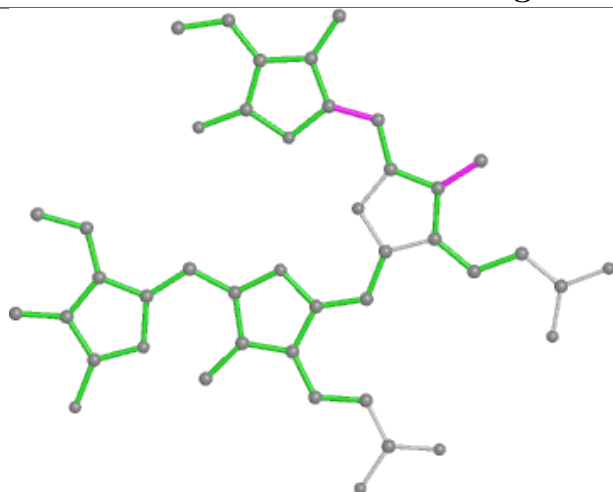


Rings

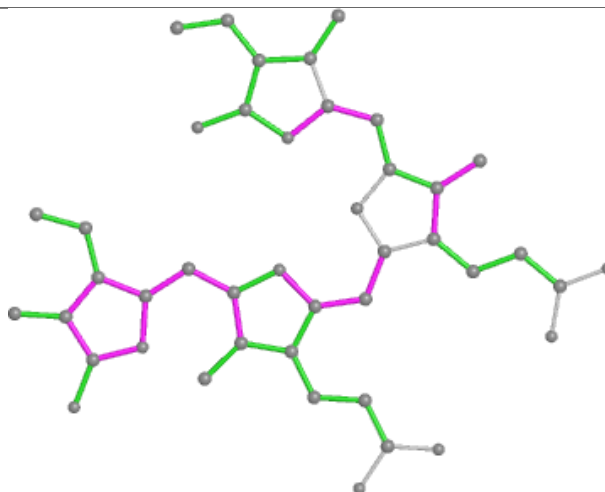




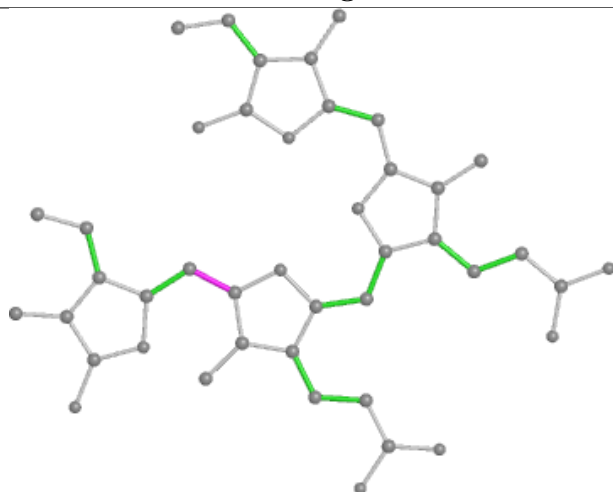
## Ligand PEB N 203



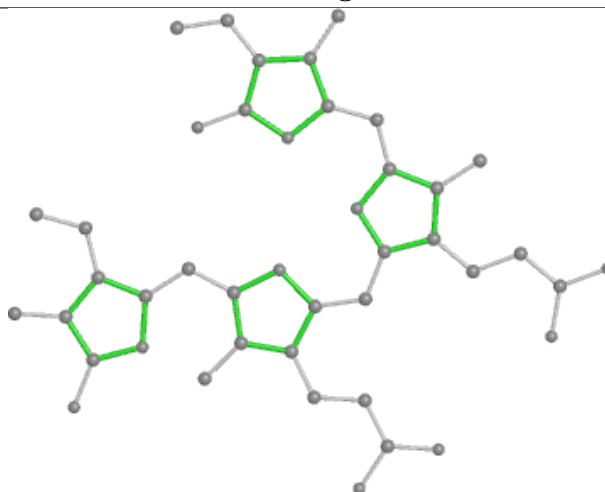
Bond lengths



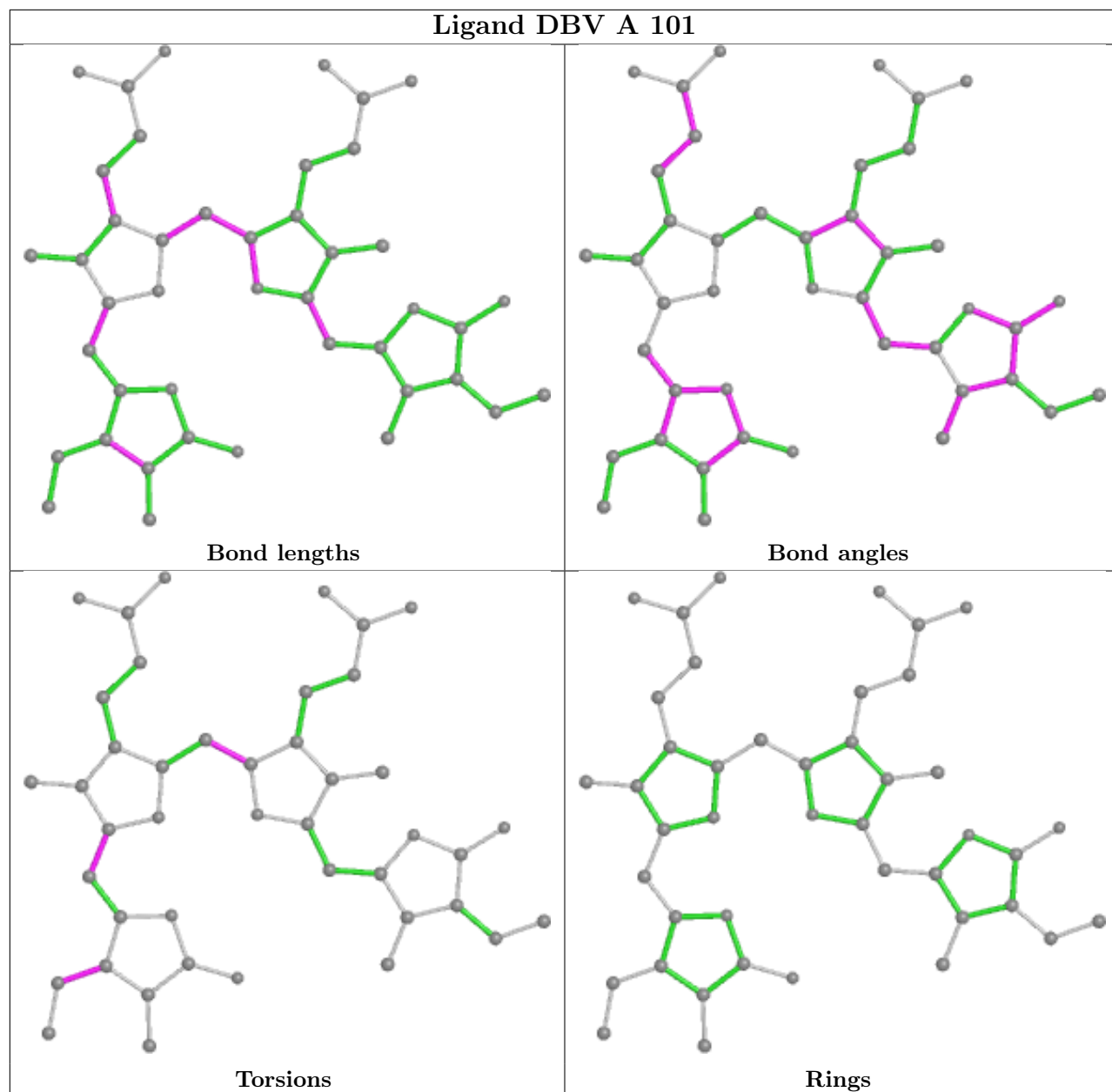
Bond angles



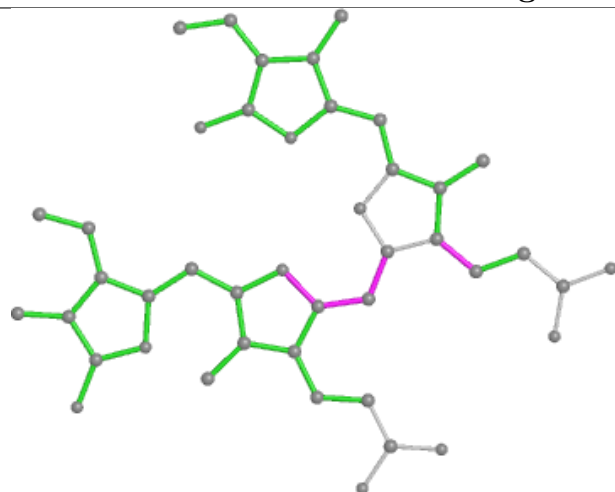
Torsions



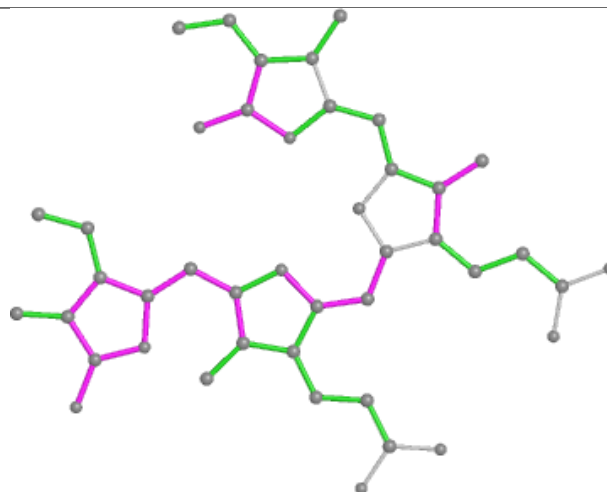
Rings



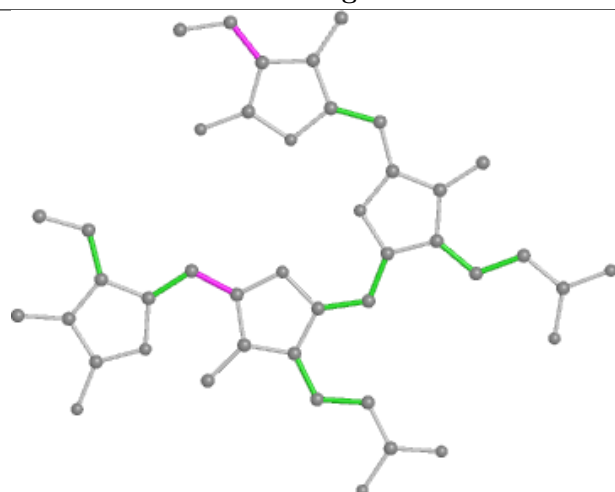
## Ligand PEB F 201



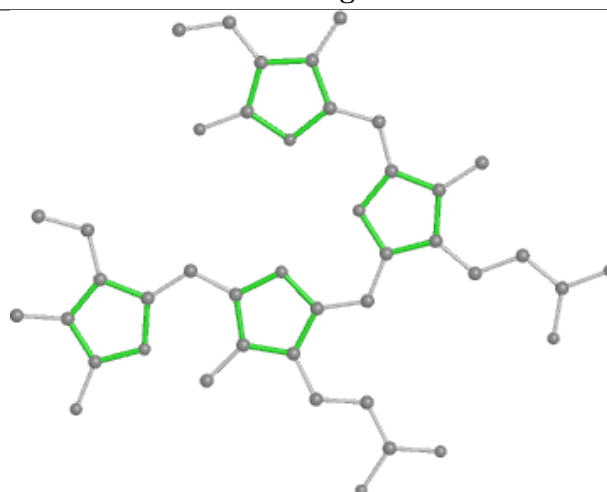
Bond lengths



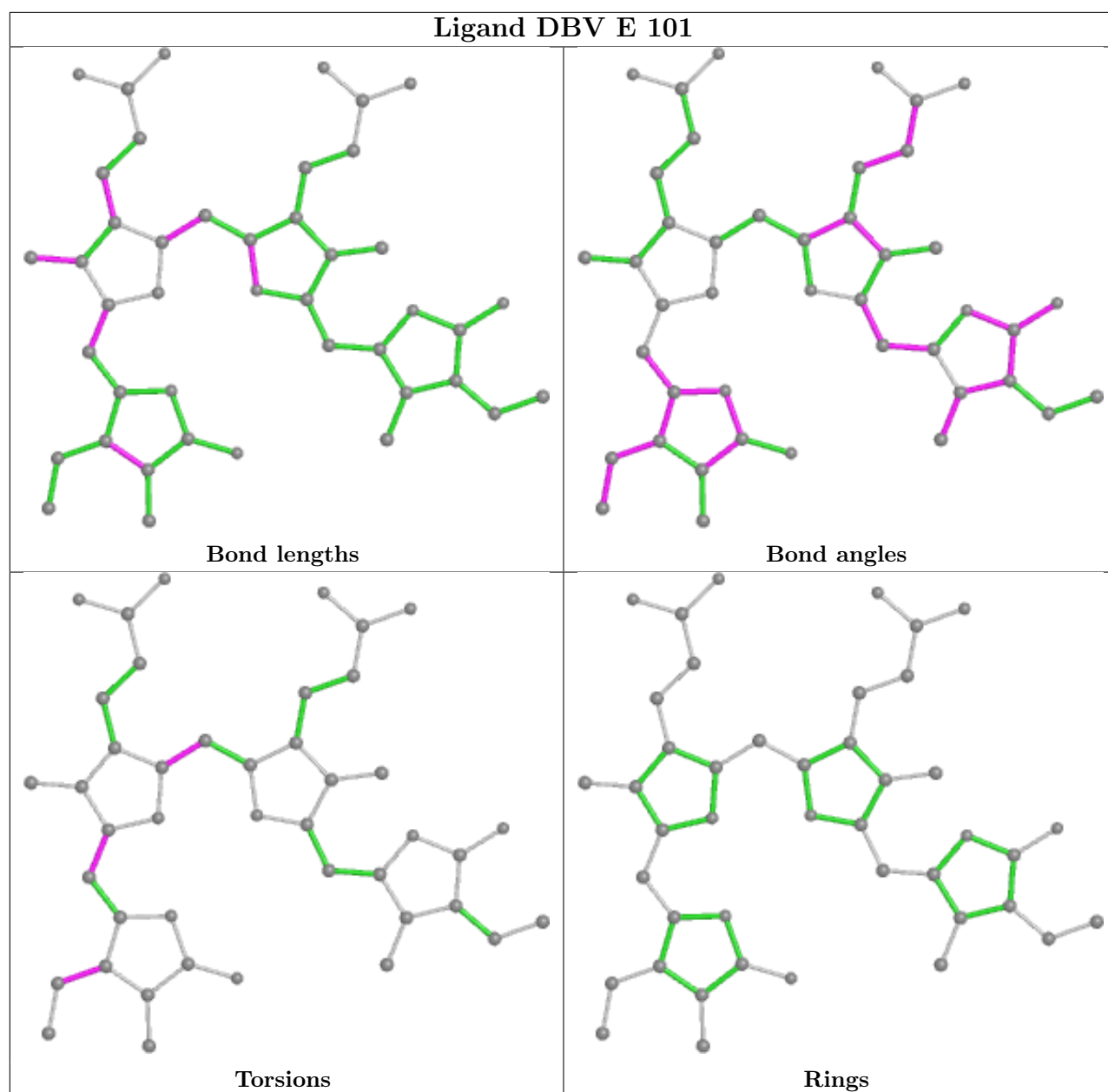
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	72/76 (94%)	1.37	19 (26%) 0 0	50, 68, 100, 141	0
1	E	74/76 (97%)	0.84	8 (10%) 5 3	28, 45, 64, 68	0
1	I	75/76 (98%)	1.04	16 (21%) 0 0	32, 54, 75, 113	0
1	M	74/76 (97%)	1.04	11 (14%) 2 1	38, 58, 74, 93	0
2	B	162/177 (91%)	1.44	44 (27%) 0 0	32, 59, 89, 116	0
2	D	173/177 (97%)	1.11	35 (20%) 1 0	32, 56, 107, 143	0
2	F	166/177 (93%)	1.08	35 (21%) 1 0	30, 47, 82, 98	0
2	H	170/177 (96%)	0.89	25 (14%) 2 1	27, 45, 78, 150	0
2	J	170/177 (96%)	1.00	24 (14%) 2 1	33, 47, 76, 124	0
2	L	172/177 (97%)	0.91	23 (13%) 3 1	33, 52, 87, 106	0
2	N	170/177 (96%)	0.90	21 (12%) 4 2	36, 55, 79, 105	0
2	P	173/177 (97%)	0.83	21 (12%) 4 2	27, 53, 89, 112	0
3	C	60/67 (89%)	1.61	17 (28%) 0 0	57, 75, 106, 145	0
3	G	67/67 (100%)	0.93	12 (17%) 1 1	32, 47, 74, 114	0
3	K	67/67 (100%)	1.02	10 (14%) 2 1	38, 53, 74, 90	0
3	O	67/67 (100%)	1.11	9 (13%) 3 1	40, 59, 78, 91	0
All	All	1912/1988 (96%)	1.05	330 (17%) 1 1	27, 53, 89, 150	0

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	167	GLY	9.9
2	D	147	SER	6.9
2	H	13	ASP	6.7
3	C	18	GLY	6.6
3	G	27	THR	6.5

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Mol	Chain	Res	Type	RSRZ
3	K	18	GLY	6.1
2	H	7	ARG	6.1
2	D	7	ARG	5.9
2	B	112	GLY	5.9
2	F	177	SER	5.8
2	H	177	SER	5.8
2	J	6	SER	5.8
2	H	74	TYR	5.5
1	A	30	SER	5.5
2	F	176	ILE	5.4
1	M	49	SER	5.2
2	F	101	ASP	5.2
3	C	5	SER	5.2
2	J	177	SER	5.1
2	B	107	ASP	5.0
2	H	14	SER	5.0
2	B	14	SER	4.9
2	F	10	THR	4.9
2	D	148	GLN	4.9
2	F	103	SER	4.7
2	H	154	PRO	4.7
2	D	149	LYS	4.6
2	F	160	GLY	4.6
2	N	162	ALA	4.6
2	P	10	THR	4.6
2	B	165	VAL	4.5
1	A	71	SER	4.5
1	A	65	GLU	4.5
2	P	147	SER	4.5
2	B	15	LYS	4.5
3	O	32	SER	4.4
1	A	27	SER	4.4
2	L	120	LEU	4.4
2	P	74	TYR	4.3
2	D	177	SER	4.3
2	J	162	ALA	4.2
1	M	6	ALA	4.2
3	G	1	ALA	4.2
2	H	103	SER	4.2
2	L	3	ASP	4.1
2	J	15	LYS	4.1
2	F	107	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	153	THR	4.1
3	K	22	ALA	4.1
2	J	101	ASP	4.0
2	F	155	GLN	4.0
2	L	74	TYR	4.0
2	B	115	GLU	4.0
3	G	26	TYR	3.9
1	A	6	ALA	3.9
2	L	8	VAL	3.9
2	L	30	PHE	3.9
2	J	163	SER	3.9
3	O	47	ILE	3.8
1	E	72	VAL	3.8
2	F	166	ALA	3.8
2	L	177	SER	3.8
2	J	174	SER	3.8
3	G	3	ASP	3.8
1	E	30	SER	3.8
1	M	23	PRO	3.8
2	B	103	SER	3.8
3	G	50	SER	3.7
1	A	31	GLY	3.7
2	F	165	VAL	3.7
2	B	162	ALA	3.7
3	G	2	MET	3.7
2	N	160	GLY	3.7
2	L	103	SER	3.7
2	J	160	GLY	3.7
2	D	74	TYR	3.7
2	F	17	ALA	3.6
2	H	75	THR	3.6
2	J	111	ASN	3.6
2	N	123	PRO	3.6
2	P	80	ALA	3.6
2	B	100	GLY	3.6
2	N	115	GLU	3.6
1	E	43	SER	3.6
2	D	108	ARG	3.6
2	B	62	GLU	3.6
2	H	152	SER	3.6
2	B	173	THR	3.5
3	G	32	SER	3.5

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Mol	Chain	Res	Type	RSRZ
2	N	124	ALA	3.5
2	D	3	ASP	3.5
2	D	13	ASP	3.5
3	C	36	ASP	3.5
2	J	7	ARG	3.4
1	M	12	THR	3.4
2	D	58	GLY	3.4
2	L	14	SER	3.4
3	C	60	ASP	3.4
2	F	106	GLU	3.4
2	B	176	ILE	3.3
2	D	155	GLN	3.3
3	K	20	SER	3.3
2	N	163	SER	3.3
2	N	118	SER	3.3
2	J	166	ALA	3.3
2	P	149	LYS	3.3
2	L	147	SER	3.2
1	A	72	VAL	3.2
2	D	154	PRO	3.2
2	N	173	THR	3.2
2	B	164	GLU	3.2
2	J	107	ASP	3.2
2	B	175	ALA	3.2
1	I	6	ALA	3.2
3	O	20	SER	3.2
2	D	14	SER	3.2
2	N	101	ASP	3.2
2	B	168	TYR	3.1
2	B	130	ALA	3.1
2	F	100	GLY	3.1
2	J	167	GLY	3.1
2	L	149	LYS	3.1
3	C	20	SER	3.1
2	F	172	VAL	3.1
2	D	115	GLU	3.1
3	K	19	CYS	3.1
1	I	75	LYS	3.1
2	D	95	TYR	3.1
2	N	107	ASP	3.1
2	H	104	VAL	3.0
2	N	17	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	159	SER	3.0
3	C	61	SER	3.0
2	D	163	SER	3.0
2	L	118	SER	3.0
2	D	41	VAL	3.0
3	C	40	VAL	3.0
2	B	117	TYR	3.0
2	B	111	ASN	3.0
1	A	42	ALA	2.9
2	F	112	GLY	2.9
2	L	112	GLY	2.9
2	J	129	ARG	2.9
1	I	49	SER	2.9
2	B	7	ARG	2.9
2	P	22	ALA	2.9
2	L	72	ASN	2.9
2	F	53	SER	2.9
2	J	63	ASN	2.9
2	N	174	SER	2.9
2	D	153	THR	2.9
2	F	168	TYR	2.9
2	B	65	SER	2.8
2	P	75	THR	2.8
3	K	32	SER	2.8
1	E	32	SER	2.8
2	F	154	PRO	2.8
2	L	75	THR	2.8
3	C	37	GLU	2.8
1	I	13	ILE	2.8
2	B	105	LEU	2.8
1	I	30	SER	2.8
2	J	140	ALA	2.8
1	A	5	SER	2.8
3	K	61	SER	2.8
3	K	3	ASP	2.8
2	P	148	GLN	2.8
1	I	23	PRO	2.7
2	D	106	GLU	2.7
1	A	70	GLY	2.7
1	A	11	ILE	2.7
2	J	103	SER	2.7
2	N	140	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	127	ASN	2.7
3	K	52	GLY	2.7
1	A	12	THR	2.7
3	O	6	ALA	2.7
3	C	26	TYR	2.7
1	E	3	ASP	2.7
2	D	24	LEU	2.7
2	B	61	CYS	2.7
2	H	145	THR	2.7
1	M	28	ALA	2.7
3	O	22	ALA	2.7
2	B	122	VAL	2.7
2	H	107	ASP	2.7
2	N	164	GLU	2.7
2	H	26	ALA	2.7
3	K	24	LYS	2.7
2	B	116	THR	2.7
2	J	106	GLU	2.6
2	N	119	SER	2.6
3	C	11	ILE	2.6
2	H	153	THR	2.6
1	I	18	GLY	2.6
2	D	43	SER	2.6
3	C	38	MET	2.6
2	P	125	ASN	2.6
2	D	152	SER	2.6
2	N	125	ASN	2.6
2	F	102	SER	2.6
2	H	147	SER	2.6
2	H	94	SER	2.5
2	P	35	ASN	2.5
1	E	73	ILE	2.5
2	B	155	GLN	2.5
3	O	19	CYS	2.5
1	E	1	GLY	2.5
1	I	74	ARG	2.5
1	M	71	SER	2.5
2	B	17	ALA	2.5
2	H	119	SER	2.5
3	C	63	SER	2.5
2	B	93	VAL	2.5
3	O	42	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	104	VAL	2.4
2	B	63	ASN	2.4
3	C	57	VAL	2.4
2	P	112	GLY	2.4
2	P	9	VAL	2.4
2	B	102	SER	2.4
2	L	125	ASN	2.4
2	F	129	ARG	2.4
2	F	62	GLU	2.4
2	D	30	PHE	2.4
1	A	3	ASP	2.4
2	B	119	SER	2.4
2	P	14	SER	2.4
2	J	5	PHE	2.4
2	H	23	ASP	2.4
2	D	6	SER	2.4
2	F	51	ILE	2.4
2	B	160	GLY	2.4
2	H	41	VAL	2.4
1	A	10	ALA	2.4
2	B	99	SER	2.4
2	D	48	ALA	2.4
2	F	162	ALA	2.4
2	F	64	PRO	2.3
2	L	116	THR	2.3
3	O	12	THR	2.3
1	I	27	SER	2.3
2	H	53	SER	2.3
1	M	36	GLU	2.3
2	D	75	THR	2.3
2	L	57	SER	2.3
2	P	101	ASP	2.3
1	I	73	ILE	2.3
2	D	21	GLY	2.3
3	C	52	GLY	2.3
2	P	108	ARG	2.3
1	I	32	SER	2.3
2	F	49	SER	2.3
2	F	111	ASN	2.3
1	A	28	ALA	2.3
1	I	10	ALA	2.3
2	J	105	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	13	ILE	2.3
2	N	6	SER	2.2
2	P	73	CYS	2.2
2	B	6	SER	2.2
2	F	173	THR	2.2
2	L	99	SER	2.2
1	I	3	ASP	2.2
2	L	69	PRO	2.2
2	P	120	LEU	2.2
2	L	73	CYS	2.2
2	L	7	ARG	2.2
2	H	46	SER	2.2
1	M	72	VAL	2.2
2	J	62	GLU	2.2
3	K	36	ASP	2.2
2	B	124	ALA	2.2
2	F	65	SER	2.2
2	B	39	ASP	2.2
2	J	146	ALA	2.2
2	D	44	ILE	2.2
2	B	134	MET	2.2
2	F	105	LEU	2.2
2	D	103	SER	2.2
2	F	132	SER	2.2
2	L	22	ALA	2.1
1	E	5	SER	2.1
2	H	6	SER	2.1
3	C	12	THR	2.1
2	N	30	PHE	2.1
2	H	89	ILE	2.1
2	J	165	VAL	2.1
2	P	116	THR	2.1
2	J	9	VAL	2.1
2	L	119	SER	2.1
2	D	105	LEU	2.1
2	D	62	GLU	2.1
3	G	52	GLY	2.1
1	A	43	SER	2.1
3	G	36	ASP	2.1
2	F	133	ILE	2.1
1	A	64	LYS	2.1
3	G	28	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	172	VAL	2.1
1	I	12	THR	2.1
2	H	115	GLU	2.1
3	C	34	GLN	2.1
2	B	26	ALA	2.1
3	C	23	PRO	2.1
3	O	64	VAL	2.1
2	B	49	SER	2.1
2	P	30	PHE	2.1
1	M	8	ALA	2.1
2	N	121	GLY	2.1
1	A	59	GLU	2.1
2	B	101	ASP	2.1
1	A	24	LYS	2.1
3	G	30	LYS	2.1
2	P	31	ILE	2.0
1	I	36	GLU	2.0
2	D	150	LYS	2.0
2	F	93	VAL	2.0
1	I	5	SER	2.0
2	D	9	VAL	2.0
2	F	104	VAL	2.0
2	B	161	LEU	2.0
1	M	74	ARG	2.0
2	N	41	VAL	2.0
2	H	73	CYS	2.0
2	B	126	GLY	2.0
2	F	85	ASP	2.0
3	G	60	ASP	2.0
2	P	118	SER	2.0
2	D	76	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

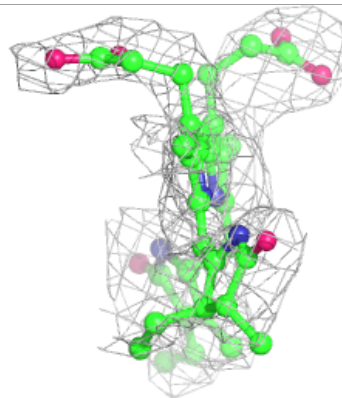
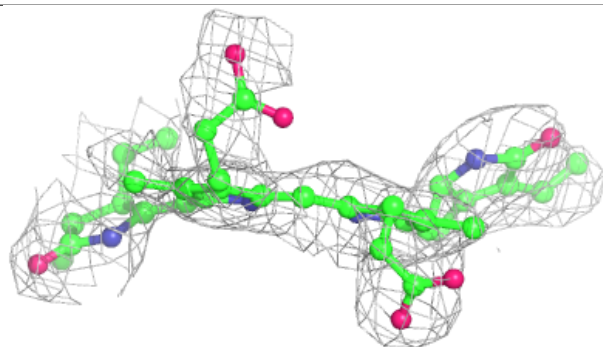
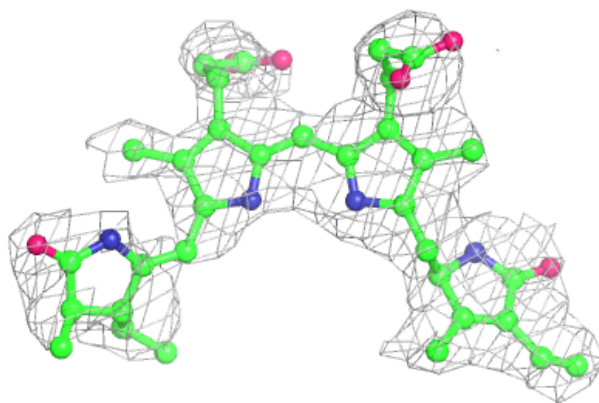
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PEB	B	202	43/43	0.76	0.33	31,51,65,80	0
5	PEB	P	203	43/43	0.77	0.29	21,59,80,85	0
5	PEB	D	202	43/43	0.80	0.35	35,61,102,108	0
4	DBV	C	101	43/43	0.80	0.27	32,53,67,78	0
5	PEB	J	203	43/43	0.81	0.29	26,41,59,66	0
5	PEB	F	202	43/43	0.82	0.30	14,41,60,63	0
5	PEB	D	201	43/43	0.83	0.28	21,45,64,66	0
5	PEB	L	203	43/43	0.83	0.26	5,53,69,84	0
5	PEB	F	203	43/43	0.83	0.30	20,38,48,61	0
5	PEB	H	201	43/43	0.84	0.25	2,36,49,80	0
5	PEB	B	201	43/43	0.84	0.32	16,44,71,73	0
4	DBV	E	101	43/43	0.84	0.30	17,42,67,86	0
4	DBV	I	101	43/43	0.84	0.29	28,51,70,76	0
5	PEB	B	203	43/43	0.85	0.32	19,48,62,66	0
5	PEB	L	202	43/43	0.85	0.27	24,56,78,84	0
4	DBV	K	101	43/43	0.85	0.28	17,46,63,77	0
5	PEB	N	203	43/43	0.85	0.29	21,48,65,67	0
5	PEB	P	202	43/43	0.85	0.29	19,49,73,102	0
5	PEB	H	202	43/43	0.85	0.29	15,54,71,80	0
4	DBV	M	101	43/43	0.86	0.27	21,52,71,82	0
5	PEB	H	203	43/43	0.87	0.29	21,45,59,75	0
5	PEB	J	201	43/43	0.87	0.24	15,36,51,69	0
5	PEB	F	201	43/43	0.88	0.22	2,28,44,64	0
5	PEB	N	202	43/43	0.88	0.23	10,39,50,71	0
4	DBV	O	101	43/43	0.88	0.23	16,40,55,59	0
5	PEB	L	201	43/43	0.88	0.22	9,32,63,69	0
4	DBV	A	101	43/43	0.88	0.26	23,39,60,74	0
5	PEB	N	201	43/43	0.89	0.22	14,34,63,68	0
5	PEB	P	201	43/43	0.90	0.23	2,30,62,92	0
4	DBV	G	101	43/43	0.90	0.21	2,32,51,72	0
5	PEB	D	203	43/43	0.90	0.25	14,40,60,70	0
5	PEB	J	202	43/43	0.91	0.20	14,36,55,58	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.

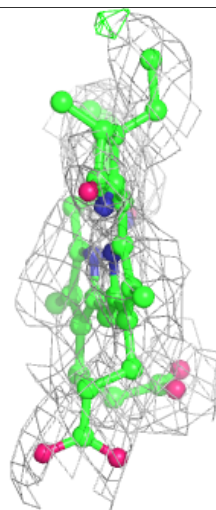
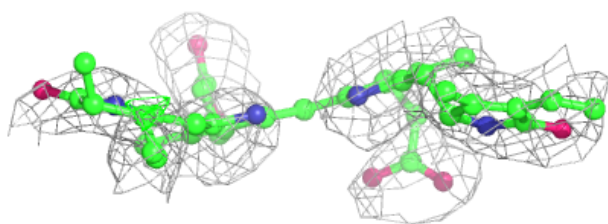
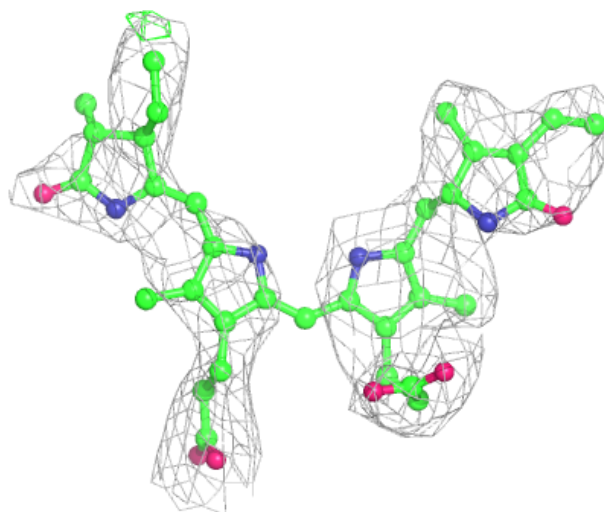
**Electron density around PEB B 202:**

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



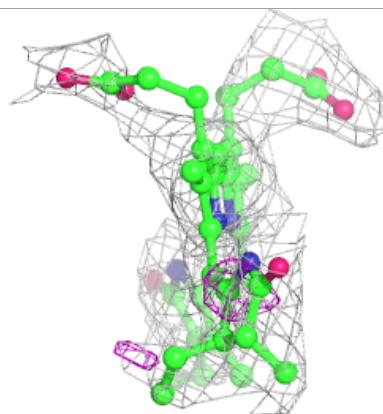
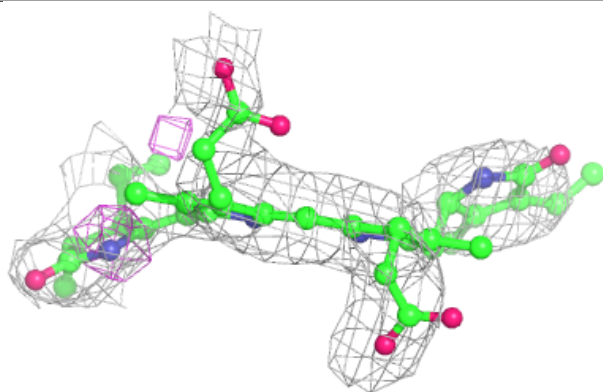
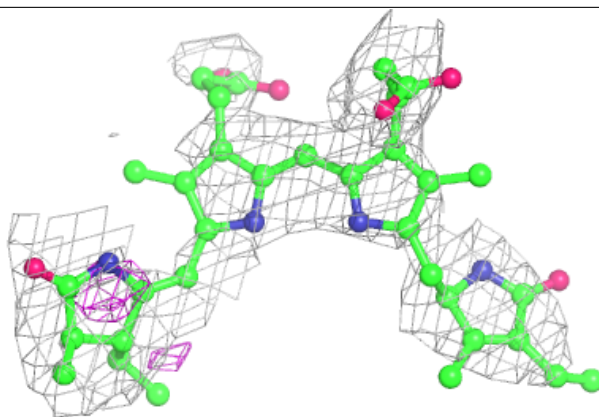
**Electron density around PEB P 203:**

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

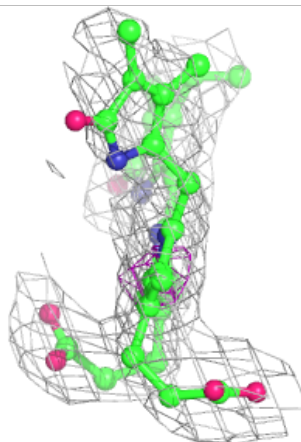
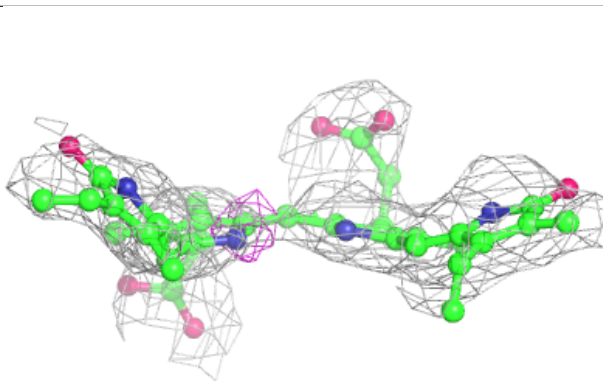
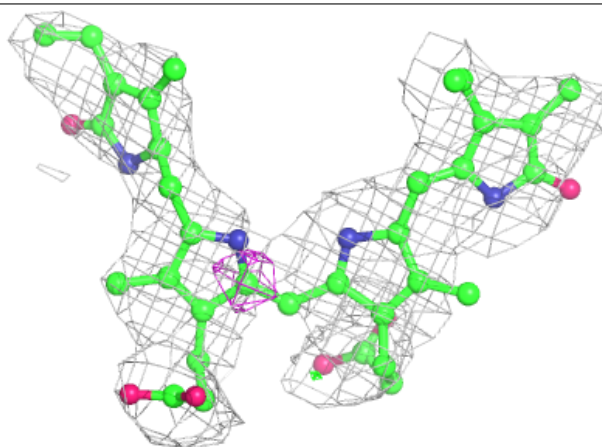


**Electron density around PEB D 202:**

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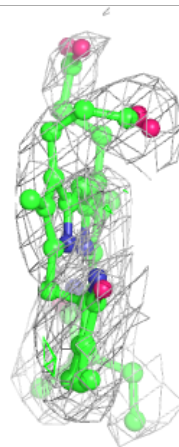
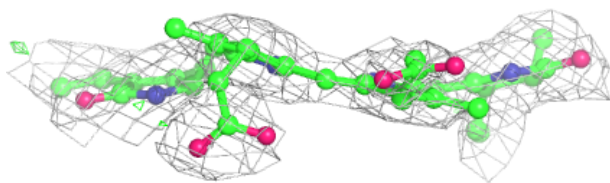
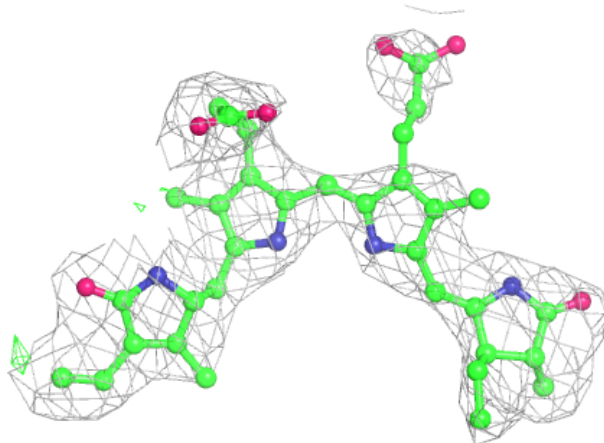
**Electron density around DBV C 101:**

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



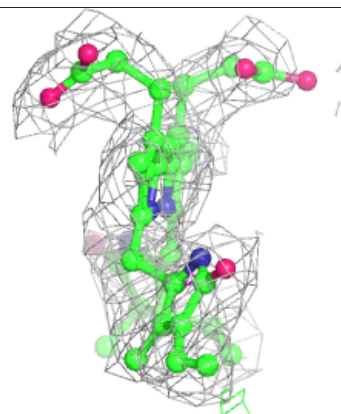
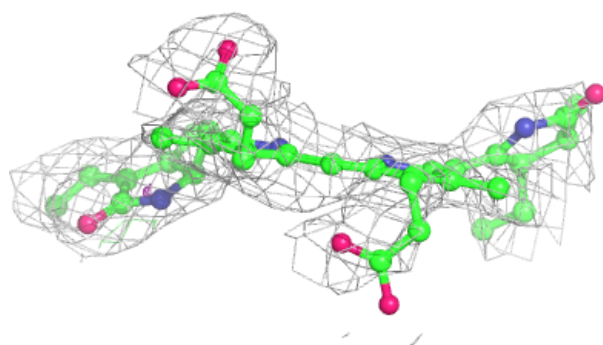
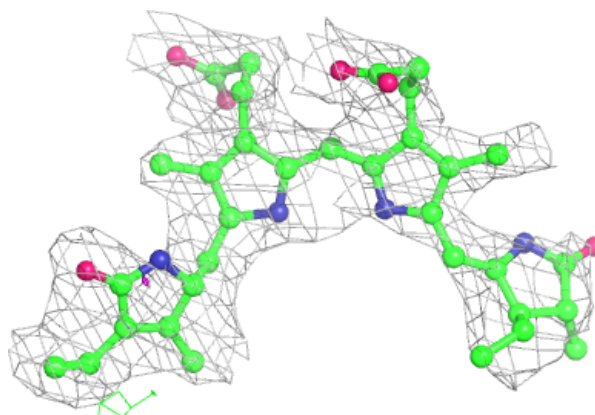
**Electron density around PEB J 203:**

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and green (positive)



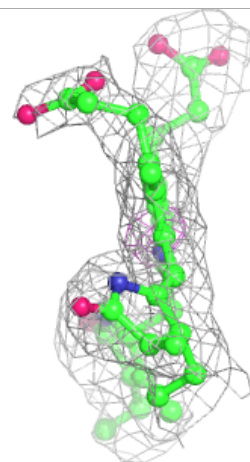
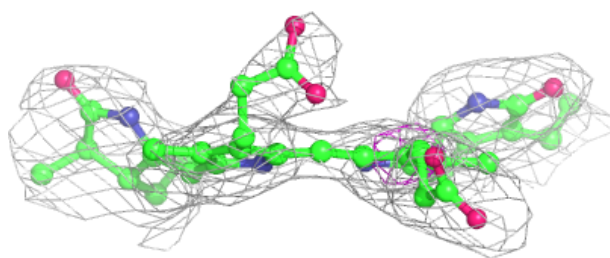
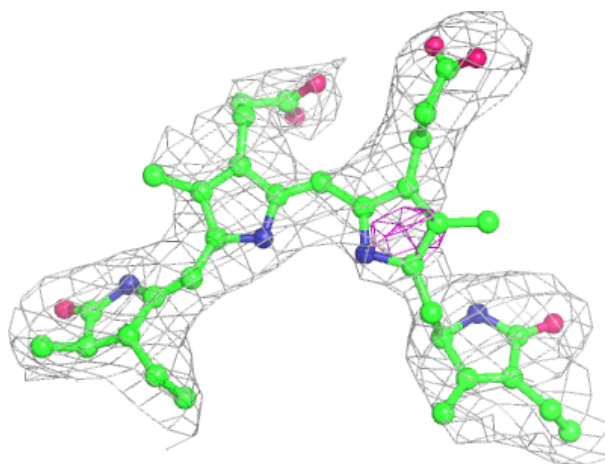
**Electron density around PEB F 202:**

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



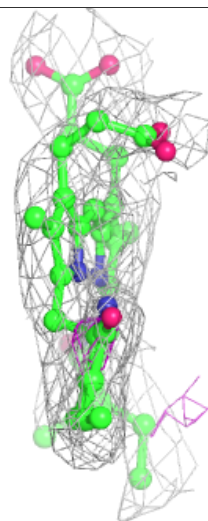
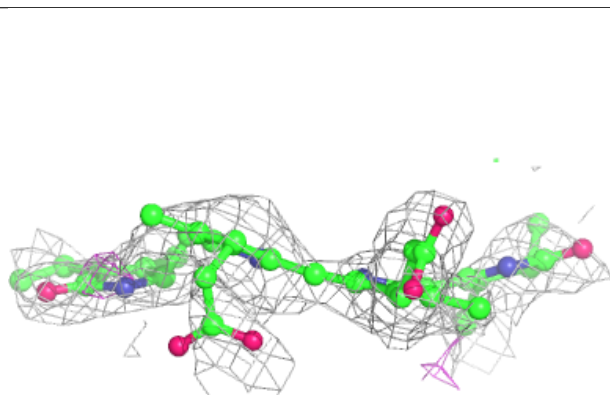
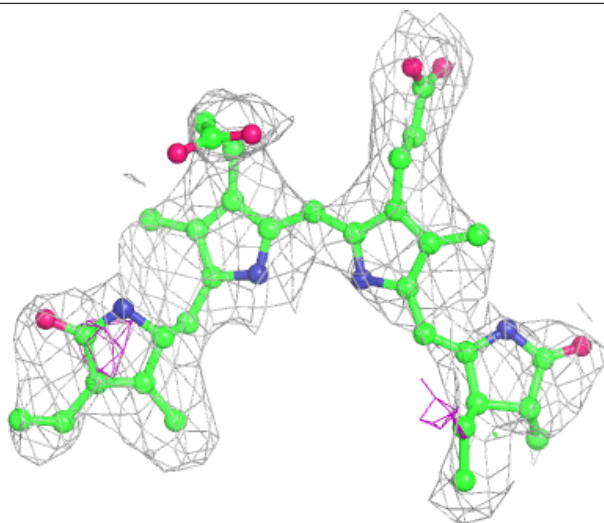
**Electron density around PEB D 201:**

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



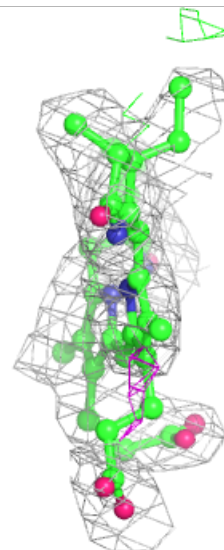
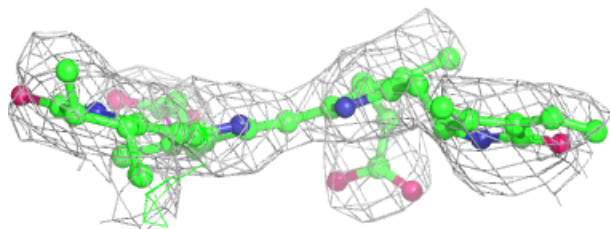
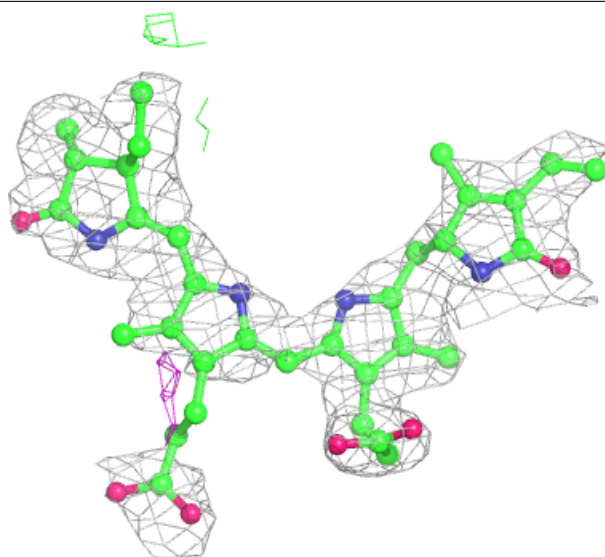
**Electron density around PEB L 203:**

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



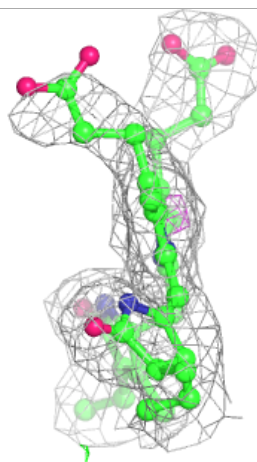
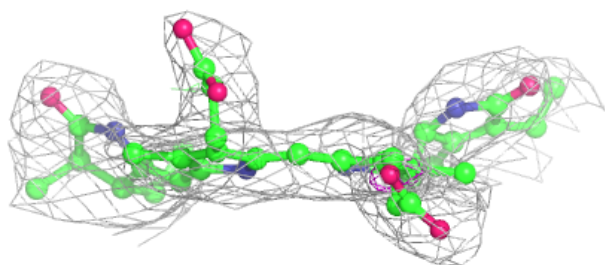
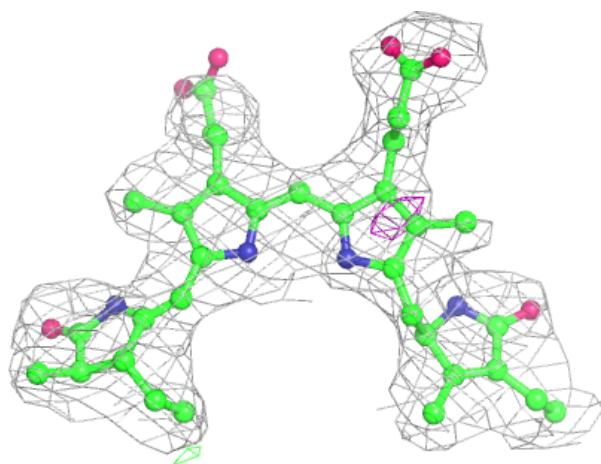
**Electron density around PEB F 203:**

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and green (positive)



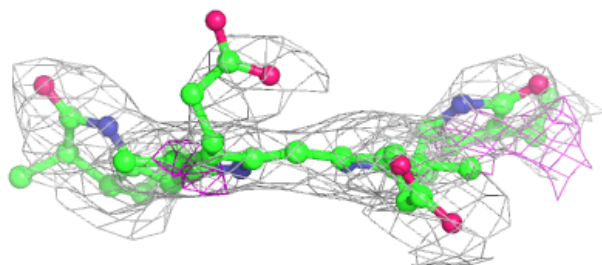
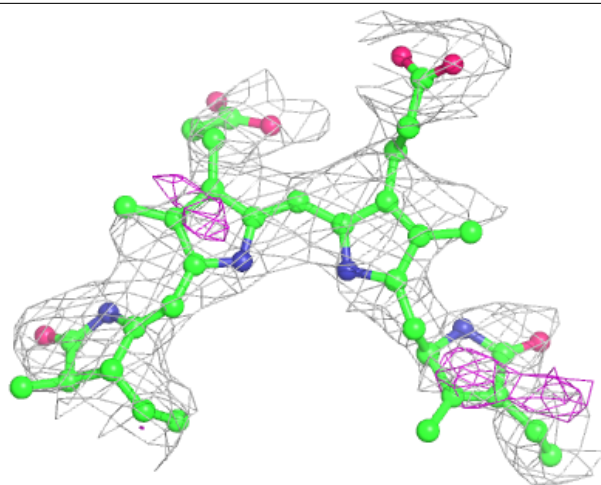
**Electron density around PEB H 201:**

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and green (positive)



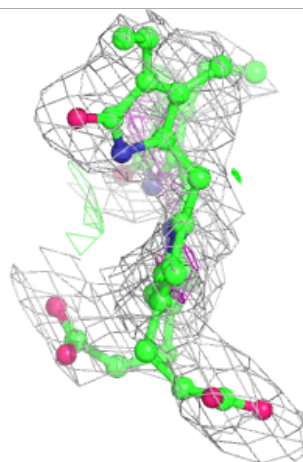
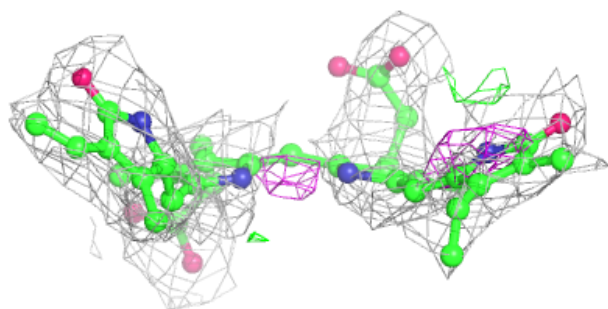
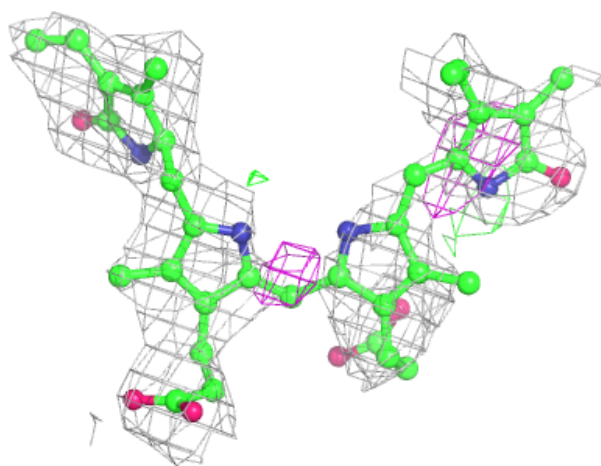
**Electron density around PEB B 201:**

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and green (positive)



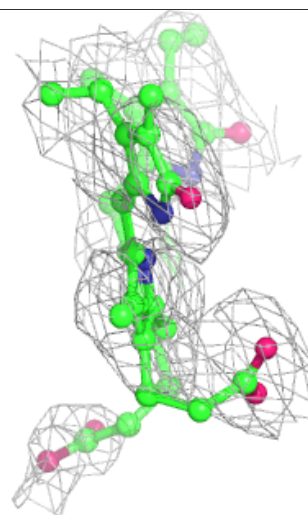
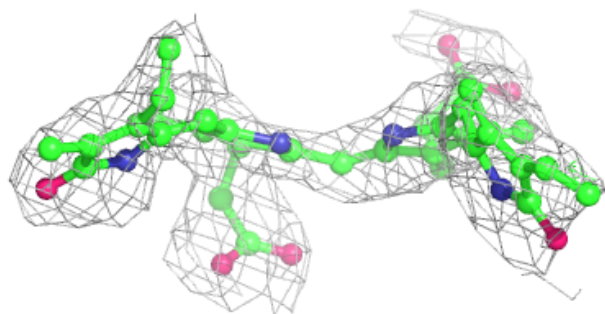
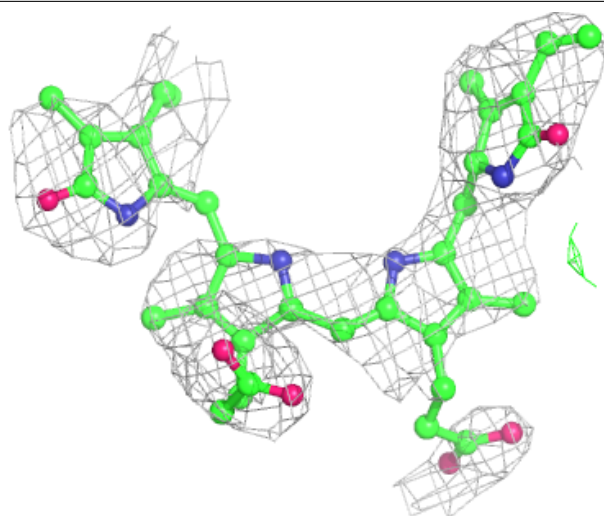
**Electron density around DBV E 101:**

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and green (positive)



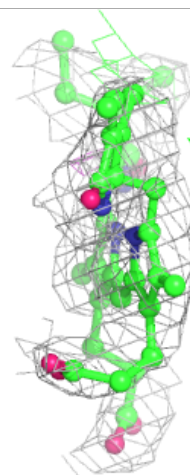
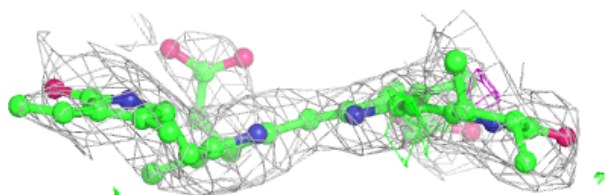
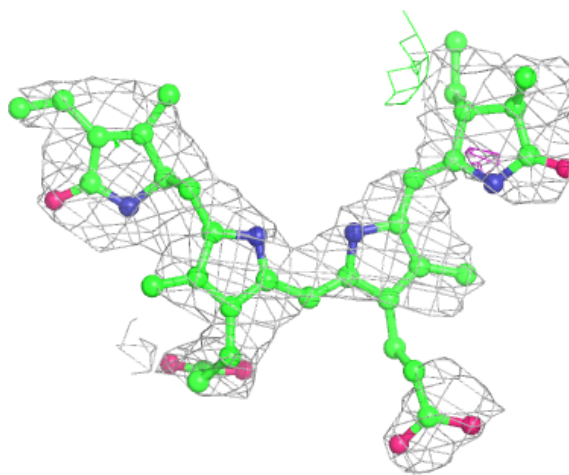
**Electron density around DBV I 101:**

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and green (positive)



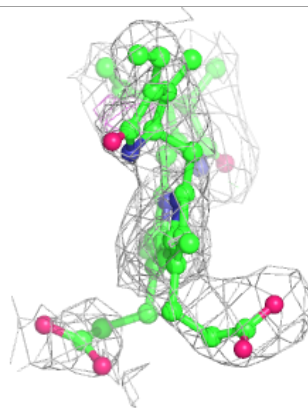
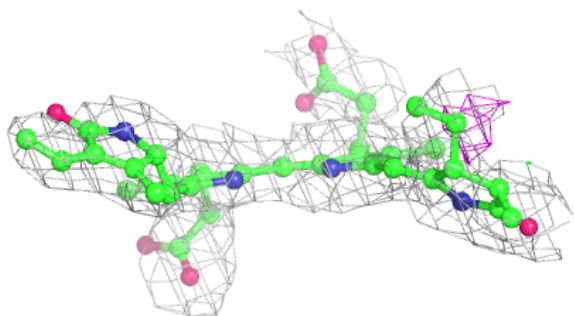
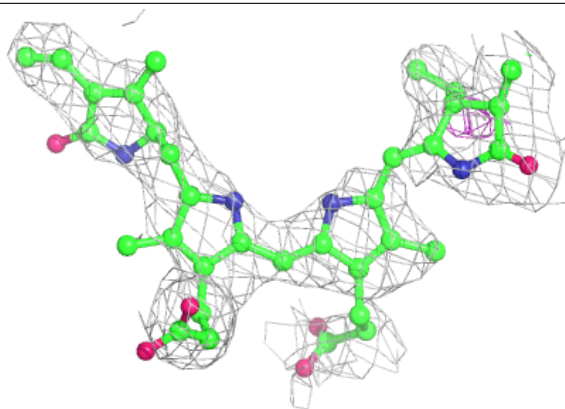
**Electron density around PEB B 203:**

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



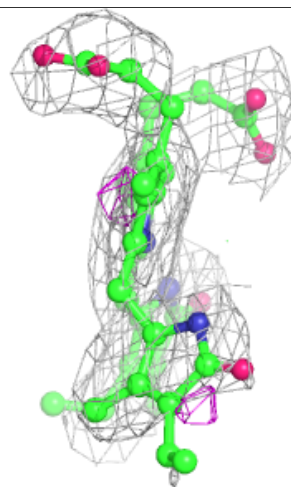
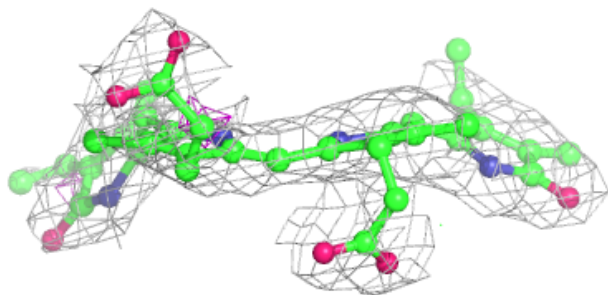
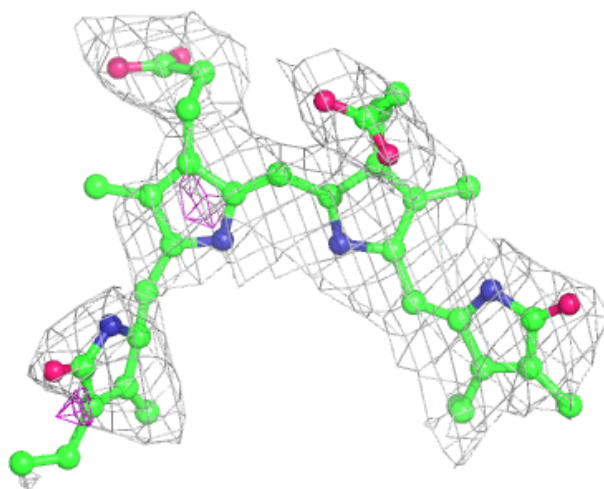
**Electron density around PEB L 202:**

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



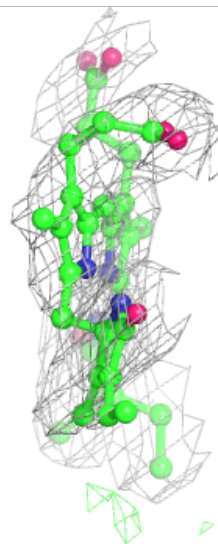
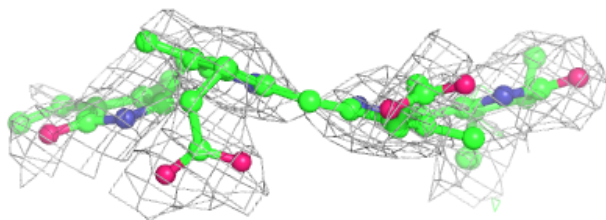
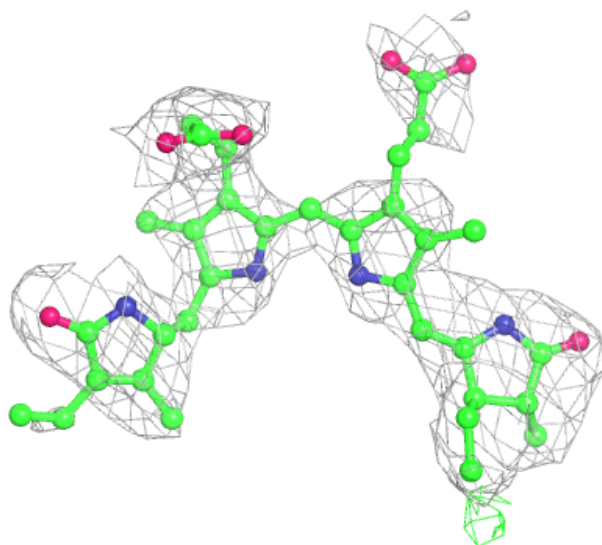
**Electron density around DBV K 101:**

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and green (positive)



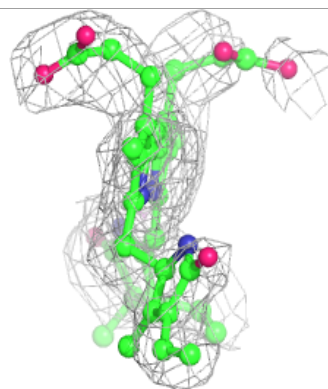
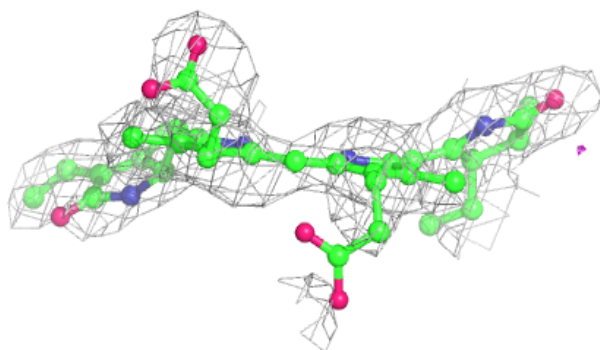
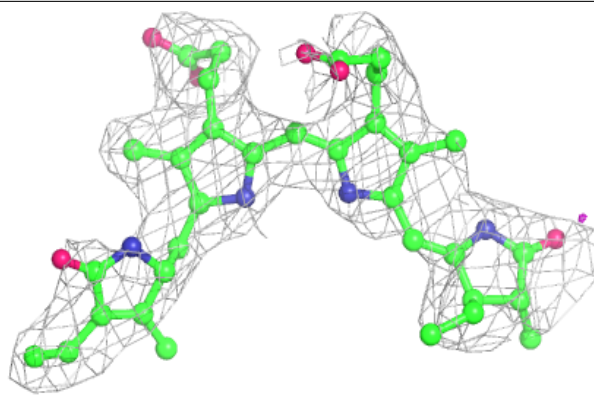
**Electron density around PEB N 203:**

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and green (positive)



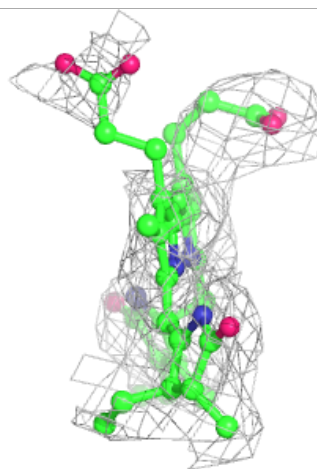
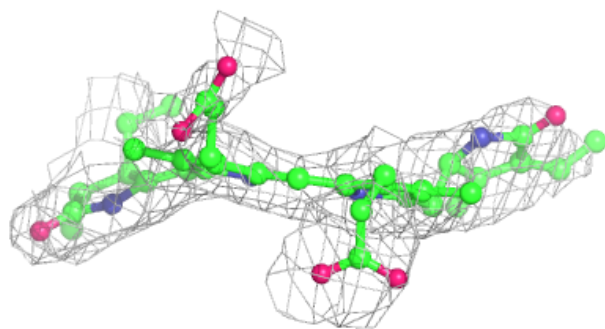
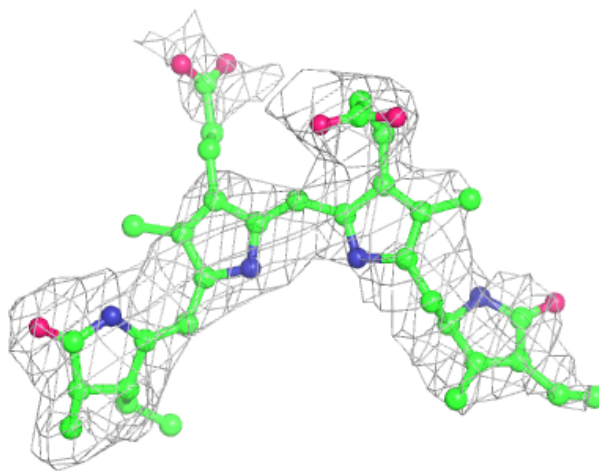
**Electron density around PEB P 202:**

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and green (positive)



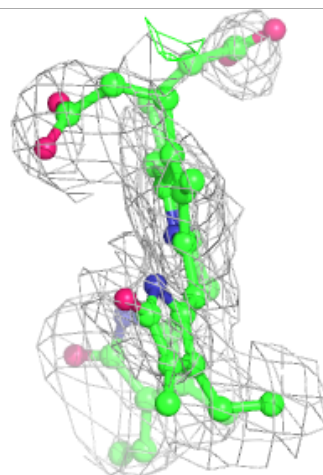
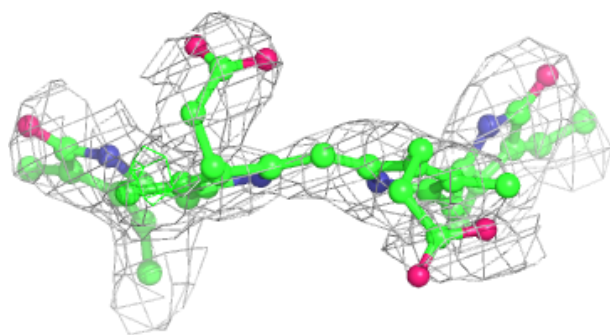
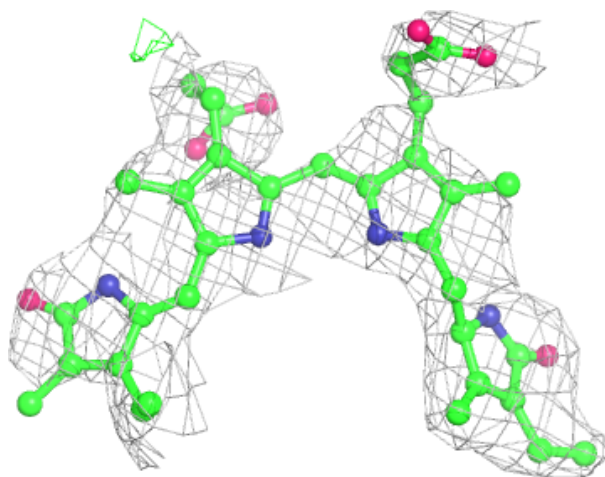
**Electron density around PEB H 202:**

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and green (positive)



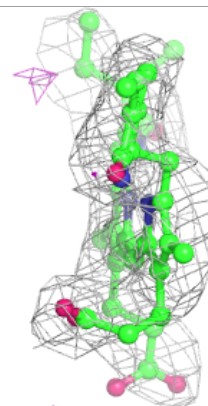
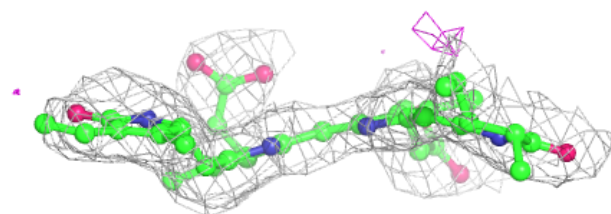
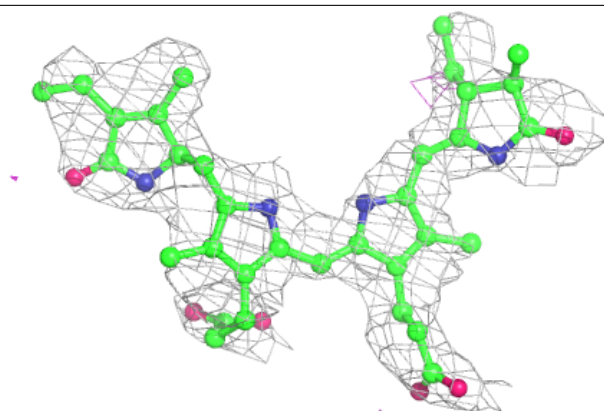
**Electron density around DBV M 101:**

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and green (positive)



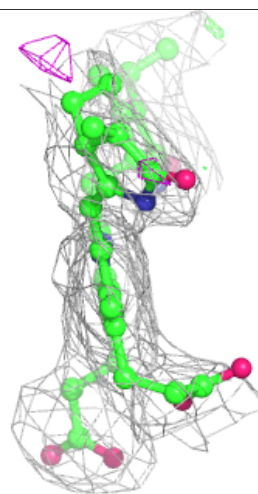
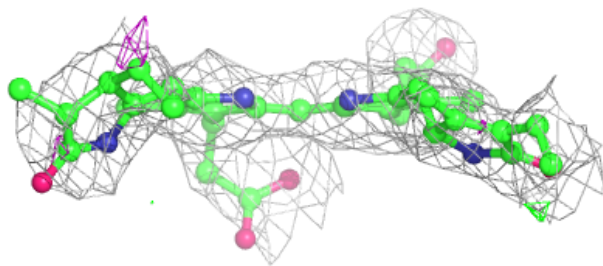
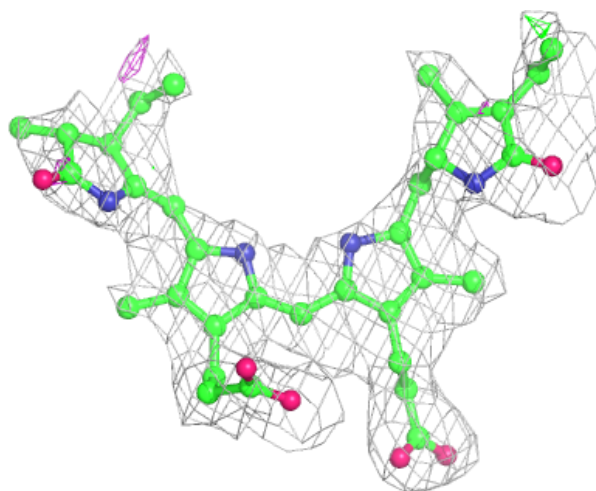
**Electron density around PEB H 203:**

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and green (positive)



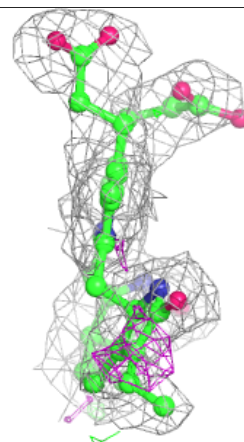
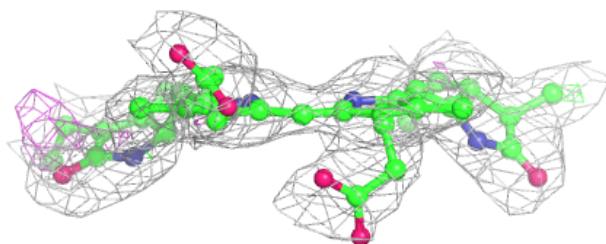
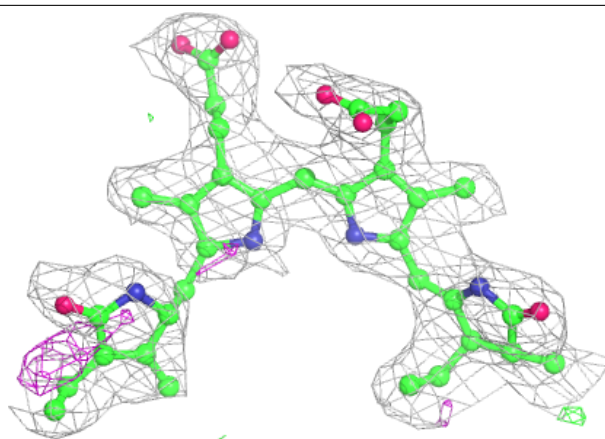
**Electron density around PEB J 201:**

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

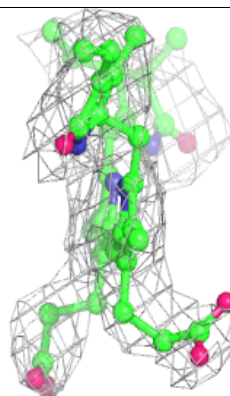
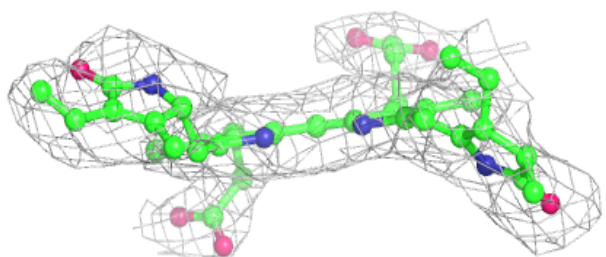
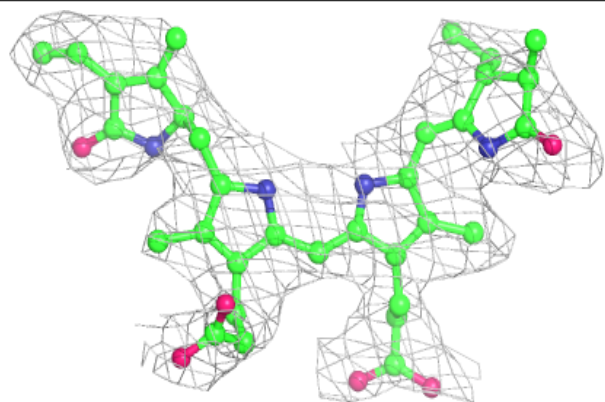


**Electron density around PEB F 201:**

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and green (positive)

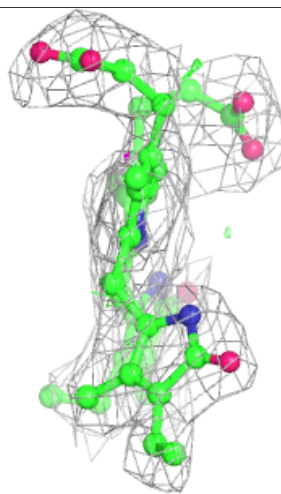
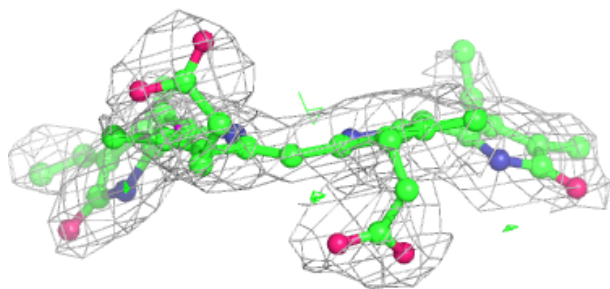
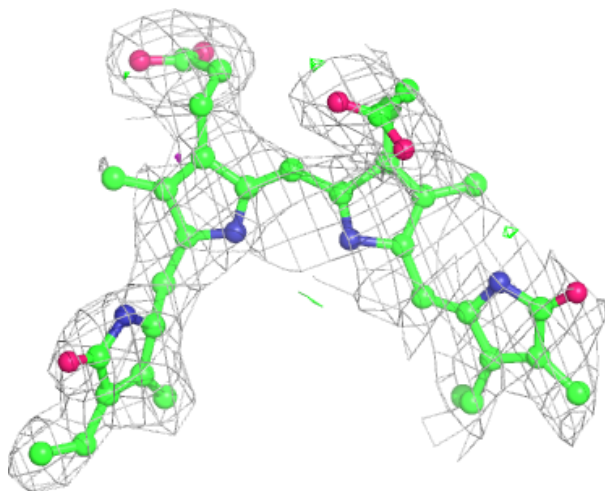
**Electron density around PEB N 202:**

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and green (positive)



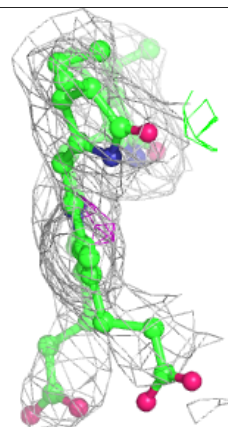
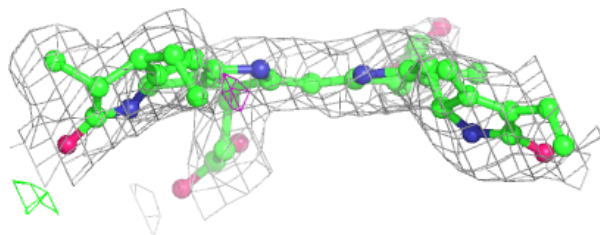
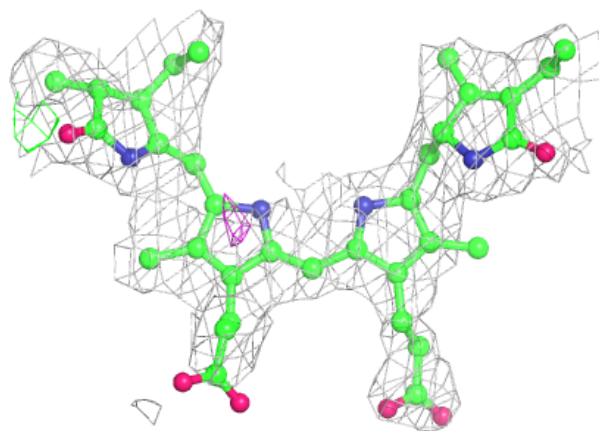
**Electron density around DBV O 101:**

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



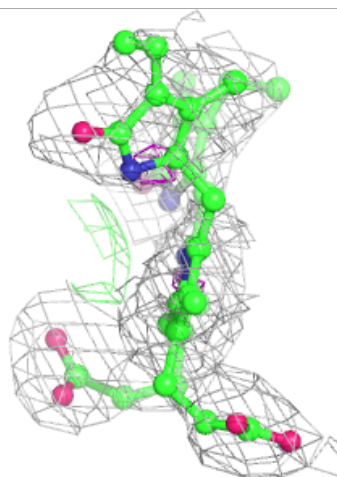
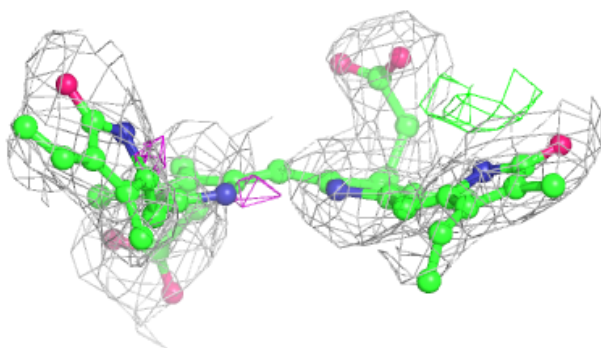
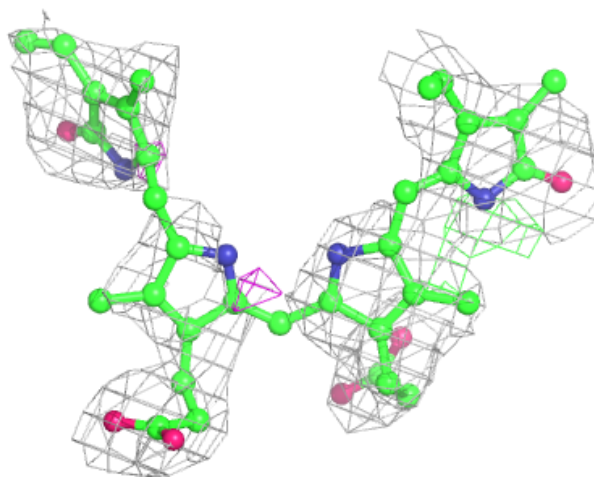
**Electron density around PEB L 201:**

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



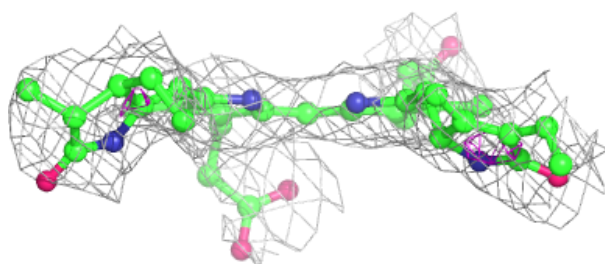
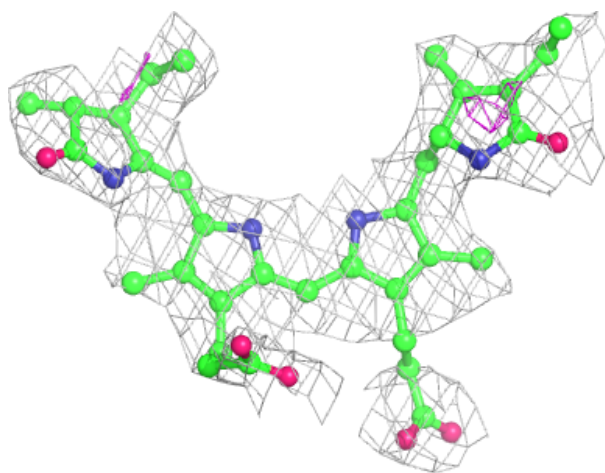
**Electron density around DBV A 101:**

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



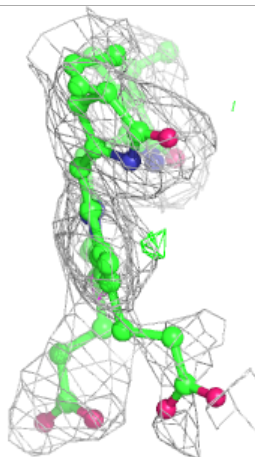
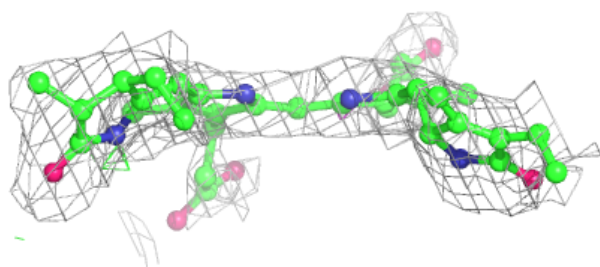
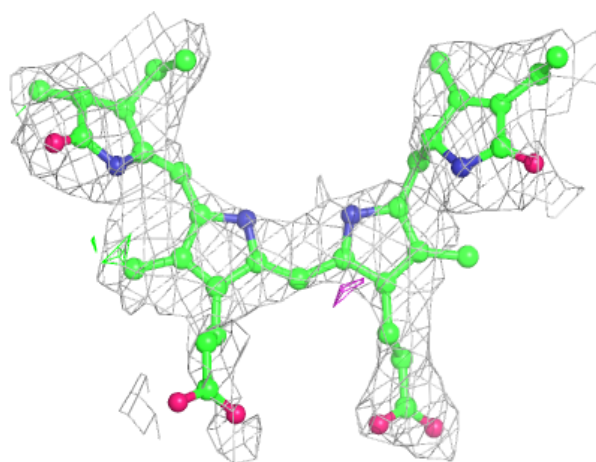
**Electron density around PEB N 201:**

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



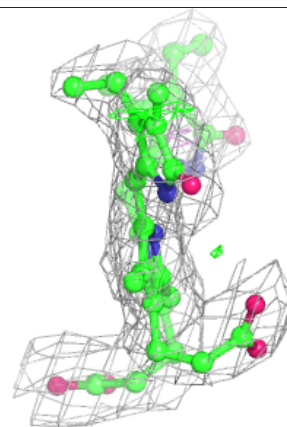
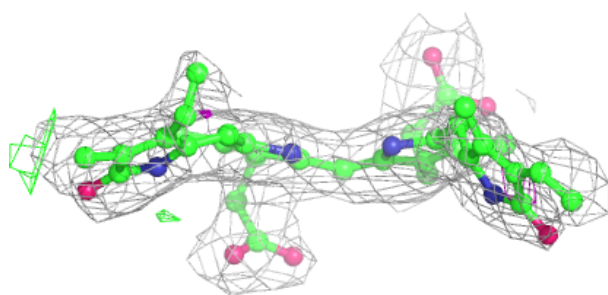
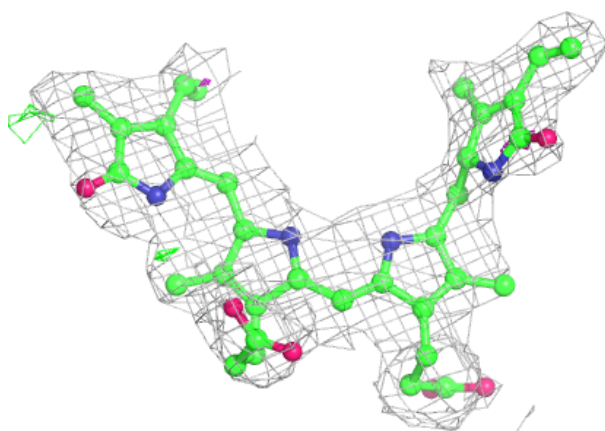
**Electron density around PEB P 201:**

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

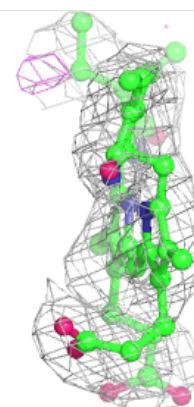
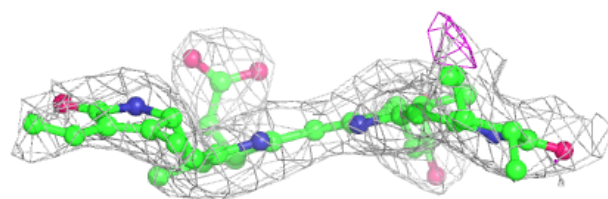
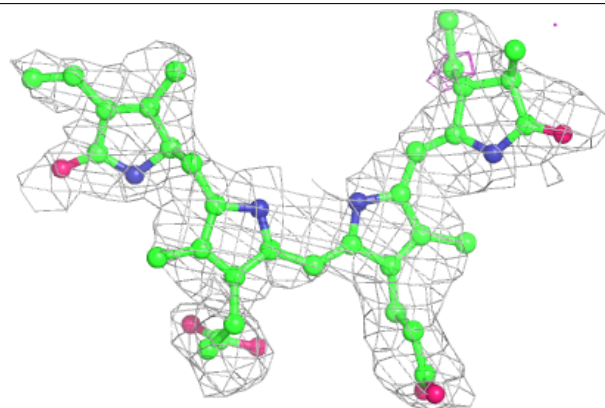


**Electron density around DBV G 101:**

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

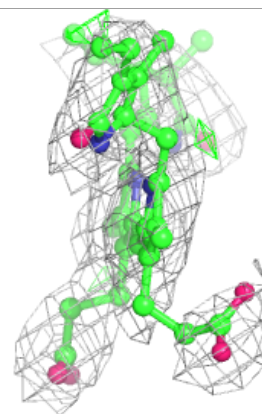
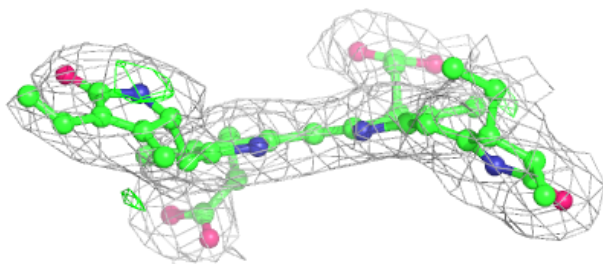
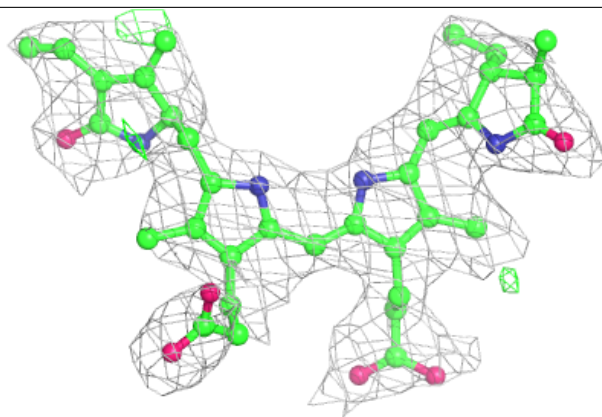
**Electron density around PEB D 203:**

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



**Electron density around PEB J 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.