



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:14 am BST

PDB ID : 3V58  
Title : Crystal Structure of the B-phycoerythrin from the red algae *Porphyridium Cruentum* at pH5  
Authors : Camara-Artigas, A.  
Deposited on : 2011-12-16  
Resolution : 1.85 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 : 2.11  
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) : 2.11

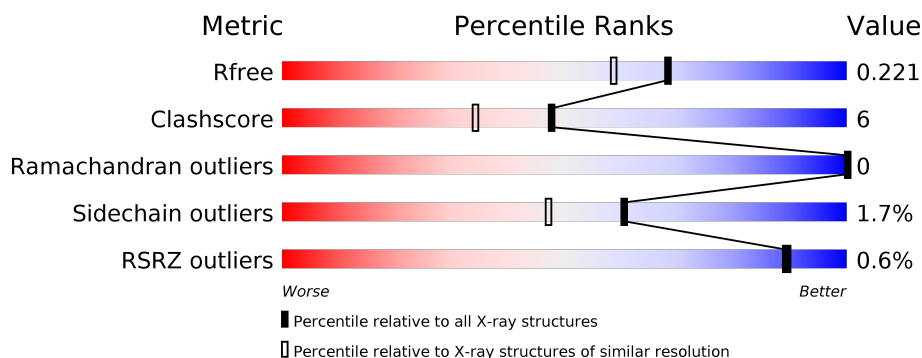
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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	164	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>88%</span> <span>12%</span> </div> </div>
1	C	164	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>88%</span> <span>12%</span> </div> </div>
2	B	177	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>94%</span> <span>6%</span> </div> </div>
2	D	177	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>90%</span> <span>10%</span> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6081 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.

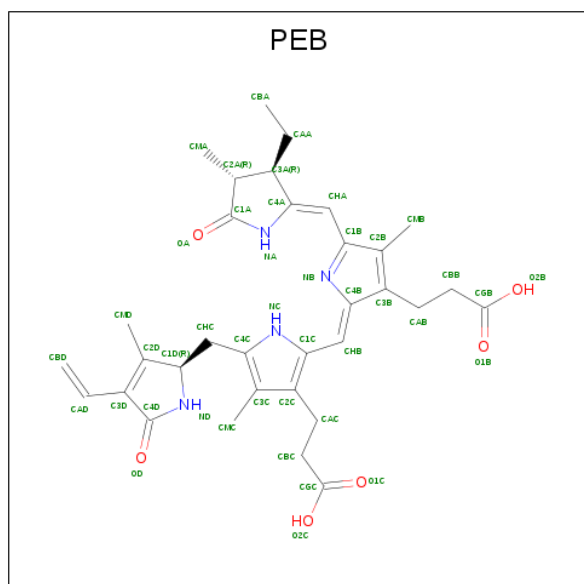
- Molecule 1 is a protein called Phycoerythrin alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1250	779	219	245	7			
1	C	164	Total	C	N	O	S	0	0	0
			1250	779	219	245	7			

- Molecule 2 is a protein called Phycoerythrin beta subunit.

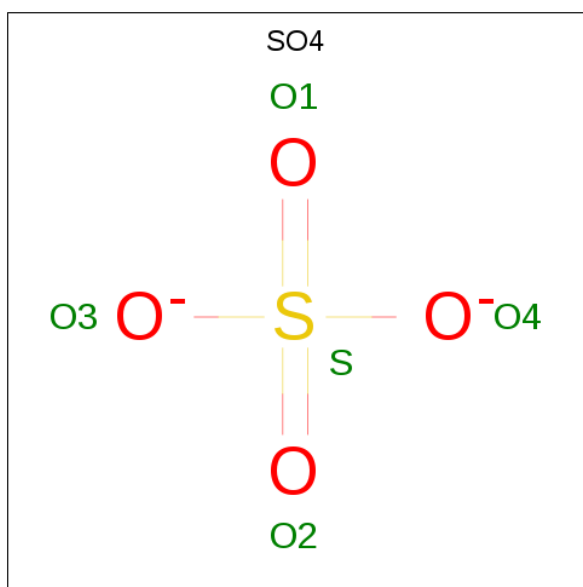
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	3	0
			1303	806	225	260	12			
2	D	177	Total	C	N	O	S	0	3	0
			1303	806	225	260	12			

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



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

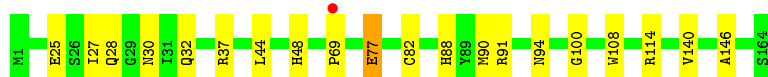
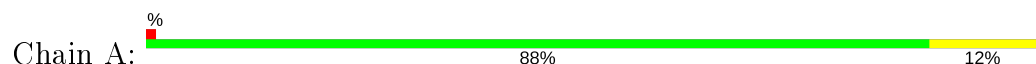
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	123	Total 123	O 123	0	0
5	B	153	Total 153	O 153	0	0
5	C	124	Total 124	O 124	0	0
5	D	140	Total 140	O 140	0	0

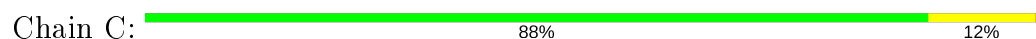
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



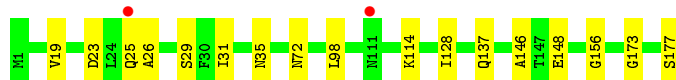
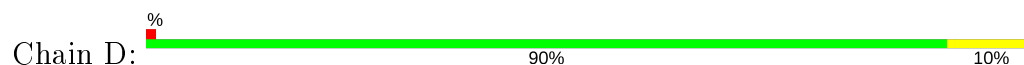
- Molecule 1: Phycoerythrin alpha subunit



- Molecule 2: Phycoerythrin beta subunit



- Molecule 2: Phycoerythrin beta subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.00 Å   187.00 Å   59.33 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	20.00 – 1.85 19.81 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-1.85) 98.0 (19.81-1.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 1.85 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.178 , 0.221 0.178 , 0.221	Depositor DCC
$R_{free}$ test set	3283 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.5	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6081	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MEN, SO4, 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	A	0.90	1/1271 (0.1%)	0.77	1/1721 (0.1%)
1	C	0.86	0/1271	0.75	0/1721
2	B	0.88	0/1315	0.74	0/1774
2	D	0.88	0/1315	0.77	0/1774
All	All	0.88	1/5172 (0.0%)	0.76	1/6990 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	TRP	CD2-CE2	5.61	1.48	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ARG	NE-CZ-NH2	-5.56	117.52	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	A	1250	0	1222	22	0
1	C	1250	0	1222	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1303	0	1310	7	0
2	D	1303	0	1310	16	0
3	A	86	0	74	4	0
3	B	129	0	109	5	0
3	C	86	0	74	6	0
3	D	129	0	110	10	0
4	A	5	0	0	0	0
5	A	123	0	0	3	0
5	B	153	0	0	1	0
5	C	124	0	0	2	0
5	D	140	0	0	3	0
All	All	6081	0	5431	66	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 6.

All (66) 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)
3:C:207:PEB:HMB3	3:C:207:PEB:HNA	1.29	0.94
2:D:35:ASN:HD22	3:D:209:PEB:HND	1.23	0.86
3:C:207:PEB:CMB	3:C:207:PEB:HNA	1.95	0.79
3:C:207:PEB:HMB3	3:C:207:PEB:NA	1.96	0.79
1:A:32:GLN:HG3	1:C:32:GLN:HG3	1.66	0.77
1:C:94:ASN:HD21	2:D:19:VAL:H	1.40	0.69
3:C:207:PEB:CMB	3:C:207:PEB:NA	2.56	0.67
2:D:35:ASN:ND2	3:D:209:PEB:HND	1.94	0.66
1:C:63:TYR:HB2	1:C:66:LEU:HD22	1.77	0.65
1:A:94:ASN:HD21	2:B:19:VAL:H	1.44	0.64
1:A:28:GLN:HE21	1:A:32:GLN:HE21	1.47	0.63
1:A:88:HIS:HD2	1:A:91:ARG:HH21	1.46	0.63
1:A:32:GLN:CG	1:C:32:GLN:HG3	2.27	0.63
1:C:48:HIS:HE1	5:C:277:HOH:O	1.82	0.63
1:A:114:ARG:HD2	5:A:182:HOH:O	1.98	0.63
2:B:72:MEN:HE22	3:B:203:PEB:HBB2	1.81	0.63
3:B:204:PEB:HMB2	3:B:204:PEB:HNA	1.65	0.60
1:C:140:VAL:HG11	1:C:146:ALA:HA	1.82	0.60
1:A:25:GLU:OE2	1:C:30:ASN:HA	2.03	0.59
1:A:27:ILE:O	1:A:30:ASN:HB2	2.03	0.59
1:A:32:GLN:HG3	1:C:32:GLN:CG	2.32	0.58
1:C:94:ASN:ND2	2:D:19:VAL:H	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:CD2	1:A:91:ARG:HH21	2.23	0.57
1:C:28:GLN:HE21	1:C:32:GLN:HE21	1.52	0.56
3:B:204:PEB:NA	3:B:204:PEB:HMB2	2.20	0.56
2:D:148:GLU:HG3	5:D:202:HOH:O	2.06	0.56
1:C:138:LEU:HA	3:C:207:PEB:HMD2	1.87	0.55
1:A:44:LEU:HD11	1:A:90:MET:HE2	1.89	0.55
1:A:140:VAL:HG11	1:A:146:ALA:HA	1.89	0.55
1:A:82:CYS:SG	3:A:201:PEB:C3A	2.93	0.55
3:D:209:PEB:HHA1	3:D:209:PEB:HBA3	1.89	0.54
2:D:26:ALA:HB3	5:D:315:HOH:O	2.08	0.53
3:B:203:PEB:HMB2	3:B:203:PEB:HNA	1.72	0.53
2:D:137:GLN:HG2	3:D:210:PEB:C1B	2.38	0.53
1:A:82:CYS:SG	3:A:201:PEB:CBA	2.92	0.52
3:A:201:PEB:CMB	3:A:201:PEB:HNA	2.22	0.52
1:C:63:TYR:CB	1:C:66:LEU:HD22	2.40	0.51
1:A:44:LEU:HD11	1:A:90:MET:CE	2.40	0.51
1:C:38:LEU:O	1:C:42:GLU:HG3	2.10	0.50
2:D:156:GLY:HA3	3:D:209:PEB:CMB	2.41	0.50
3:D:208:PEB:HNA	3:D:208:PEB:HMB2	1.77	0.49
2:B:81:ALA:HA	2:B:84:ARG:NH1	2.27	0.49
2:D:23:ASP:O	5:D:315:HOH:O	2.20	0.49
1:A:69:PRO:HD3	5:A:278:HOH:O	2.13	0.48
1:A:30:ASN:HA	1:C:25:GLU:OE2	2.14	0.47
3:C:207:PEB:HNA	3:C:207:PEB:C2B	2.26	0.47
1:C:72:ALA:HA	5:C:300:HOH:O	2.15	0.46
2:D:146:ALA:HA	3:D:210:PEB:O1B	2.16	0.46
2:D:72:MEN:HE22	3:D:208:PEB:HBB2	1.97	0.46
5:A:276:HOH:O	2:B:108:ARG:HD3	2.14	0.46
3:A:201:PEB:HNA	3:A:201:PEB:HMB2	1.80	0.45
2:B:137:GLN:HG2	3:B:205:PEB:C1B	2.46	0.45
1:A:77:GLU:O	1:A:77:GLU:HG3	2.17	0.44
1:A:100:GLY:O	1:C:22:SER:HB3	2.16	0.44
1:C:1:MET:CE	1:C:108:TRP:CZ2	3.01	0.44
1:A:94:ASN:ND2	2:B:19:VAL:H	2.14	0.44
3:D:209:PEB:HMB2	3:D:209:PEB:HNA	1.83	0.43
1:A:48:HIS:HE1	5:B:504:HOH:O	2.02	0.42
2:D:128:ILE:HG12	2:D:173:GLY:HA2	2.01	0.42
1:C:27:ILE:HD13	2:D:98:LEU:HD11	2.01	0.42
1:A:25:GLU:O	1:C:29:GLY:HA3	2.20	0.42
2:B:134:MET:HA	2:B:137:GLN:OE1	2.20	0.42
1:C:27:ILE:O	1:C:30:ASN:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:LYS:HE2	2:D:177:SER:OXT	2.20	0.41
2:D:156:GLY:HA3	3:D:209:PEB:HMB1	2.03	0.41
2:D:31:ILE:HA	2:D:31:ILE:HD13	1.92	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	C	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
2	B	177/177 (100%)	175 (99%)	2 (1%)	0	100	100
2	D	177/177 (100%)	175 (99%)	2 (1%)	0	100	100
All	All	678/682 (99%)	668 (98%)	10 (2%)	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	A	128/128 (100%)	127 (99%)	1 (1%)	81	76
1	C	128/128 (100%)	126 (98%)	2 (2%)	62	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	140/137 (102%)	136 (97%)	4 (3%)	42	26
2	D	140/137 (102%)	138 (99%)	2 (1%)	67	55
All	All	536/530 (101%)	527 (98%)	9 (2%)	60	47

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

Mol	Chain	Res	Type
1	A	77	GLU
2	B	22	SER
2	B	23	ASP
2	B	25	GLN
2	B	165	VAL
1	C	43	LYS
1	C	66	LEU
2	D	25	GLN
2	D	29	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	48	HIS
1	A	88	HIS
1	A	94	ASN
2	B	111	ASN
1	C	28	GLN
1	C	32	GLN
1	C	94	ASN
2	D	25	GLN
2	D	35	ASN
2	D	76	ASN

### 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	D	72	2	7,8,9	0.82	0	6,9,11	1.44	1 (16%)
2	MEN	B	72	2	7,8,9	0.58	0	6,9,11	1.29	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	D	72	2	-	3/7/8/10	-
2	MEN	B	72	2	-	2/7/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	72	MEN	CB-CG-ND2	3.05	119.58	115.48
2	B	72	MEN	CB-CG-ND2	2.94	119.43	115.48

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	72	MEN	CA-CB-CG-OD1
2	D	72	MEN	CA-CB-CG-OD1
2	D	72	MEN	CA-CB-CG-ND2
2	B	72	MEN	CA-CB-CG-ND2
2	D	72	MEN	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	72	MEN	1	0
2	B	72	MEN	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

11 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	B	203	2	37,46,46	3.37	9 (24%)	39,67,67	2.56	14 (35%)
3	PEB	C	207	1	37,46,46	3.79	13 (35%)	39,67,67	2.13	17 (43%)
3	PEB	A	202	1	37,46,46	3.40	9 (24%)	39,67,67	2.47	15 (38%)
3	PEB	B	204	2	37,46,46	3.48	9 (24%)	39,67,67	2.55	15 (38%)
3	PEB	C	206	1	37,46,46	3.83	10 (27%)	39,67,67	2.45	17 (43%)
3	PEB	A	201	1	37,46,46	3.62	9 (24%)	39,67,67	2.54	16 (41%)
3	PEB	D	209	2	37,46,46	3.66	13 (35%)	39,67,67	1.99	13 (33%)
3	PEB	B	205	2	37,46,46	3.58	9 (24%)	39,67,67	2.92	18 (46%)
4	SO4	A	165	-	4,4,4	0.41	0	6,6,6	0.58	0
3	PEB	D	208	2	37,46,46	3.66	9 (24%)	39,67,67	2.65	17 (43%)
3	PEB	D	210	2	37,46,46	3.44	10 (27%)	39,67,67	2.11	14 (35%)

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	B	203	2	-	2/20/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	C	207	1	-	3/20/74/74	0/4/4/4
3	PEB	A	202	1	-	4/20/74/74	0/4/4/4
3	PEB	B	204	2	-	4/20/74/74	0/4/4/4
3	PEB	C	206	1	-	3/20/74/74	0/4/4/4
3	PEB	A	201	1	-	3/20/74/74	0/4/4/4
3	PEB	D	209	2	-	3/20/74/74	0/4/4/4
3	PEB	B	205	2	-	4/20/74/74	0/4/4/4
3	PEB	D	208	2	-	2/20/74/74	0/4/4/4
3	PEB	D	210	2	-	4/20/74/74	0/4/4/4

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	208	PEB	CHB-C4B	17.54	1.49	1.35
3	C	206	PEB	CHB-C4B	17.51	1.49	1.35
3	C	207	PEB	CHB-C4B	17.06	1.49	1.35
3	B	205	PEB	CHB-C4B	16.86	1.49	1.35
3	A	201	PEB	CHB-C4B	15.94	1.48	1.35
3	D	209	PEB	CHB-C4B	15.80	1.48	1.35
3	A	202	PEB	CHB-C4B	15.22	1.47	1.35
3	B	203	PEB	CHB-C4B	14.79	1.47	1.35
3	B	204	PEB	CHB-C4B	14.70	1.47	1.35
3	D	210	PEB	CHB-C4B	14.60	1.47	1.35
3	C	207	PEB	C2D-C3D	9.54	1.46	1.34
3	C	206	PEB	C2D-C3D	9.54	1.46	1.34
3	A	201	PEB	C2D-C3D	9.39	1.46	1.34
3	B	203	PEB	C2D-C3D	9.02	1.46	1.34
3	A	202	PEB	C2D-C3D	8.67	1.45	1.34
3	B	204	PEB	C2D-C3D	8.46	1.45	1.34
3	D	208	PEB	C2D-C3D	8.41	1.45	1.34
3	B	205	PEB	C2D-C3D	8.40	1.45	1.34
3	D	210	PEB	C2D-C3D	7.73	1.44	1.34
3	B	204	PEB	C3C-C4C	7.51	1.53	1.42
3	D	210	PEB	C3C-C4C	7.46	1.53	1.42
3	D	209	PEB	C2D-C3D	7.24	1.43	1.34
3	C	206	PEB	C3C-C4C	6.92	1.52	1.42
3	A	201	PEB	C3B-C2B	6.14	1.49	1.36
3	D	209	PEB	C1A-NA	-6.04	1.29	1.37
3	A	201	PEB	C3C-C4C	6.01	1.51	1.42
3	D	209	PEB	C3C-C4C	5.95	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	204	PEB	C3B-C2B	5.88	1.49	1.36
3	B	205	PEB	C3C-C4C	5.54	1.50	1.42
3	D	210	PEB	C3B-C2B	5.33	1.48	1.36
3	A	202	PEB	C3B-C2B	5.32	1.48	1.36
3	C	207	PEB	C3C-C4C	5.24	1.50	1.42
3	D	209	PEB	C3B-C2B	5.18	1.47	1.36
3	C	207	PEB	C3B-C2B	5.09	1.47	1.36
3	B	203	PEB	C3C-C4C	5.03	1.49	1.42
3	B	203	PEB	CHA-C1B	4.92	1.51	1.40
3	B	204	PEB	CHA-C1B	4.89	1.51	1.40
3	A	202	PEB	C3C-C4C	4.86	1.49	1.42
3	D	208	PEB	C3C-C4C	4.81	1.49	1.42
3	B	205	PEB	CHA-C1B	4.72	1.51	1.40
3	C	206	PEB	C3B-C2B	4.52	1.46	1.36
3	D	210	PEB	CHA-C1B	4.38	1.50	1.40
3	B	203	PEB	C3B-C2B	4.36	1.46	1.36
3	D	208	PEB	C3B-C2B	4.31	1.45	1.36
3	B	205	PEB	C3B-C2B	4.26	1.45	1.36
3	D	208	PEB	CHA-C1B	4.26	1.50	1.40
3	D	209	PEB	CHA-C1B	4.25	1.50	1.40
3	C	207	PEB	CHA-C1B	4.23	1.50	1.40
3	D	209	PEB	C2C-C3C	4.06	1.49	1.37
3	A	202	PEB	CHA-C1B	3.94	1.49	1.40
3	C	207	PEB	C2C-C3C	3.88	1.49	1.37
3	D	210	PEB	OD-C4D	3.87	1.30	1.23
3	A	201	PEB	CHA-C1B	3.74	1.49	1.40
3	D	208	PEB	C2C-C3C	3.71	1.48	1.37
3	C	206	PEB	CHA-C1B	3.65	1.49	1.40
3	D	210	PEB	C2C-C3C	3.63	1.48	1.37
3	A	201	PEB	C2C-C3C	3.63	1.48	1.37
3	D	209	PEB	OD-C4D	3.60	1.30	1.23
3	C	206	PEB	OD-C4D	3.54	1.30	1.23
3	A	202	PEB	C2C-C3C	3.49	1.48	1.37
3	C	206	PEB	C2C-C3C	3.44	1.47	1.37
3	B	205	PEB	C1D-ND	3.31	1.50	1.45
3	B	203	PEB	C2C-C3C	3.24	1.47	1.37
3	A	201	PEB	OD-C4D	3.18	1.29	1.23
3	C	206	PEB	C1D-ND	3.12	1.50	1.45
3	D	210	PEB	C1D-ND	3.08	1.50	1.45
3	C	207	PEB	OD-C4D	3.07	1.29	1.23
3	C	207	PEB	C1B-C2B	3.04	1.52	1.45
3	B	204	PEB	C2C-C3C	3.01	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	209	PEB	C4D-ND	2.99	1.39	1.35
3	B	204	PEB	OD-C4D	2.98	1.29	1.23
3	A	201	PEB	C1D-ND	2.95	1.50	1.45
3	B	203	PEB	C1C-CHB	2.89	1.52	1.41
3	B	203	PEB	C4D-ND	2.83	1.38	1.35
3	C	207	PEB	C4B-C3B	2.80	1.50	1.45
3	B	205	PEB	C2C-C3C	2.79	1.45	1.37
3	C	207	PEB	C4D-ND	2.72	1.38	1.35
3	D	209	PEB	C4B-C3B	2.69	1.50	1.45
3	A	202	PEB	C4D-ND	2.67	1.38	1.35
3	A	201	PEB	C3A-C4A	2.64	1.54	1.50
3	C	207	PEB	C2A-C1A	-2.64	1.49	1.52
3	D	209	PEB	C1C-CHB	2.56	1.51	1.41
3	D	208	PEB	C4D-ND	2.49	1.38	1.35
3	C	207	PEB	C1A-NA	-2.48	1.34	1.37
3	D	209	PEB	C1D-ND	2.44	1.49	1.45
3	A	202	PEB	C1B-C2B	2.39	1.51	1.45
3	C	206	PEB	C1C-CHB	2.31	1.50	1.41
3	D	210	PEB	C1A-NA	-2.27	1.34	1.37
3	A	202	PEB	OD-C4D	2.25	1.27	1.23
3	B	204	PEB	C3A-C4A	2.20	1.54	1.50
3	B	205	PEB	OD-C4D	2.20	1.27	1.23
3	C	206	PEB	CMD-C2D	2.19	1.54	1.50
3	B	204	PEB	C1A-NA	-2.18	1.34	1.37
3	B	203	PEB	OD-C4D	2.17	1.27	1.23
3	D	209	PEB	C1B-C2B	2.16	1.50	1.45
3	C	207	PEB	C1D-ND	2.16	1.49	1.45
3	D	210	PEB	C1C-CHB	2.13	1.49	1.41
3	D	208	PEB	C2A-C1A	-2.10	1.50	1.52
3	D	208	PEB	C1C-CHB	2.08	1.49	1.41
3	B	205	PEB	CMD-C2D	2.01	1.53	1.50

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	205	PEB	OA-C1A-C2A	-10.45	117.87	126.17
3	B	204	PEB	OA-C1A-C2A	-8.10	119.73	126.17
3	D	208	PEB	OA-C1A-C2A	-6.80	120.77	126.17
3	A	201	PEB	OA-C1A-C2A	-6.51	120.99	126.17
3	B	205	PEB	C2A-C1A-NA	6.20	113.61	108.27
3	B	203	PEB	CHC-C1D-ND	-6.17	106.79	113.95
3	B	203	PEB	OA-C1A-C2A	-6.03	121.38	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	208	PEB	C2A-C1A-NA	5.77	113.25	108.27
3	B	204	PEB	CHC-C1D-ND	-5.75	107.27	113.95
3	D	208	PEB	CHC-C1D-ND	-5.63	107.41	113.95
3	C	206	PEB	CHC-C1D-ND	-5.52	107.54	113.95
3	B	203	PEB	C2A-C1A-NA	5.39	112.92	108.27
3	A	202	PEB	C2A-C1A-NA	5.34	112.88	108.27
3	A	201	PEB	CHB-C4B-NB	-5.14	121.70	128.83
3	B	203	PEB	C1C-CHB-C4B	4.94	134.71	128.81
3	A	201	PEB	CHA-C1B-NB	-4.93	114.63	124.93
3	D	210	PEB	OA-C1A-C2A	-4.80	122.36	126.17
3	C	206	PEB	CHA-C1B-NB	-4.69	115.12	124.93
3	C	207	PEB	CMB-C2B-C1B	4.67	132.25	125.06
3	A	202	PEB	OA-C1A-C2A	-4.64	122.48	126.17
3	D	208	PEB	C3D-C4D-ND	4.60	116.29	107.26
3	B	203	PEB	C3D-C4D-ND	4.58	116.24	107.26
3	B	205	PEB	CBC-CAC-C2C	-4.57	104.07	112.49
3	B	204	PEB	C2A-C1A-NA	4.54	112.19	108.27
3	A	202	PEB	CHC-C4C-C3C	-4.54	122.60	130.34
3	B	205	PEB	CHC-C1D-ND	-4.53	108.69	113.95
3	A	202	PEB	CMB-C2B-C1B	4.52	132.02	125.06
3	A	202	PEB	OD-C4D-ND	-4.50	119.26	125.93
3	A	201	PEB	OD-C4D-C3D	-4.41	119.47	129.46
3	A	201	PEB	C2A-C1A-NA	4.31	111.98	108.27
3	D	209	PEB	CHC-C1D-ND	-4.23	109.04	113.95
3	A	201	PEB	CHC-C4C-C3C	-4.23	123.13	130.34
3	D	210	PEB	C4B-C3B-C2B	-4.19	102.14	106.78
3	C	207	PEB	OA-C1A-C2A	-4.16	122.87	126.17
3	C	206	PEB	OA-C1A-C2A	-4.15	122.88	126.17
3	A	202	PEB	C3D-C4D-ND	4.14	115.38	107.26
3	B	205	PEB	C3D-C4D-ND	4.14	115.38	107.26
3	C	206	PEB	C3D-C4D-ND	4.06	115.23	107.26
3	A	202	PEB	C3B-C4B-NB	4.05	115.94	110.05
3	C	206	PEB	CMD-C2D-C3D	4.00	135.70	130.06
3	B	204	PEB	C3D-C4D-ND	3.99	115.09	107.26
3	C	206	PEB	CHA-C4A-NA	3.99	129.95	125.20
3	B	205	PEB	OD-C4D-C3D	-3.96	120.48	129.46
3	D	210	PEB	OD-C4D-C3D	-3.89	120.65	129.46
3	D	208	PEB	CMB-C2B-C1B	3.87	131.03	125.06
3	D	209	PEB	C3D-C4D-ND	3.85	114.81	107.26
3	A	201	PEB	C3D-C4D-ND	3.84	114.79	107.26
3	B	204	PEB	C4B-C3B-C2B	-3.83	102.54	106.78
3	B	204	PEB	CHB-C4B-NB	-3.83	123.52	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	PEB	CHC-C1D-ND	-3.76	109.58	113.95
3	B	203	PEB	OD-C4D-ND	-3.74	120.39	125.93
3	C	206	PEB	C2A-C1A-NA	3.67	111.44	108.27
3	D	210	PEB	CHB-C4B-NB	-3.60	123.83	128.83
3	D	210	PEB	C3D-C4D-ND	3.53	114.19	107.26
3	D	210	PEB	C3B-C4B-NB	3.48	115.12	110.05
3	D	209	PEB	CHC-C4C-C3C	-3.48	124.40	130.34
3	D	208	PEB	OD-C4D-C3D	-3.47	121.59	129.46
3	C	207	PEB	C3D-C4D-ND	3.47	114.06	107.26
3	D	209	PEB	OD-C4D-C3D	-3.40	121.75	129.46
3	C	207	PEB	CHB-C4B-NB	-3.39	124.12	128.83
3	C	206	PEB	CHB-C4B-NB	-3.39	124.12	128.83
3	A	202	PEB	CHB-C4B-NB	-3.39	124.13	128.83
3	B	204	PEB	C3B-C4B-NB	3.37	114.96	110.05
3	D	208	PEB	C3B-C4B-NB	3.34	114.91	110.05
3	B	205	PEB	C3B-C4B-NB	3.34	114.91	110.05
3	A	202	PEB	C4B-C3B-C2B	-3.31	103.12	106.78
3	D	208	PEB	CHB-C4B-C3B	-3.30	117.69	125.32
3	D	208	PEB	CAB-CBB-CGB	-3.29	107.15	112.67
3	B	203	PEB	CAC-CBC-CGC	-3.28	107.16	112.67
3	B	204	PEB	OD-C4D-C3D	-3.27	122.04	129.46
3	B	203	PEB	OD-C4D-C3D	-3.25	122.08	129.46
3	B	205	PEB	CHC-C4C-C3C	-3.25	124.79	130.34
3	D	208	PEB	CHA-C1B-NB	-3.24	118.16	124.93
3	C	206	PEB	CMB-C2B-C1B	3.22	130.02	125.06
3	C	206	PEB	OD-C4D-C3D	-3.21	122.19	129.46
3	C	207	PEB	C3B-C4B-NB	3.17	114.67	110.05
3	D	208	PEB	CHC-C4C-C3C	-3.16	124.95	130.34
3	D	210	PEB	CHA-C1B-NB	-3.14	118.36	124.93
3	C	207	PEB	C4B-C3B-C2B	-3.10	103.35	106.78
3	D	209	PEB	CMB-C2B-C1B	3.07	129.79	125.06
3	C	207	PEB	C2A-C1A-NA	3.05	110.91	108.27
3	B	205	PEB	C4B-C3B-C2B	-3.02	103.44	106.78
3	D	208	PEB	CAC-CBC-CGC	-3.01	107.61	112.67
3	C	207	PEB	OD-C4D-ND	-2.96	121.54	125.93
3	D	209	PEB	C4B-C3B-C2B	-2.96	103.51	106.78
3	B	205	PEB	OA-C1A-NA	2.95	128.52	124.94
3	D	209	PEB	CHB-C4B-NB	-2.95	124.73	128.83
3	C	207	PEB	CHC-C1D-ND	-2.95	110.52	113.95
3	A	202	PEB	CHA-C1B-NB	-2.94	118.78	124.93
3	D	210	PEB	C2A-C1A-NA	2.91	110.78	108.27
3	A	202	PEB	C1C-CHB-C4B	2.89	132.26	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	PEB	CHA-C1B-C2B	2.89	132.32	124.90
3	B	203	PEB	CHA-C1B-NB	-2.88	118.91	124.93
3	C	207	PEB	CHC-C4C-C3C	-2.83	125.51	130.34
3	A	201	PEB	C1B-C2B-C3B	-2.80	103.29	106.51
3	C	206	PEB	CMA-C2A-C1A	-2.80	106.36	112.40
3	A	202	PEB	CHC-C1D-ND	-2.78	110.71	113.95
3	B	203	PEB	CHC-C4C-C3C	-2.77	125.61	130.34
3	C	206	PEB	CHC-C4C-C3C	-2.75	125.64	130.34
3	D	209	PEB	C3B-C4B-NB	2.73	114.02	110.05
3	A	201	PEB	C3B-C4B-NB	2.72	114.01	110.05
3	A	201	PEB	CMB-C2B-C1B	2.72	129.26	125.06
3	D	209	PEB	C1C-CHB-C4B	2.71	132.05	128.81
3	D	208	PEB	C4B-C3B-C2B	-2.70	103.79	106.78
3	B	205	PEB	CHA-C1B-NB	-2.70	119.28	124.93
3	B	203	PEB	CHB-C4B-NB	-2.70	125.08	128.83
3	D	208	PEB	C1C-CHB-C4B	2.67	132.00	128.81
3	D	209	PEB	CHA-C1B-NB	-2.66	119.37	124.93
3	D	208	PEB	OD-C4D-ND	-2.65	122.01	125.93
3	B	205	PEB	CMB-C2B-C1B	2.64	129.13	125.06
3	B	205	PEB	CMA-C2A-C1A	-2.62	106.75	112.40
3	B	204	PEB	CAC-CBC-CGC	-2.59	108.32	112.67
3	A	201	PEB	C4B-C3B-C2B	-2.57	103.93	106.78
3	B	204	PEB	CAA-C3A-C2A	-2.56	107.87	114.26
3	B	205	PEB	C2A-C3A-C4A	2.54	105.14	101.34
3	B	204	PEB	CMB-C2B-C1B	2.53	128.96	125.06
3	C	207	PEB	CHA-C1B-NB	-2.53	119.65	124.93
3	C	206	PEB	C1B-C2B-C3B	-2.49	103.65	106.51
3	B	203	PEB	C2A-C3A-C4A	2.49	105.06	101.34
3	A	202	PEB	CHB-C4B-C3B	-2.49	119.58	125.32
3	D	210	PEB	CMB-C2B-C1B	2.48	128.89	125.06
3	A	202	PEB	CBA-CAA-C3A	-2.48	107.94	113.47
3	B	205	PEB	CHB-C4B-C3B	-2.47	119.61	125.32
3	C	206	PEB	OD-C4D-ND	-2.46	122.29	125.93
3	B	203	PEB	C1B-C2B-C3B	-2.46	103.69	106.51
3	A	202	PEB	C1B-C2B-C3B	-2.46	103.69	106.51
3	D	209	PEB	CAC-CBC-CGC	-2.44	108.57	112.67
3	D	210	PEB	CBC-CAC-C2C	-2.44	108.00	112.49
3	B	204	PEB	OA-C1A-NA	2.43	127.89	124.94
3	B	205	PEB	CHB-C4B-NB	-2.41	125.48	128.83
3	D	210	PEB	CBD-CAD-C3D	-2.41	115.65	127.62
3	C	207	PEB	CAB-C3B-C4B	2.37	129.20	125.01
3	D	208	PEB	C1B-C2B-C3B	-2.37	103.79	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	206	PEB	CHA-C1B-C2B	2.35	130.95	124.90
3	C	206	PEB	CBA-CAA-C3A	-2.33	108.29	113.47
3	D	209	PEB	C1B-C2B-C3B	-2.32	103.84	106.51
3	C	206	PEB	C4B-C3B-C2B	-2.32	104.21	106.78
3	D	210	PEB	C1C-CHB-C4B	2.32	131.58	128.81
3	C	207	PEB	C1B-C2B-C3B	-2.32	103.85	106.51
3	A	201	PEB	CAB-C3B-C4B	2.31	129.10	125.01
3	D	209	PEB	C2A-C1A-NA	2.31	110.27	108.27
3	D	208	PEB	C2A-C3A-C4A	2.31	104.80	101.34
3	C	207	PEB	C1C-CHB-C4B	2.28	131.54	128.81
3	C	207	PEB	OD-C4D-C3D	-2.28	124.30	129.46
3	D	210	PEB	CHC-C1D-ND	-2.24	111.35	113.95
3	B	203	PEB	C3B-C4B-NB	2.23	113.30	110.05
3	C	207	PEB	CHA-C4A-NA	-2.23	122.55	125.20
3	B	204	PEB	CMC-C3C-C2C	-2.21	120.77	124.94
3	D	210	PEB	CHC-C4C-C3C	-2.19	126.60	130.34
3	A	201	PEB	CMA-C2A-C1A	-2.16	107.74	112.40
3	A	201	PEB	CAC-CBC-CGC	-2.14	109.08	112.67
3	C	207	PEB	CAC-CBC-CGC	-2.09	109.17	112.67
3	B	204	PEB	OD-C4D-ND	-2.08	122.86	125.93
3	B	204	PEB	C1B-C2B-C3B	-2.04	104.17	106.51
3	B	205	PEB	CHA-C4A-NA	2.03	127.62	125.20
3	B	205	PEB	C1B-C2B-C3B	-2.02	104.19	106.51

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	203	PEB	NB-C1B-CHA-C4A
3	B	203	PEB	C2B-C1B-CHA-C4A
3	C	207	PEB	NB-C1B-CHA-C4A
3	C	207	PEB	C2B-C1B-CHA-C4A
3	A	202	PEB	NB-C1B-CHA-C4A
3	A	202	PEB	C2B-C1B-CHA-C4A
3	B	204	PEB	C2A-C3A-CAA-CBA
3	B	204	PEB	C4A-C3A-CAA-CBA
3	B	204	PEB	NB-C1B-CHA-C4A
3	B	204	PEB	C2B-C1B-CHA-C4A
3	C	206	PEB	C2B-C1B-CHA-C4A
3	A	201	PEB	C2C-C1C-CHB-C4B
3	A	201	PEB	C2B-C1B-CHA-C4A
3	D	209	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
3	D	209	PEB	C2B-C1B-CHA-C4A
3	B	205	PEB	C2D-C3D-CAD-CBD
3	B	205	PEB	C4D-C3D-CAD-CBD
3	B	205	PEB	NB-C1B-CHA-C4A
3	B	205	PEB	C2B-C1B-CHA-C4A
3	D	210	PEB	C2D-C3D-CAD-CBD
3	D	210	PEB	C4D-C3D-CAD-CBD
3	D	210	PEB	NB-C1B-CHA-C4A
3	D	210	PEB	C2B-C1B-CHA-C4A
3	D	208	PEB	NB-C1B-CHA-C4A
3	D	208	PEB	C2B-C1B-CHA-C4A
3	C	206	PEB	NB-C1B-CHA-C4A
3	A	201	PEB	NB-C1B-CHA-C4A
3	C	207	PEB	C3B-CAB-CBB-CGB
3	D	209	PEB	C4A-C3A-CAA-CBA
3	A	202	PEB	NB-C4B-CHB-C1C
3	C	206	PEB	NA-C4A-CHA-C1B
3	A	202	PEB	C2B-C3B-CAB-CBB

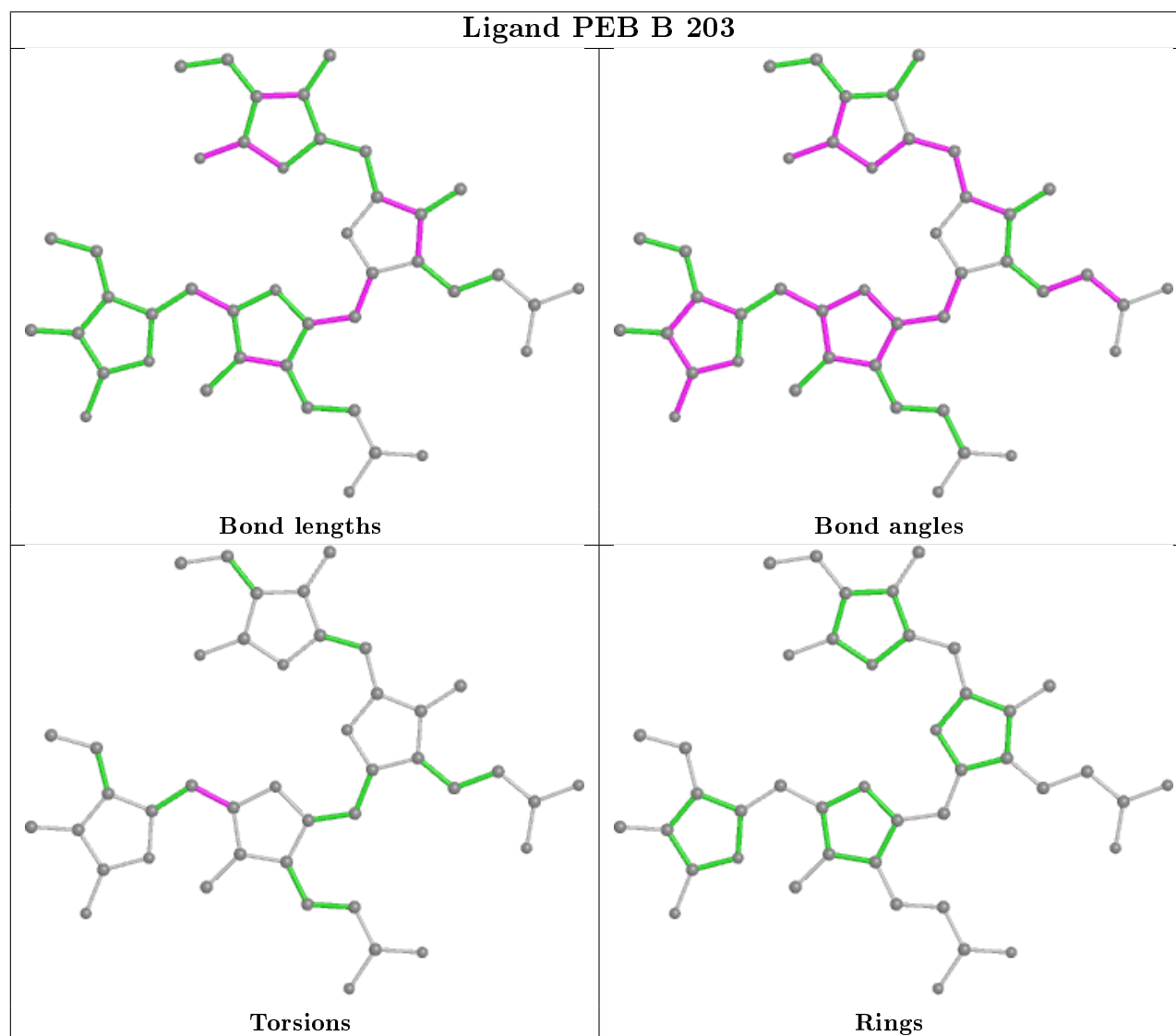
There are no ring outliers.

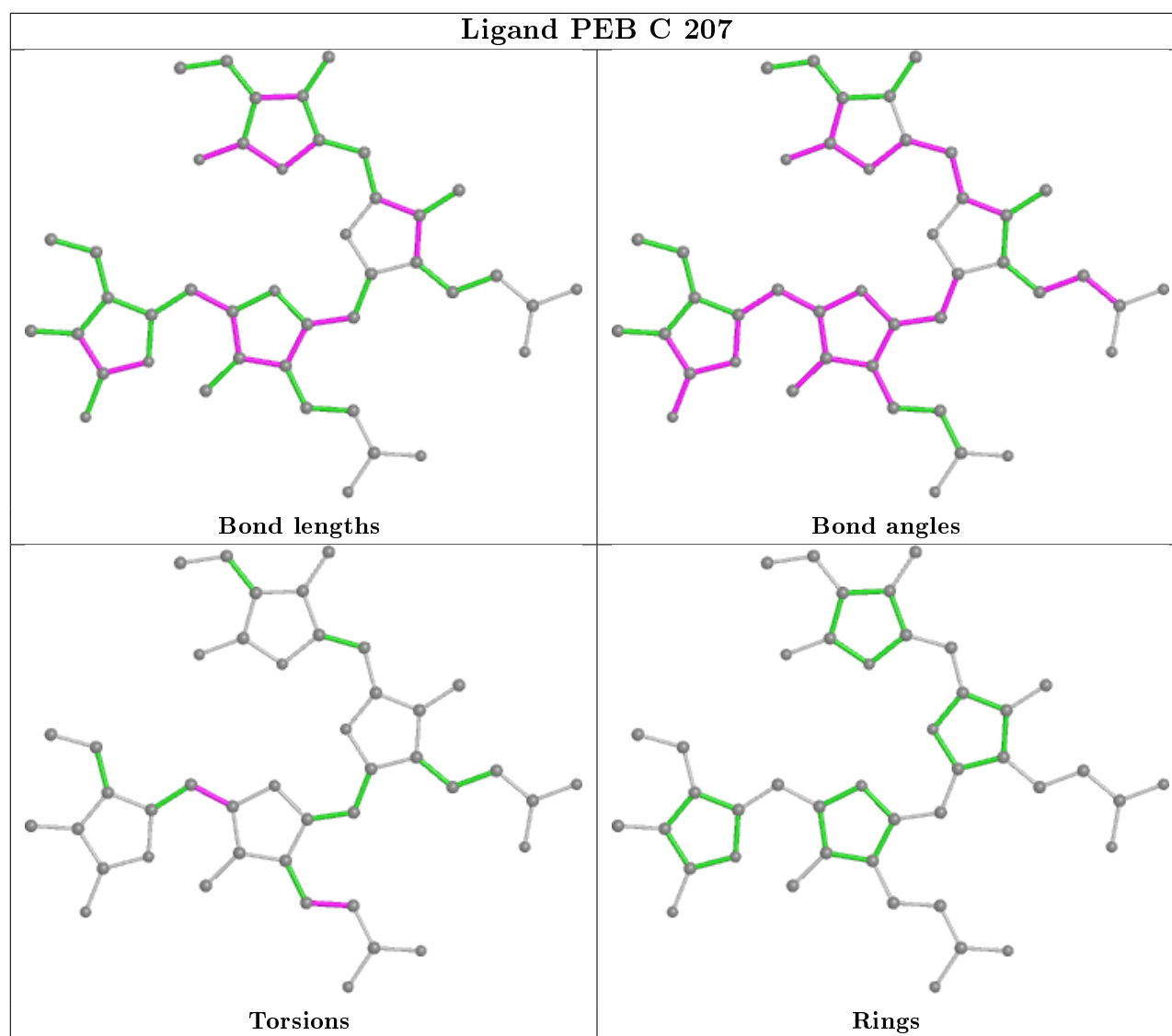
8 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	203	PEB	2	0
3	C	207	PEB	6	0
3	B	204	PEB	2	0
3	A	201	PEB	4	0
3	D	209	PEB	6	0
3	B	205	PEB	1	0
3	D	208	PEB	2	0
3	D	210	PEB	2	0

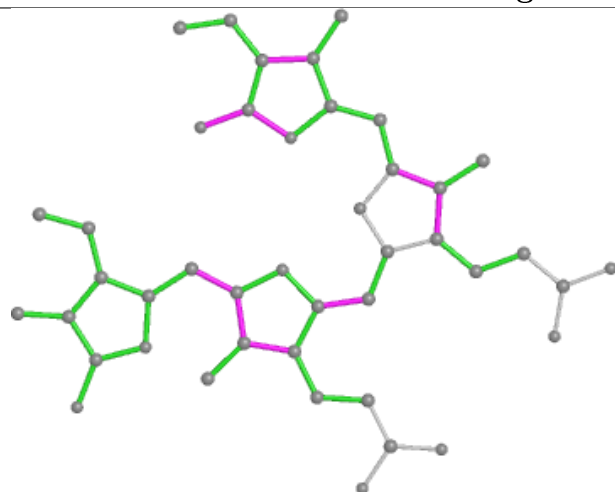
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

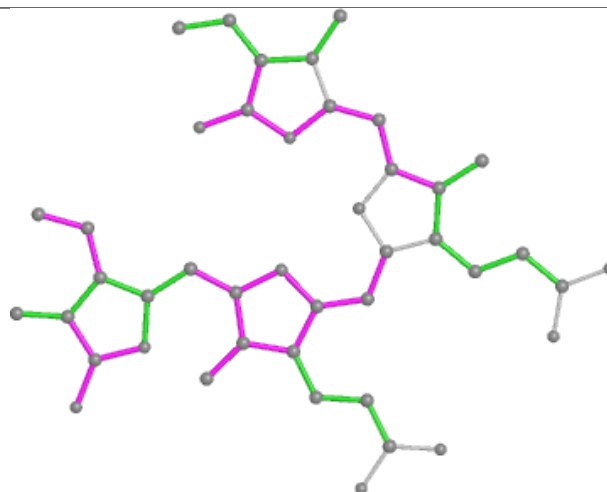




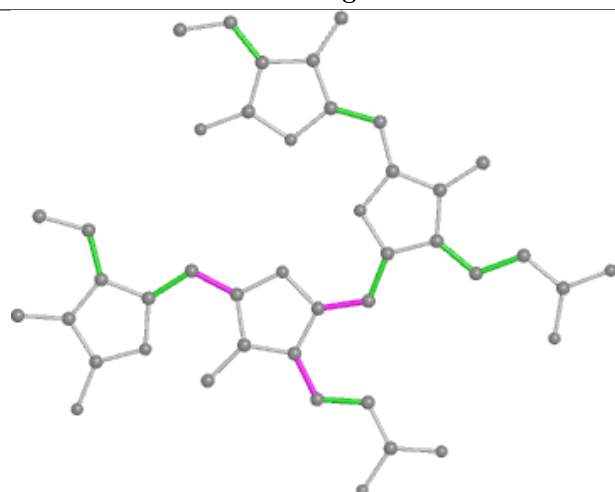
## Ligand PEB A 202



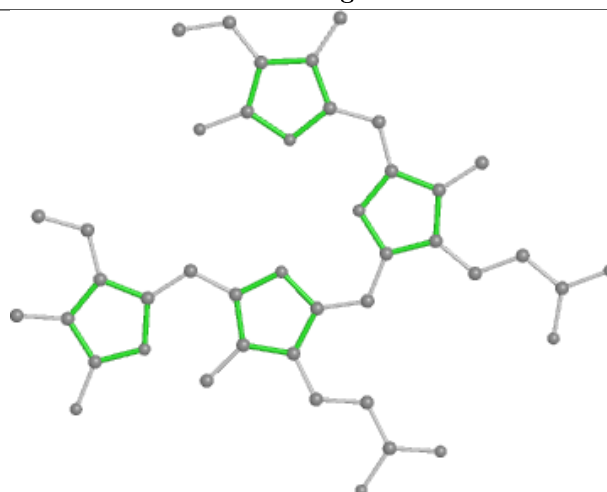
Bond lengths



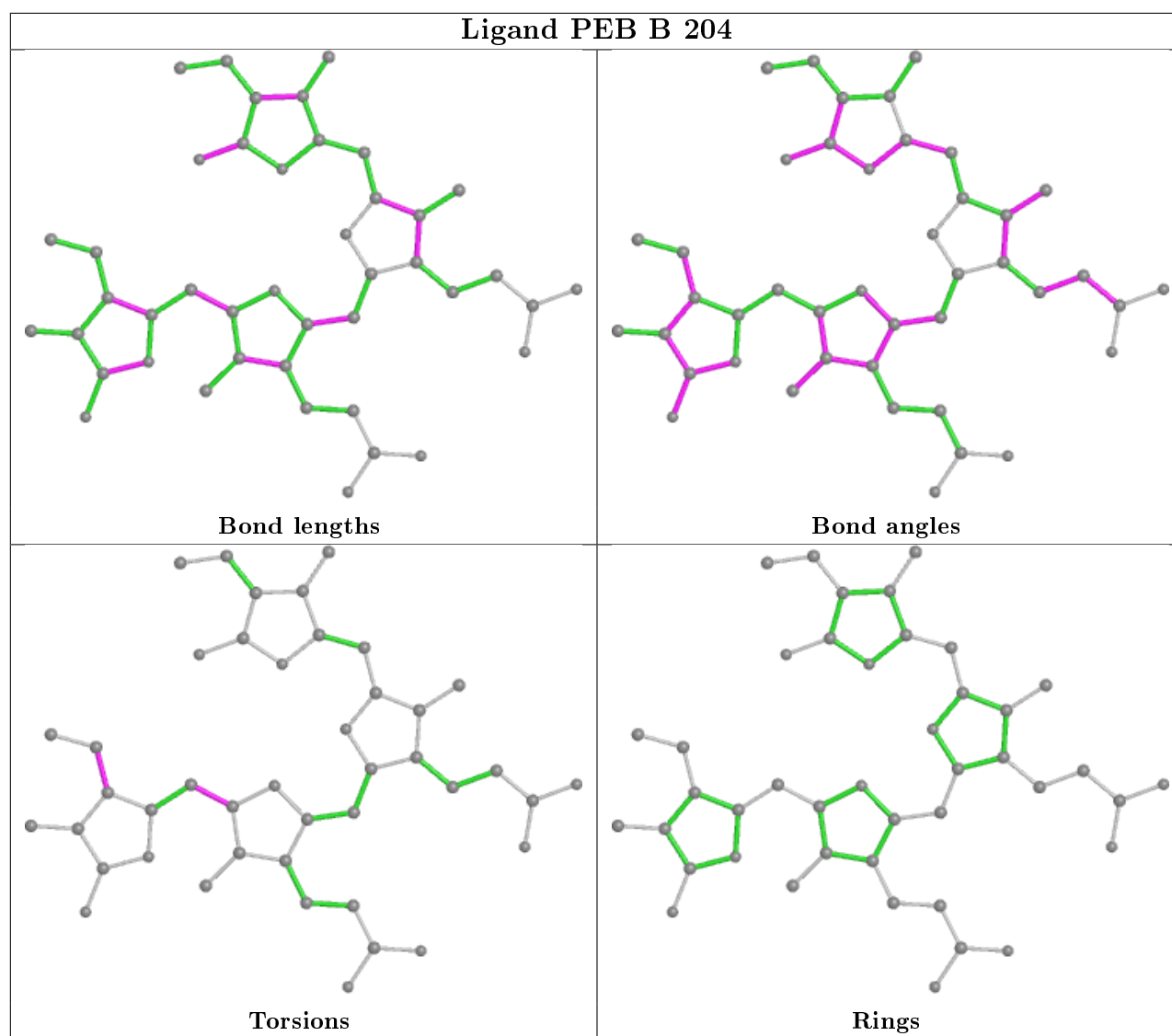
Bond angles

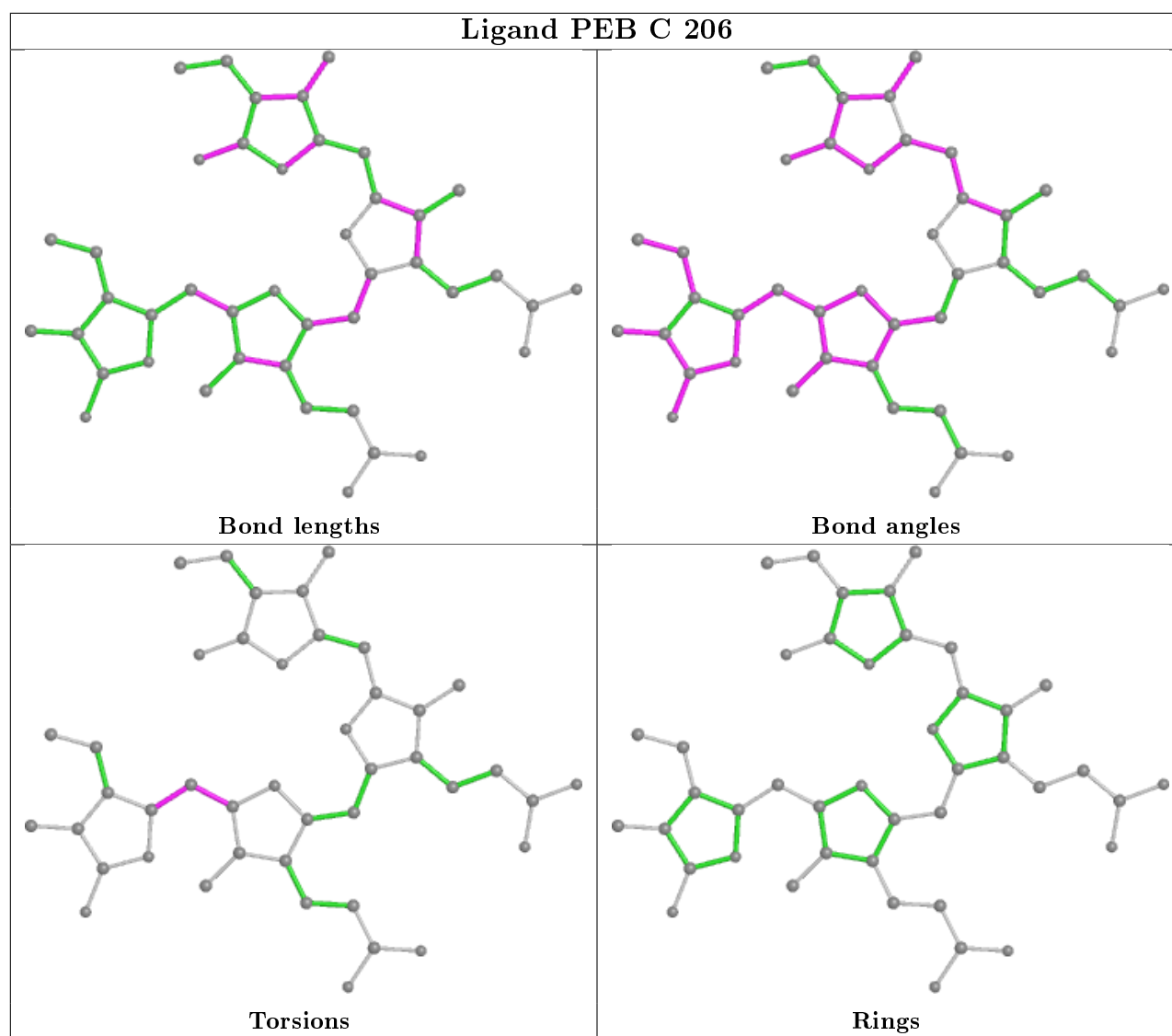


Torsions

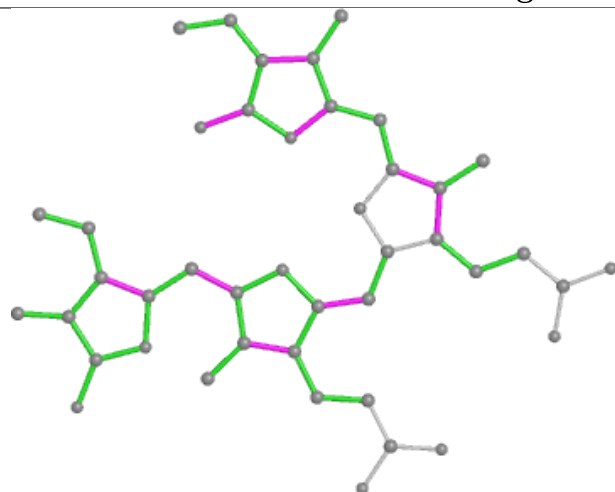


Rings

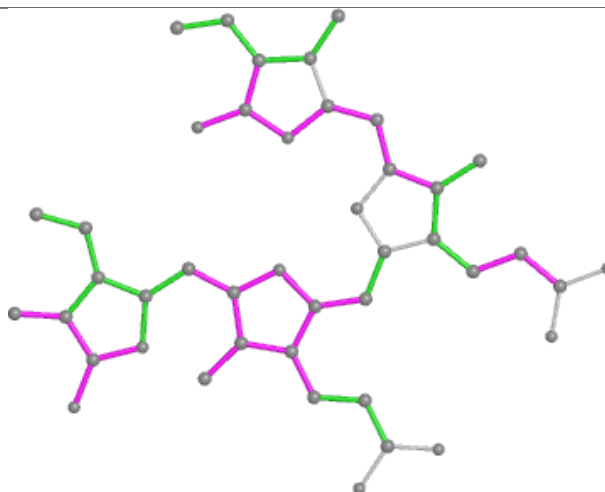




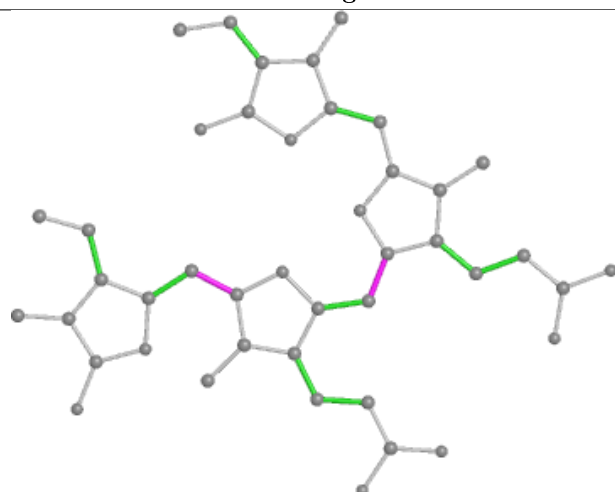
## Ligand PEB A 201



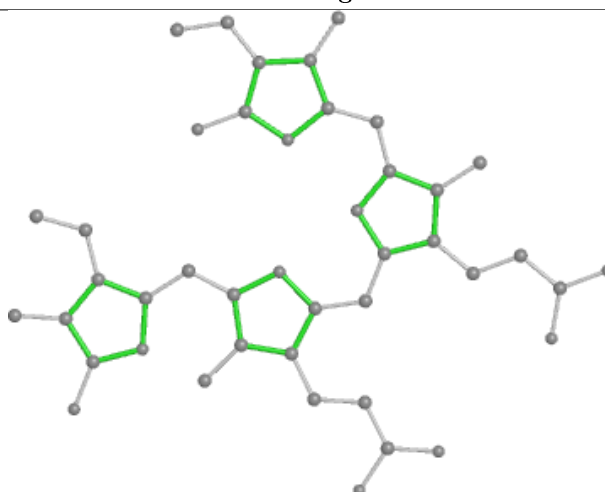
Bond lengths



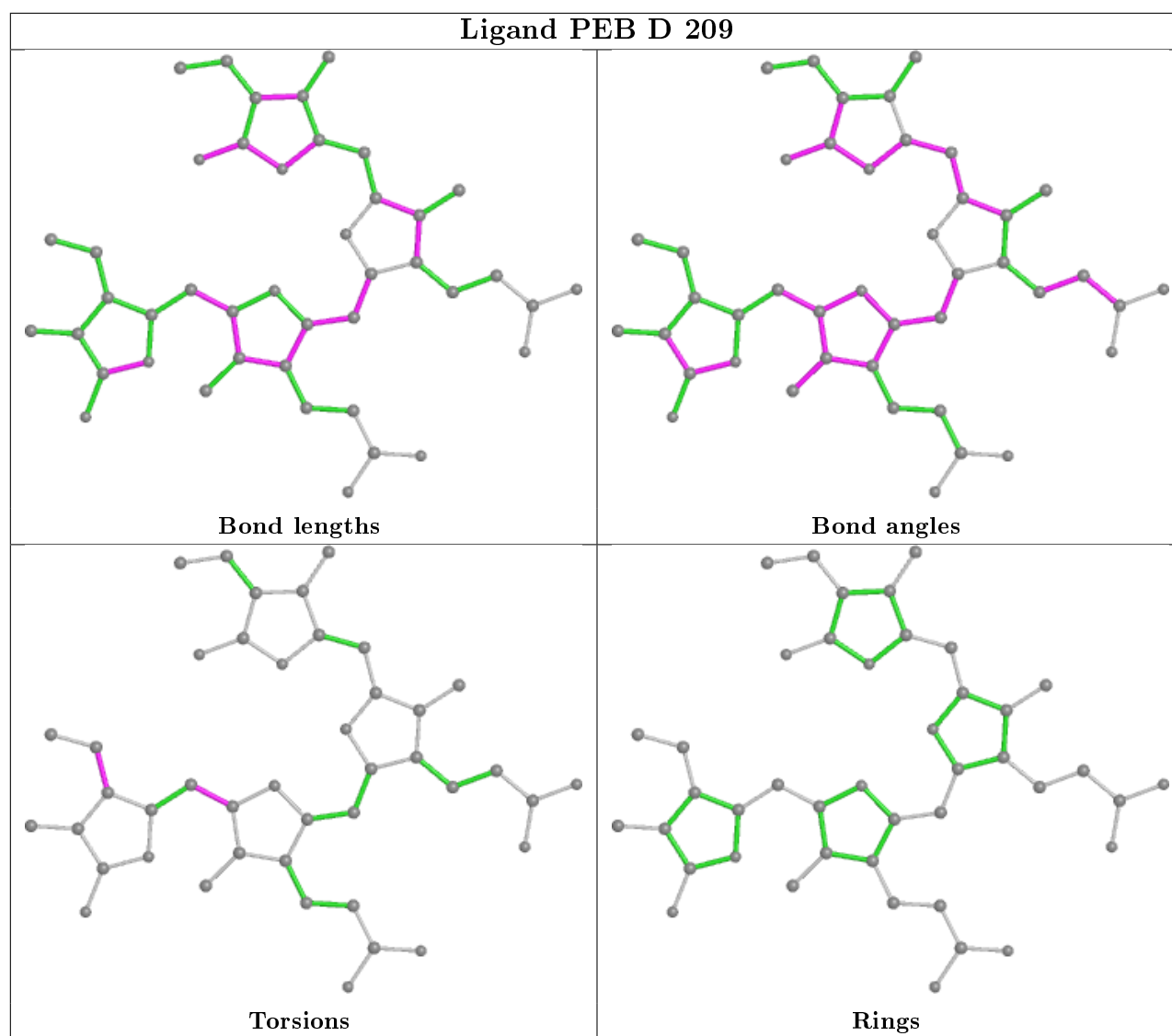
Bond angles

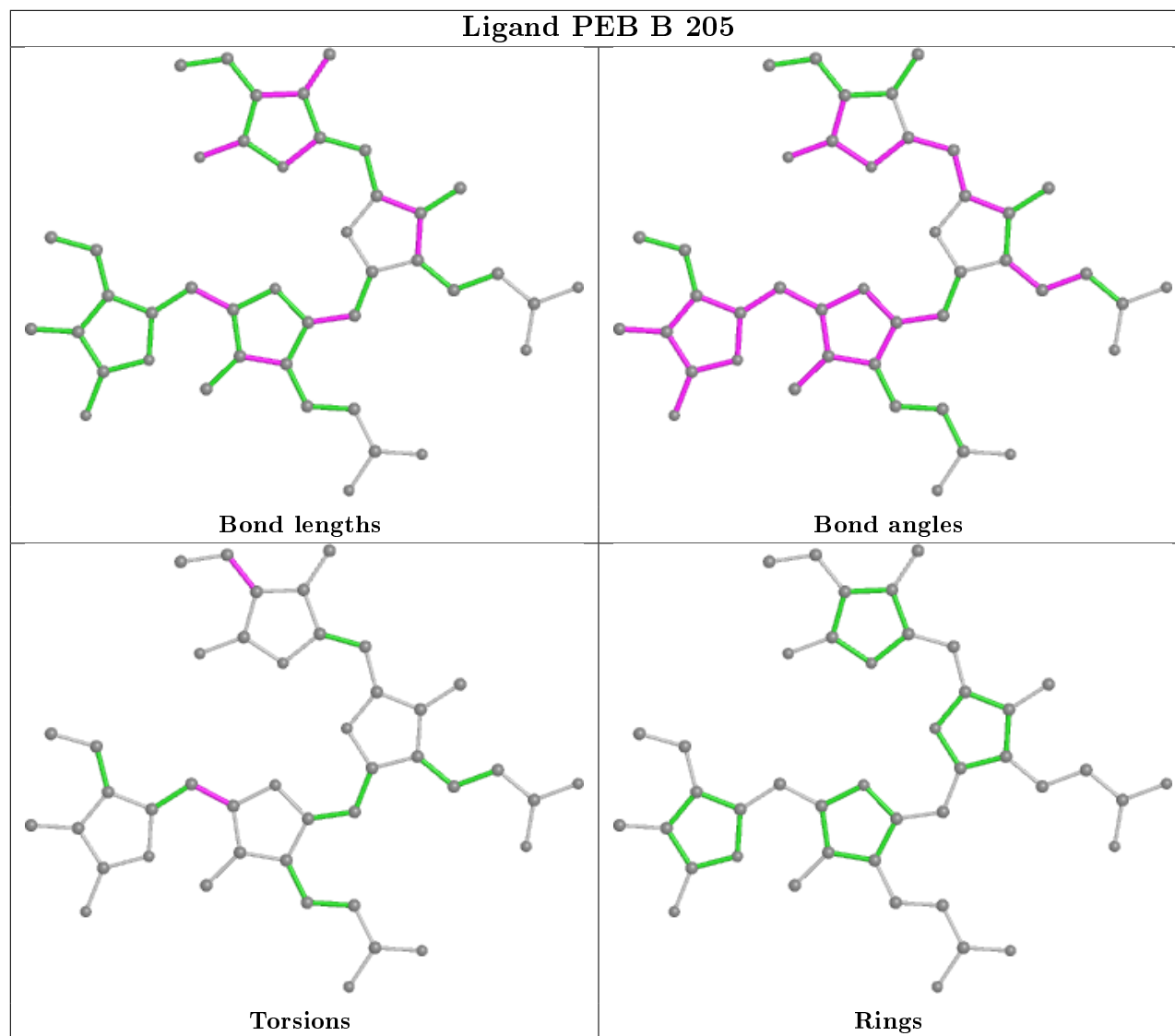


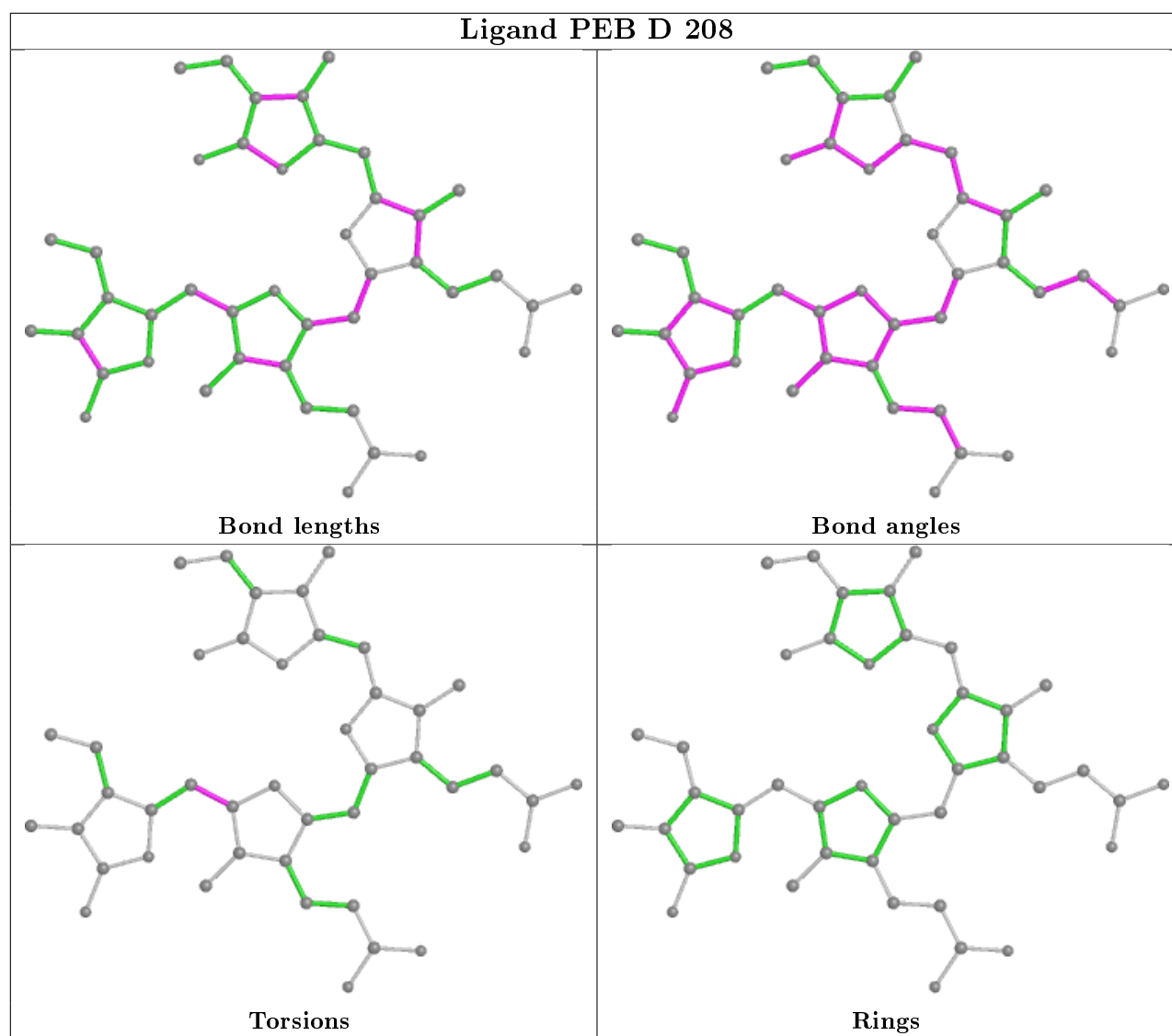
Torsions

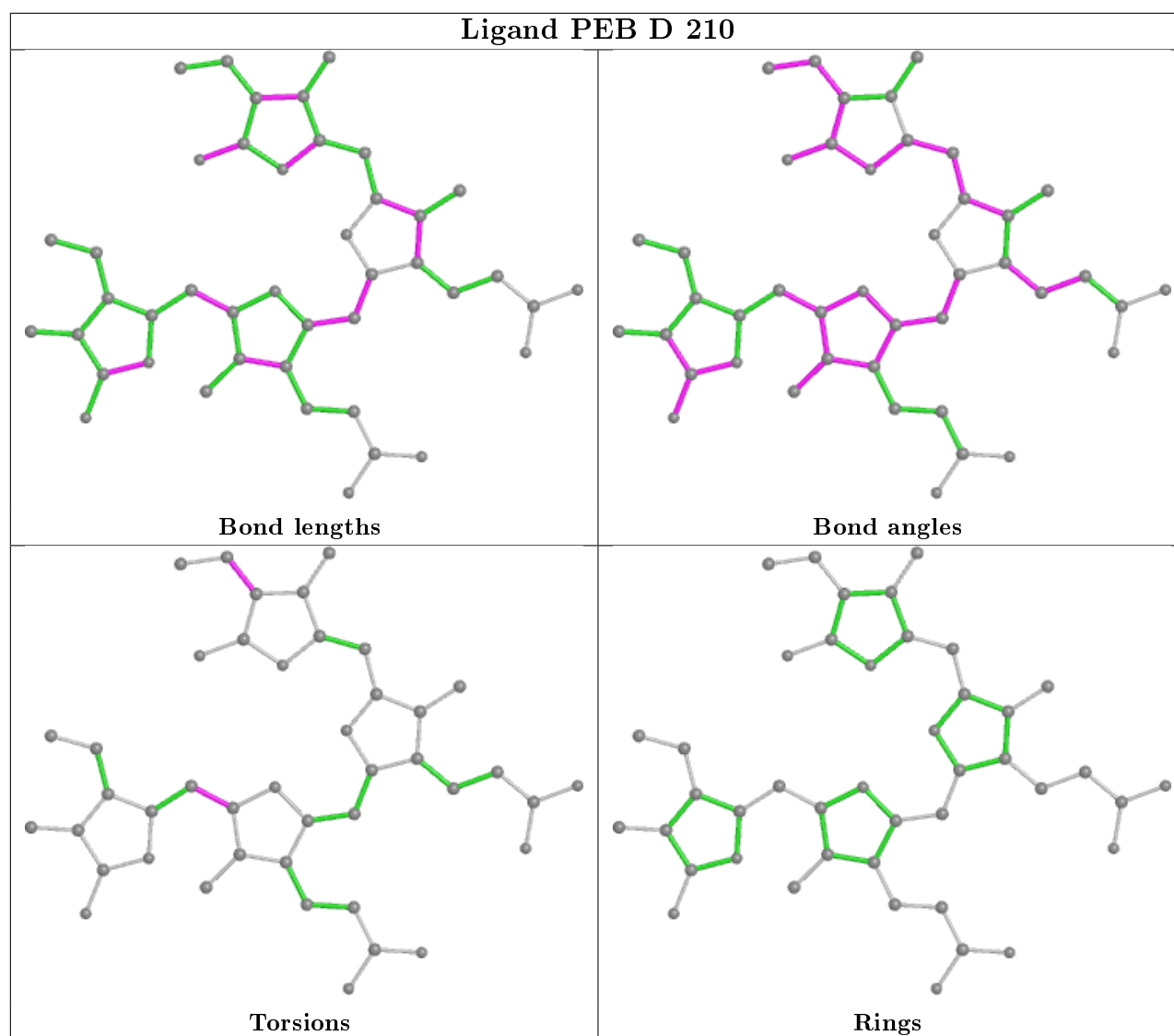


Rings









## 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 [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, 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	164/164 (100%)	-0.56	1 (0%) 89 89	10, 16, 31, 42	0
1	C	164/164 (100%)	-0.47	0 100 100	10, 18, 33, 49	0
2	B	176/177 (99%)	-0.51	1 (0%) 89 89	10, 16, 31, 49	0
2	D	176/177 (99%)	-0.49	2 (1%) 80 81	10, 17, 32, 52	0
All	All	680/682 (99%)	-0.51	4 (0%) 89 89	10, 17, 32, 52	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	111	ASN	2.6
2	D	25	GLN	2.1
1	A	69	PRO	2.0
2	B	25	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	MEN	D	72	9/10	0.97	0.08	15,15,18,19	0
2	MEN	B	72	9/10	0.98	0.06	14,16,18,18	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

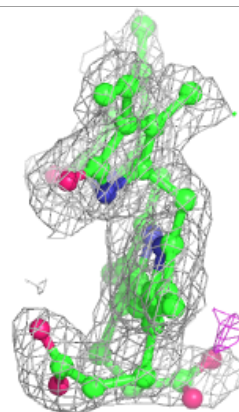
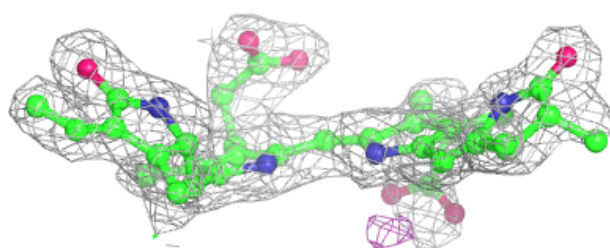
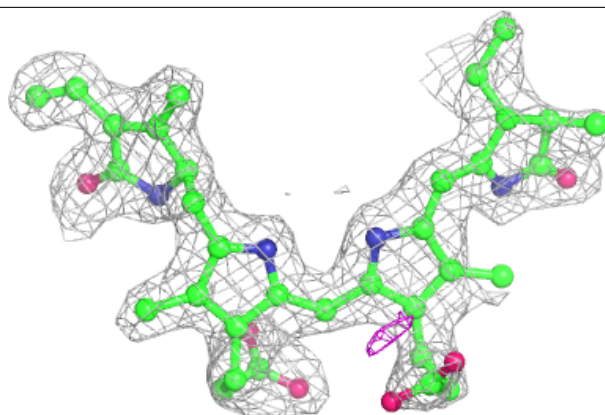
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEB	C	207	43/43	0.82	0.18	22,38,53,69	0
3	PEB	A	202	43/43	0.92	0.10	14,19,29,42	0
3	PEB	D	209	43/43	0.93	0.09	13,17,28,39	0
3	PEB	D	208	43/43	0.93	0.09	13,17,31,36	0
3	PEB	B	203	43/43	0.94	0.10	10,16,31,34	0
3	PEB	B	205	43/43	0.94	0.09	12,17,22,26	0
3	PEB	B	204	43/43	0.94	0.09	15,18,26,44	0
3	PEB	D	210	43/43	0.94	0.09	13,19,27,29	0
3	PEB	C	206	43/43	0.95	0.10	11,15,22,29	0
3	PEB	A	201	43/43	0.96	0.09	13,16,24,31	0
4	SO4	A	165	5/5	0.98	0.09	27,33,41,42	0

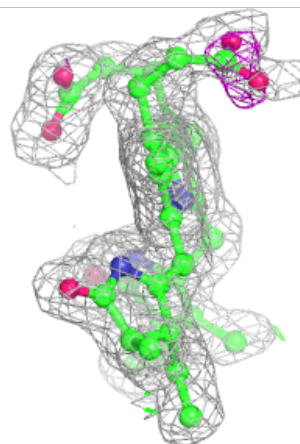
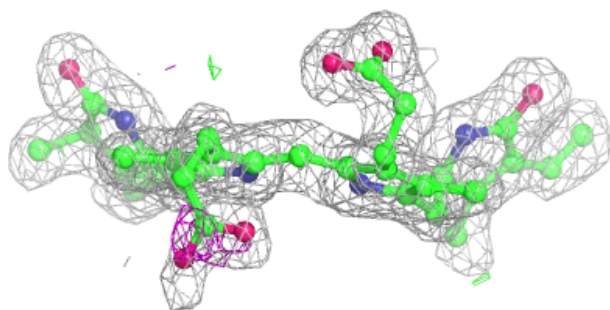
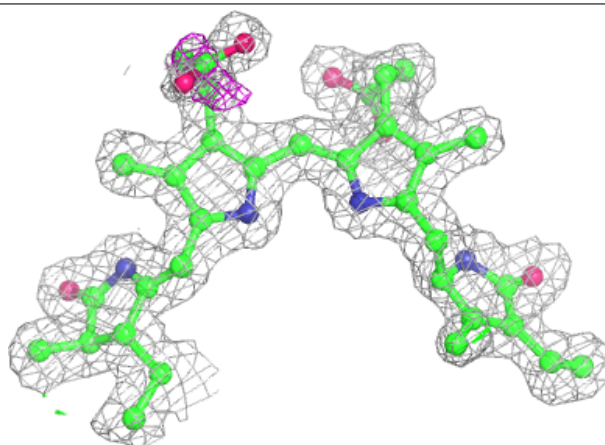
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PEB C 207:**

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

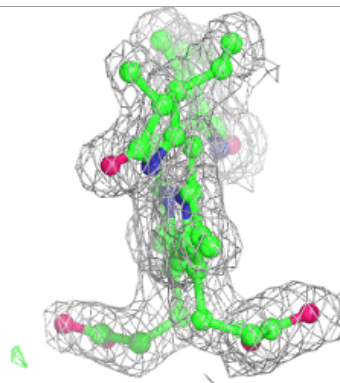
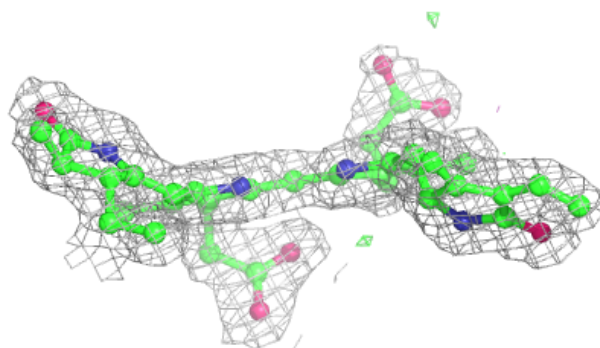
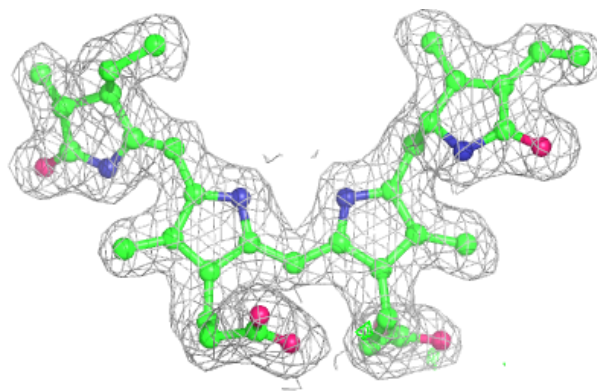
**Electron density around PEB A 202:**

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



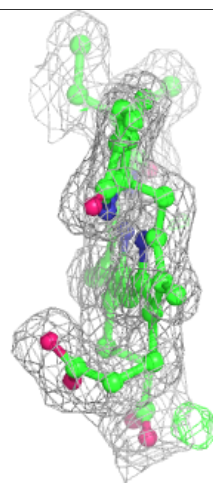
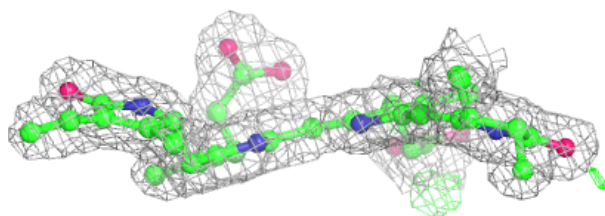
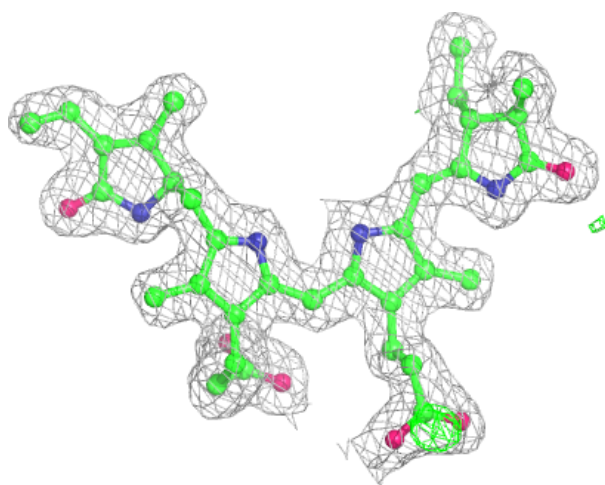
**Electron density around PEB D 209:**

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



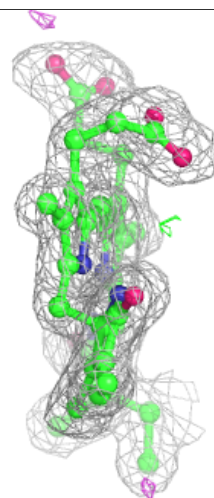
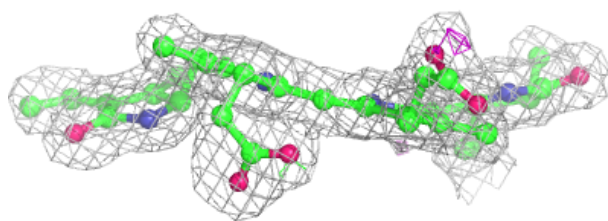
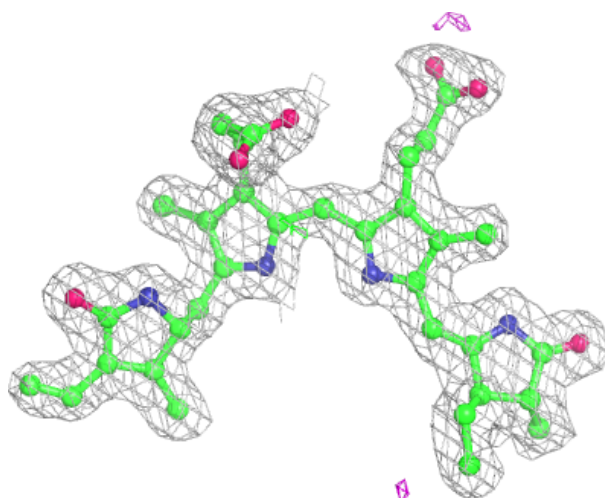
**Electron density around PEB D 208:**

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



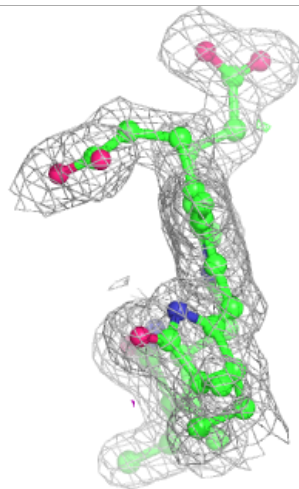
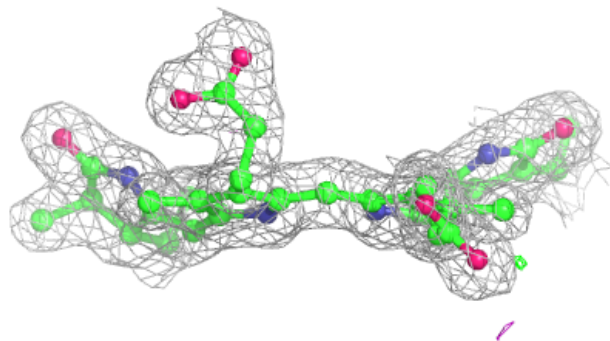
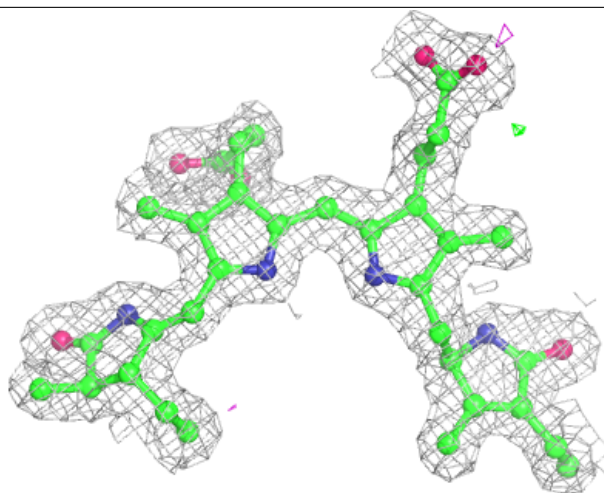
**Electron density around PEB B 203:**

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



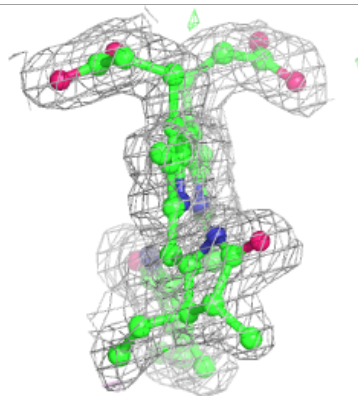
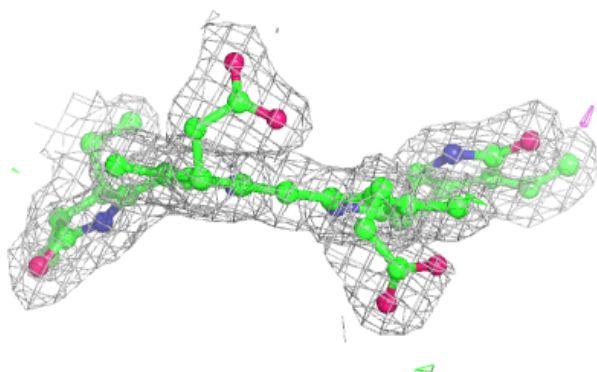
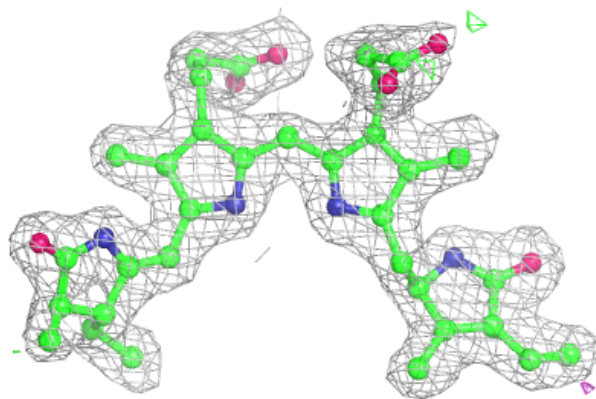
**Electron density around PEB B 205:**

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



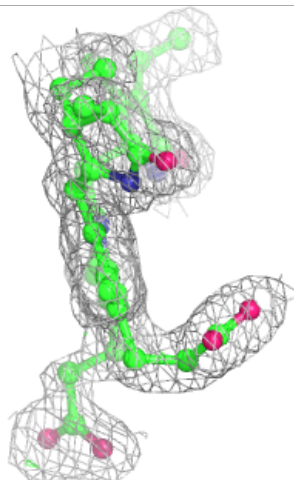
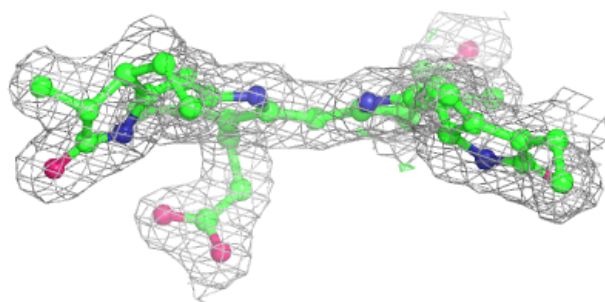
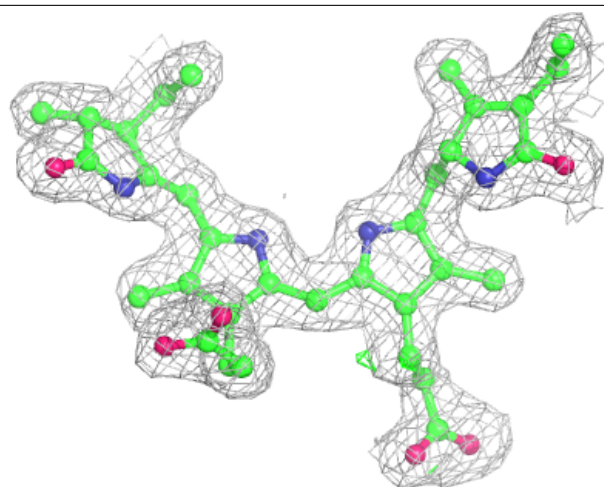
**Electron density around PEB B 204:**

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



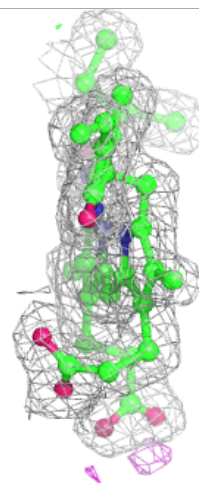
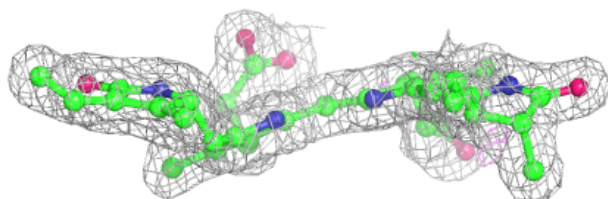
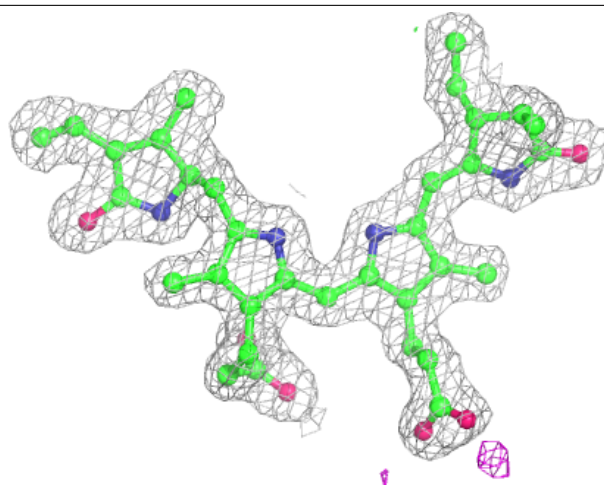
**Electron density around PEB D 210:**

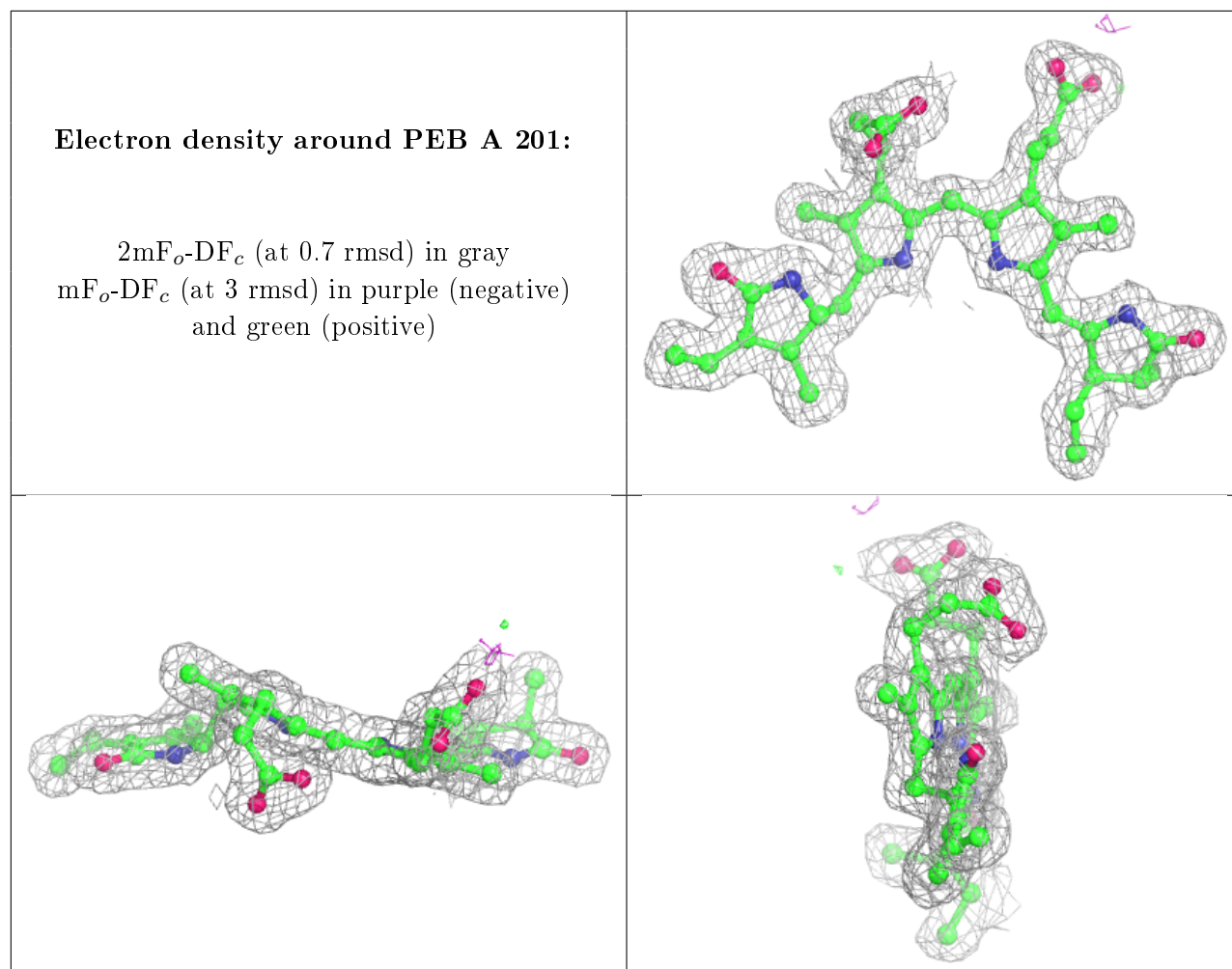
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PEB C 206:**

$2mF_o-DF_c$  (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.