



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:59 PM UTC

PDB ID : 8B4N / pdb_00008b4n
Title : X-ray structure of phycoerythrin from *Porphyridium cruentum*
Authors : Merlino, A.; Ferraro, G.
Deposited on : 2022-09-20
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

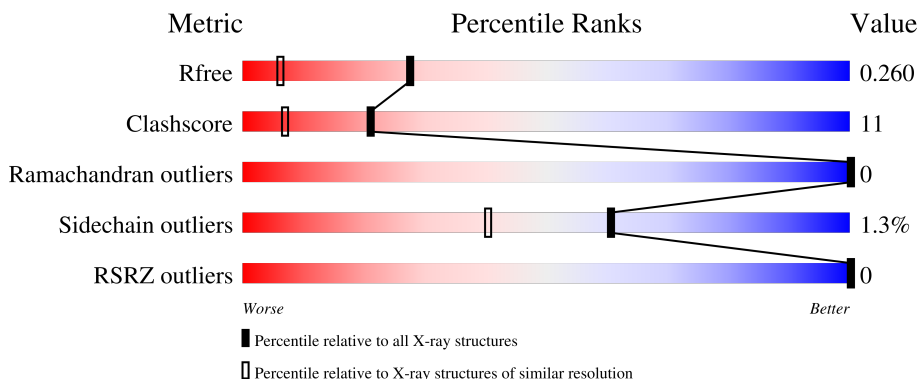
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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

Mol	Chain	Length	Quality of chain
1	AAA	164	85% 15%
1	CCC	164	84% 14% .
2	BBB	177	93% 6% .
2	DDD	177	90% 8% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5990 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 B-phycoerythrin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	164	Total	C	N	O	S	0	2	0
			1266	788	223	248	7			
1	CCC	164	Total	C	N	O	S	0	4	0
			1283	797	228	251	7			

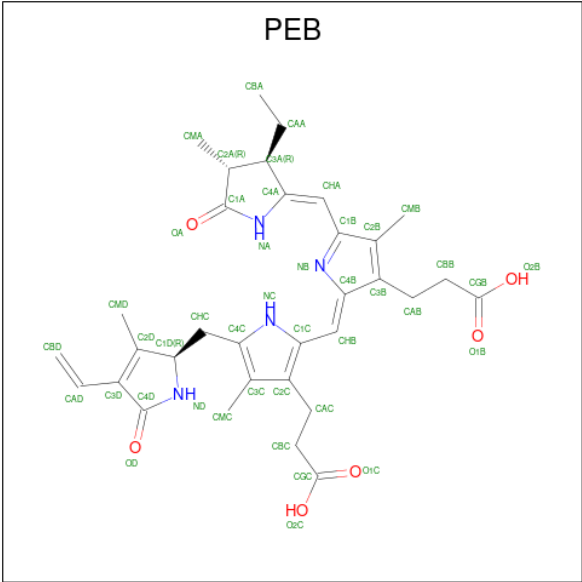
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	96	CYS	ASP	conflict	UNP P11392
CCC	96	CYS	ASP	conflict	UNP P11392

- Molecule 2 is a protein called B-phycoerythrin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	177	Total	C	N	O	S	0	4	0
			1314	812	229	261	12			
2	DDD	177	Total	C	N	O	S	0	5	0
			1320	815	230	263	12			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	0	1
			86	66	8	12		
3	AAA	1	Total	C	N	O	0	0
			43	33	4	6		
3	BBB	1	Total	C	N	O	0	0
			43	33	4	6		
3	BBB	1	Total	C	N	O	0	0
			43	33	4	6		
3	BBB	1	Total	C	N	O	0	0
			43	33	4	6		
3	CCC	1	Total	C	N	O	0	0
			43	33	4	6		
3	CCC	1	Total	C	N	O	0	0
			43	33	4	6		
3	DDD	1	Total	C	N	O	0	0
			43	33	4	6		
3	DDD	1	Total	C	N	O	0	0
			43	33	4	6		
3	DDD	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	O	S	0	0
			5	4	1		
4	DDD	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

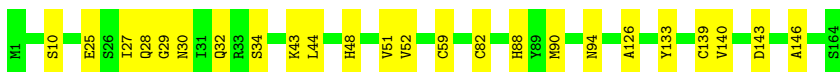
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	93	Total	O	0	0
			93	93		
5	BBB	72	Total	O	0	0
			72	72		
5	CCC	79	Total	O	0	0
			79	79		
5	DDD	80	Total	O	0	0
			80	80		

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: B-phycoerythrin alpha chain

Chain AAA: 



- Molecule 1: B-phycoerythrin alpha chain

Chain CCC: 



- Molecule 2: B-phycoerythrin beta chain

Chain BBB: 



- Molecule 2: B-phycoerythrin beta chain

Chain DDD: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	186.59Å 186.59Å 59.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.65 – 1.60 46.65 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.65-1.60) 99.0 (46.65-1.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.222 , 0.256 0.226 , 0.260	Depositor DCC
R_{free} test set	4971 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 25.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.245 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5990	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEB, MEN, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AAA	1.06	0/1288	1.31	0/1744
1	CCC	1.05	0/1305	1.35	2/1766 (0.1%)
2	BBB	1.15	1/1326 (0.1%)	1.43	2/1788 (0.1%)
2	DDD	1.11	0/1332	1.30	1/1797 (0.1%)
All	All	1.09	1/5251 (0.0%)	1.35	5/7095 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	BBB	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	40	ALA	C-O	5.17	1.30	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	30	ASN	CB-CA-C	-7.36	99.22	110.92
2	DDD	159	THR	CB-CA-C	5.40	120.03	110.85
1	CCC	30	ASN	N-CA-CB	5.33	117.92	109.82
2	BBB	33	ASP	CA-C-N	5.22	125.88	120.03
2	BBB	33	ASP	C-N-CA	5.22	125.88	120.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BBB	72	MEN	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1266	0	1233	34	0
1	CCC	1283	0	1249	34	0
2	BBB	1314	0	1326	23	0
2	DDD	1320	0	1332	28	0
3	AAA	129	0	113	22	0
3	BBB	129	0	112	12	0
3	CCC	86	0	75	8	0
3	DDD	129	0	113	19	0
4	AAA	5	0	0	0	0
4	DDD	5	0	0	0	0
5	AAA	93	0	0	3	0
5	BBB	72	0	0	2	1
5	CCC	79	0	0	0	0
5	DDD	80	0	0	0	1
All	All	5990	0	5553	115	1

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 11.

The worst 5 of 115 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:DDD:82:CYS:SG	3:DDD:202:PEB:HAA2	1.25	1.76
2:BBB:50:CYS:SG	3:BBB:201:PEB:HAA1	1.23	1.75
2:DDD:50:CYS:SG	3:DDD:201:PEB:HAA1	1.18	1.64
1:AAA:82:CYS:SG	3:AAA:201[A]:PEB:HAA2	1.52	1.45
1:AAA:82:CYS:SG	3:AAA:201[B]:PEB:HAA2	1.61	1.39

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BBB:315:HOH:O	5:DDD:371:HOH:O[2_554]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	164/164 (100%)	161 (98%)	3 (2%)	0	100	100
1	CCC	166/164 (101%)	164 (99%)	2 (1%)	0	100	100
2	BBB	178/177 (101%)	176 (99%)	2 (1%)	0	100	100
2	DDD	179/177 (101%)	178 (99%)	1 (1%)	0	100	100
All	All	687/682 (101%)	679 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	130/128 (102%)	130 (100%)	0	100	100
1	CCC	132/128 (103%)	130 (98%)	2 (2%)	57	35
2	BBB	141/137 (103%)	140 (99%)	1 (1%)	76	63
2	DDD	142/137 (104%)	138 (97%)	4 (3%)	38	15
All	All	545/530 (103%)	538 (99%)	7 (1%)	61	40

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	DDD	1	MET
2	DDD	22	SER
2	DDD	165	VAL
2	DDD	25	GLN
1	CCC	164	SER

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MEN	DDD	72	2	7,8,9	0.69	0	4,9,11	0.44	0
2	MEN	BBB	72	2	7,8,9	0.39	0	4,9,11	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	DDD	72	2	-	2/7/8/10	-
2	MEN	BBB	72	2	-	3/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	72	MEN	O-C-CA-CB
2	DDD	72	MEN	CA-CB-CG-OD1
2	BBB	72	MEN	CA-CB-CG-OD1
2	BBB	72	MEN	CA-CB-CG-ND2
2	DDD	72	MEN	CA-CB-CG-ND2

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	DDD	72	MEN	4	0
2	BBB	72	MEN	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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
3	PEB	BBB	201	2	46,46,46	0.88	4 (8%)	56,67,67	0.84	1 (1%)
3	PEB	DDD	203	2	46,46,46	0.98	2 (4%)	56,67,67	0.81	1 (1%)
4	SO4	AAA	203	-	4,4,4	0.37	0	6,6,6	0.11	0
4	SO4	DDD	204	-	4,4,4	0.32	0	6,6,6	0.22	0
3	PEB	AAA	201[B]	-	46,46,46	0.67	0	56,67,67	0.86	0
3	PEB	AAA	201[A]	-	46,46,46	0.74	1 (2%)	56,67,67	0.97	2 (3%)
3	PEB	CCC	201	1	46,46,46	0.84	1 (2%)	56,67,67	1.02	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEB	DDD	201	2	46,46,46	0.79	2 (4%)	56,67,67	1.03	2 (3%)
3	PEB	CCC	202	-	46,46,46	0.84	1 (2%)	56,67,67	0.82	1 (1%)
3	PEB	AAA	202	1	46,46,46	0.82	2 (4%)	56,67,67	0.92	2 (3%)
3	PEB	BBB	202	2	46,46,46	0.81	0	56,67,67	1.72	8 (14%)
3	PEB	BBB	203	2	46,46,46	0.66	0	56,67,67	0.74	0
3	PEB	DDD	202	2	46,46,46	0.80	1 (2%)	56,67,67	1.15	2 (3%)

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
3	PEB	BBB	201	2	-	3/26/74/74	0/4/4/4
3	PEB	DDD	203	2	-	8/26/74/74	0/4/4/4
3	PEB	AAA	201[B]	-	-	6/26/74/74	0/4/4/4
3	PEB	AAA	201[A]	-	-	7/26/74/74	0/4/4/4
3	PEB	CCC	201	1	-	6/26/74/74	0/4/4/4
3	PEB	DDD	201	2	-	5/26/74/74	0/4/4/4
3	PEB	CCC	202	-	-	11/26/74/74	0/4/4/4
3	PEB	AAA	202	1	-	6/26/74/74	0/4/4/4
3	PEB	BBB	202	2	-	7/26/74/74	0/4/4/4
3	PEB	BBB	203	2	-	8/26/74/74	0/4/4/4
3	PEB	DDD	202	2	-	6/26/74/74	0/4/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DDD	203	PEB	CHA-C4A	3.98	1.43	1.36
3	CCC	202	PEB	CHA-C4A	3.03	1.41	1.36
3	CCC	201	PEB	CHA-C4A	2.79	1.41	1.36
3	BBB	201	PEB	CHA-C4A	2.68	1.41	1.36
3	AAA	201[A]	PEB	CHA-C4A	2.49	1.40	1.36

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	202	PEB	CHC-C1D-ND	-7.38	104.67	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	202	PEB	CHA-C4A-NA	4.94	131.79	125.63
3	BBB	202	PEB	OD-C4D-ND	-4.15	120.31	126.02
3	DDD	202	PEB	CHA-C4A-NA	3.99	130.61	125.63
3	CCC	201	PEB	CHA-C4A-NA	3.28	129.72	125.63

There are no chirality outliers.

5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	201[A]	PEB	NA-C4A-CHA-C1B
3	AAA	201[A]	PEB	C3A-C4A-CHA-C1B
3	AAA	201[A]	PEB	NB-C1B-CHA-C4A
3	AAA	201[A]	PEB	C2B-C1B-CHA-C4A
3	AAA	201[B]	PEB	NA-C4A-CHA-C1B

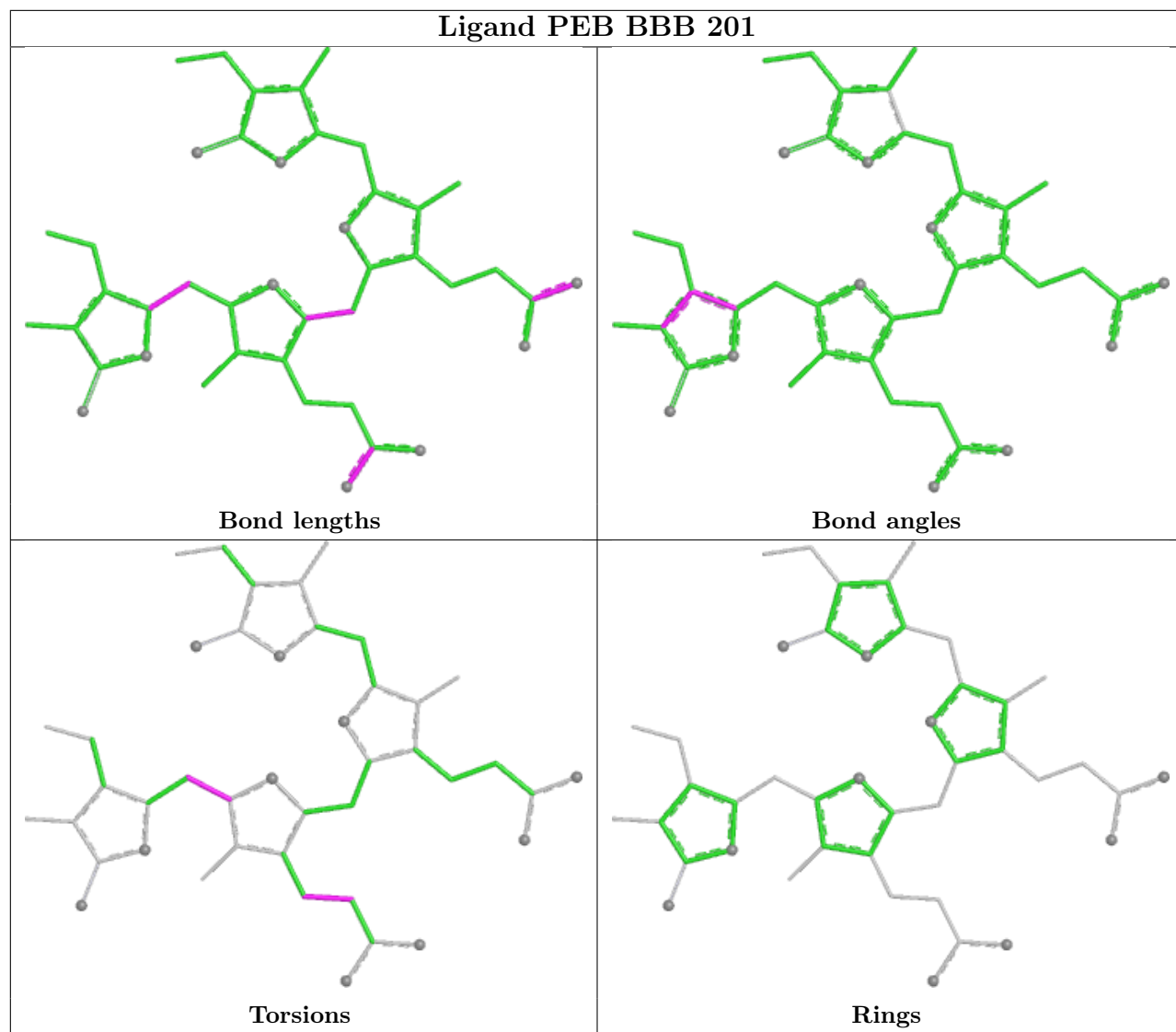
There are no ring outliers.

10 monomers are involved in 61 short contacts:

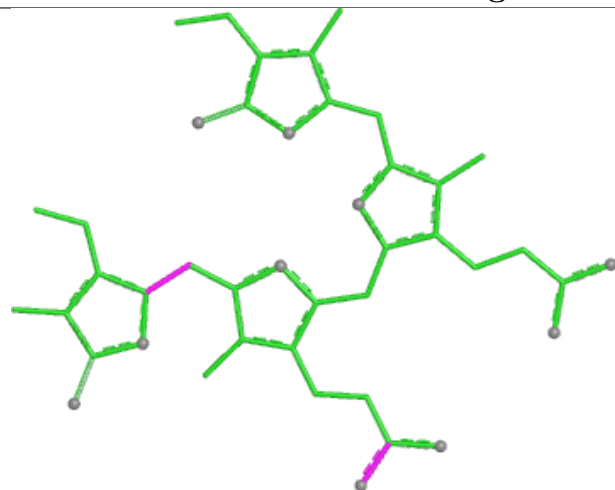
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	201	PEB	10	0
3	DDD	203	PEB	3	0
3	AAA	201[B]	PEB	10	0
3	AAA	201[A]	PEB	9	0
3	CCC	201	PEB	6	0
3	DDD	201	PEB	10	0
3	CCC	202	PEB	2	0
3	AAA	202	PEB	3	0
3	BBB	203	PEB	2	0
3	DDD	202	PEB	6	0

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

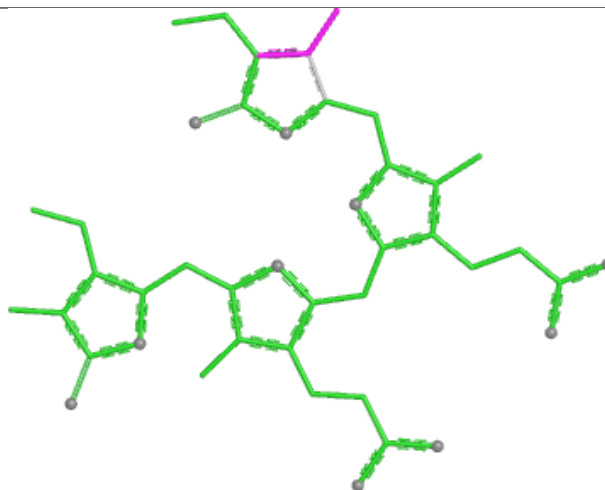
Ligand PEB BBB 201



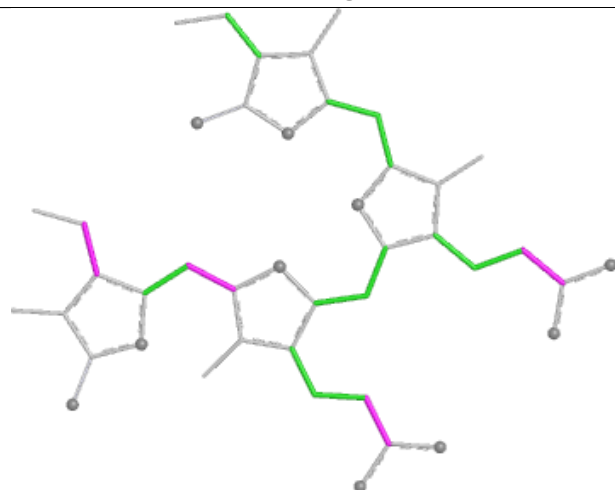
Ligand PEB DDD 203



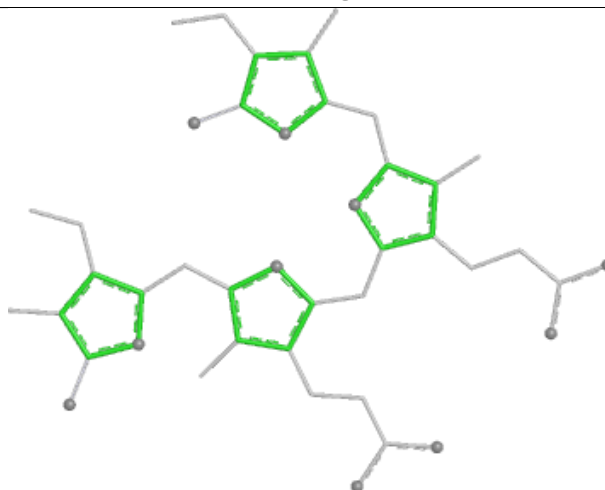
Bond lengths



Bond angles

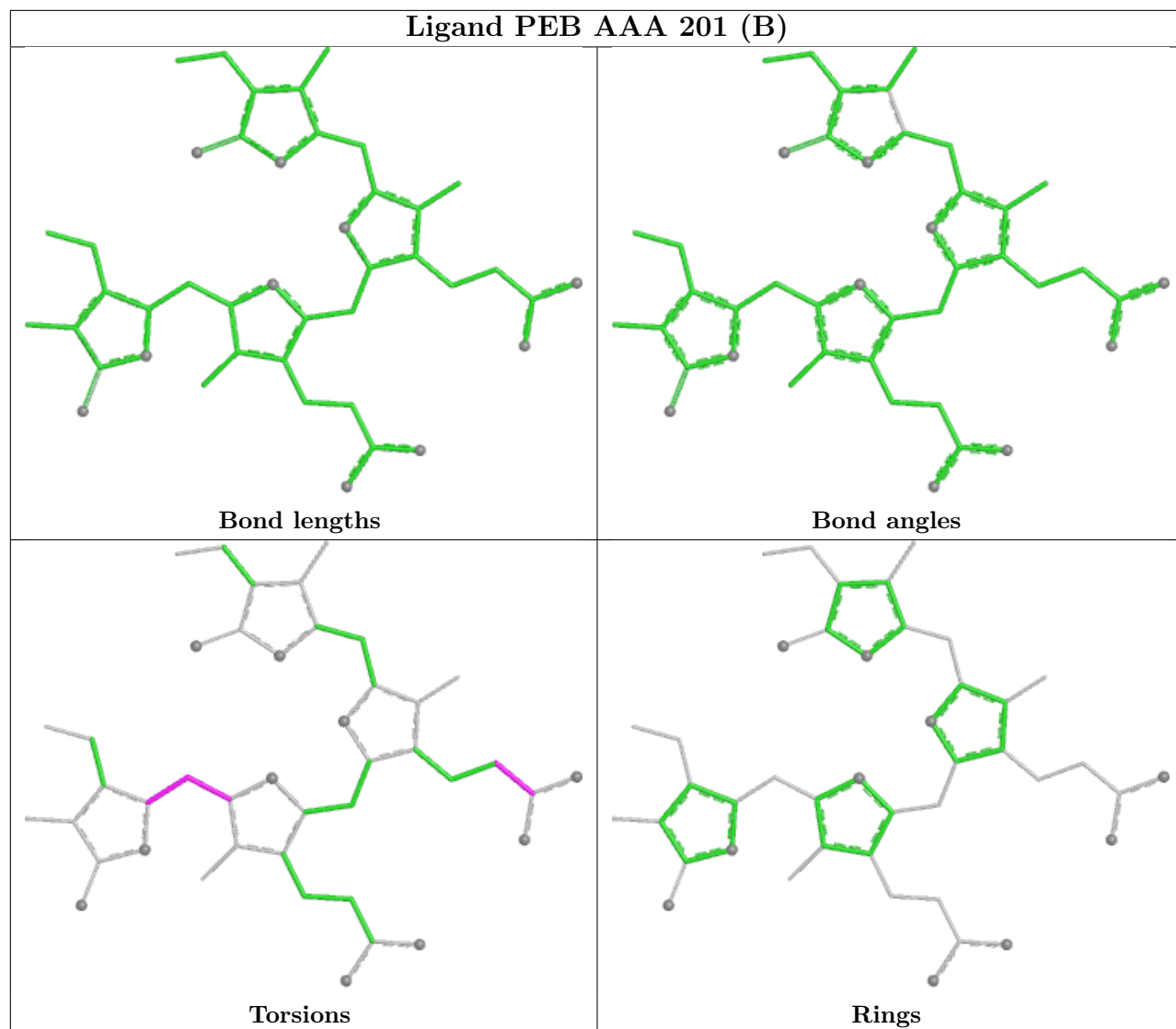


Torsions

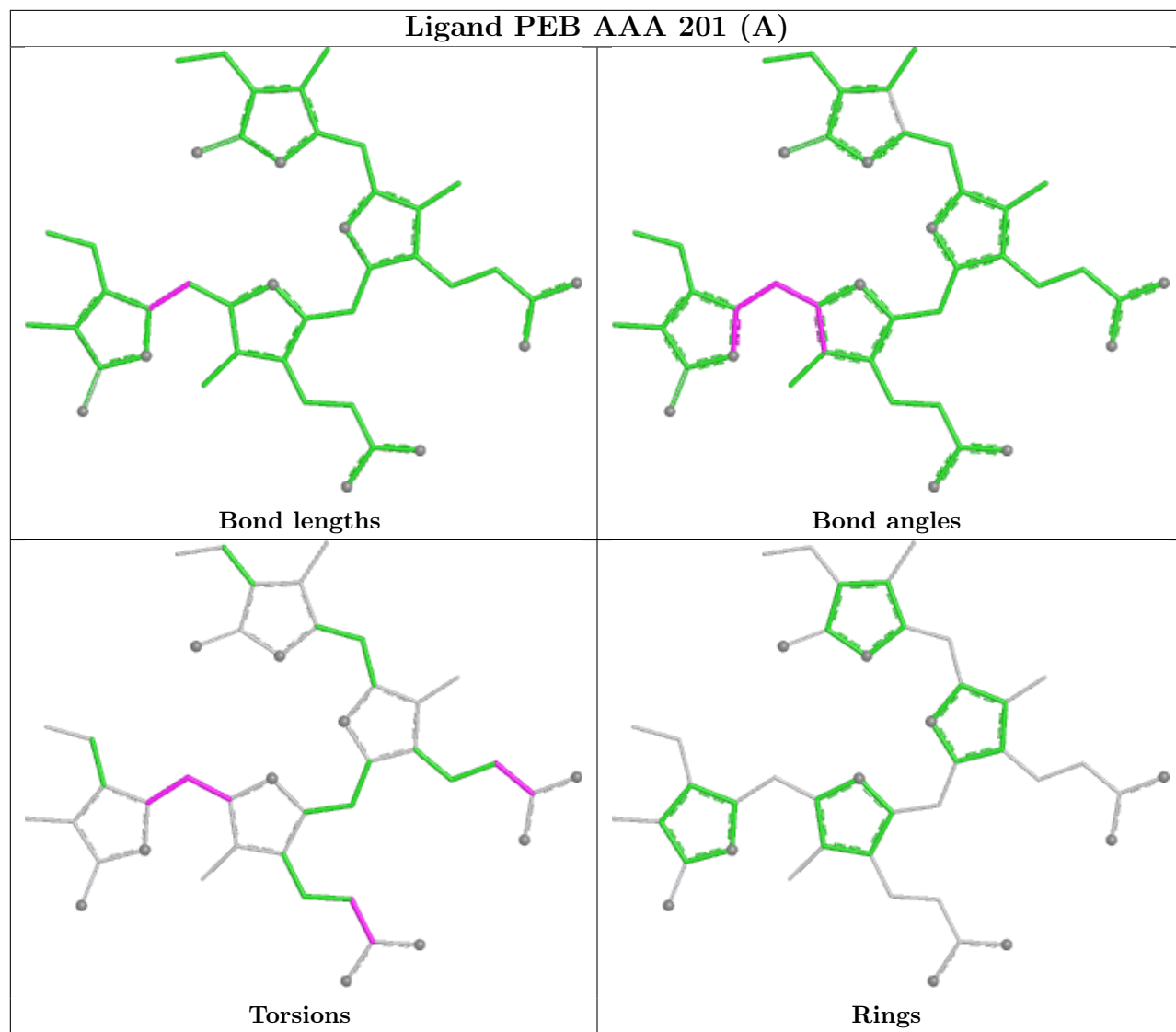


Rings

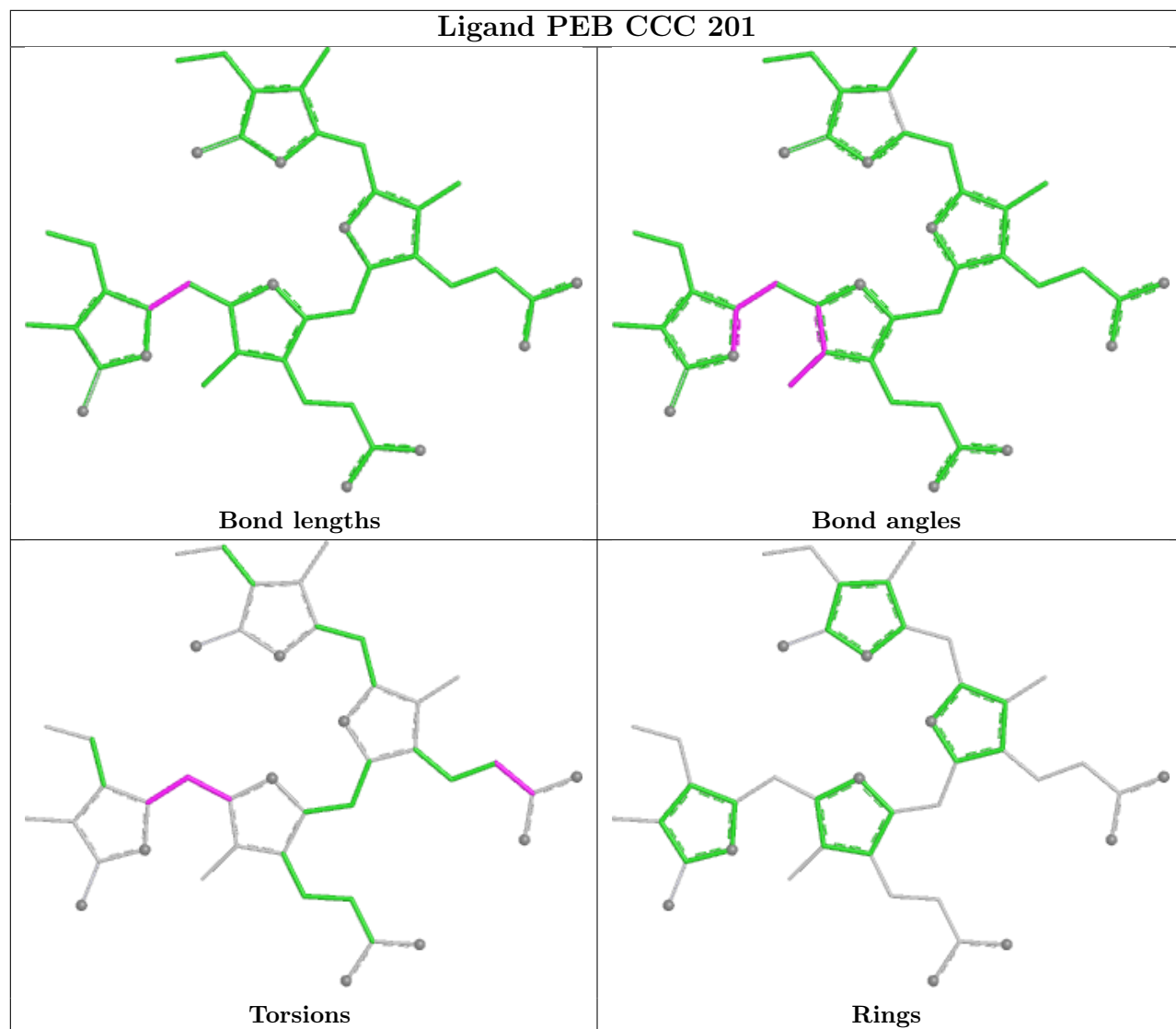
Ligand PEB AAA 201 (B)



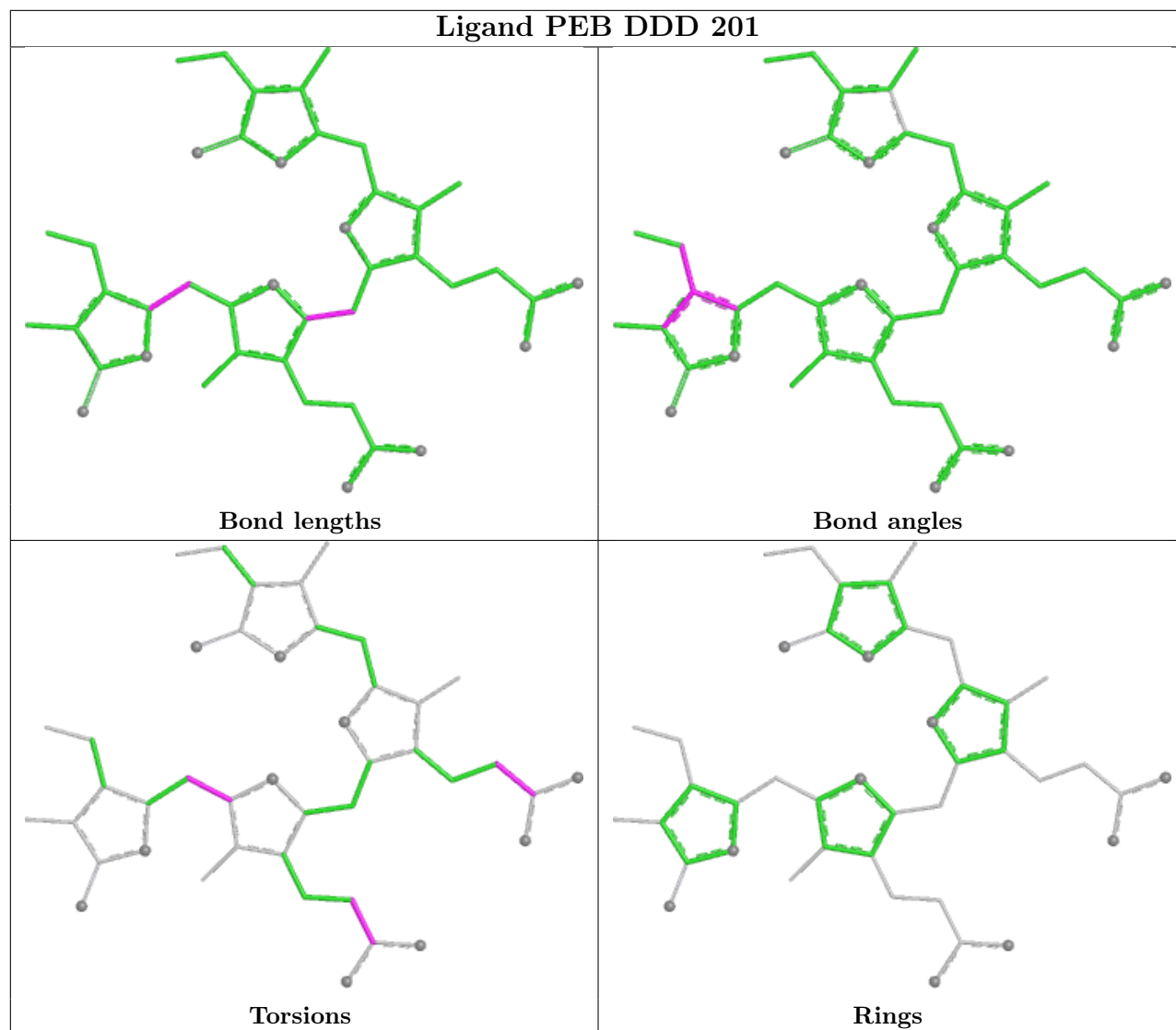
Ligand PEB AAA 201 (A)



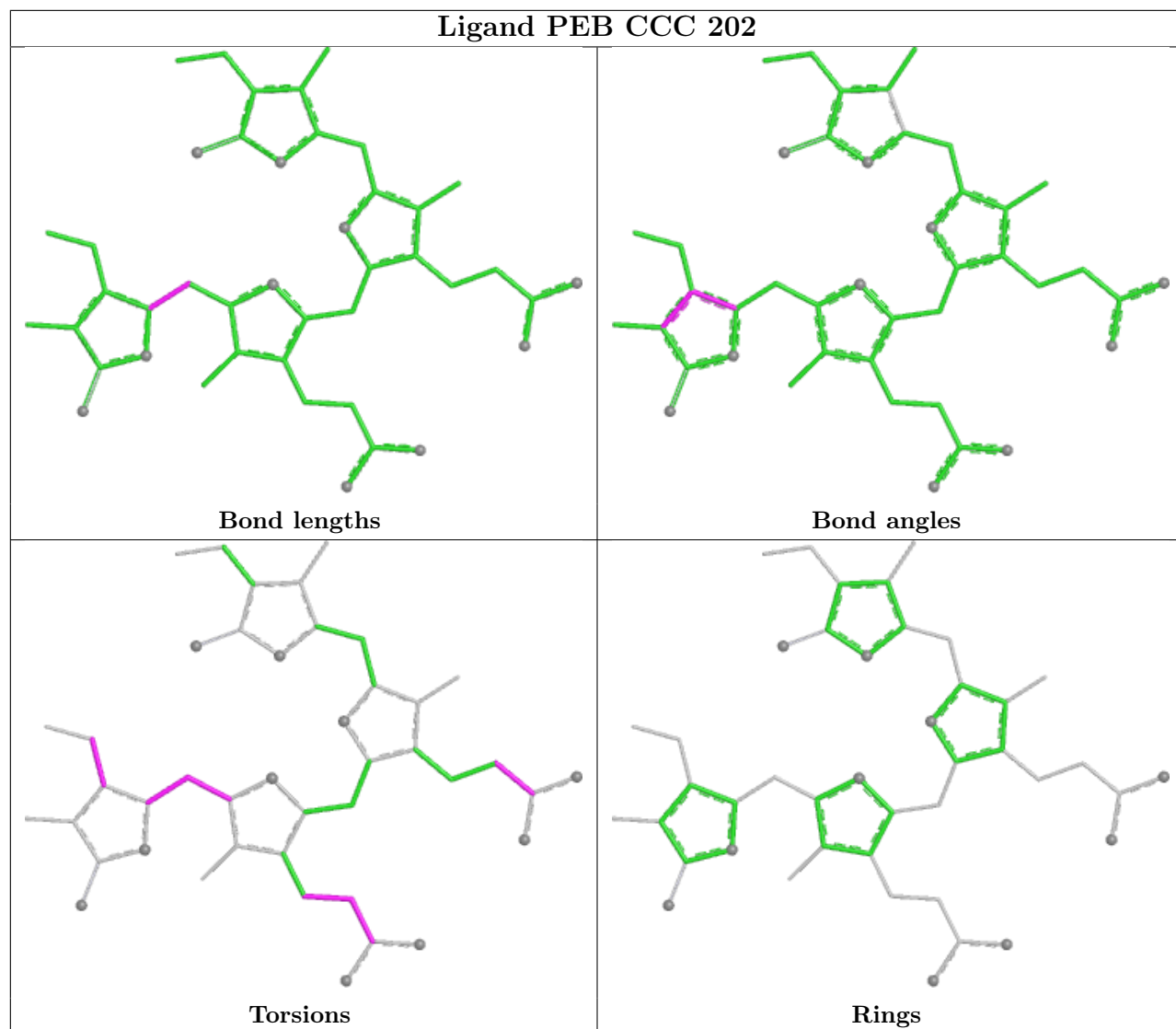
Ligand PEB CCC 201

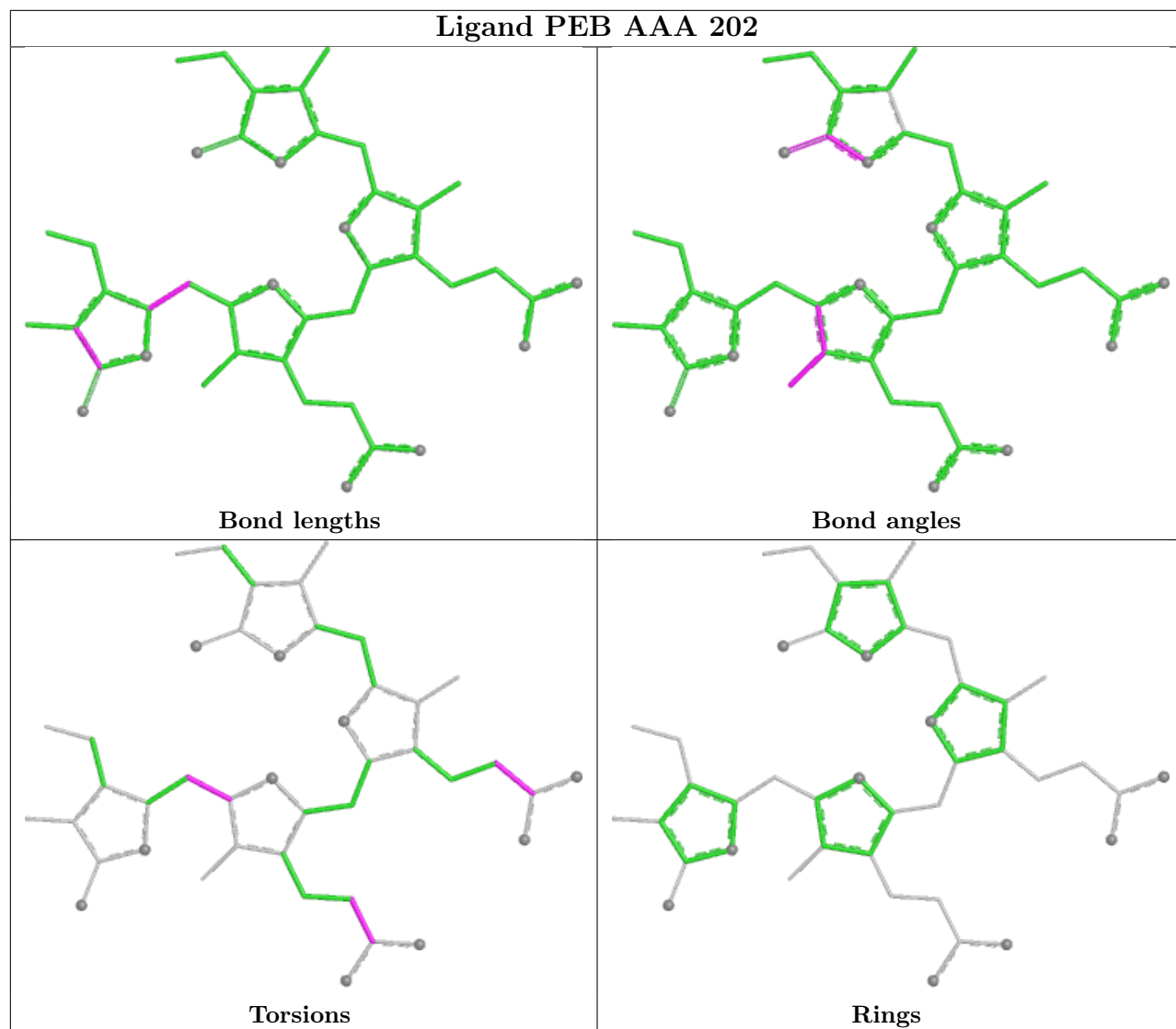


Ligand PEB DDD 201

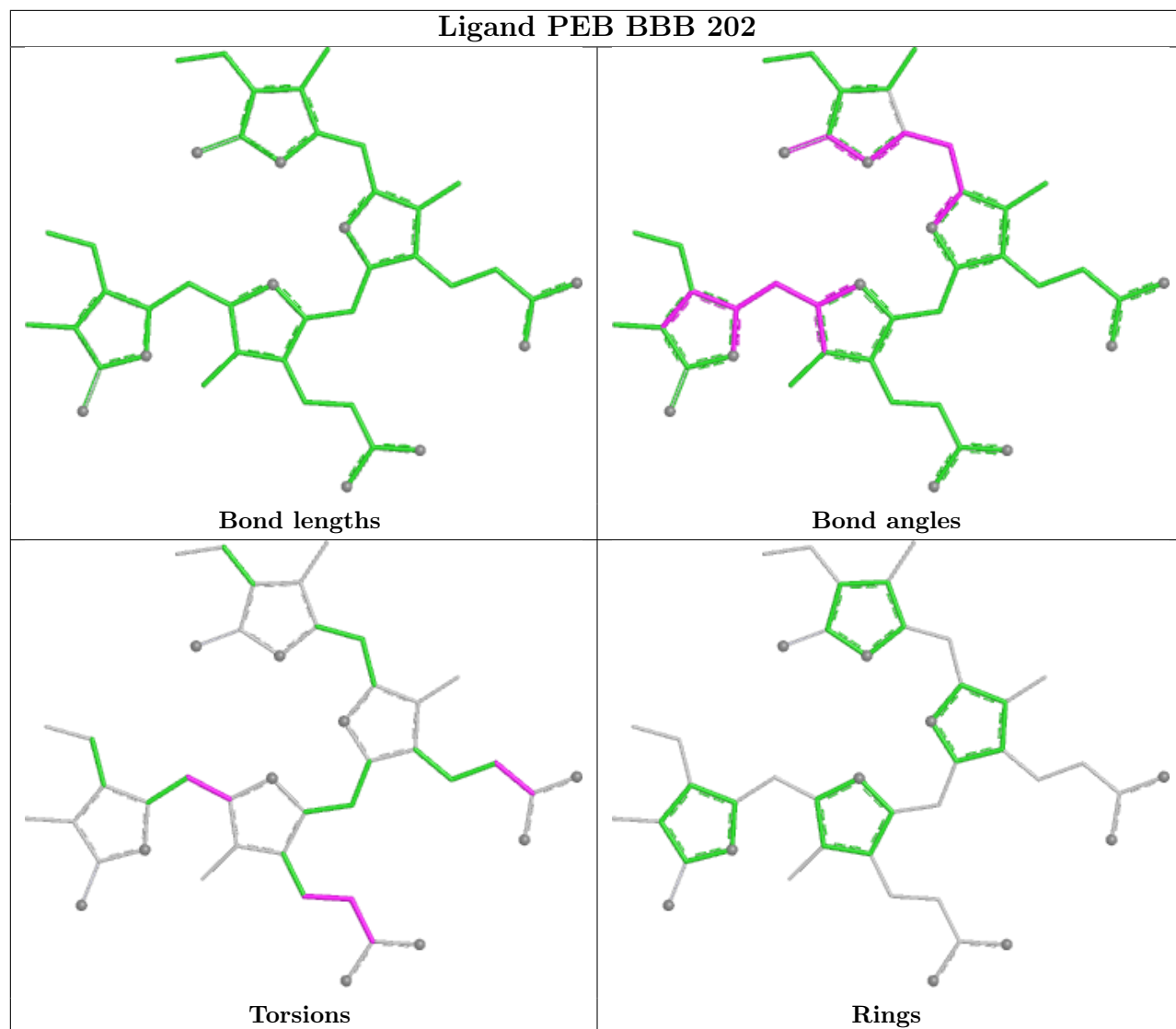


Ligand PEB CCC 202

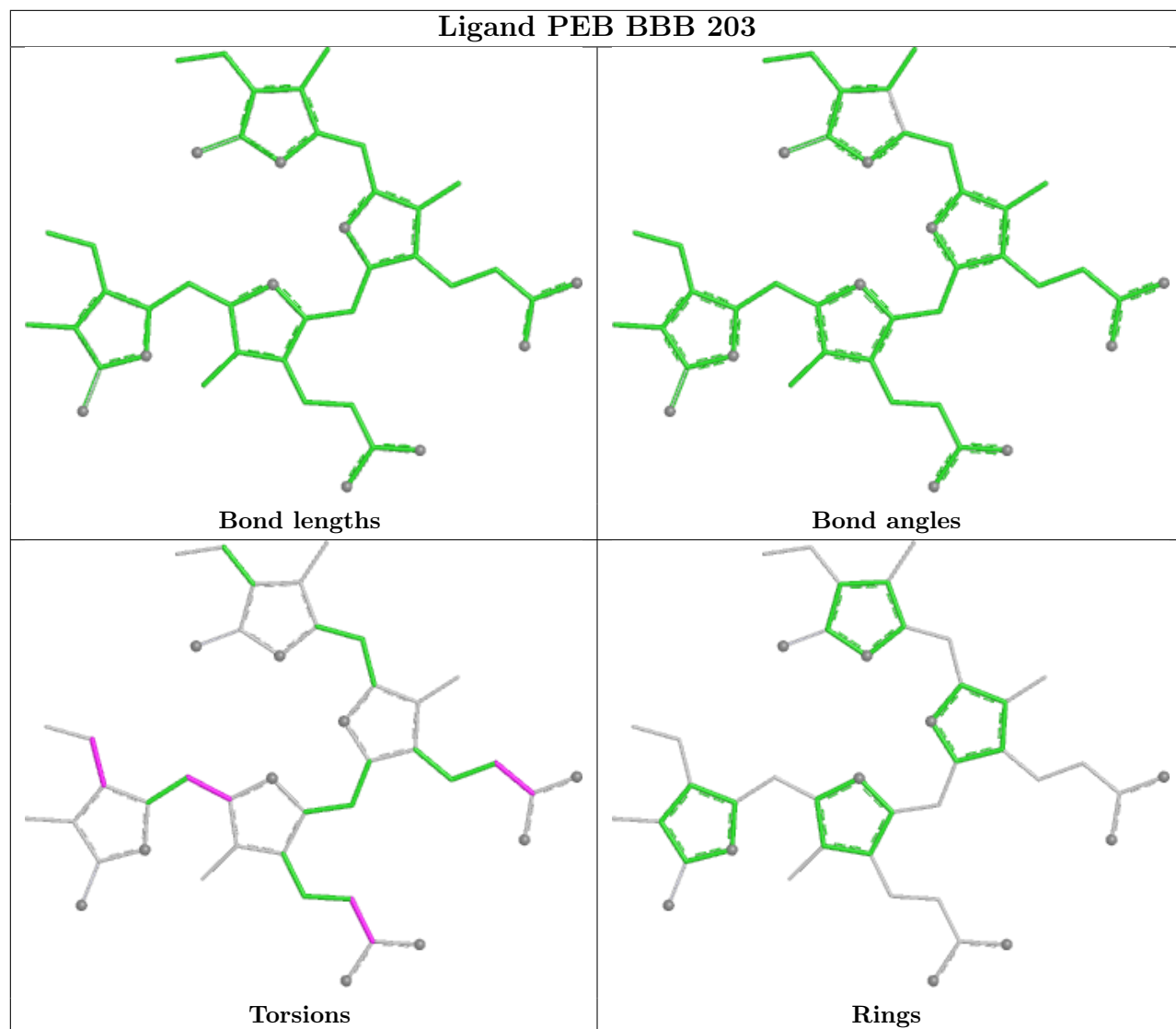


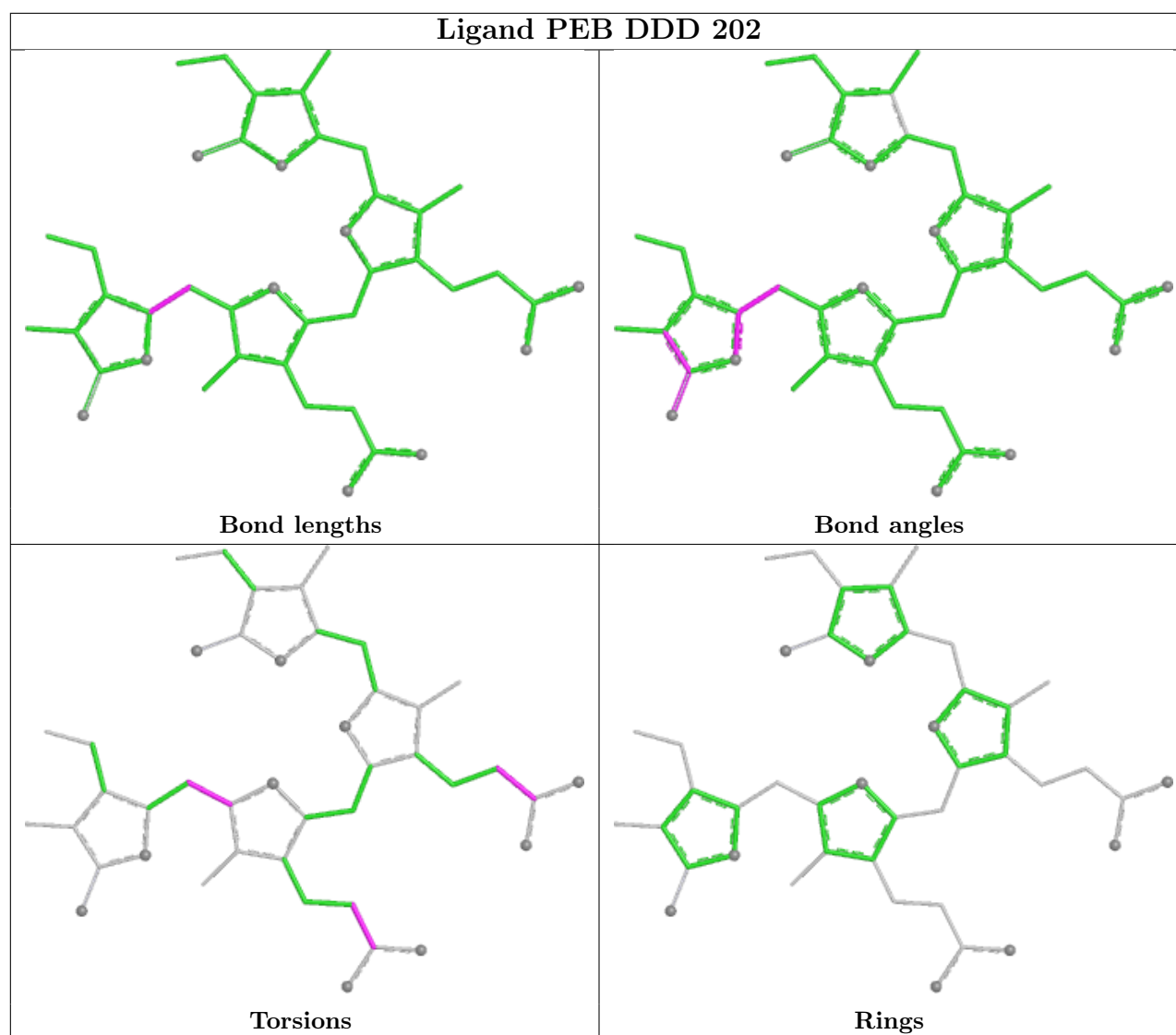


Ligand PEB BBB 202



Ligand PEB BBB 203





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	DDD	2
2	BBB	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DDD	71:GLY	C	72:MEN	N	1.73
1	BBB	71:GLY	C	72:MEN	N	1.69
1	DDD	72:MEN	C	73:CYS	N	1.63

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	164/164 (100%)	-0.90	0 100 100	11, 24, 38, 47	2 (1%)
1	CCC	164/164 (100%)	-0.96	0 100 100	10, 24, 37, 43	4 (2%)
2	BBB	176/177 (99%)	-0.94	0 100 100	12, 23, 36, 51	4 (2%)
2	DDD	176/177 (99%)	-0.96	0 100 100	12, 22, 35, 47	5 (2%)
All	All	680/682 (99%)	-0.94	0 100 100	10, 23, 38, 51	15 (2%)

There are no RSRZ outliers to report.

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MEN	DDD	72	9/10	0.98	0.04	20,23,26,26	0
2	MEN	BBB	72	9/10	0.99	0.04	22,23,25,25	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

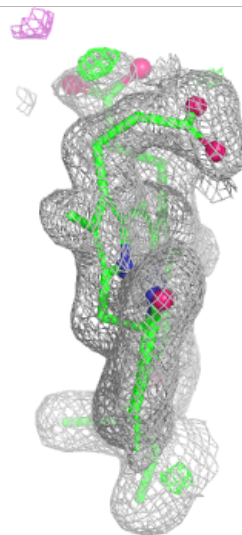
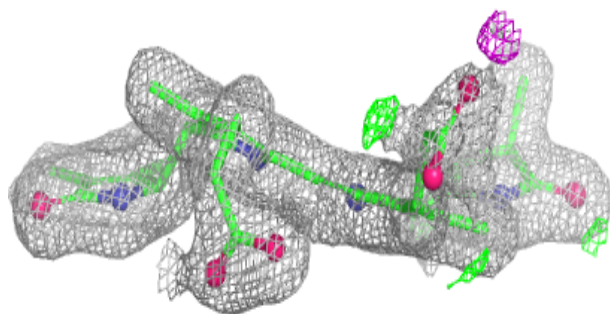
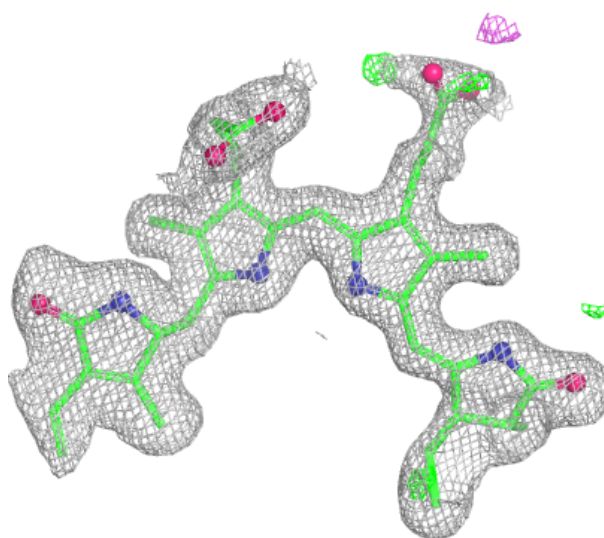
labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	DDD	204	5/5	0.96	0.06	41,42,49,50	0
3	PEB	AAA	201[B]	43/43	0.98	0.05	23,26,34,41	43
3	PEB	AAA	202	43/43	0.98	0.05	24,28,40,56	0
3	PEB	BBB	201	43/43	0.98	0.04	21,24,29,31	0
3	PEB	BBB	203	43/43	0.98	0.05	23,26,37,49	0
3	PEB	CCC	201	43/43	0.98	0.05	20,24,33,45	0
3	PEB	CCC	202	43/43	0.98	0.05	28,38,50,57	0
3	PEB	DDD	202	43/43	0.98	0.05	19,24,34,41	0
4	SO4	AAA	203	5/5	0.98	0.05	38,43,47,52	0
3	PEB	AAA	201[A]	43/43	0.98	0.05	22,25,33,39	43
3	PEB	DDD	203	43/43	0.99	0.04	19,23,35,52	0
3	PEB	DDD	201	43/43	0.99	0.04	20,24,31,34	0
3	PEB	BBB	202	43/43	0.99	0.04	19,24,34,42	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.

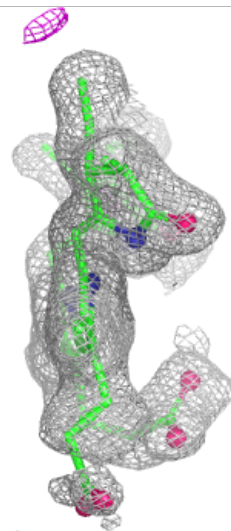
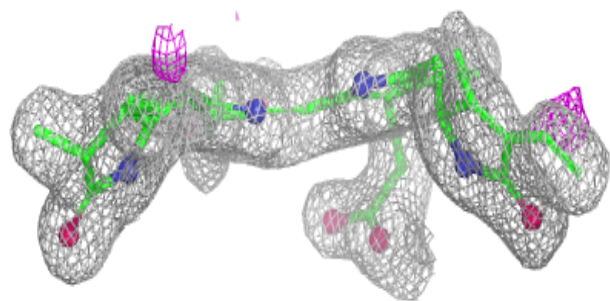
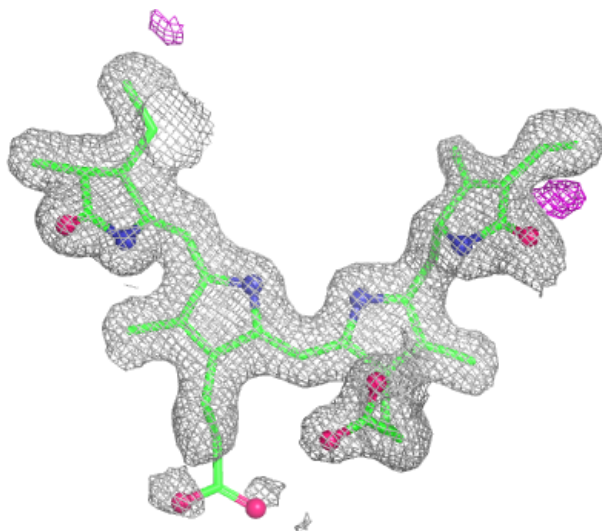
Electron density around PEB AAA 201 (B):

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



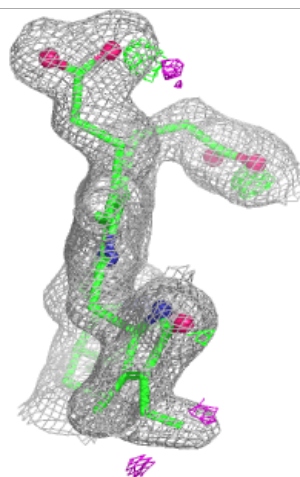
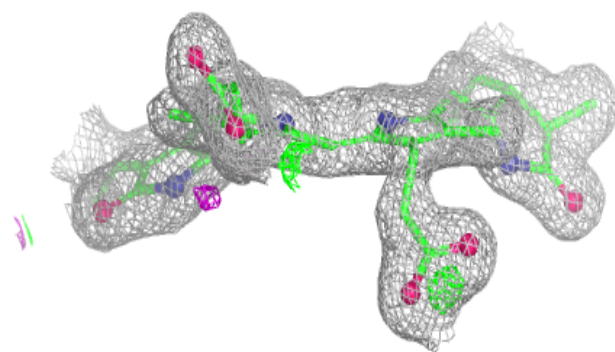
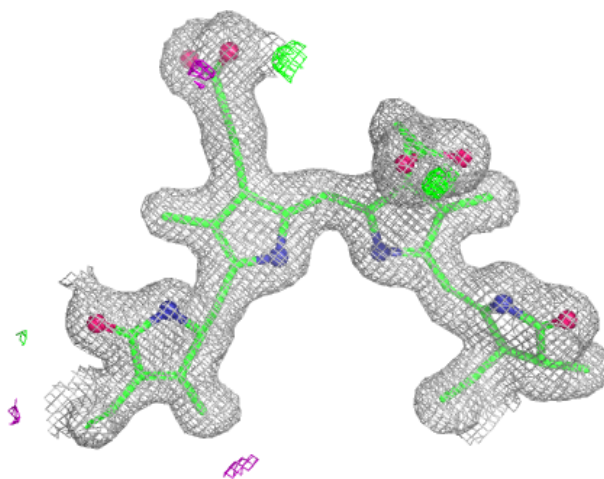
Electron density around PEB AAA 202:

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



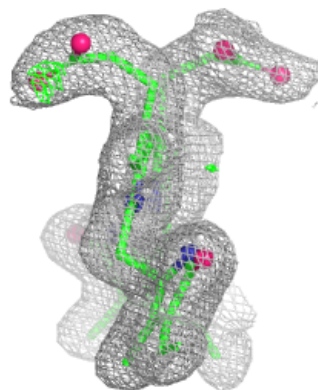
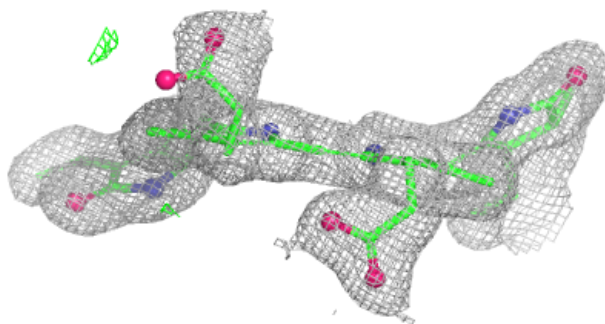
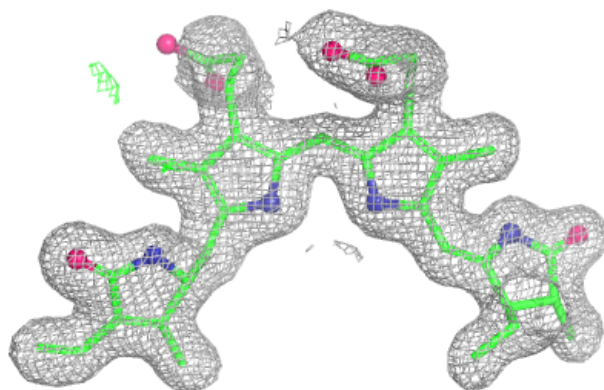
Electron density around PEB BBB 201:

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



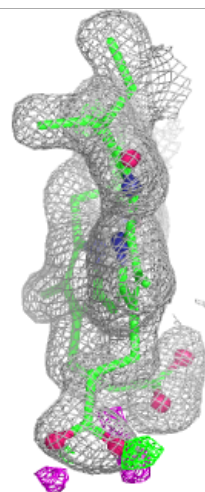
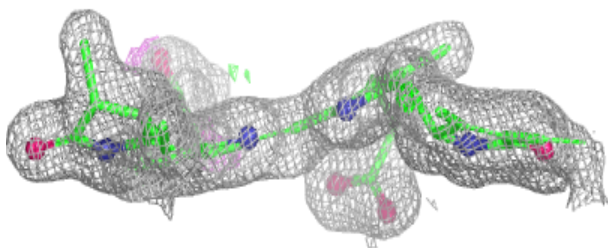
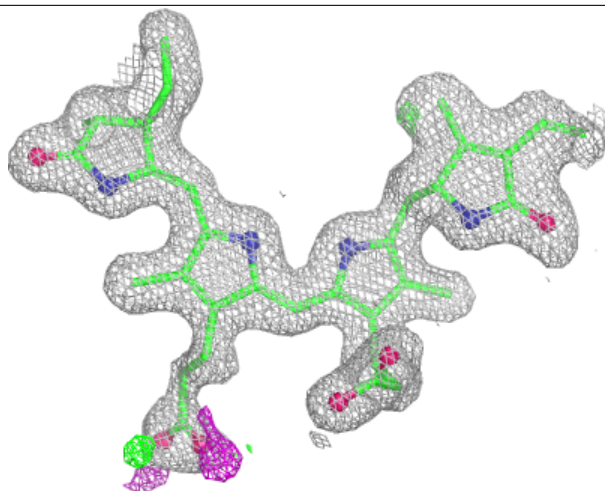
Electron density around PEB BBB 203:

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



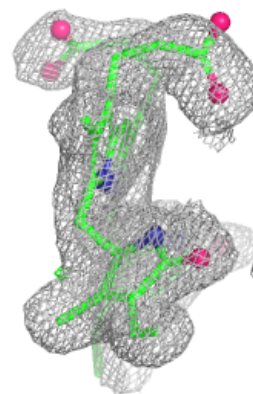
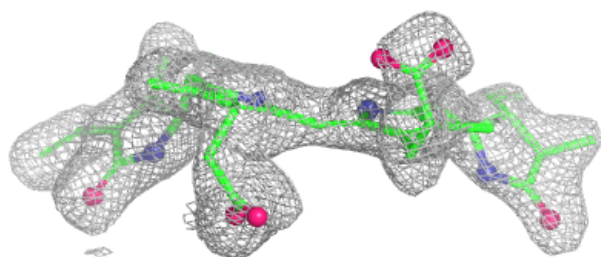
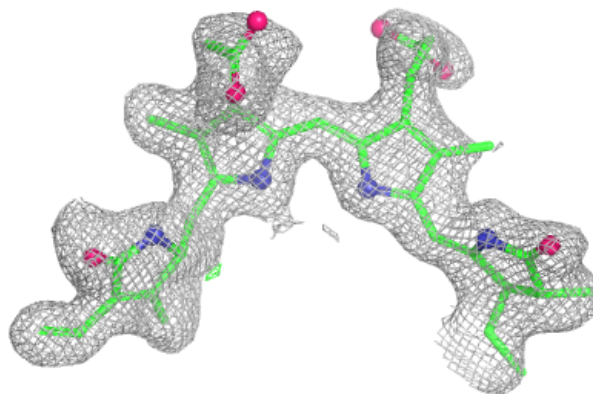
Electron density around PEB CCC 201:

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



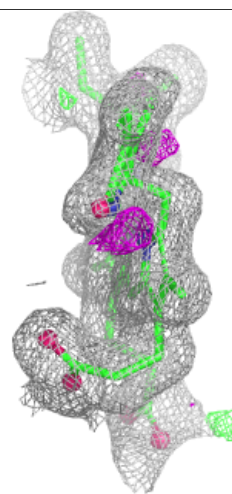
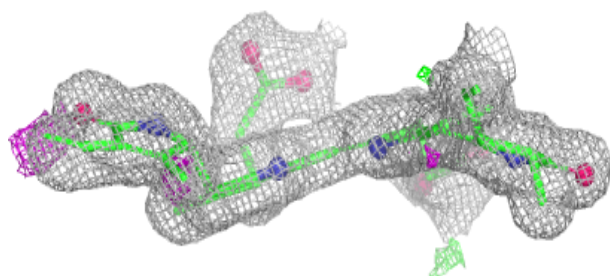
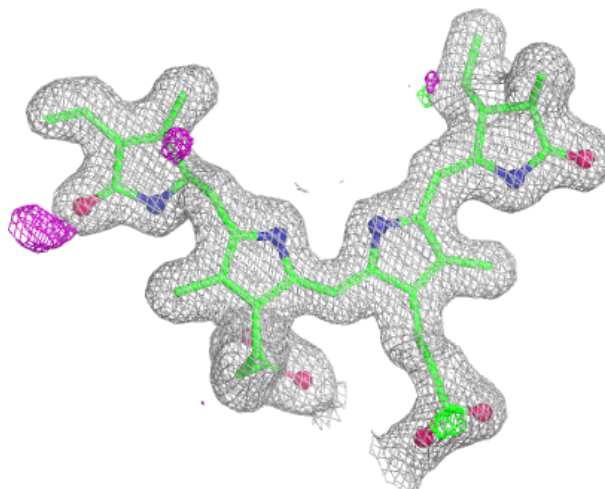
Electron density around PEB CCC 202:

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



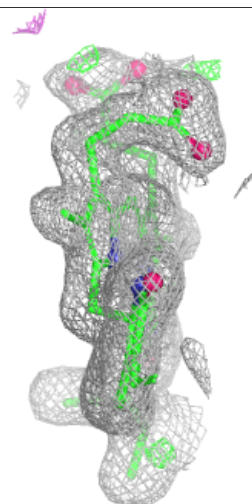
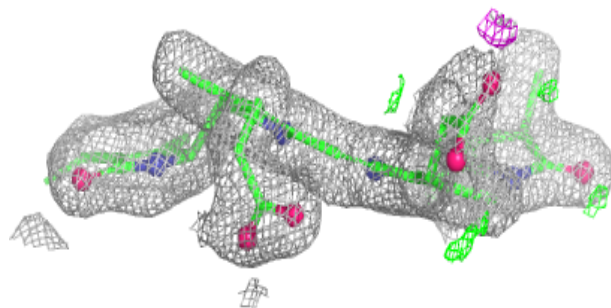
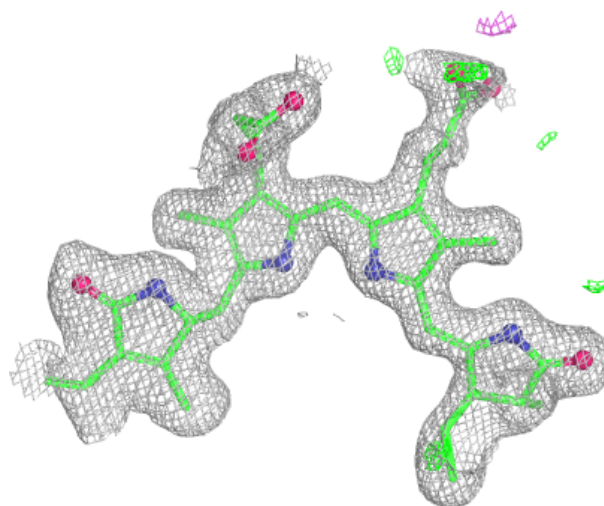
Electron density around PEB DDD 202:

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



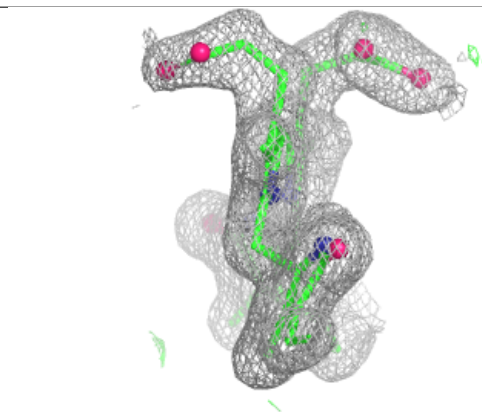
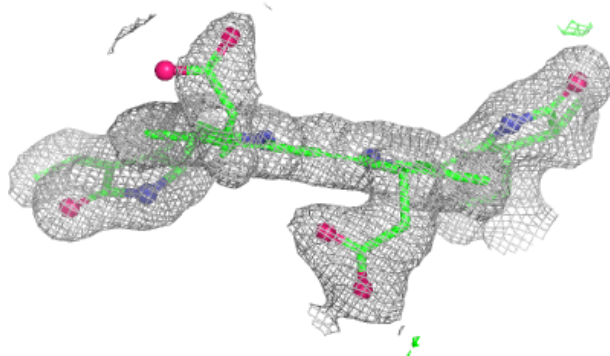
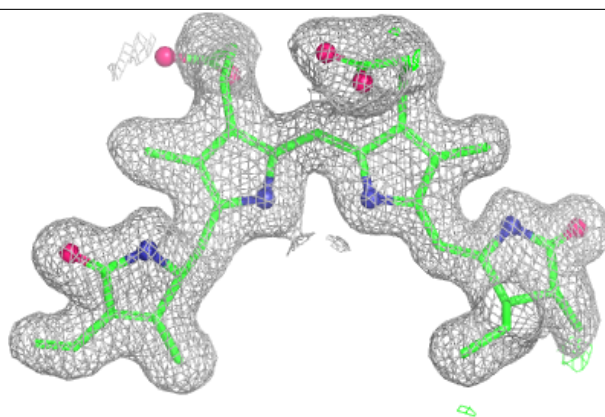
Electron density around PEB AAA 201 (A):

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and green (positive)

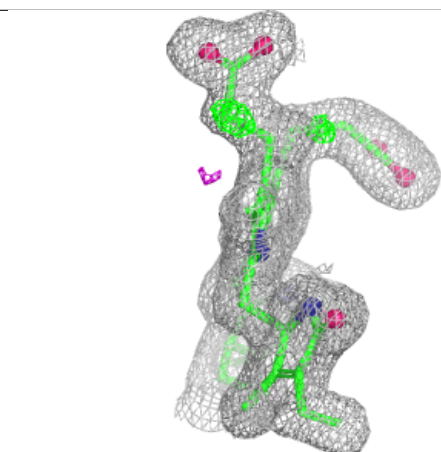
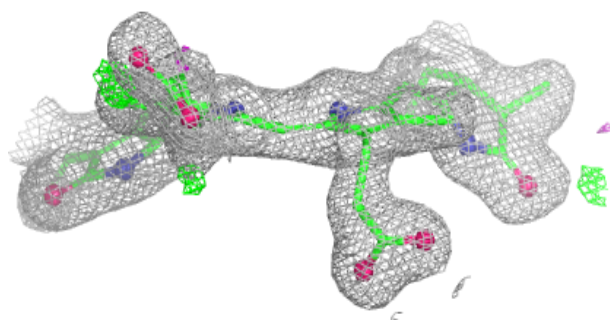
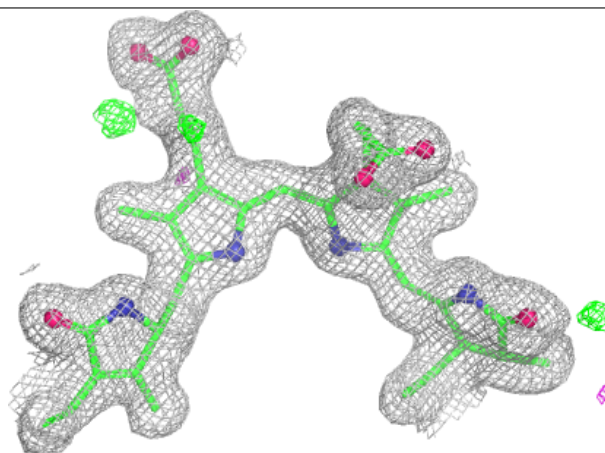


Electron density around PEB DDD 203:

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and green (positive)

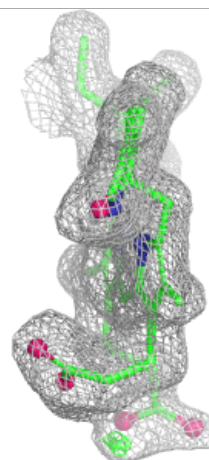
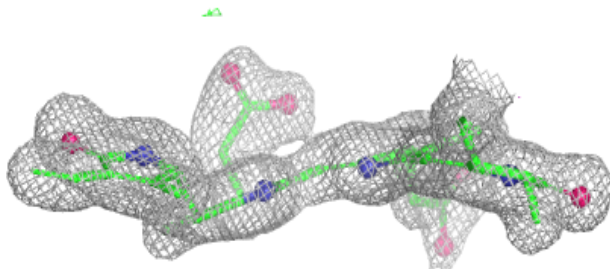
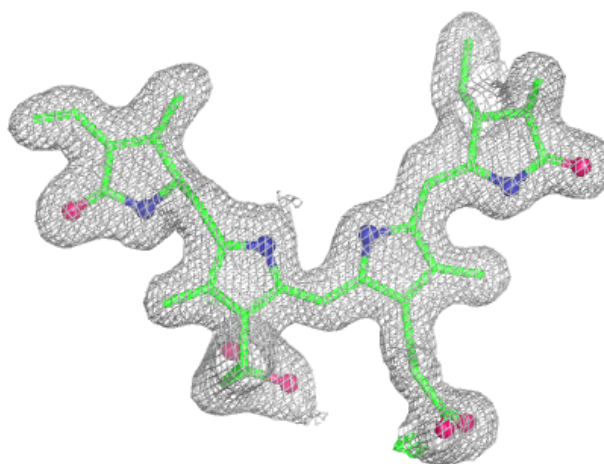
**Electron density around PEB DDD 201:**

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



Electron density around PEB BBB 202:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.