



wwPDB X-ray Structure Validation Summary Report

Dec 14, 2023 – 05:16 am GMT

PDB ID : 3ZOO
Title : Structure of the Y46F mutant of human cytochrome c
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Deposited on : 2013-02-22
Resolution : 1.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 Å.

There are no overall percentile quality scores available for this entry.

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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	104	 96% .
1	B	104	 96% .
1	C	104	 97% .
1	D	104	 94% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3983 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 CYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	104	848	542	148	153	5	22	5	0
1	B	104	836	537	145	149	5	11	4	0
1	C	104	858	549	150	153	6	19	8	0
1	D	104	840	536	145	153	6	16	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PHE	TYR	engineered mutation	UNP P99999
B	46	PHE	TYR	engineered mutation	UNP P99999
C	46	PHE	TYR	engineered mutation	UNP P99999
D	46	PHE	TYR	engineered mutation	UNP P99999

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	145	Total	O	0	1
			146	146		
4	B	88	Total	O	0	0
			88	88		
4	C	92	Total	O	0	1
			93	93		
4	D	92	Total	O	0	0
			92	92		

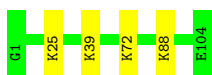
3 Residue-property plots [i](#)

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 failed to run properly.

- Molecule 1: CYTOCHROME C

Chain A:  96%



- Molecule 1: CYTOCHROME C

Chain B:  96%



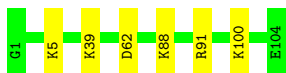
- Molecule 1: CYTOCHROME C

Chain C:  97%



- Molecule 1: CYTOCHROME C

Chain D:  94% 6%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	36.37Å 53.95Å 58.95Å 76.55° 88.73° 71.86°	Depositor
Resolution (Å)	30.59 – 1.35	Depositor
% Data completeness (in resolution range)	94.7 (30.59-1.35)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.35Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.138 , 0.179	Depositor
Wilson B-factor (Å ²)	14.9	Xtrriage
Anisotropy	0.456	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.025 for h,h-k,-l	Xtrriage
Total number of atoms	3983	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, PO4

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	0.85	3/870 (0.3%)	0.95	2/1153 (0.2%)
1	B	1.04	5/864 (0.6%)	1.18	4/1148 (0.3%)
1	C	0.88	2/890 (0.2%)	0.90	1/1185 (0.1%)
1	D	1.04	4/862 (0.5%)	1.02	7/1147 (0.6%)
All	All	0.96	14/3486 (0.4%)	1.02	14/4633 (0.3%)

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
1	C	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	LYS	CD-CE	-12.78	1.19	1.51
1	B	87	LYS	CG-CD	-12.08	1.11	1.52
1	D	5	LYS	CE-NZ	-11.72	1.19	1.49
1	C	89	GLU	CB-CG	-9.87	1.33	1.52
1	D	39	LYS	CD-CE	-9.53	1.27	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	LYS	CB-CG-CD	20.03	163.69	111.60
1	B	87	LYS	CG-CD-CE	14.46	155.28	111.90
1	B	88	LYS	CD-CE-NZ	11.83	138.90	111.70
1	D	5	LYS	CD-CE-NZ	11.53	138.22	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	72	LYS	CD-CE-NZ	9.34	133.19	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	24[A]	GLY	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

6 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
2	HEC	C	105	1	32,50,50	1.21	3 (9%)	24,82,82	2.02	12 (50%)
3	PO4	A	1105	-	4,4,4	1.00	0	6,6,6	1.00	0
3	PO4	A	1106	-	4,4,4	0.92	0	6,6,6	0.64	0
2	HEC	A	105	1	32,50,50	1.72	5 (15%)	24,82,82	2.20	11 (45%)
2	HEC	B	105	1	32,50,50	1.79	6 (18%)	24,82,82	2.01	9 (37%)
2	HEC	D	105	1	32,50,50	1.73	9 (28%)	24,82,82	1.75	8 (33%)

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	HEC	B	105	1	-	3/10/54/54	-
2	HEC	C	105	1	-	4/10/54/54	-
2	HEC	D	105	1	-	2/10/54/54	-
2	HEC	A	105	1	-	4/10/54/54	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	105	HEC	C2B-C3B	-5.34	1.35	1.40
2	B	105	HEC	C4B-C3B	4.86	1.51	1.43
2	A	105	HEC	C3C-C2C	-3.78	1.36	1.40
2	B	105	HEC	C2B-C3B	-3.78	1.36	1.40
2	B	105	HEC	CBC-CAC	-3.70	1.35	1.49

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	105	HEC	CMB-C2B-C1B	-4.46	121.61	128.46
2	B	105	HEC	CBD-CAD-C3D	-3.72	106.27	112.62
2	A	105	HEC	CBD-CAD-C3D	-3.65	106.40	112.62
2	A	105	HEC	CMB-C2B-C1B	-3.57	122.97	128.46
2	C	105	HEC	CMC-C2C-C3C	3.54	129.98	125.82

There are no chirality outliers.

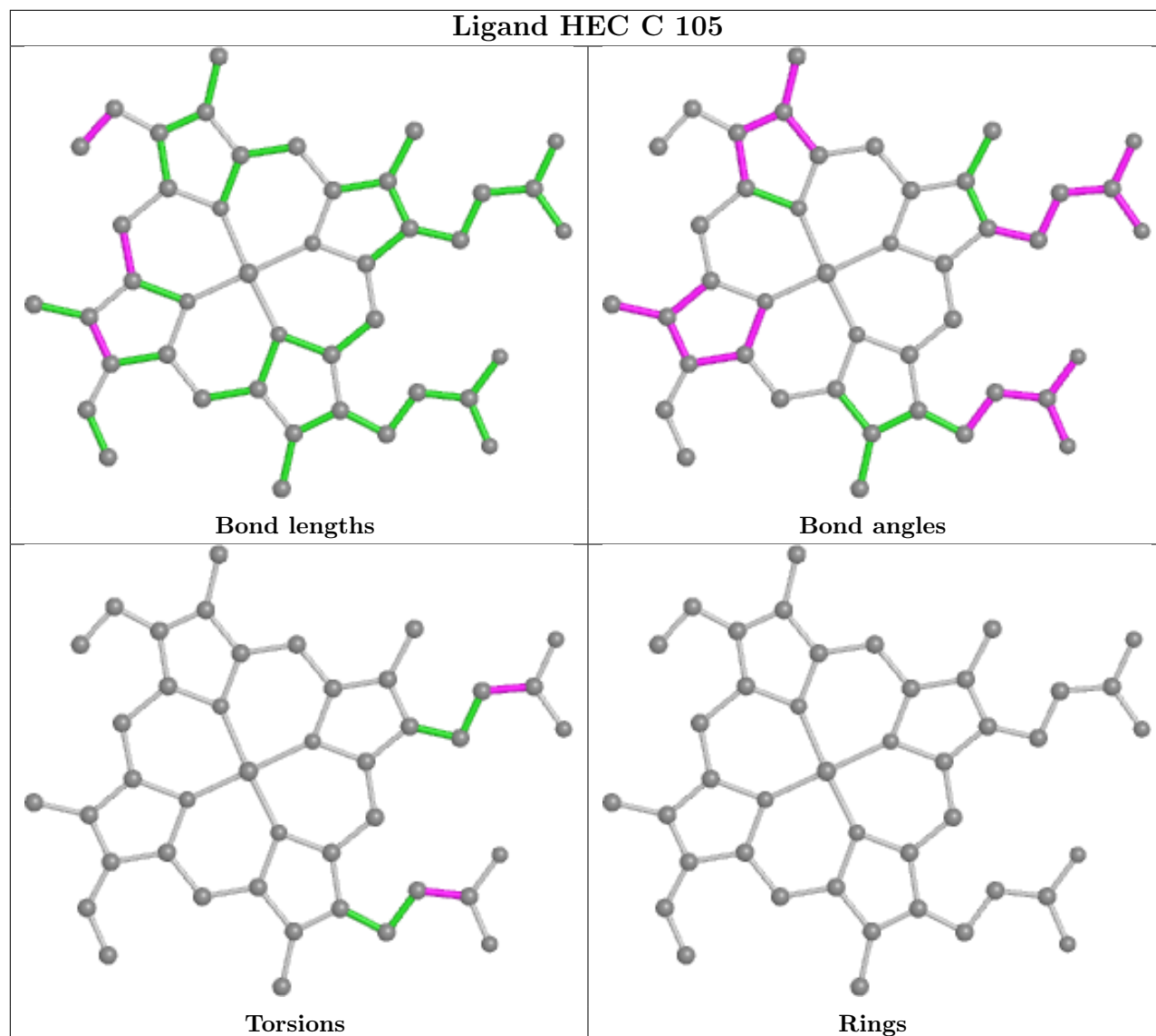
5 of 13 torsion outliers are listed below:

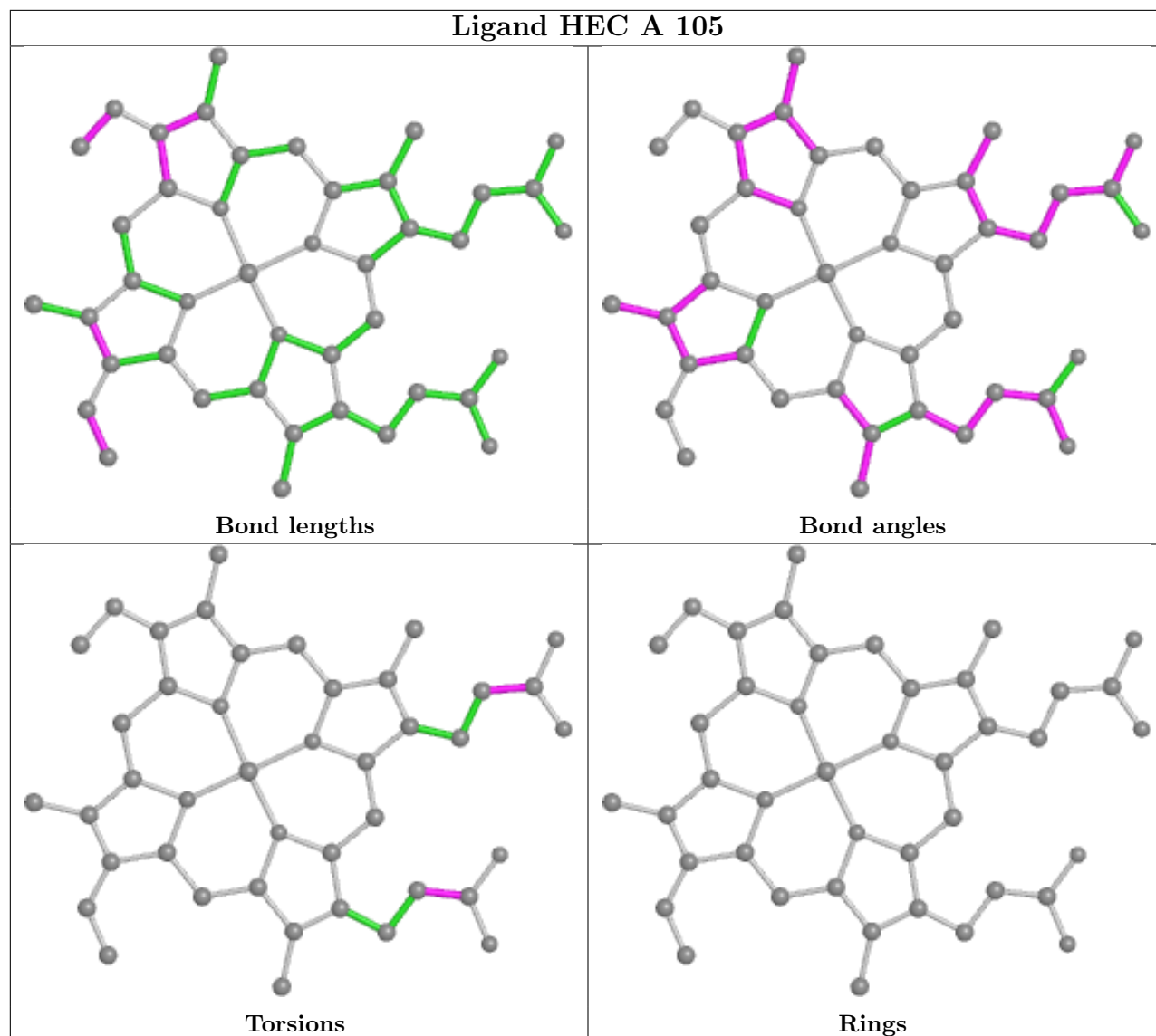
Mol	Chain	Res	Type	Atoms
2	C	105	HEC	CAA-CBA-CGA-O2A
2	A	105	HEC	CAA-CBA-CGA-O2A
2	A	105	HEC	CAD-CBD-CGD-O2D
2	D	105	HEC	CAA-CBA-CGA-O1A
2	D	105	HEC	CAA-CBA-CGA-O2A

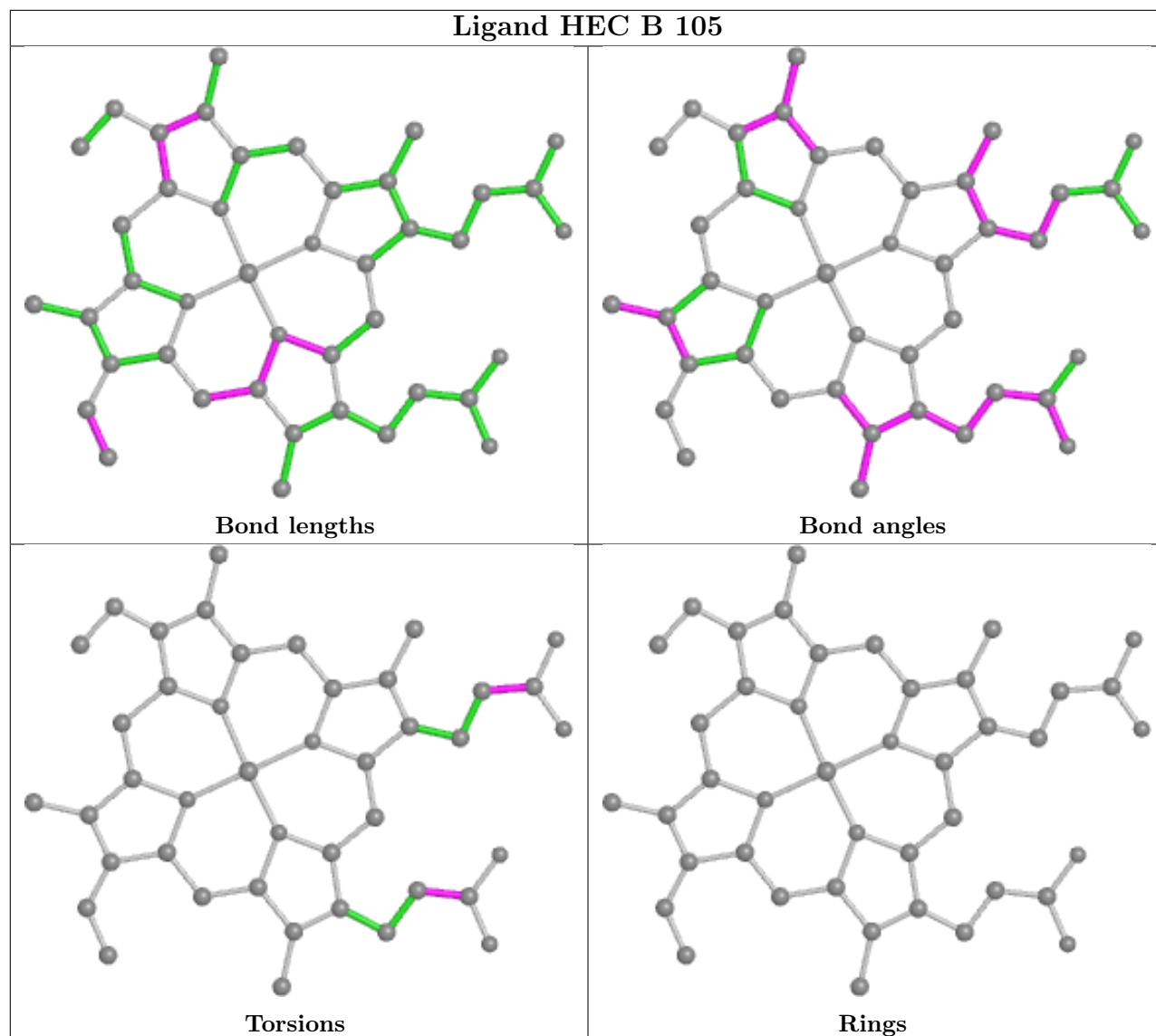
There are no ring outliers.

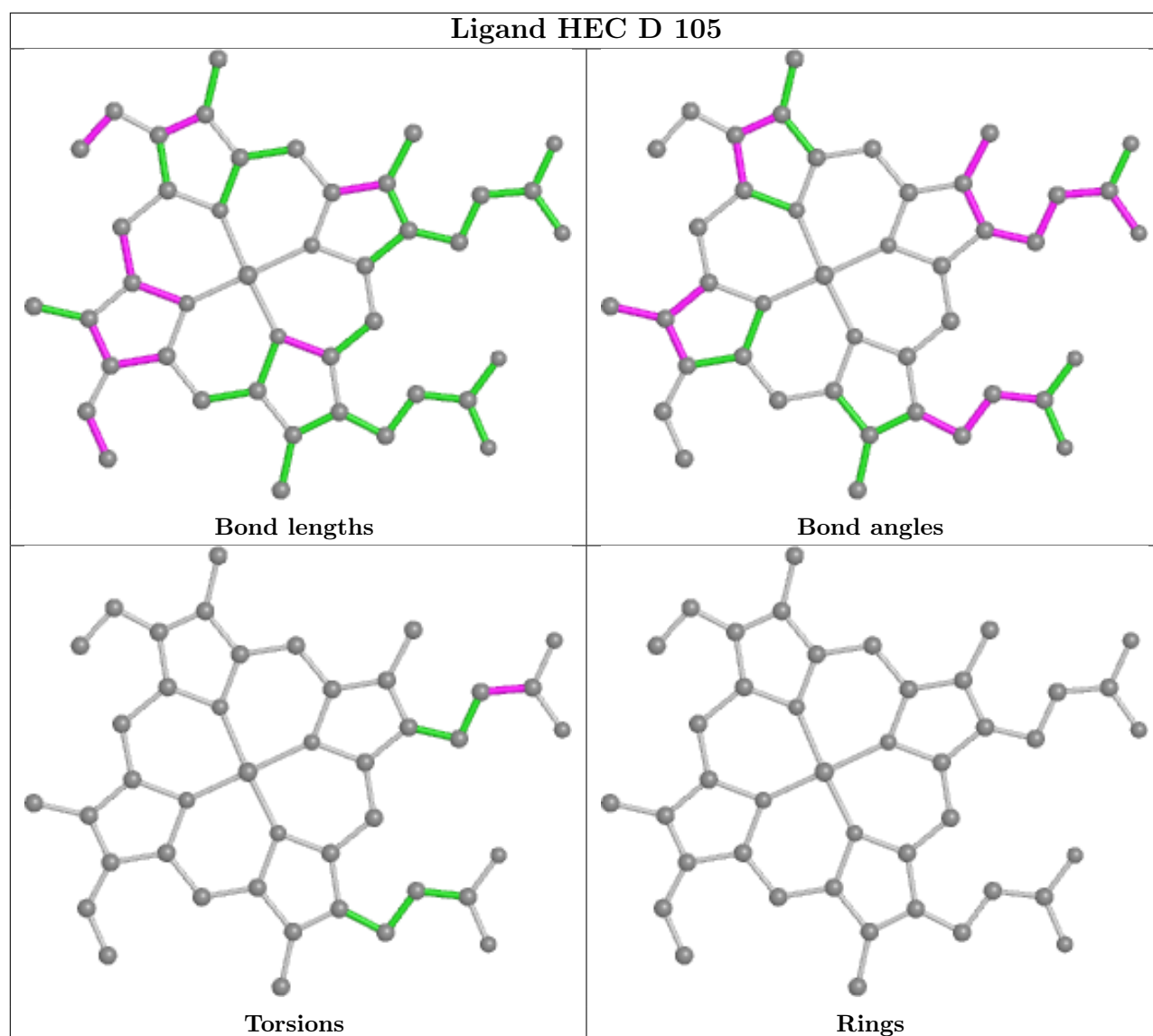
No monomer is involved in short contacts.

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.









5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.