wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2023 – 11:23 PM EDT

PDB ID	:	1XG0
Title	:	High resolution crystal structure of phycoerythrin 545 from the marine cryptophyte rhodomonas CS24
Authors	:	Doust, A.B.; Marai, C.N.J.; Harrop, S.J.; Wilk, K.E.; Curmi, P.M.G.; Scholes, G.D.
Deposited on	:	2004-09-16
Resolution	:	0.97 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 (1)) were used in the production of this report:

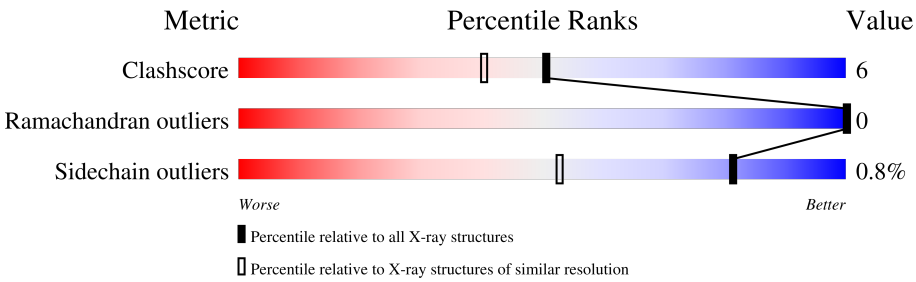
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 0.97 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))
Clashscore	141614	1241 (1.06-0.90)
Ramachandran outliers	138981	1159 (1.06-0.90)
Sidechain outliers	138945	1161 (1.06-0.90)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	76	97% .
2	B	67	90% 10%
3	C	177	93% 5% . .
3	D	177	94% . .

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5126 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-3 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	76	579	357	99	119	4	4	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	LYZ	LYS	modified residue	UNP Q00433

- Molecule 2 is a protein called Phycoerythrin alpha-2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	67	508	317	87	98	6	0	4	0

- Molecule 3 is a protein called B-phycoerythrin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	174	1303	802	223	268	10	14	9	0
3	D	177	1337	828	228	270	11	7	11	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	50	CYS	VAL	conflict	UNP P27198
C	56	VAL	TYR	conflict	UNP P27198
C	61	CYS	GLU	conflict	UNP P27198
C	65	SER	HIS	conflict	UNP P27198
C	72	MEN	ASN	modified residue	UNP P27198
C	73	CYS	GLU	conflict	UNP P27198
D	50	CYS	VAL	conflict	UNP P27198

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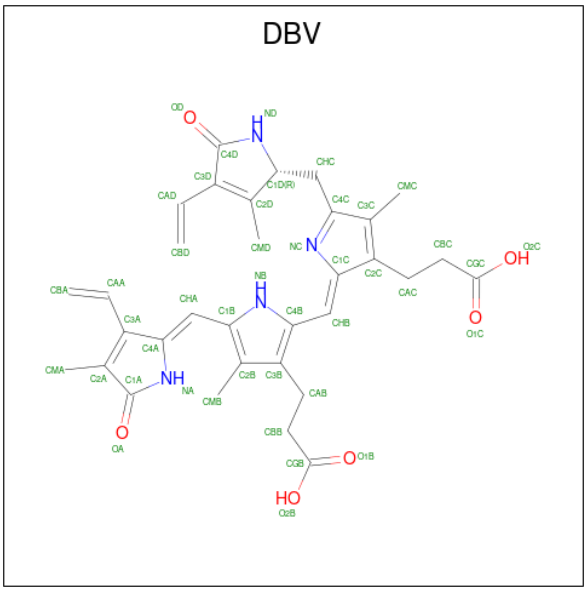
Chain	Residue	Modelled	Actual	Comment	Reference
D	56	VAL	TYR	conflict	UNP P27198
D	61	CYS	GLU	conflict	UNP P27198
D	65	SER	HIS	conflict	UNP P27198
D	72	MEN	ASN	modified residue	UNP P27198
D	73	CYS	GLU	conflict	UNP P27198

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
			Total	Mg		
4	D	1	1	1	0	0

- Molecule 5 is 15,16-DIHYDROBILIVERDIN (three-letter code: DBV) (formula: $C_{33}H_{36}N_4O_6$).

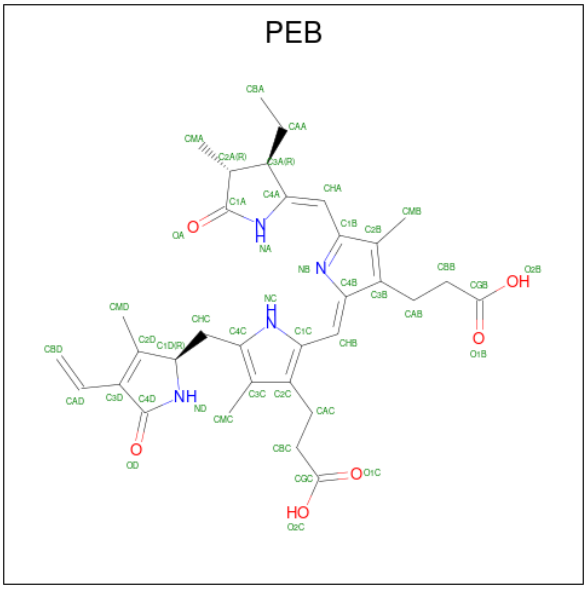


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	43	33	4	6	0	0
			Total	C	N	O		
5	B	1	43	33	4	6	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
6	C	1	1	1	0	0

- Molecule 7 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: $C_{33}H_{40}N_4O_6$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	199	199	199	0	0
			Total	O		
8	B	169	169	169	0	0
			Total	O		
8	C	301	301	301	1	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	D	383	383	383	0	0

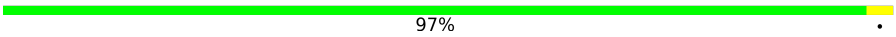
3 Residue-property plots (i)

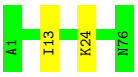
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: Phycoerythrin alpha-3 chain

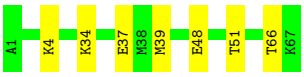
Chain A:





• Molecule 2: Phycoerythrin alpha-2 chain

Chain B:

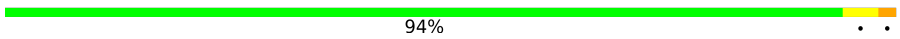


• Molecule 3: B-phycoerythrin beta chain

Chain C:

• Molecule 3: B-phycoerythrin beta chain

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.98Å 82.76Å 89.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.86 – 0.97	Depositor
% Data completeness (in resolution range)	89.5 (60.86-0.97)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.107 , 0.126	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5126	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

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: CL, DBV, PEB, MEN, MG, LYZ

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	0.83	0/588	0.90	2/782 (0.3%)
2	B	0.82	1/524 (0.2%)	0.81	0/696
3	C	0.81	1/1337 (0.1%)	0.87	3/1801 (0.2%)
3	D	0.78	1/1373 (0.1%)	0.87	2/1849 (0.1%)
All	All	0.80	3/3822 (0.1%)	0.86	7/5128 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	GLU	CD-OE1	-6.13	1.19	1.25
3	D	31	ILE	CA-C	5.80	1.68	1.52
3	C	91	ARG	NE-CZ	5.23	1.39	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	77	ARG	NE-CZ-NH2	-7.42	116.59	120.30
3	C	30	PHE	CB-CG-CD2	-6.61	116.17	120.80
3	C	91	ARG	NE-CZ-NH1	-6.04	117.28	120.30
3	C	30	PHE	CB-CG-CD1	5.86	124.90	120.80
1	A	13[A]	ILE	CA-CB-CG1	5.69	121.81	111.00

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	579	0	584	3	0
2	B	508	0	549	9	0
3	C	1303	0	1312	9	2
3	D	1337	0	1370	13	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	43	0	33	2	0
5	B	43	0	33	2	0
6	C	1	0	0	1	0
7	C	129	0	110	5	0
7	D	129	0	111	3	0
8	A	199	0	0	6	0
8	B	169	0	0	5	0
8	C	301	0	0	8	2
8	D	383	0	0	10	0
All	All	5126	0	4102	46	2

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.

The worst 5 of 46 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24[B]:LYS:HE3	8:A:2190:HOH:O	1.22	1.30
3:C:155[A]:GLN:HG2	8:C:3146:HOH:O	1.33	1.28
8:A:2065:HOH:O	3:D:149[B]:LYS:HE3	1.32	1.27
3:C:108:ARG:HD2	8:C:3197:HOH:O	1.67	0.95
2:B:34[B]:LYS:CE	8:B:1167:HOH:O	2.14	0.94

All (2) 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)
3:C:7:ARG:NH1	8:C:3255:HOH:O[2_564]	1.60	0.60
3:C:7:ARG:CZ	8:C:3255:HOH:O[2_564]	1.90	0.30

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	76/76 (100%)	74 (97%)	2 (3%)	0	100	100
2	B	69/67 (103%)	66 (96%)	3 (4%)	0	100	100
3	C	179/177 (101%)	178 (99%)	1 (1%)	0	100	100
3	D	185/177 (104%)	184 (100%)	1 (0%)	0	100	100
All	All	509/497 (102%)	502 (99%)	7 (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	A	63/60 (105%)	63 (100%)	0	100	100
2	B	55/51 (108%)	55 (100%)	0	100	100
3	C	148/141 (105%)	146 (99%)	2 (1%)	67	33
3	D	152/141 (108%)	149 (98%)	3 (2%)	55	20
All	All	418/393 (106%)	413 (99%)	5 (1%)	81	38

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	155[A]	GLN
3	C	155[B]	GLN

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Mol	Chain	Res	Type
3	D	111	ASN
3	D	149[A]	LYS
3	D	149[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	111	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 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	$\#\|Z\| > 2$
3	MEN	C	72	3	7,8,9	0.76	0	6,9,11	0.48	0
3	MEN	D	72	3	7,8,9	1.00	1 (14%)	6,9,11	0.35	0
1	LYZ	A	4	1	7,9,10	0.71	0	4,10,12	0.63	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
3	MEN	C	72	3	-	2/7/8/10	-
3	MEN	D	72	3	-	2/7/8/10	-
1	LYZ	A	4	1	-	0/8/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	72	MEN	CE2-ND2	2.41	1.49	1.45

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	72	MEN	CA-CB-CG-OD1
3	D	72	MEN	CA-CB-CG-OD1
3	D	72	MEN	CA-CB-CG-ND2
3	C	72	MEN	CA-CB-CG-ND2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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	$\#\|Z\| > 2$
7	PEB	D	282	3	43,46,46	1.34	4 (9%)	45,67,67	1.57	9 (20%)
5	DBV	A	219	1	42,46,46	1.21	2 (4%)	42,67,67	1.11	4 (9%)
7	PEB	C	282	3	43,46,46	1.44	3 (6%)	45,67,67	1.68	6 (13%)
7	PEB	D	258	3	43,46,46	2.18	8 (18%)	45,67,67	1.54	6 (13%)
7	PEB	D	250	3	43,46,46	1.60	5 (11%)	45,67,67	1.30	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DBV	B	219	2	42,46,46	1.44	2 (4%)	42,67,67	1.32	5 (11%)
7	PEB	C	258	3	43,46,46	1.61	4 (9%)	45,67,67	1.47	8 (17%)
7	PEB	C	250	3	43,46,46	1.84	7 (16%)	45,67,67	1.43	6 (13%)

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
7	PEB	D	282	3	-	2/24/74/74	0/4/4/4
5	DBV	A	219	1	-	6/26/74/74	0/4/4/4
7	PEB	C	282	3	-	4/24/74/74	0/4/4/4
7	PEB	D	258	3	-	6/24/74/74	0/4/4/4
7	PEB	D	250	3	-	6/24/74/74	0/4/4/4
5	DBV	B	219	2	-	6/26/74/74	0/4/4/4
7	PEB	C	258	3	-	7/24/74/74	0/4/4/4
7	PEB	C	250	3	-	4/24/74/74	0/4/4/4

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	250	PEB	CHB-C4B	8.62	1.42	1.35
7	D	258	PEB	CBB-CGB	-7.58	1.32	1.50
7	D	250	PEB	CHB-C4B	6.60	1.40	1.35
7	C	258	PEB	CHB-C4B	6.55	1.40	1.35
7	D	258	PEB	C3A-C4A	6.33	1.60	1.50

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	282	PEB	C1C-CHB-C4B	5.30	135.14	128.81
7	D	258	PEB	C1C-CHB-C4B	4.95	134.72	128.81
7	C	282	PEB	CHA-C4A-NA	4.33	130.35	125.20
7	C	258	PEB	C1C-CHB-C4B	4.20	133.82	128.81
7	D	282	PEB	C1C-CHB-C4B	4.18	133.80	128.81

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	219	DBV	C2A-C3A-CAA-CBA
5	A	219	DBV	C4A-C3A-CAA-CBA
5	A	219	DBV	NB-C1B-CHA-C4A
5	A	219	DBV	C2B-C1B-CHA-C4A
5	B	219	DBV	C2A-C3A-CAA-CBA

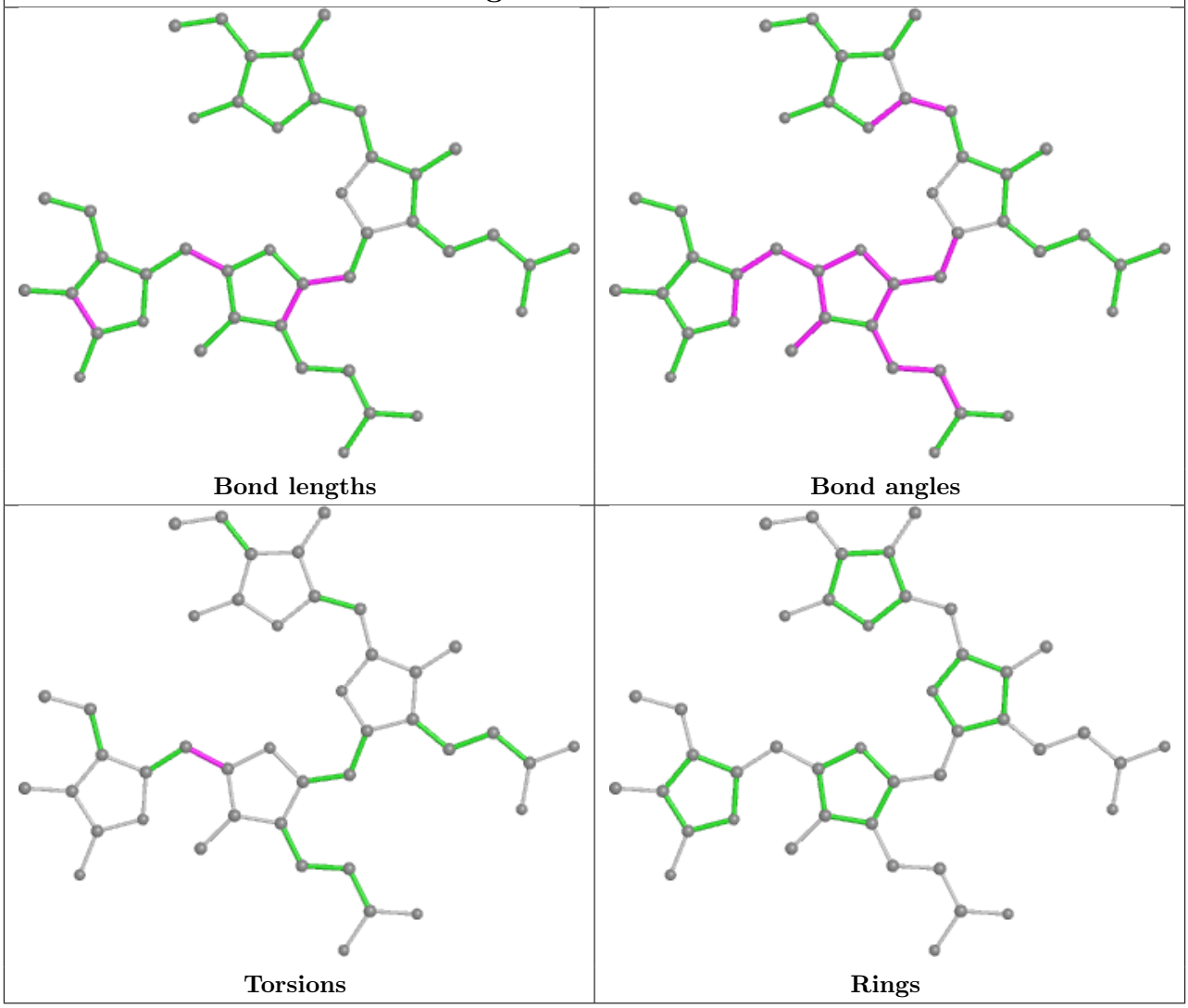
There are no ring outliers.

8 monomers are involved in 12 short contacts:

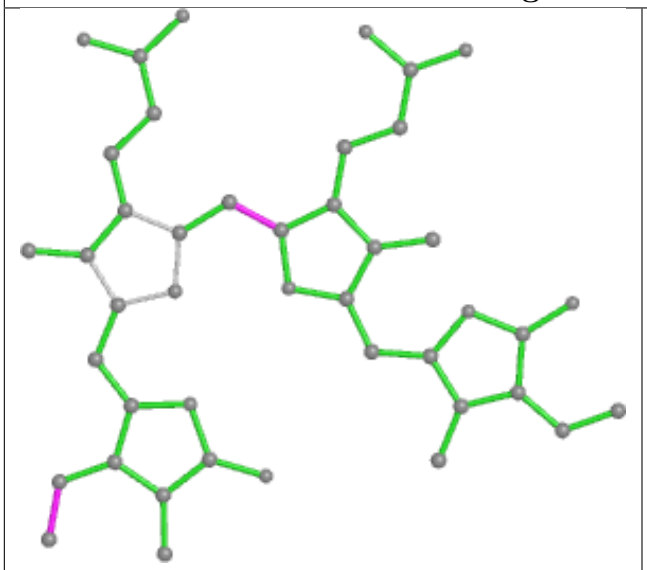
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	282	PEB	1	0
5	A	219	DBV	2	0
7	C	282	PEB	1	0
7	D	258	PEB	1	0
7	D	250	PEB	1	0
5	B	219	DBV	2	0
7	C	258	PEB	3	0
7	C	250	PEB	1	0

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.

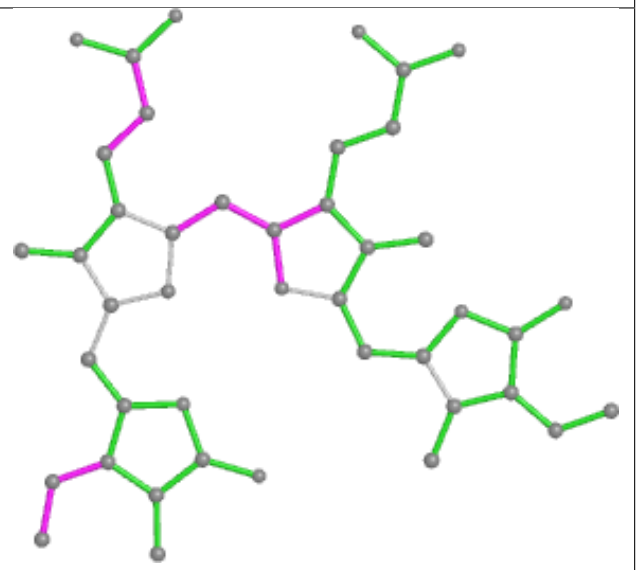
Ligand PEB D 282



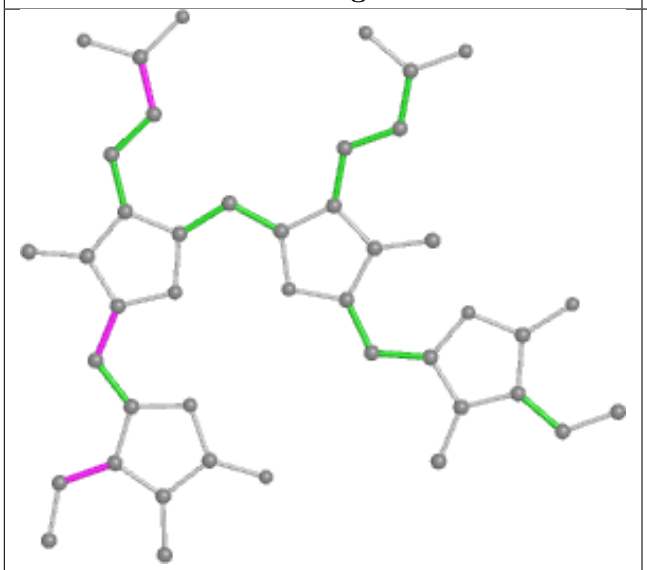
Ligand DBV A 219



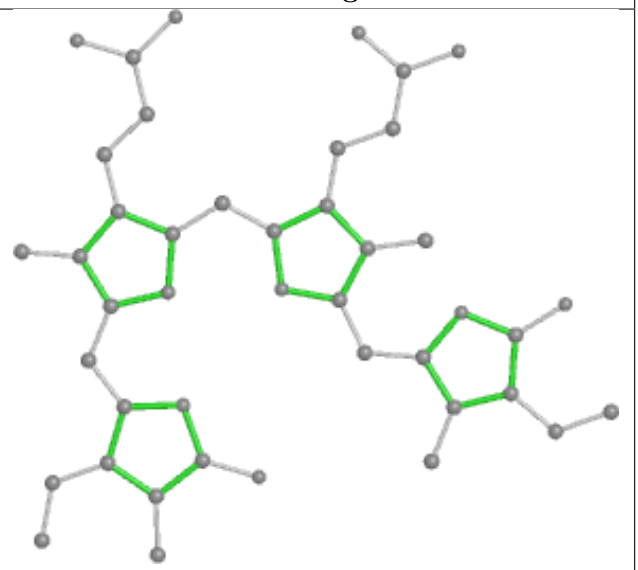
Bond lengths



Bond angles

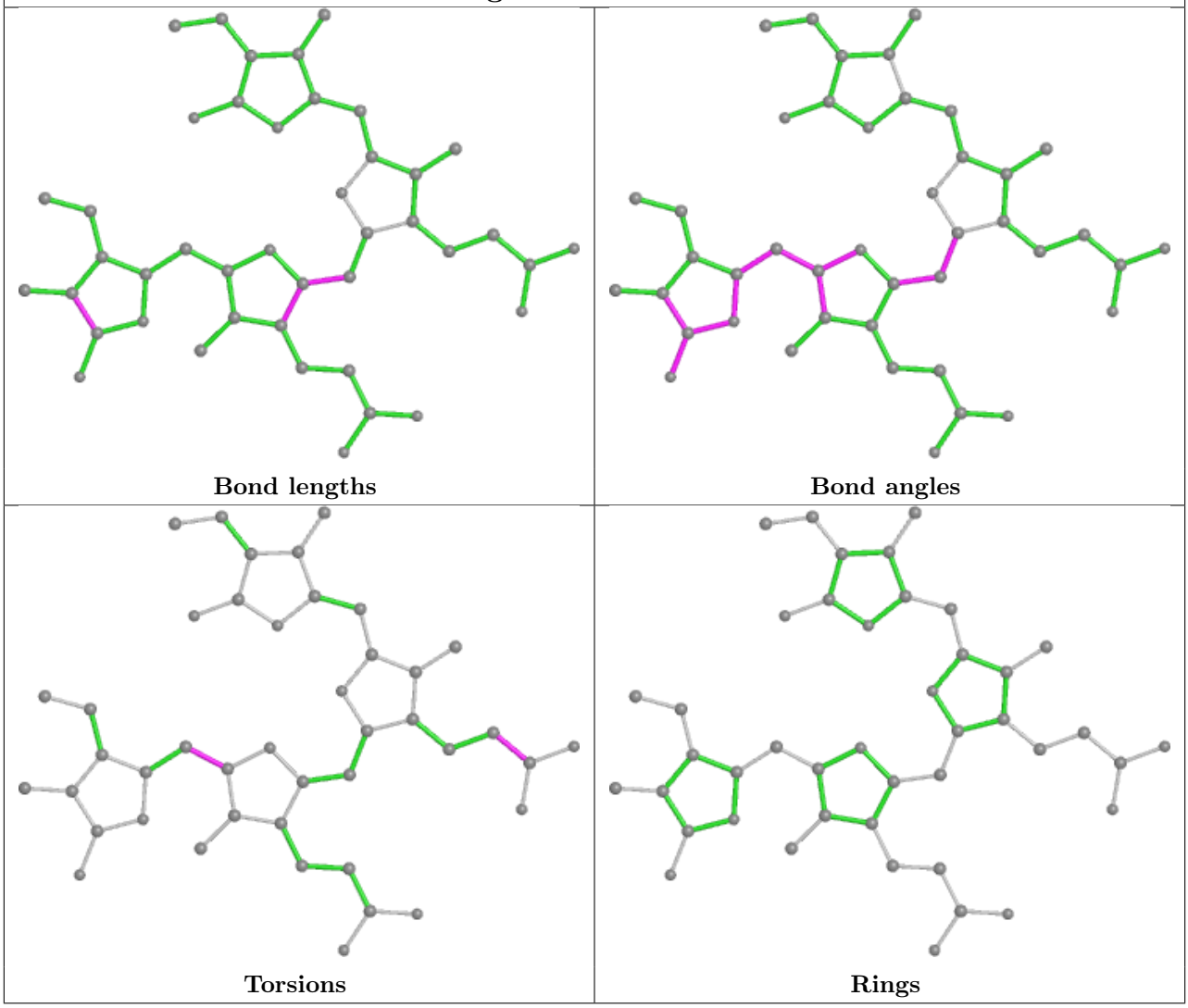


Torsions

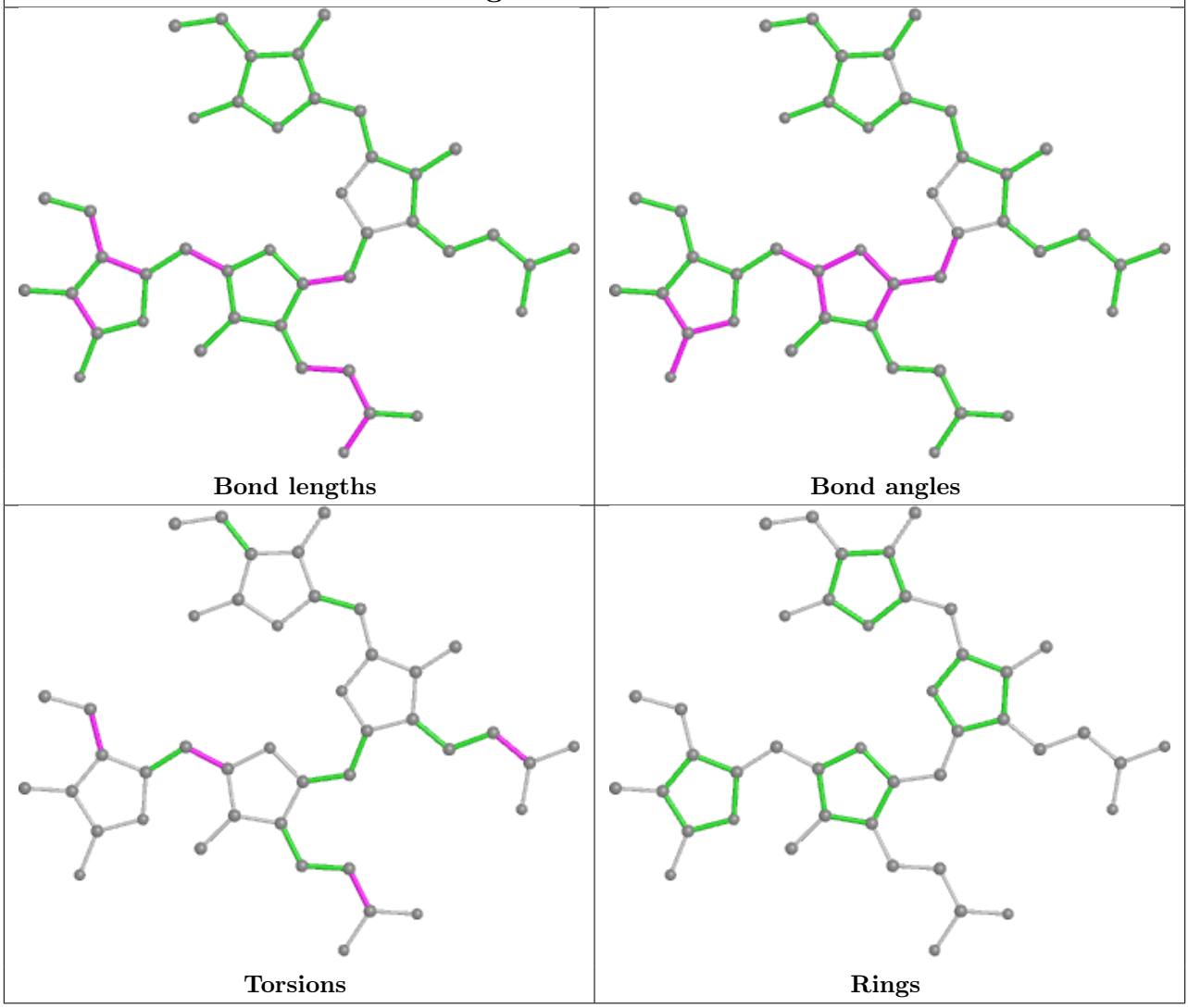


Rings

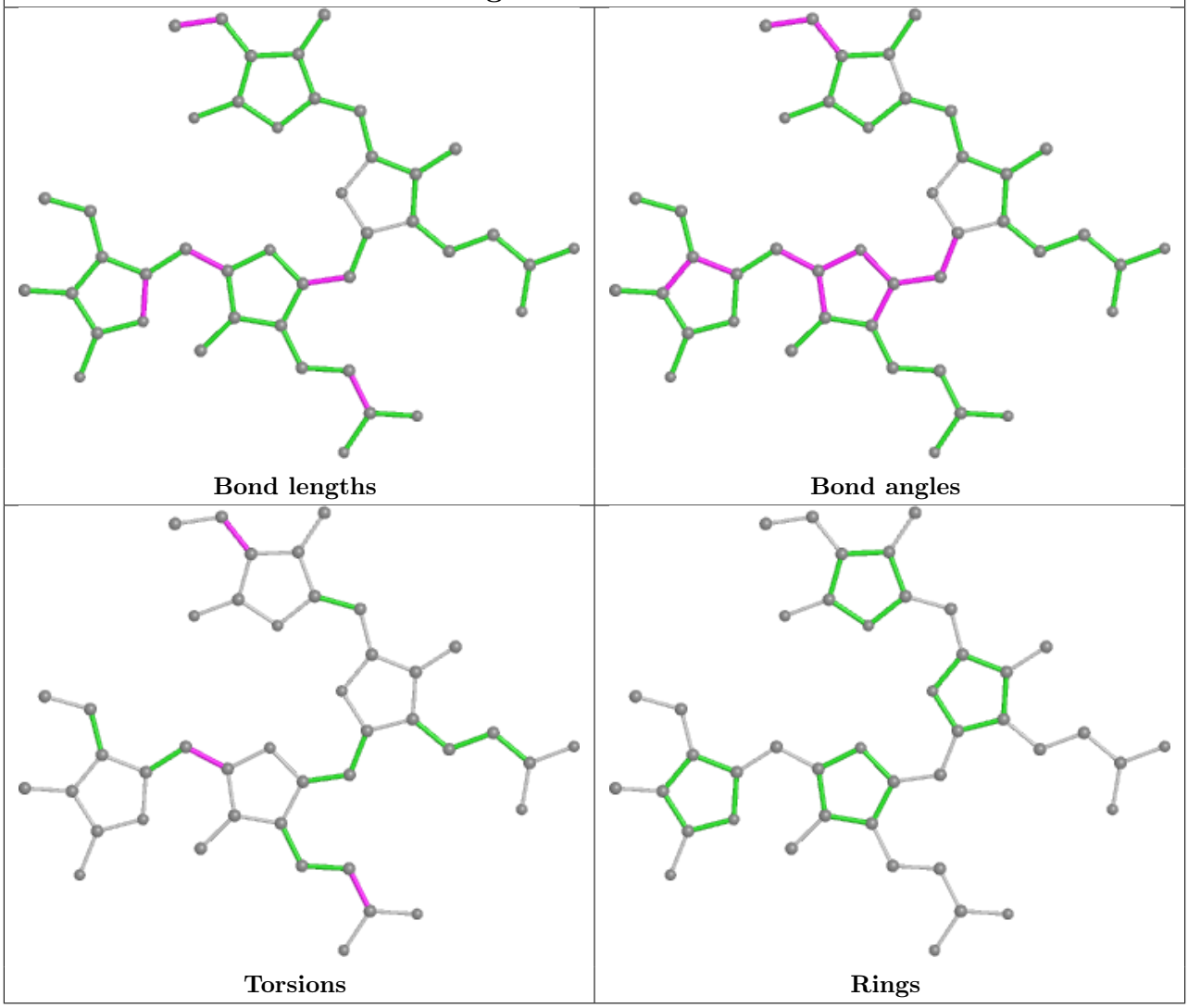
Ligand PEB C 282



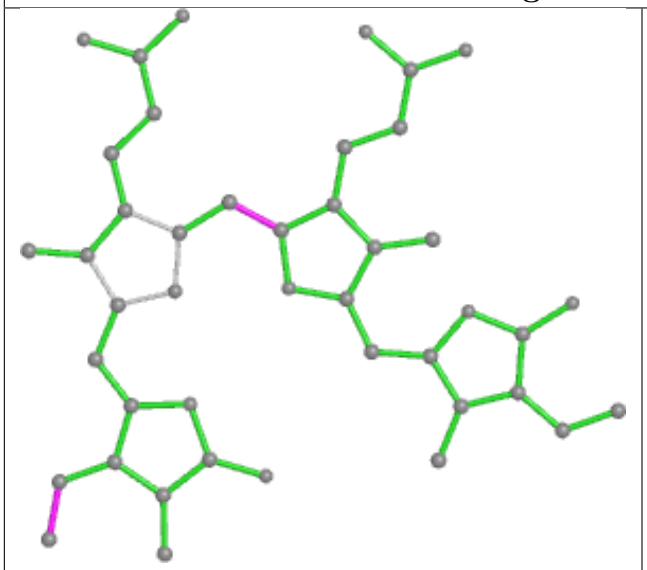
Ligand PEB D 258



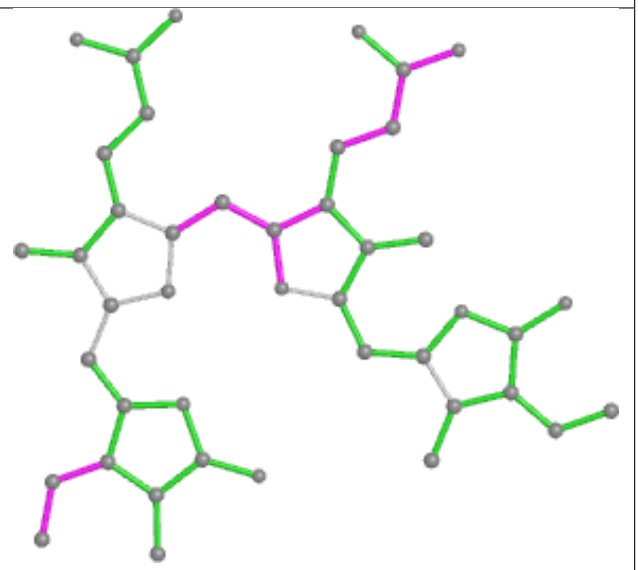
Ligand PEB D 250



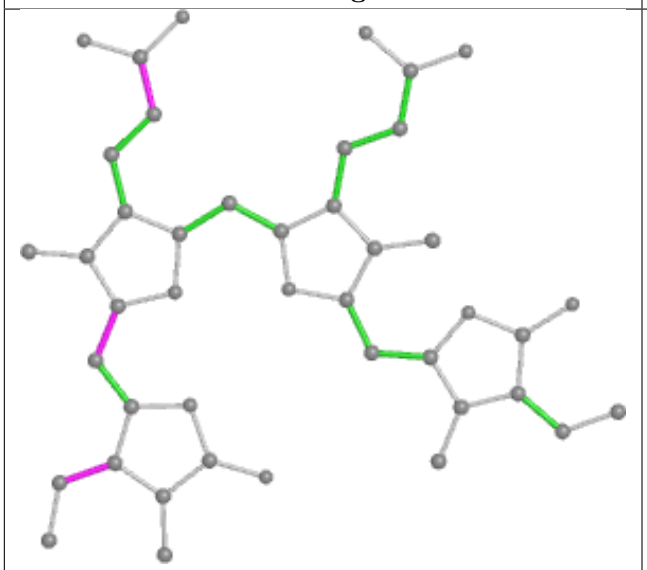
Ligand DBV B 219



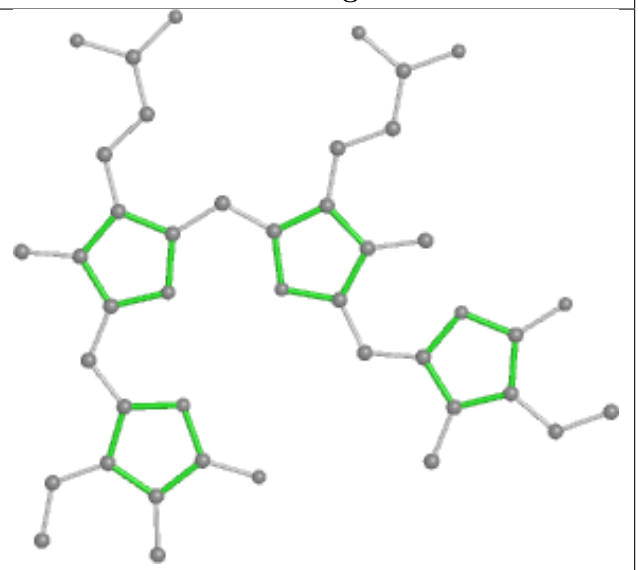
Bond lengths



Bond angles

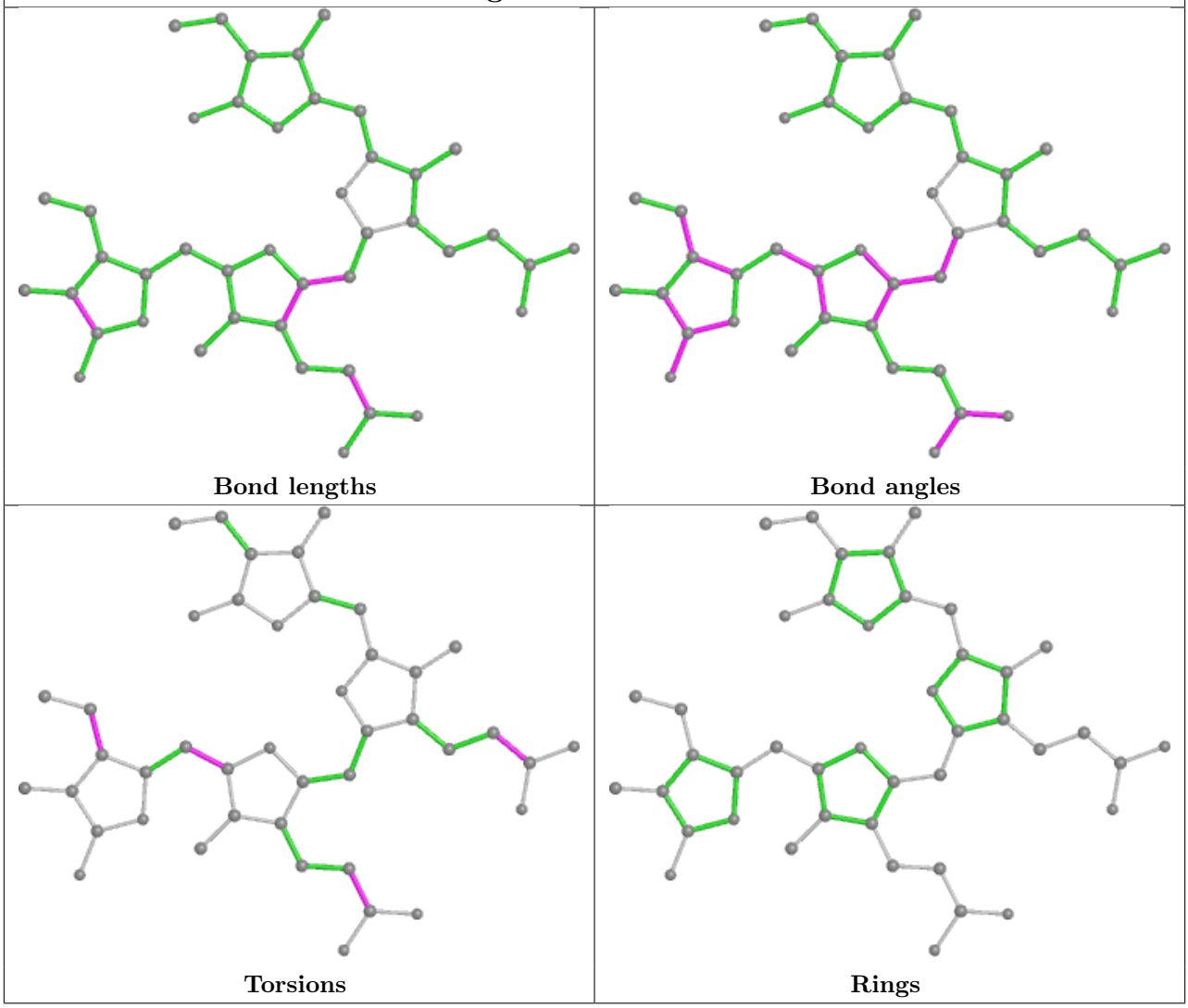


Torsions

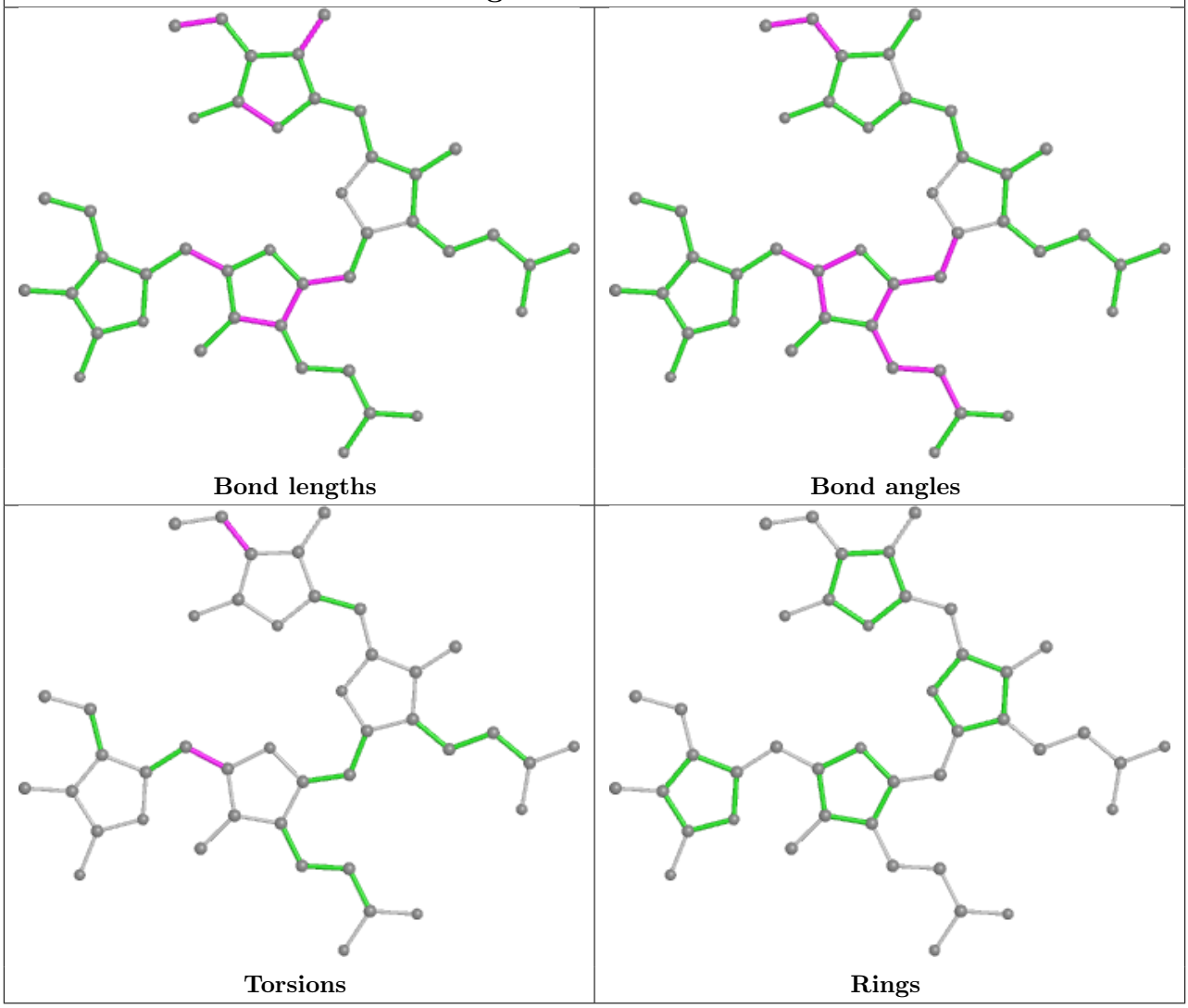


Rings

Ligand PEB C 258



Ligand PEB C 250



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.