wwPDB X-ray Structure Validation Summary Report (i)

Jul 16, 2024 – 02:37 pm BST

PDB ID	:	8B4N
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 (i) 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 (i)) were used in the production of this report:

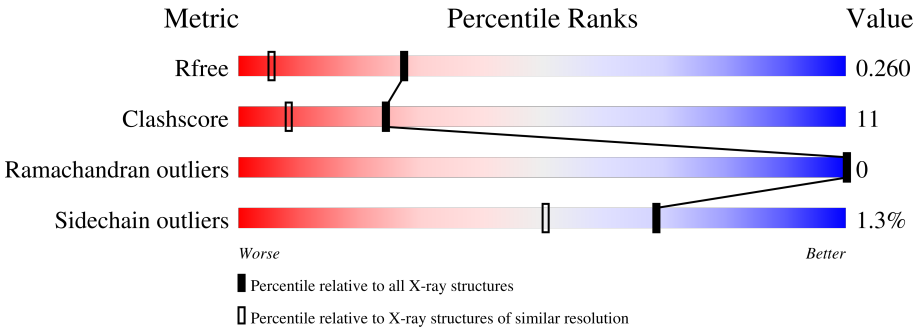
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (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 <=5%

Mol	Chain	Length	Quality of chain
1	AAA	164	87% 13%
1	CCC	164	85% 13%
2	BBB	177	94% 5%
2	DDD	177	90% 10%

2 Entry composition (i)

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			

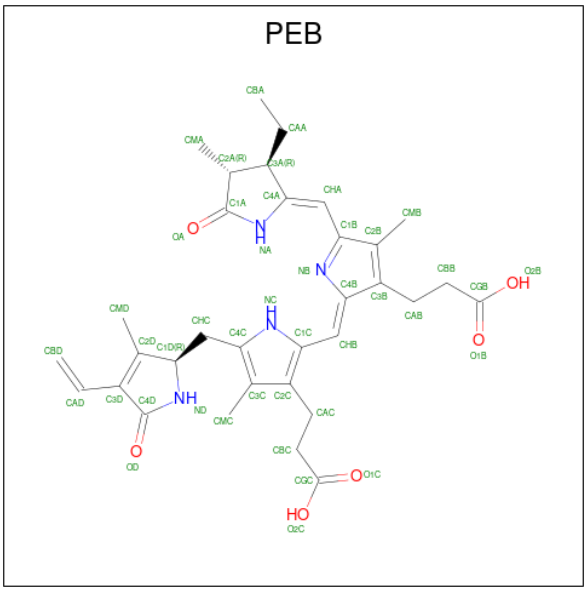
There are 2 discrepancies between the modelled and reference sequences:

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.

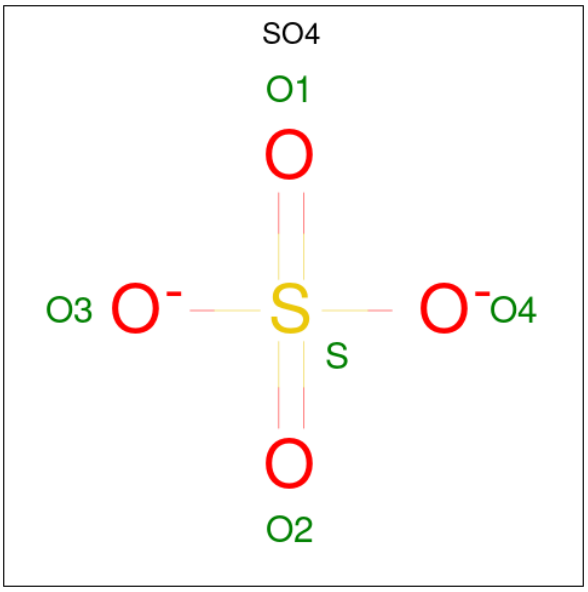
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	177	Total	C	N	O	S	0	4	0
			1314	812	229	261	12			
2	DDD	177	Total	C	N	O	S	0	5	0
			1320	815	230	263	12			

- Molecule 3 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: $C_{33}H_{40}N_4O_6$) (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 (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

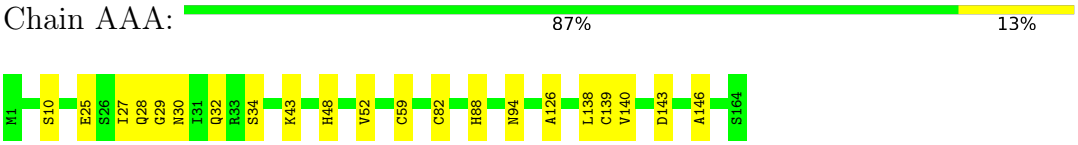
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	93	Total O 93 93	0	0
5	BBB	72	Total O 72 72	0	0
5	CCC	79	Total O 79 79	0	0
5	DDD	80	Total O 80 80	0	0

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. 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. 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.

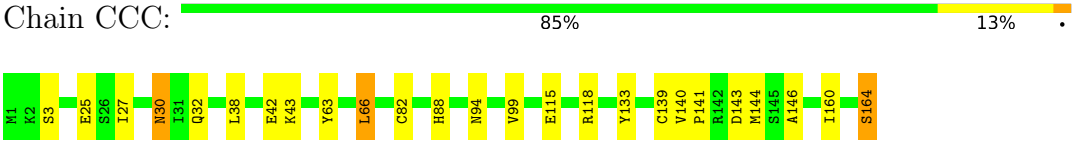
• Molecule 1: B-phycoerythrin alpha chain

Chain AAA:



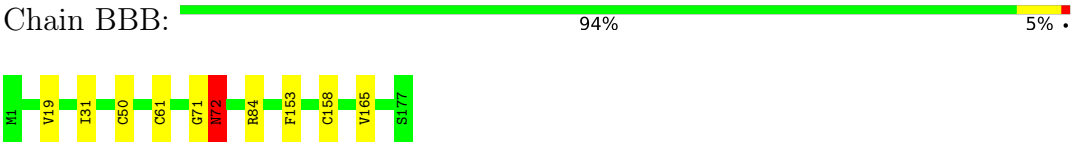
• Molecule 1: B-phycoerythrin alpha chain

Chain CCC:



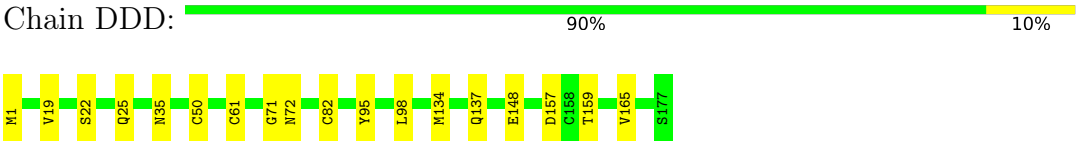
• Molecule 2: B-phycoerythrin beta chain

Chain BBB:



• Molecule 2: B-phycoerythrin beta chain

Chain DDD:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (4.95%)	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 , 26.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, MEN, PEB

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	0.73	0/1288	0.80	0/1744
1	CCC	0.73	0/1305	0.82	1/1766 (0.1%)
2	BBB	0.79	0/1326	0.87	0/1788
2	DDD	0.78	0/1332	0.83	2/1797 (0.1%)
All	All	0.76	0/5251	0.83	3/7095 (0.0%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DDD	95	TYR	CB-CG-CD1	6.27	124.76	121.00
1	CCC	30	ASN	CB-CA-C	-5.59	99.22	110.40
2	DDD	95	TYR	CB-CG-CD2	-5.01	118.00	121.00

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1266	0	1233	34	0
1	CCC	1283	0	1249	32	0
2	BBB	1314	0	1324	19	0
2	DDD	1320	0	1332	29	0
3	AAA	129	0	113	24	0
3	BBB	129	0	112	12	0
3	CCC	86	0	75	8	0
3	DDD	129	0	113	23	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	5551	114	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 114 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%)	65	44
2	BBB	141/137 (103%)	140 (99%)	1 (1%)	84	73
2	DDD	142/137 (104%)	138 (97%)	4 (3%)	43	18
All	All	545/530 (103%)	538 (99%)	7 (1%)	69	50

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

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Mol	Chain	Res	Type
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 (i)

There are no RNA molecules in this entry.

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

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	0.66	0	6,9,11	0.53	0
2	MEN	BBB	72	2	7,8,9	0.37	0	6,9,11	1.07	1 (16%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	72	MEN	CB-CA-C	2.07	115.36	111.47

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	BBB	72	MEN	CA-CB-CG-OD1
2	DDD	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 7 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	CCC	202	-	43,46,46	1.15	3 (6%)	45,67,67	0.94	3 (6%)
3	PEB	BBB	202	2	43,46,46	1.39	2 (4%)	45,67,67	1.97	7 (15%)
3	PEB	AAA	202	1	43,46,46	1.19	2 (4%)	45,67,67	0.97	2 (4%)
3	PEB	CCC	201	1	43,46,46	1.46	3 (6%)	45,67,67	1.20	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PEB	DDD	202	2	43,46,46	1.39	1 (2%)	45,67,67	1.30	4 (8%)
3	PEB	BBB	203	2	43,46,46	1.08	2 (4%)	45,67,67	0.85	0
3	PEB	AAA	201[B]	-	43,46,46	1.13	2 (4%)	45,67,67	1.10	1 (2%)
3	PEB	DDD	203	2	43,46,46	1.51	4 (9%)	45,67,67	0.99	3 (6%)
3	PEB	BBB	201	2	43,46,46	1.61	5 (11%)	45,67,67	1.01	1 (2%)
4	SO4	AAA	203	-	4,4,4	0.46	0	6,6,6	0.09	0
3	PEB	DDD	201	2	43,46,46	1.57	1 (2%)	45,67,67	1.26	6 (13%)
4	SO4	DDD	204	-	4,4,4	0.33	0	6,6,6	0.20	0
3	PEB	AAA	201[A]	-	43,46,46	1.09	2 (4%)	45,67,67	1.24	4 (8%)

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	CCC	202	-	-	11/24/74/74	0/4/4/4
3	PEB	BBB	202	2	-	7/24/74/74	0/4/4/4
3	PEB	AAA	202	1	-	7/24/74/74	0/4/4/4
3	PEB	CCC	201	1	-	6/24/74/74	0/4/4/4
3	PEB	DDD	202	2	-	6/24/74/74	0/4/4/4
3	PEB	BBB	203	2	-	8/24/74/74	0/4/4/4
3	PEB	AAA	201[B]	-	-	6/24/74/74	0/4/4/4
3	PEB	DDD	203	2	-	8/24/74/74	0/4/4/4
3	PEB	BBB	201	2	-	3/24/74/74	0/4/4/4
3	PEB	DDD	201	2	-	6/24/74/74	0/4/4/4
3	PEB	AAA	201[A]	-	-	8/24/74/74	0/4/4/4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DDD	201	PEB	CHB-C4B	9.03	1.42	1.35
3	BBB	201	PEB	CHB-C4B	8.84	1.42	1.35
3	DDD	203	PEB	CHB-C4B	7.63	1.41	1.35
3	CCC	201	PEB	CHB-C4B	7.59	1.41	1.35
3	DDD	202	PEB	CHB-C4B	7.51	1.41	1.35

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BBB	202	PEB	CHC-C1D-ND	-7.99	104.67	113.95
3	BBB	202	PEB	CHA-C4A-NA	5.54	131.79	125.20
3	DDD	202	PEB	CHA-C4A-NA	4.54	130.61	125.20
3	AAA	201[A]	PEB	CHB-C4B-NB	-3.88	123.45	128.83
3	CCC	201	PEB	CHA-C4A-NA	3.80	129.72	125.20

There are no chirality outliers.

5 of 76 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.

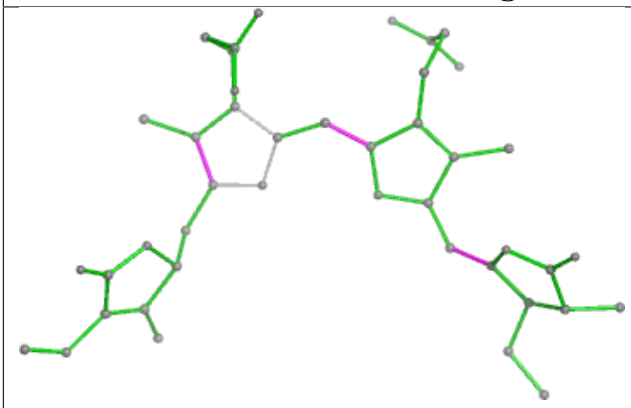
11 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	CCC	202	PEB	3	0
3	BBB	202	PEB	1	0
3	AAA	202	PEB	4	0
3	CCC	201	PEB	5	0
3	DDD	202	PEB	7	0
3	BBB	203	PEB	2	0
3	AAA	201[B]	PEB	11	0
3	DDD	203	PEB	5	0
3	BBB	201	PEB	9	0
3	DDD	201	PEB	11	0
3	AAA	201[A]	PEB	9	0

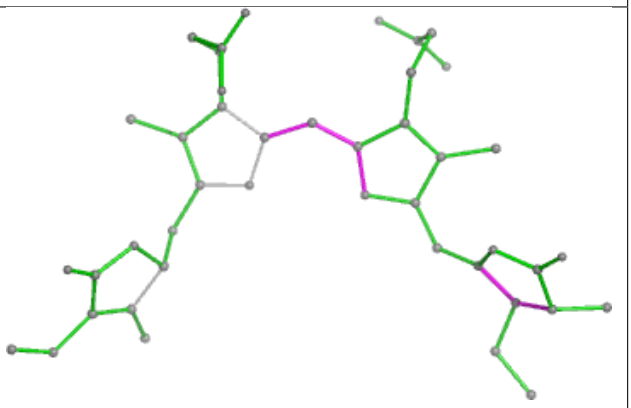
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

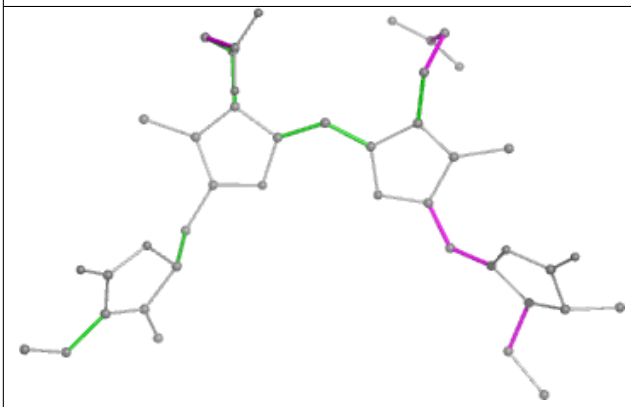
Ligand PEB CCC 202



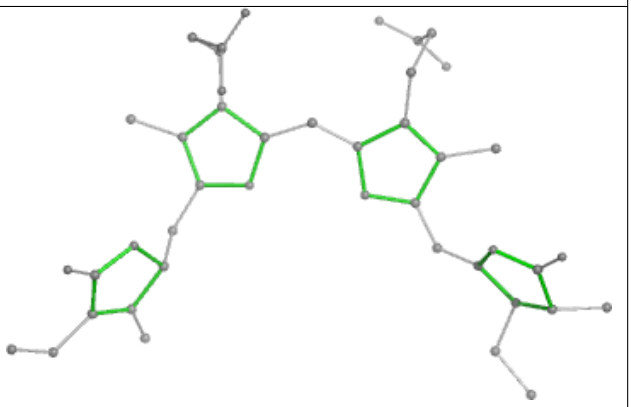
Bond lengths



Bond angles

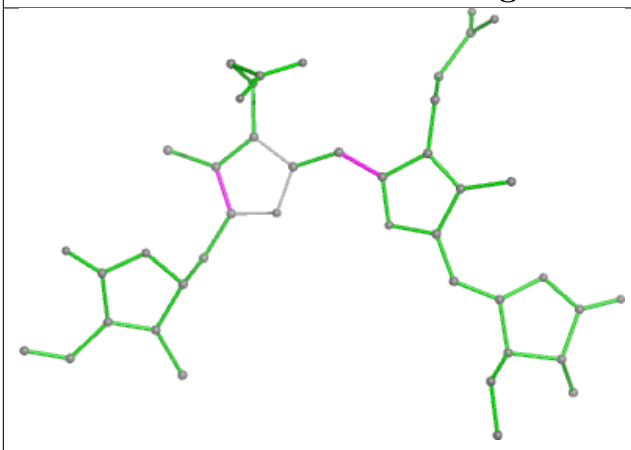


Torsions

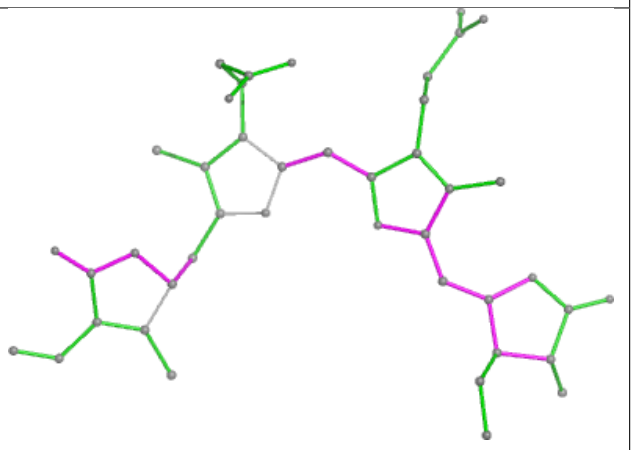


Rings

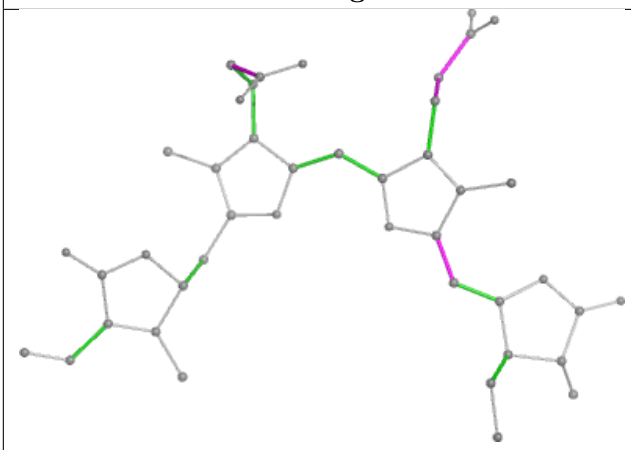
Ligand PEB BBB 202



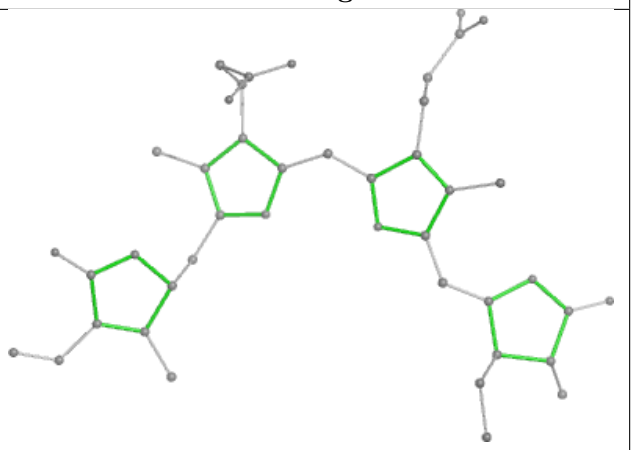
Bond lengths



Bond angles

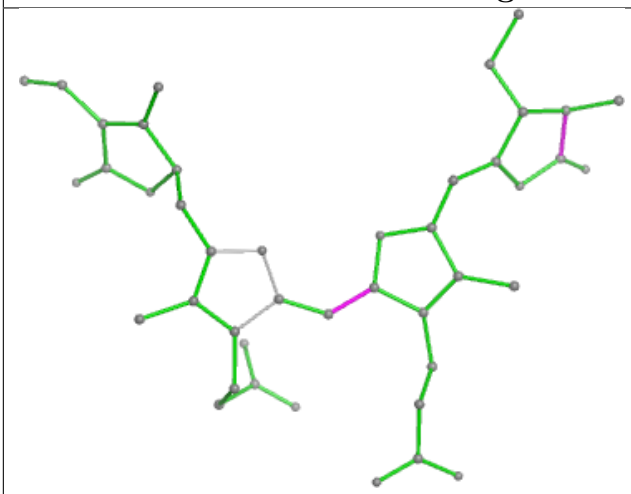


Torsions

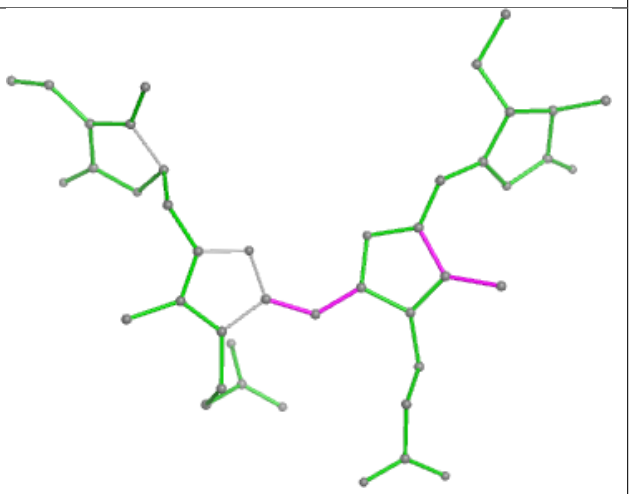


Rings

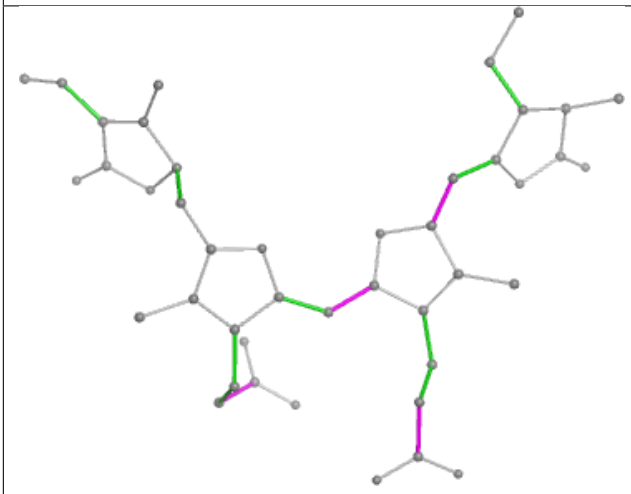
Ligand PEB AAA 202



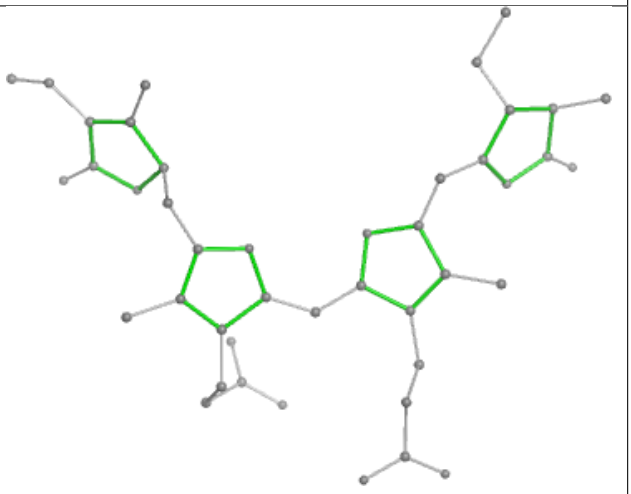
Bond lengths



Bond angles

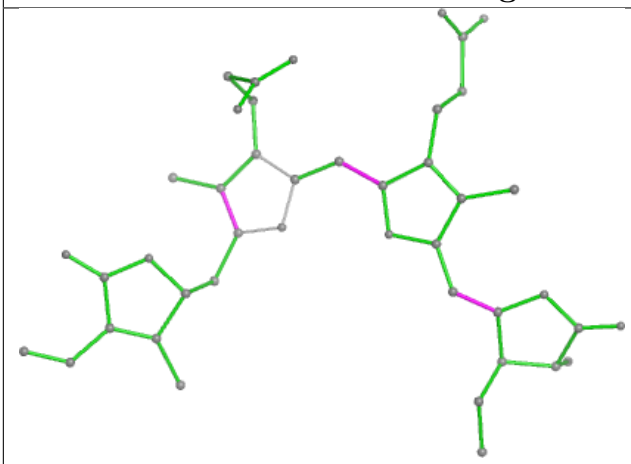


Torsions

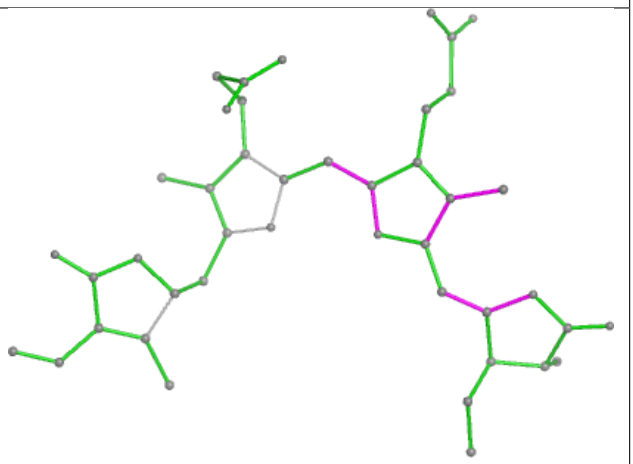


Rings

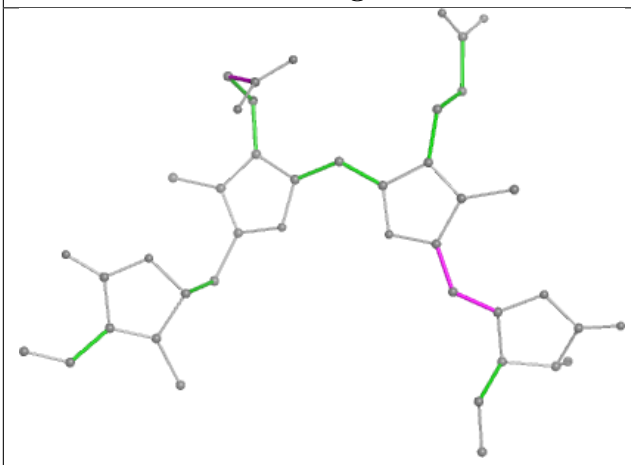
Ligand PEB CCC 201



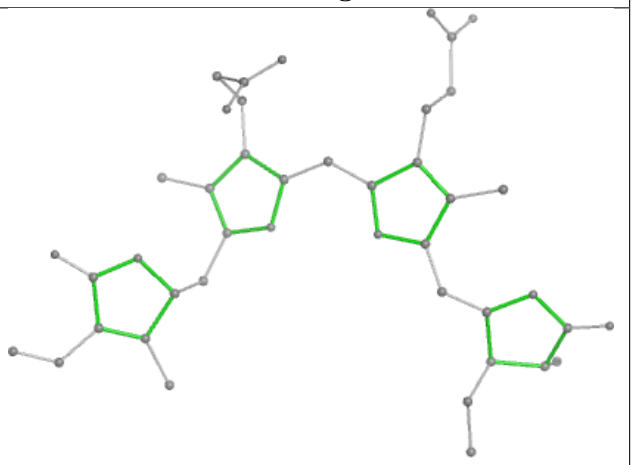
Bond lengths



Bond angles

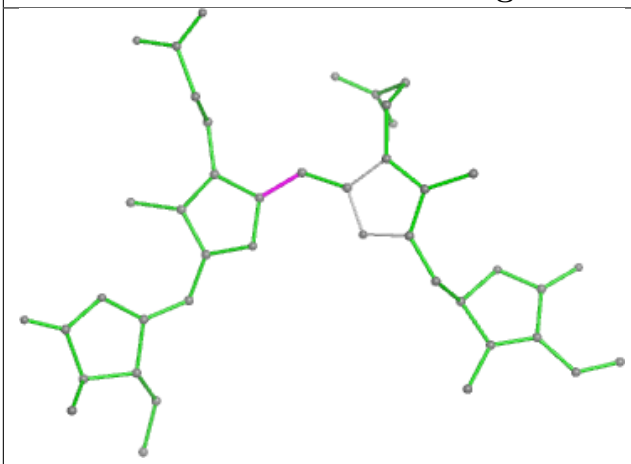


Torsions

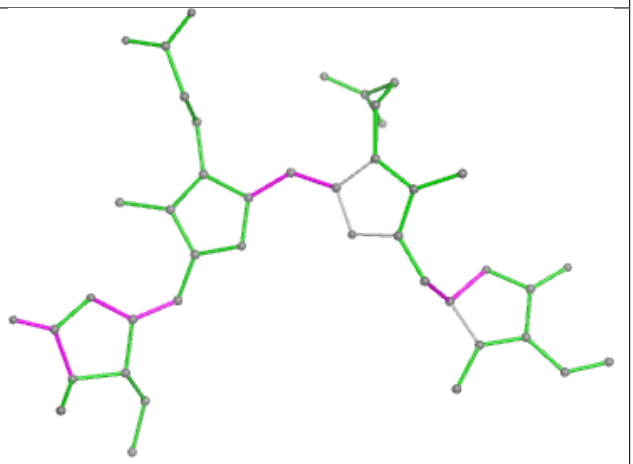


Rings

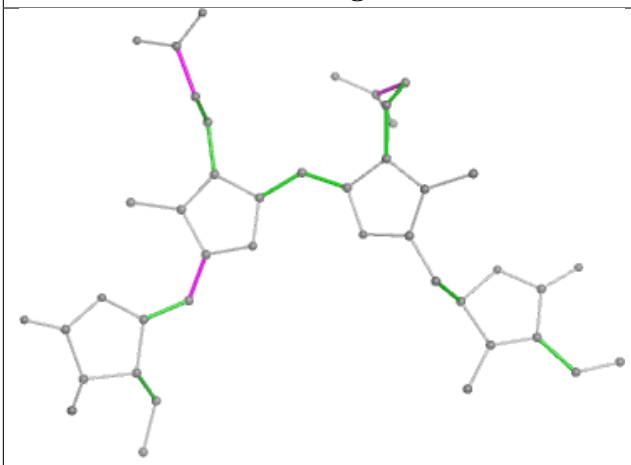
Ligand PEB DDD 202



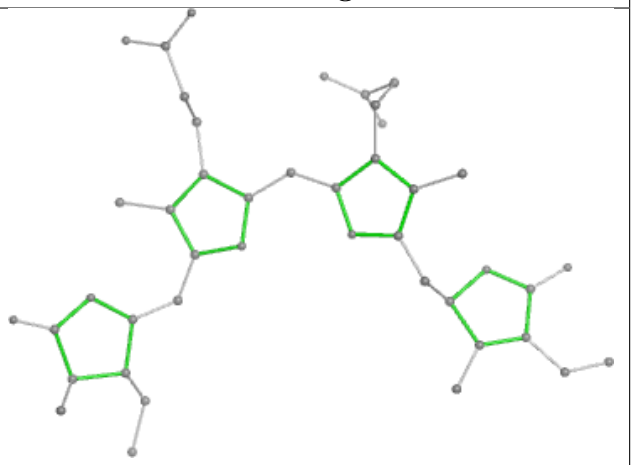
Bond lengths



Bond angles

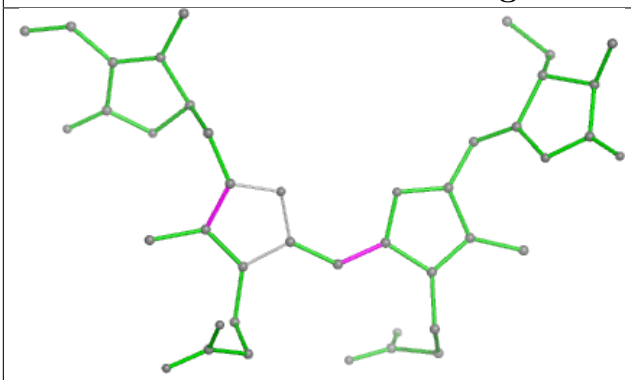


Torsions

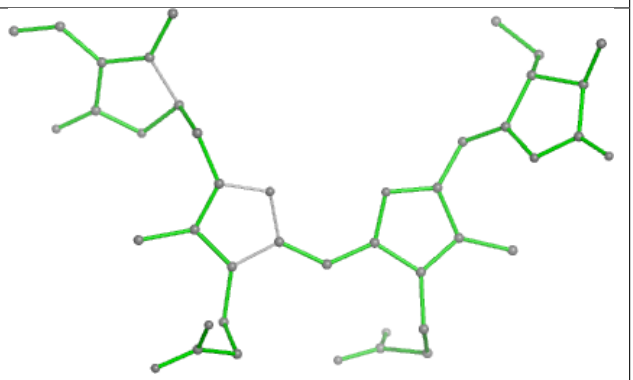


Rings

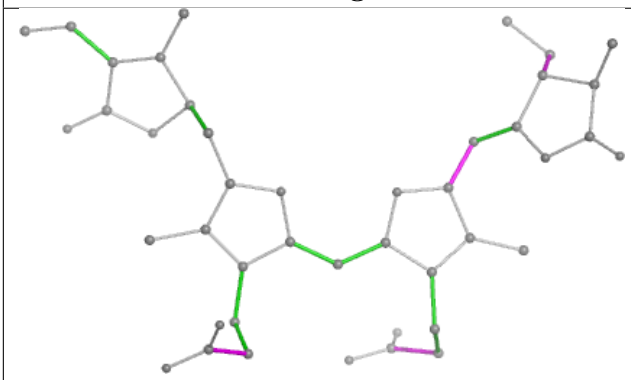
Ligand PEB BBB 203



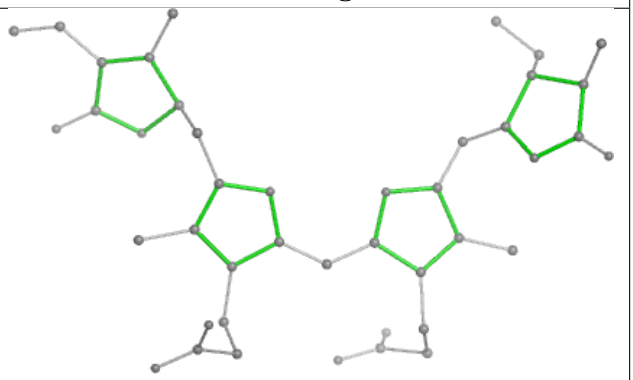
Bond lengths



Bond angles

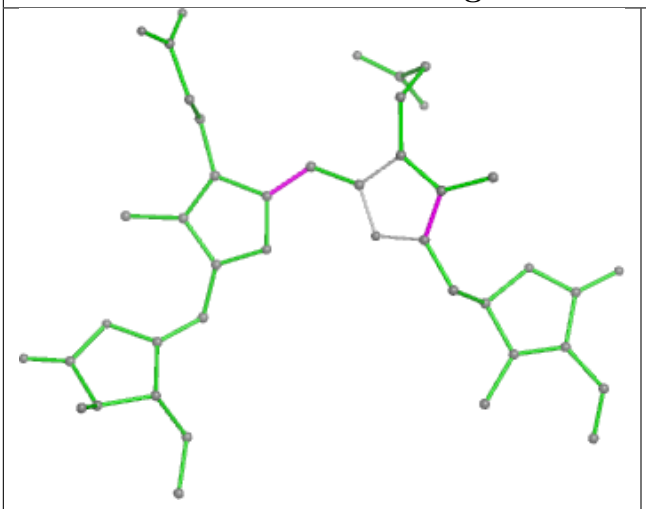


Torsions

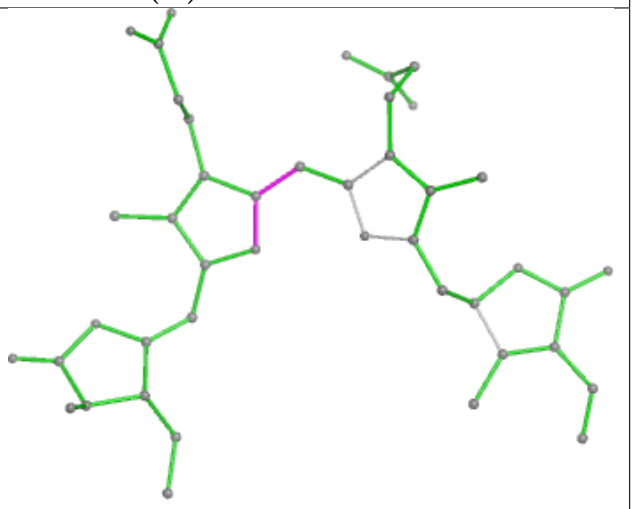


Rings

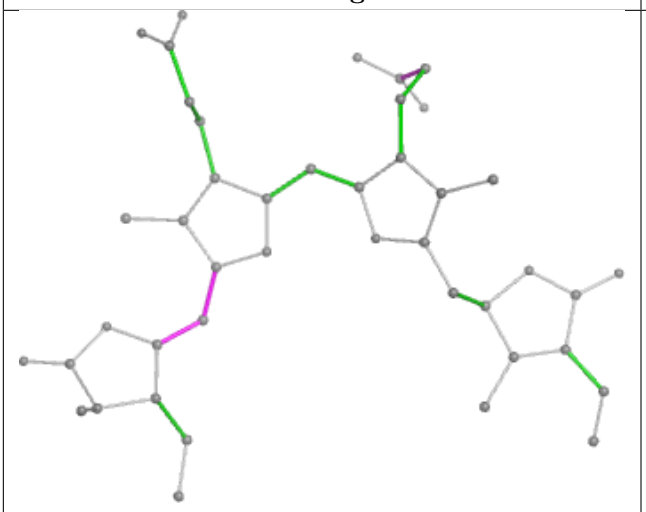
Ligand PEB AAA 201 (B)



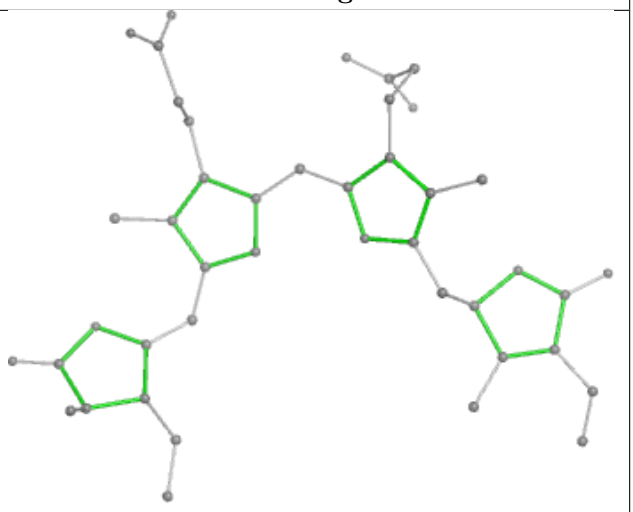
Bond lengths



Bond angles

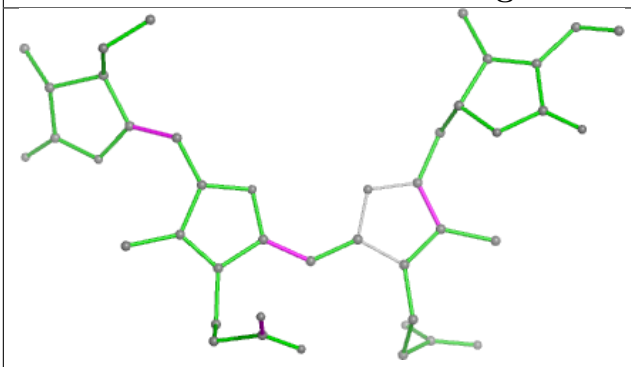


Torsions

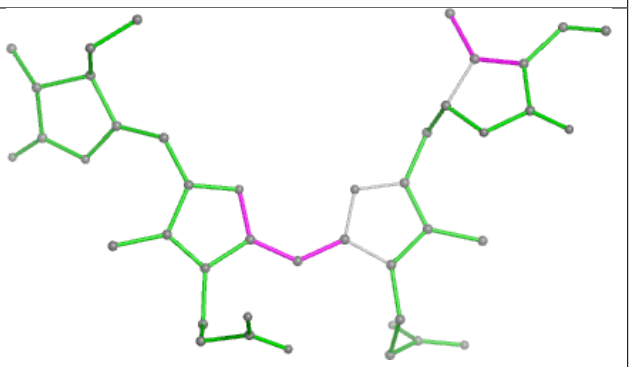


Rings

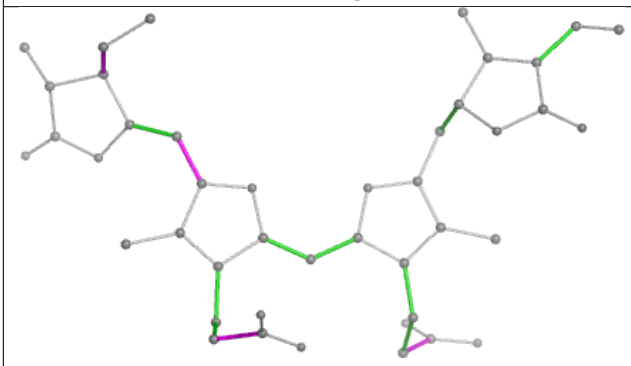
Ligand PEB DDD 203



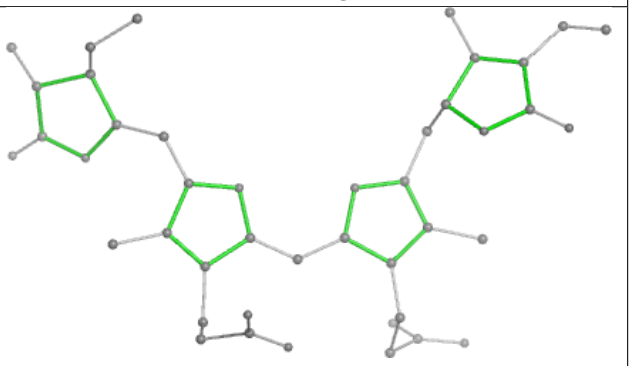
Bond lengths



Bond angles

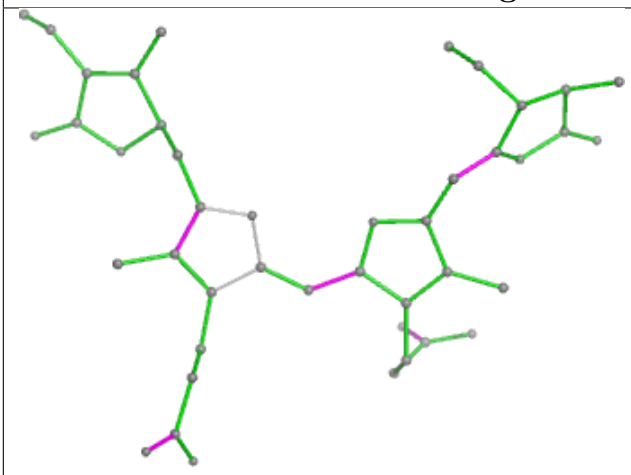


Torsions

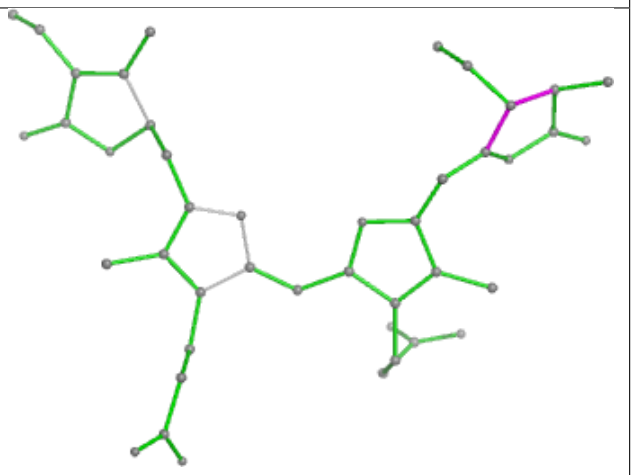


Rings

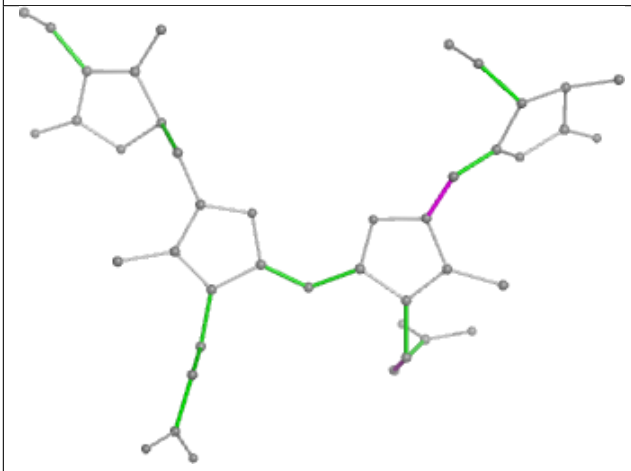
Ligand PEB BBB 201



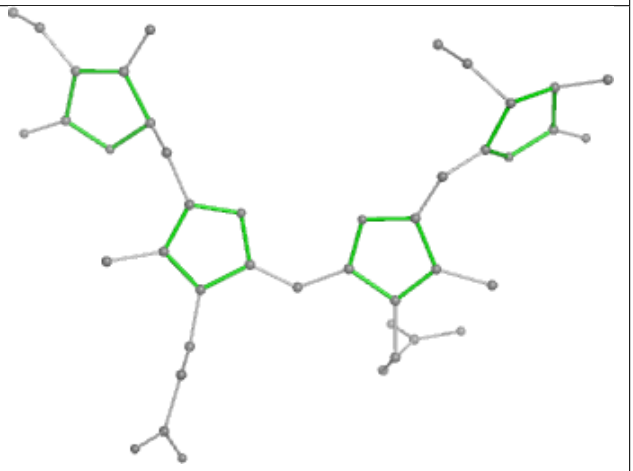
Bond lengths



Bond angles

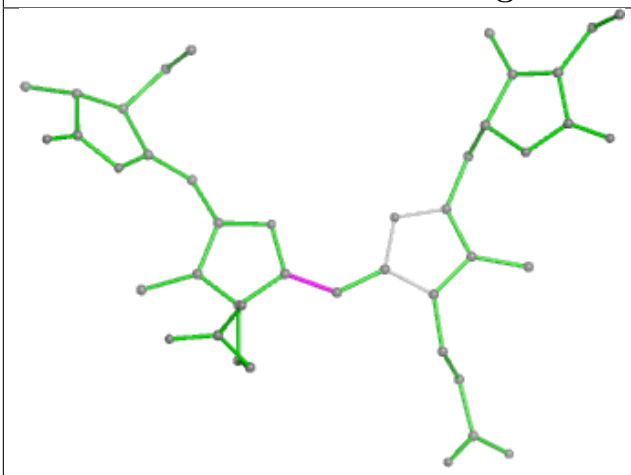


Torsions

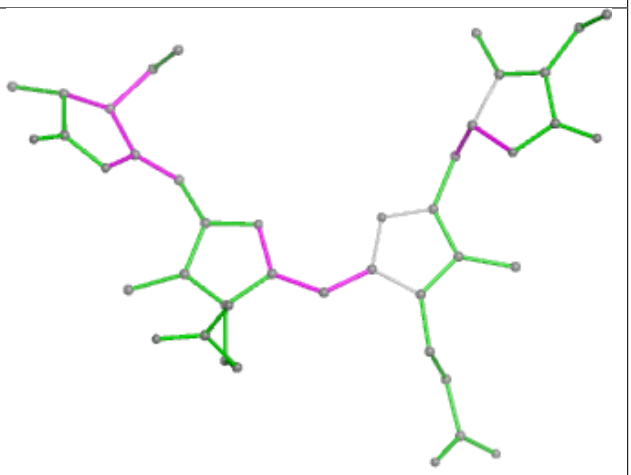


Rings

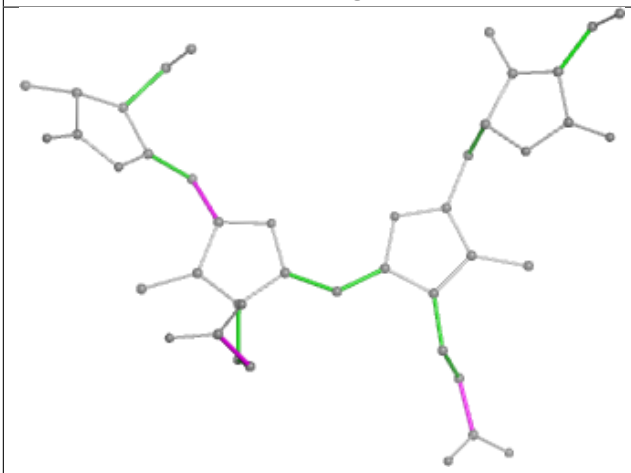
Ligand PEB DDD 201



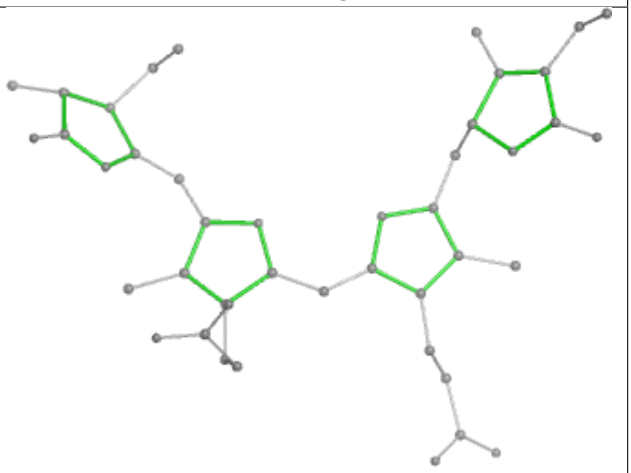
Bond lengths



Bond angles

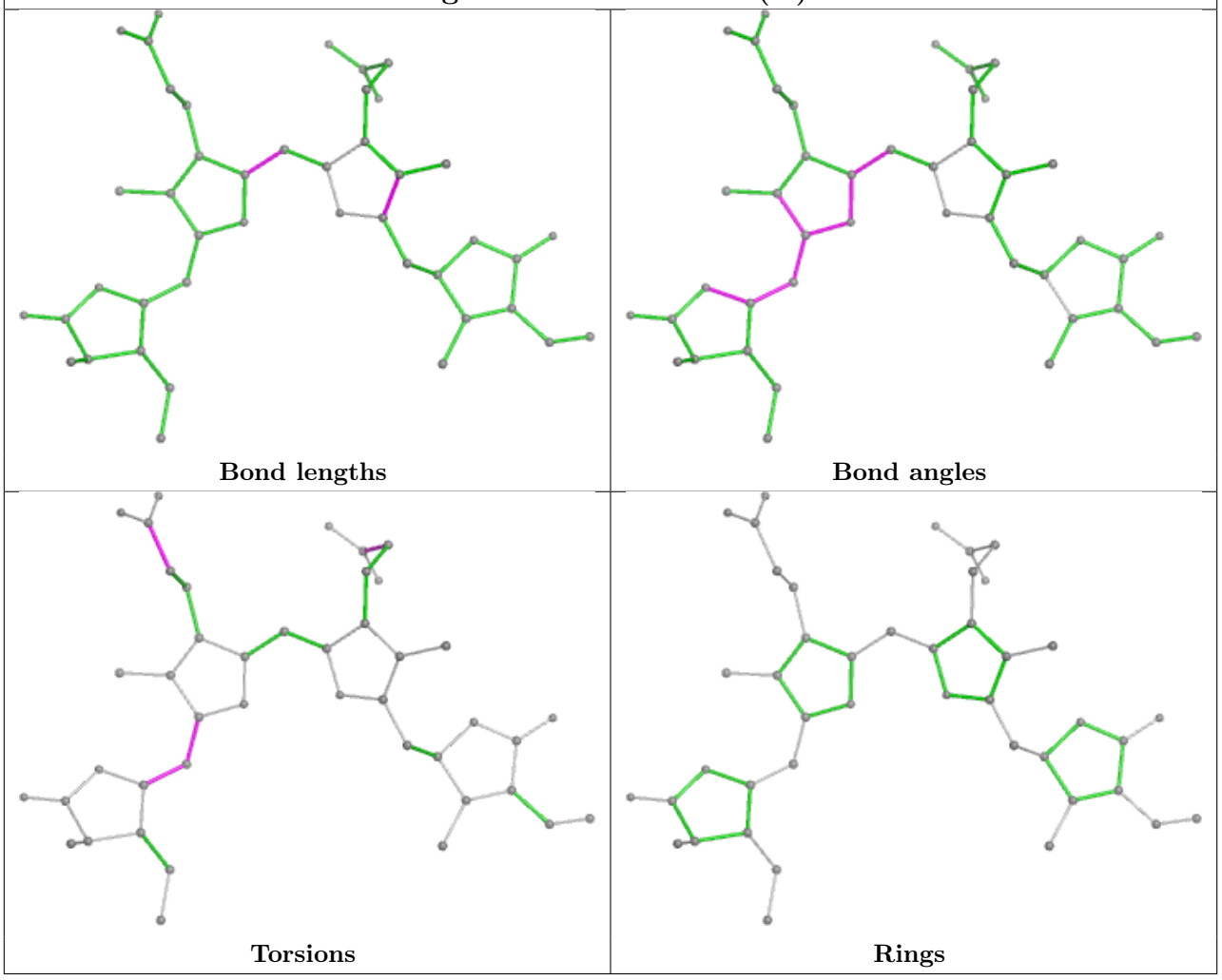


Torsions



Rings

Ligand PEB AAA 201 (A)



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

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

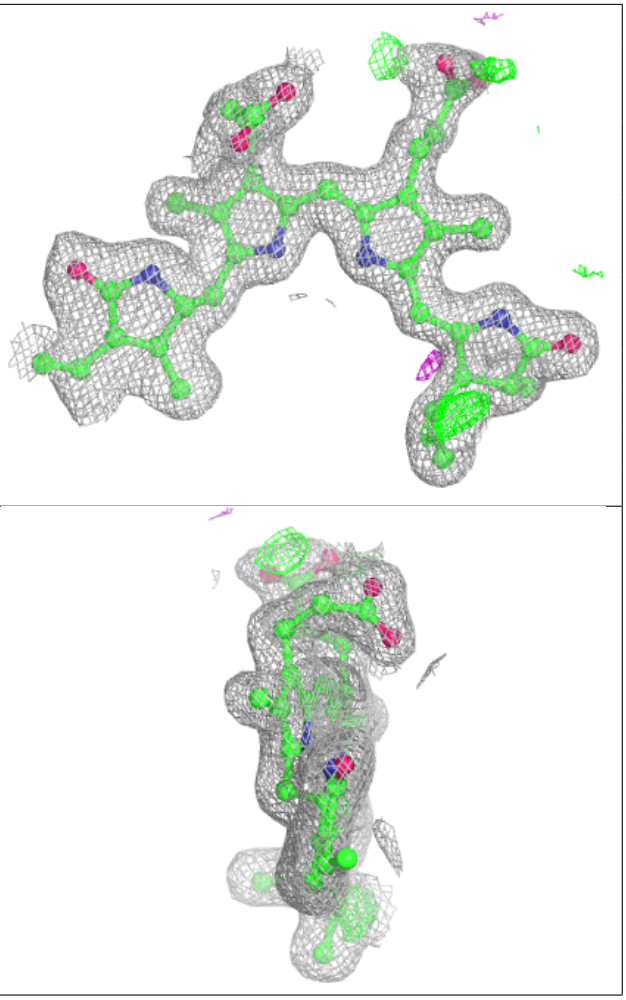
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

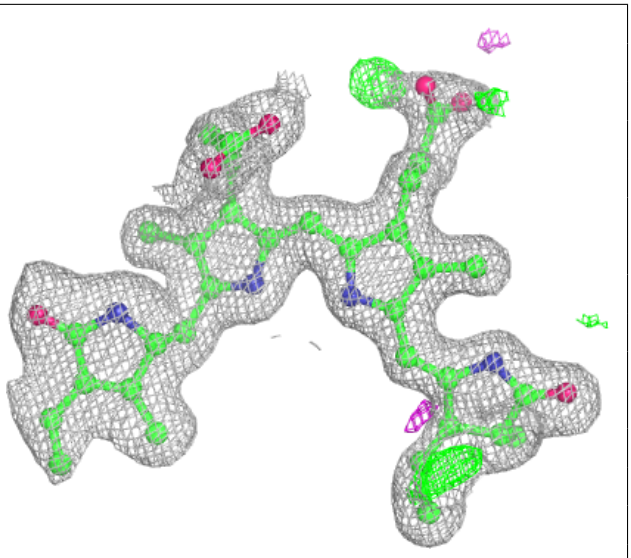
Electron density around PEB AAA 201 (A):

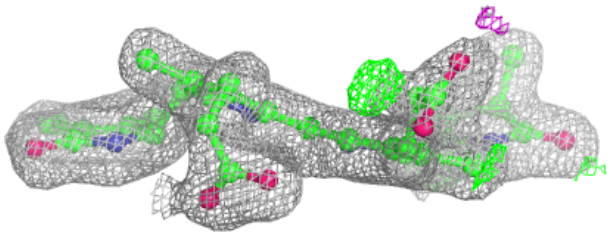
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

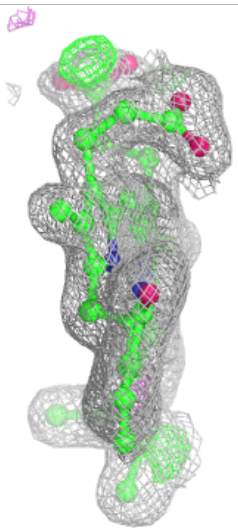


Electron density around PEB AAA 201 (B):

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

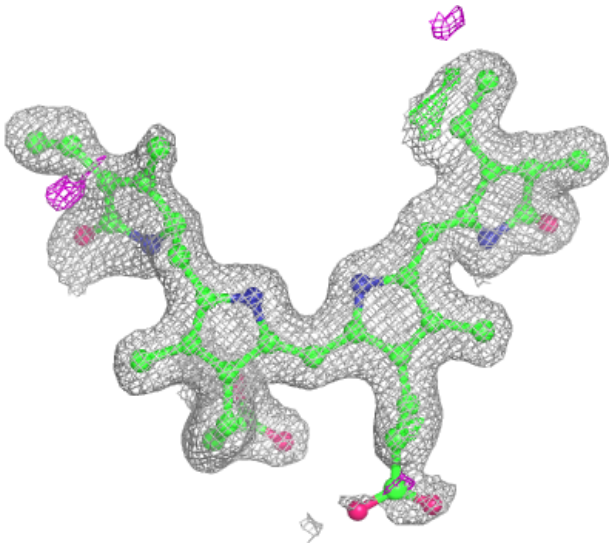


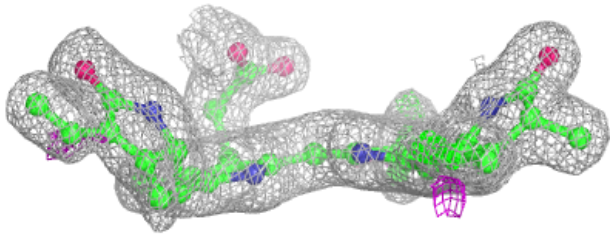


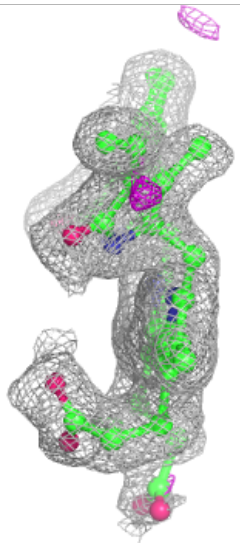


Electron density around PEB AAA 202:

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

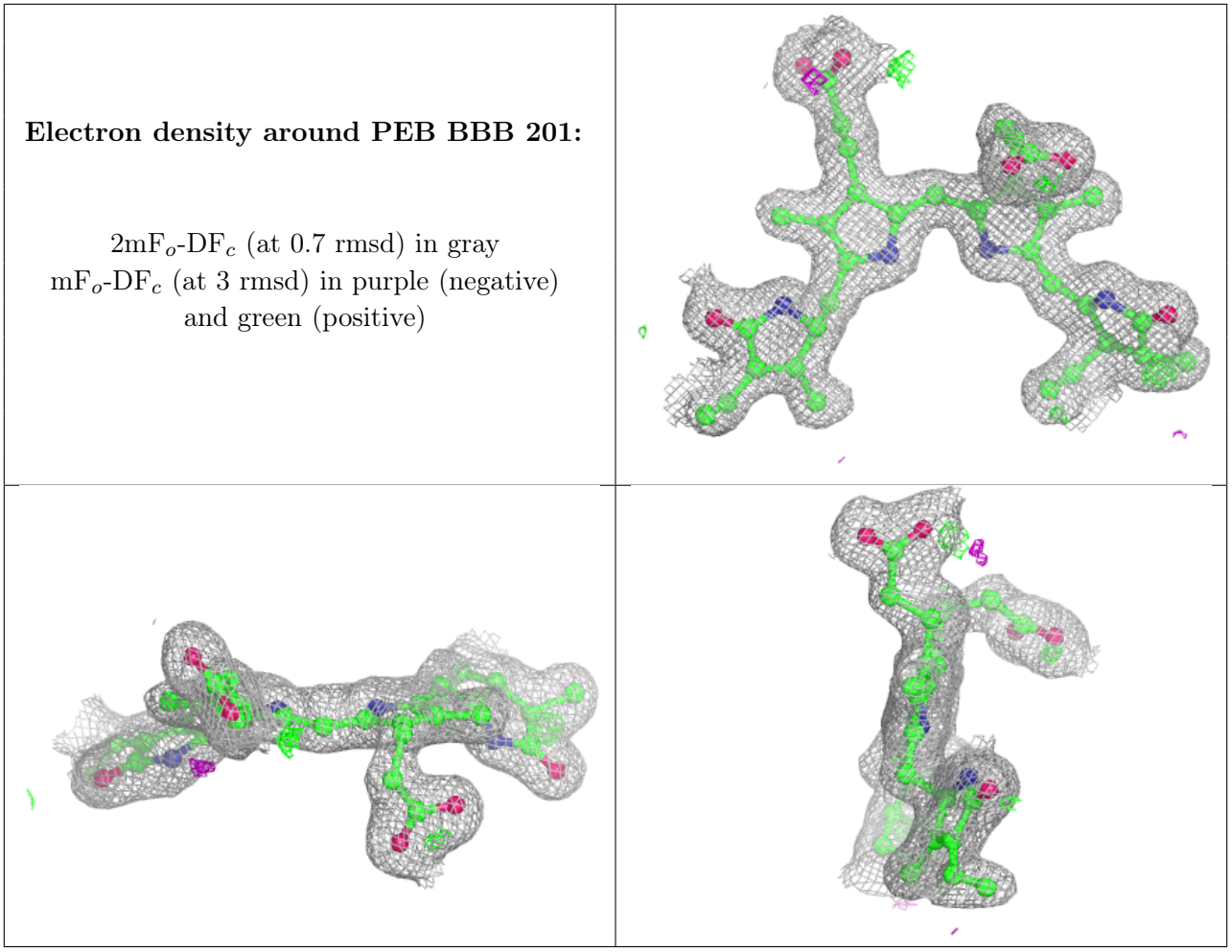






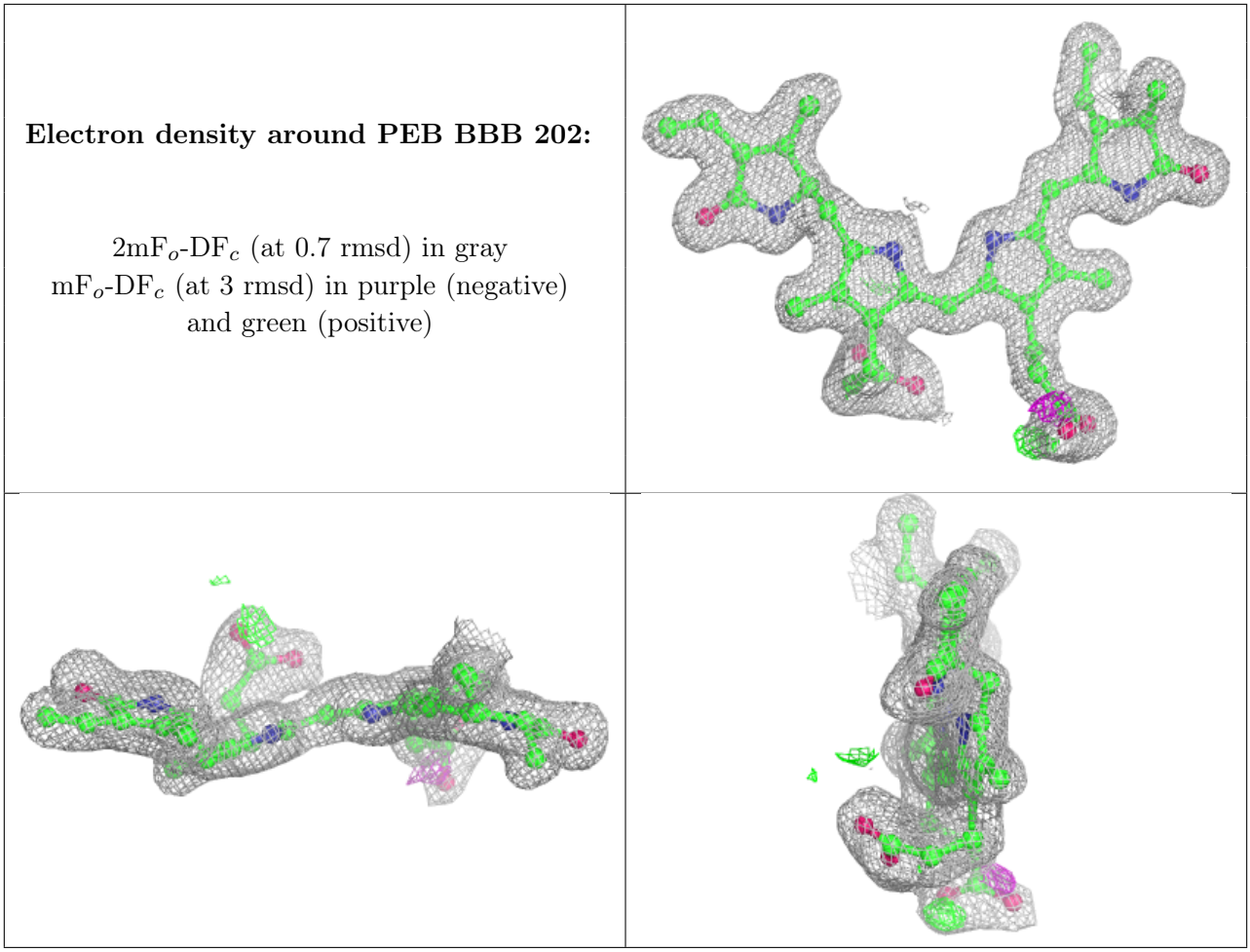
Electron density around PEB BBB 201:

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



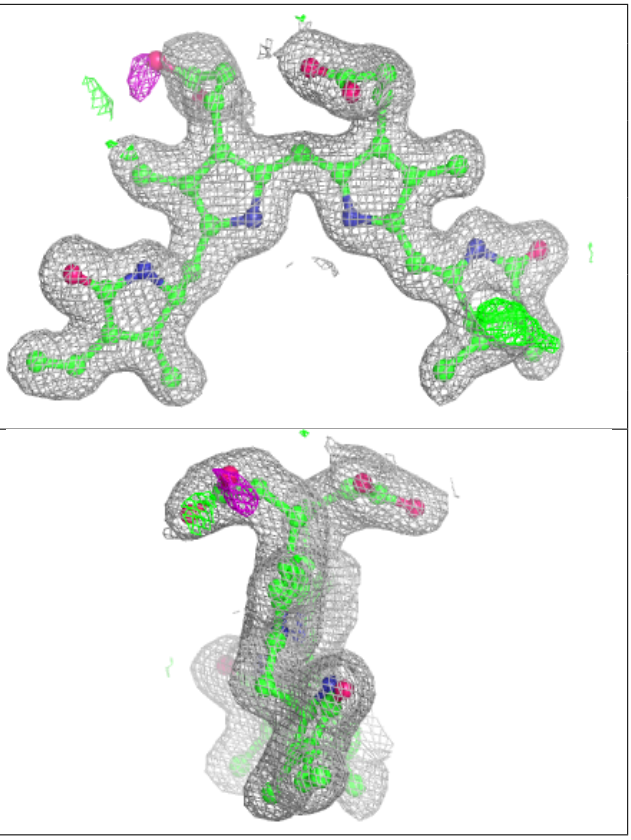
Electron density around PEB BBB 202:

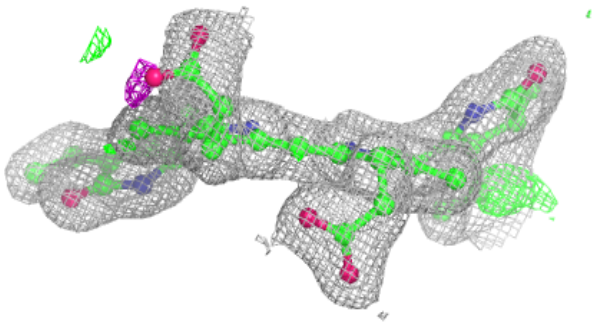
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PEB BBB 203:

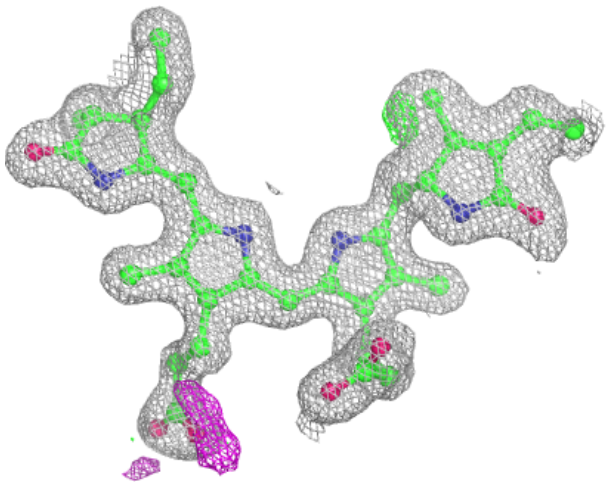
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

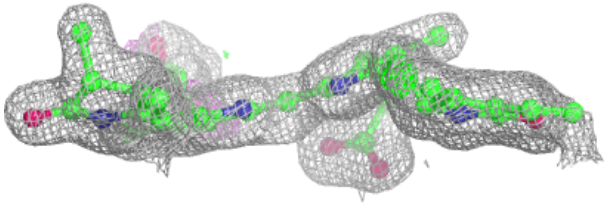


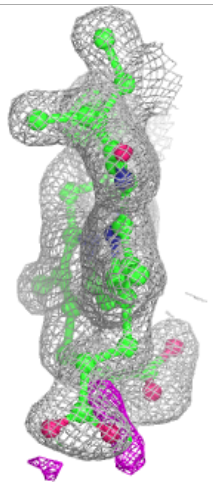


Electron density around PEB CCC 201:

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

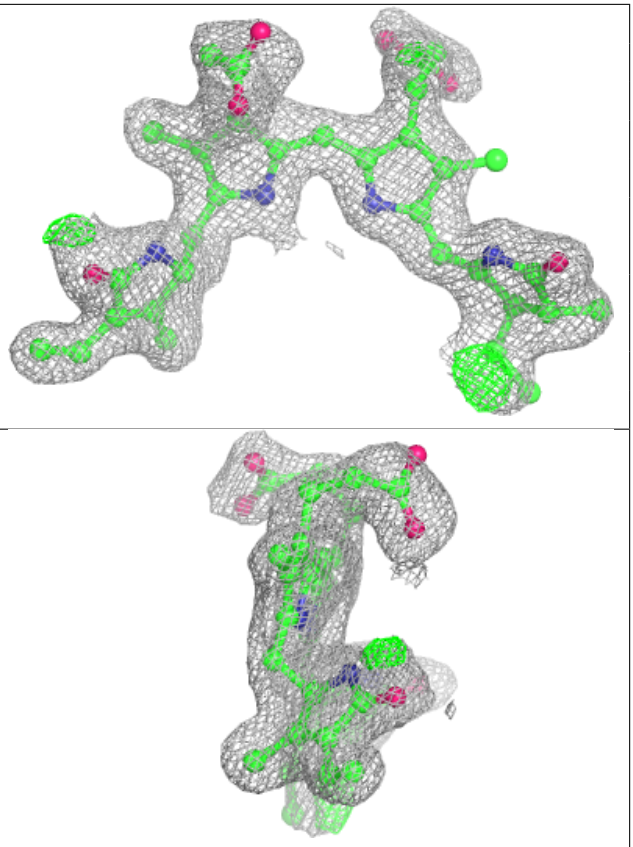


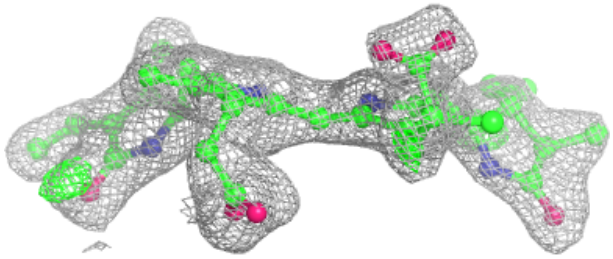




Electron density around PEB CCC 202:

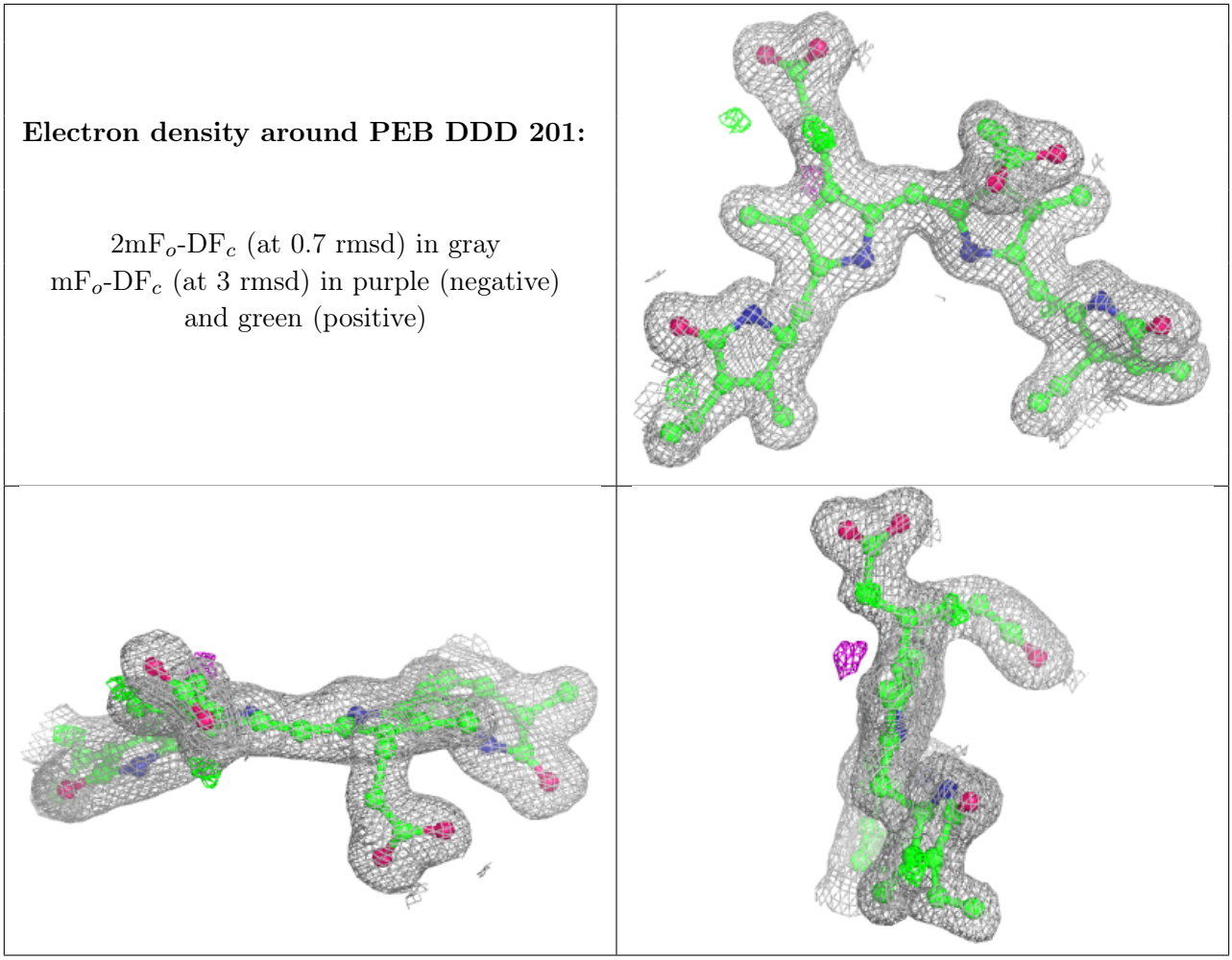
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





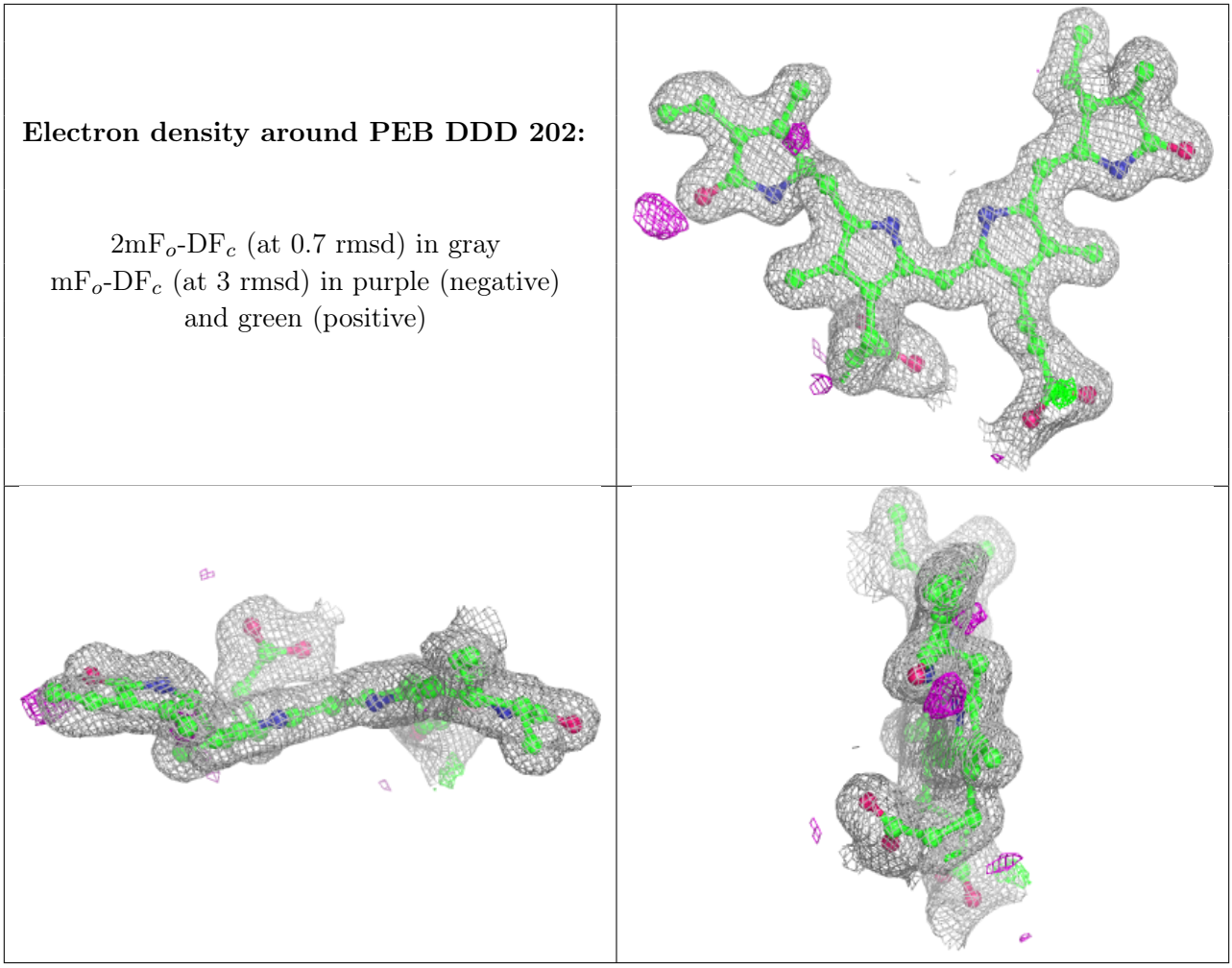
Electron density around PEB DDD 201:

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



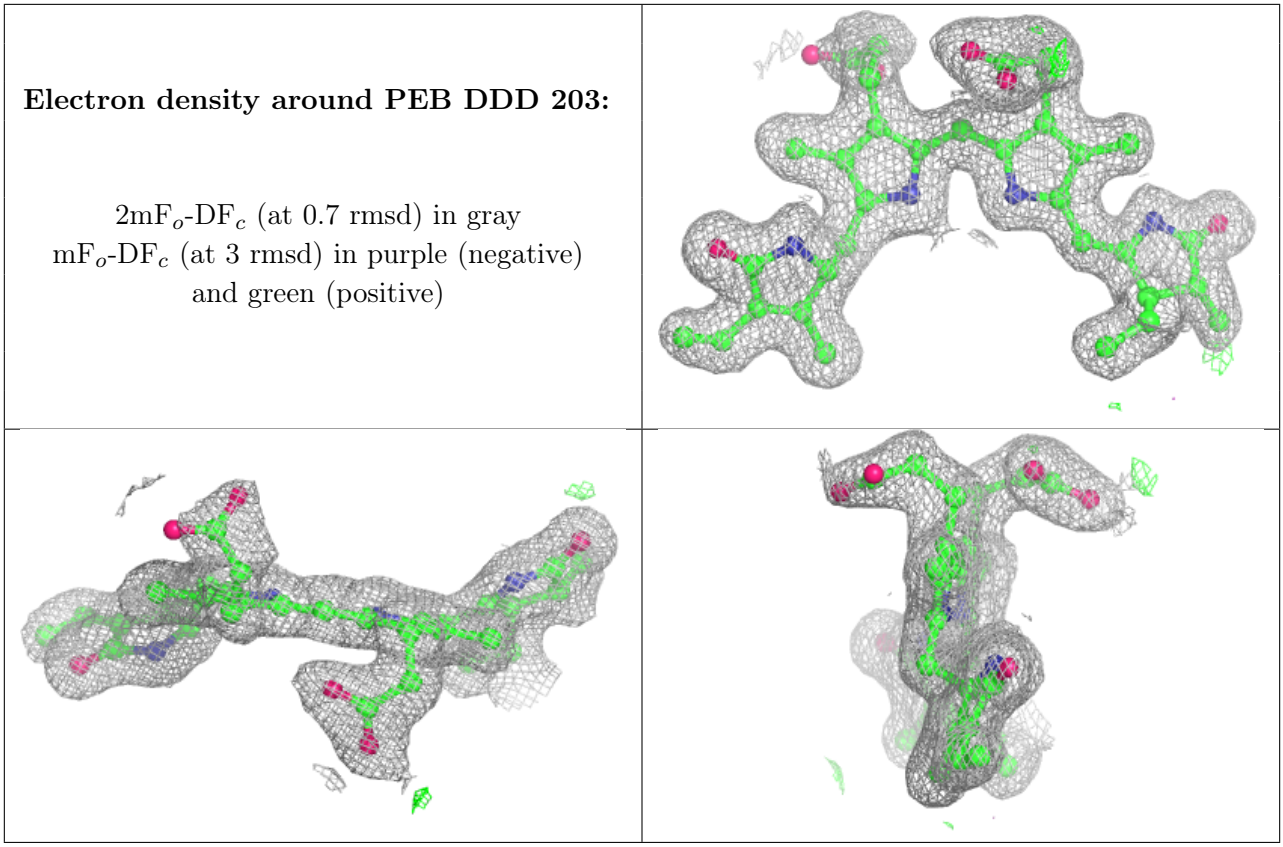
Electron density around PEB DDD 202:

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



Electron density around PEB DDD 203:

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



6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.