



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:53 PM UTC

PDB ID : 1LCO / pdb_00001lco
Title : X-RAY STRUCTURE OF TWO COMPLEXES OF THE Y143F FLAVO-CYTOCHROME B2 MUTANT CRYSTALLIZED IN THE PRESENCE OF LACTATE OR PHENYL-LACTATE
Authors : Tegoni, M.; Cambillau, C.
Deposited on : 1995-03-30
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

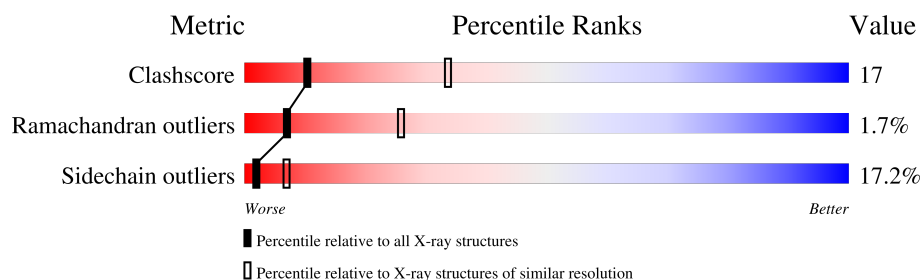
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	511	
1	B	511	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMN	A	570	X	-	-	-
3	FMN	B	570	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8915 atoms, of which 1840 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 L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	480	Total	C	H	N	O	S	0	0	0
			4547	2384	811	631	707	14			
1	B	391	Total	C	H	N	O	S	0	0	0
			3732	1930	687	521	583	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	PHE	TYR	conflict	UNP P00175
B	143	PHE	TYR	conflict	UNP P00175

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



-
- The image displays the chemical structure of Flavin Mononucleotide (FMN). It features an isoalloxazine ring system, which is a tricyclic aromatic heterocycle consisting of a benzene ring fused to two pyrimidine rings. The ring atoms are labeled: N1, N3, N5, N10 for nitrogen atoms and C2, C4, C5A, C6, C7, C8, C9 for carbon atoms. A ribityl chain is attached to the N10 position of the isoalloxazine ring. The ribityl chain consists of three carbon atoms (C1, C2, C3) and a phosphate group. The C1 atom is bonded to a hydroxyl group (OH) and a hydrogen atom (H). The C2 atom is bonded to a hydroxyl group (OH) and a hydrogen atom (H). The C3 atom is bonded to a hydroxyl group (OH) and a hydrogen atom (H). The phosphate group is attached to the C3 atom via an oxygen atom (O5) and consists of a phosphorus atom (P) bonded to four oxygen atoms: one double-bonded (O1P), one single-bonded to a hydroxyl group (OH), and two single-bonded to other oxygen atoms (O2P, O3P).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 35	C 17	H 4	N 4	O 9	P 1	0	0
3	B	1	Total 35	C 17	H 4	N 4	O 9	P 1	0	0

- PPY
-
- The chemical structure of PPY (Phenylpyruvate) is shown. It consists of a phenyl ring (labeled C1' to C6') attached to a pyruvate group (labeled C2, C3, C1, O1, O2, O3). The pyruvate group is a three-carbon chain with a carboxylic acid group at the end (C1-C2-C3) and a ketone group (C2=O3). The phenyl ring is attached to C2. The atoms are labeled as follows: C1, C2, C3, C1', C2', C3', C4', C5', C6' for the carbon atoms; O1, O2, O3 for the oxygen atoms. The structure is drawn in a skeletal format with red lines for the bonds.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	9	3		



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	9	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	152	Total	H	O	0	0
			456	304	152		
5	B	13	Total	H	O	0	0
			39	26	13		



L480	L483	K484	A485	R486	T487	V488	G489	V490	P491	M492	L495	V499	T504	F508	E509	D510	A511	L338	K339	K340	K341	T342	K343	L344	P345	I346	V347	I348	K349	G350	V351	Q352	R353	T354	E355	D356	V357	I358	A361	E362	G367	V368	V369	L370	S371	R372	R373	G374	G375	R376	Q377	L378	D379	F380	A383	E386	V387	L388	T391	M392	P393	I394	N399	L400	K403	L404	E405	V406	F407	V408	D409	G410	G411	V412	R413	R414	G415	T416	D417	V418	L419	K420	C423	L424	V429	R433	P434	F435	L436	Y437	A438	M439	S440	G441	Y442	G443	R444	M445	G446	V447	E448	K449	A450	I451	L454	R455	D456	E457	I458	E459	M460	S461	M462	R463	L464	L465	T468	L473	K474	P475	D476	L477	L478	D479	V269	E270	K271	L272	K275	A276	L277	F278	V281	D282	A283	F284	S285	L286	G287	Q288	R289	E290	R291	D292	M293	K294	L295	K296	PHE	SER	ASN	THR	LYS	ALA	GLY	PRO	LYS	ALA	A242	P243	S244	D245	K246	Q247	I248	Q249	V250	Y251	Q252	L253	Y254	V255	R256	S257	D258	R259	T262	D263	D264	K267	N268	E337	E336	I335	T331	L330	S329	P328	I326	F325	S319	Q316	SER	GLU	GLU	VAL	ASN	THR	LYS	LYS	MET	ALA	LYS	THR	ASN	VAL	GLU	GLU	K226	M226	Q225	K222	G217	A213	V212	D211	K210	E209	L206	P205	R204	G203	L202	K201	C200	L199	A198	L197	A196
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.50Å 164.50Å 114.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.90)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8915	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: FMN, HEM, PPY

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	1.25	14/3810 (0.4%)	2.24	182/5161 (3.5%)
1	B	1.26	11/3093 (0.4%)	2.19	144/4177 (3.4%)
All	All	1.25	25/6903 (0.4%)	2.22	326/9338 (3.5%)

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	A	0	2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	373	HIS	CD2-NE2	-7.58	1.29	1.37
1	A	212	VAL	CA-CB	7.54	1.64	1.54
1	B	490	VAL	CA-CB	7.12	1.63	1.54
1	B	194	VAL	CA-CB	-6.83	1.45	1.54
1	A	158	HIS	CG-ND1	-6.83	1.30	1.38

The worst 5 of 326 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ASP	CA-CB-CG	19.33	131.93	112.60
1	A	190	VAL	N-CA-CB	-13.59	97.09	111.64
1	A	379	ASP	CA-C-O	-13.33	104.00	119.60
1	B	372	ASN	CB-CG-ND2	12.09	134.53	116.40
1	B	149	ASN	CA-CB-CG	11.76	124.36	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	ASP	Peptide
1	A	492	ASN	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3736	811	3793	120	0
1	B	3045	687	3112	127	0
2	A	43	4	30	3	0
3	A	31	4	19	4	0
3	B	31	4	19	7	0
4	A	12	0	7	1	0
4	B	12	0	7	2	0
5	A	152	304	0	9	0
5	B	13	26	0	0	0
All	All	7075	1840	6987	236	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 17.

The worst 5 of 236 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:B:143:PHE:HA	1:B:289:ARG:HH22	1.45	0.79
1:B:290:GLU:HA	1:B:293:MET:HG3	1.64	0.79
1:A:226:MET:HE1	1:A:349:LYS:HE3	1.66	0.76
1:A:40:LEU:HG	1:A:47:GLN:HB2	1.67	0.76
1:B:197:THR:HG21	1:B:436:LEU:HG	1.67	0.75

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	476/511 (93%)	428 (90%)	39 (8%)	9 (2%)	6	23
1	B	387/511 (76%)	348 (90%)	33 (8%)	6 (2%)	7	27
All	All	863/1022 (84%)	776 (90%)	72 (8%)	15 (2%)	7	26

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	ASN
1	A	104	GLU
1	A	114	SER
1	A	119	LEU
1	A	493	ASP

5.3.2 Protein sidechains

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	412/440 (94%)	341 (83%)	71 (17%)	2	7
1	B	336/440 (76%)	278 (83%)	58 (17%)	2	7
All	All	748/880 (85%)	619 (83%)	129 (17%)	2	7

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	378	LEU

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Mol	Chain	Res	Type
1	B	413	ARG
1	A	330	LEU
1	A	329	SER
1	B	429	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	121	ASN
1	B	218	GLN
1	B	492	ASN
1	B	149	ASN
1	B	225	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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
4	PPY	B	580	-	12,12,12	2.61	3 (25%)	14,15,15	1.48	4 (28%)
4	PPY	A	580	-	12,12,12	2.28	2 (16%)	14,15,15	1.73	2 (14%)
2	HEM	A	560	1	50,50,50	1.24	5 (10%)	67,82,82	1.03	2 (2%)
3	FMN	A	570	-	33,33,33	2.13	9 (27%)	48,50,50	2.45	20 (41%)
3	FMN	B	570	-	33,33,33	2.01	11 (33%)	48,50,50	2.26	18 (37%)

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
4	PPY	B	580	-	-	0/8/8/8	0/1/1/1
4	PPY	A	580	-	-	1/8/8/8	0/1/1/1
2	HEM	A	560	1	-	11/14/54/54	-
3	FMN	A	570	-	2/2/4/4	12/18/18/18	0/3/3/3
3	FMN	B	570	-	2/2/4/4	8/18/18/18	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	580	PPY	C2-C1	-7.62	1.42	1.53
4	A	580	PPY	C2-C1	-6.68	1.43	1.53
3	A	570	FMN	C1'-N10	-6.05	1.33	1.47
3	B	570	FMN	C1'-N10	-5.40	1.34	1.47
3	A	570	FMN	C2'-C3'	-5.12	1.44	1.53

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	570	FMN	O4'-C4'-C5'	5.62	122.38	109.99
3	A	570	FMN	C4A-C10-N1	-5.56	110.96	124.59
3	B	570	FMN	C4'-C3'-C2'	5.20	122.22	113.57
3	B	570	FMN	C10-N1-C2	4.86	127.38	116.85
3	B	570	FMN	C4A-C10-N1	-4.76	112.92	124.59

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	570	FMN	C2'

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Mol	Chain	Res	Type	Atom
3	A	570	FMN	C4'
3	B	570	FMN	C2'
3	B	570	FMN	C4'

5 of 32 torsion outliers are listed below:

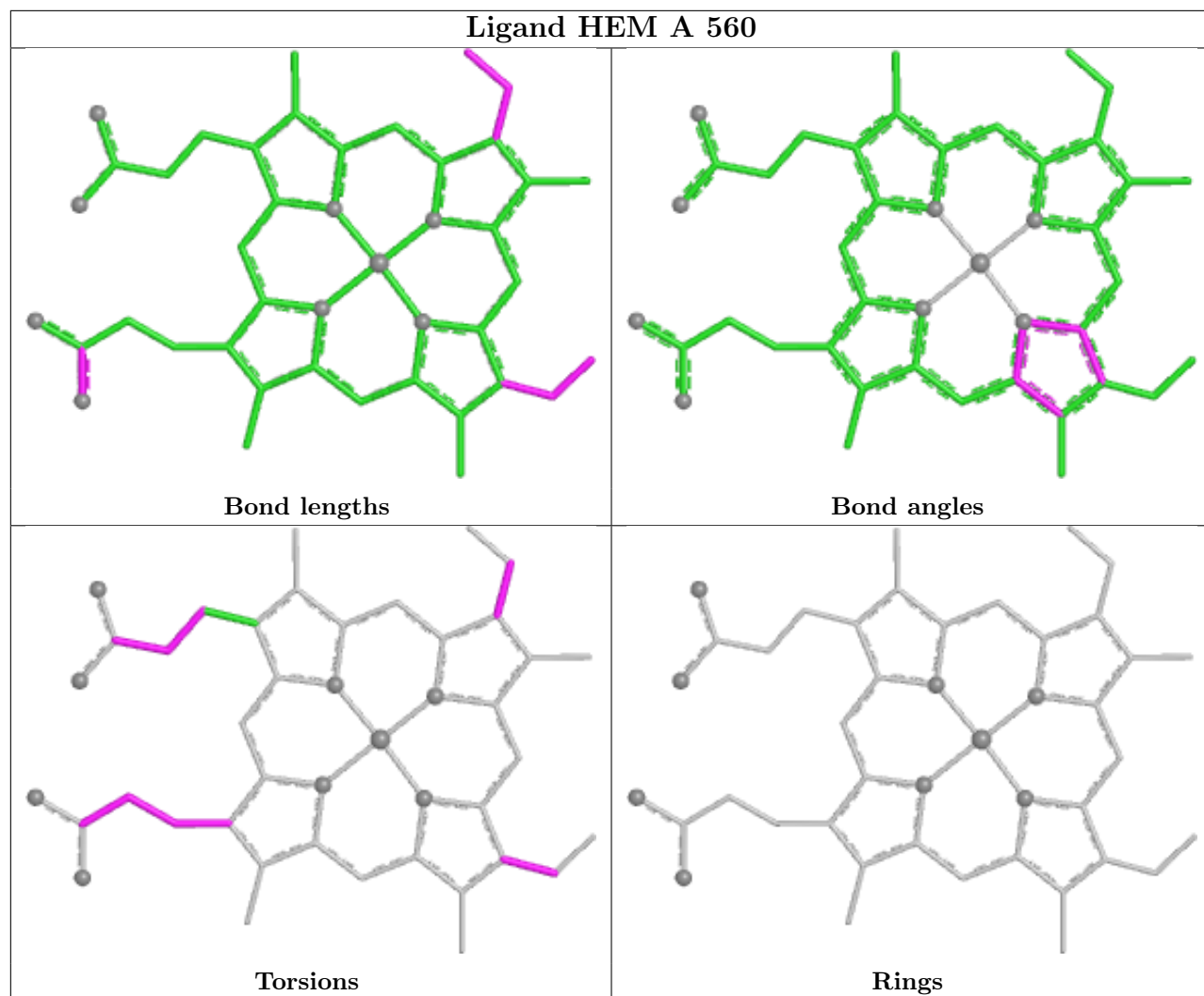
Mol	Chain	Res	Type	Atoms
2	A	560	HEM	C3A-C2A-CAA-CBA
2	A	560	HEM	C2C-C3C-CAC-CBC
2	A	560	HEM	C4C-C3C-CAC-CBC
3	A	570	FMN	N10-C1'-C2'-O2'
3	A	570	FMN	C1'-C2'-C3'-O3'

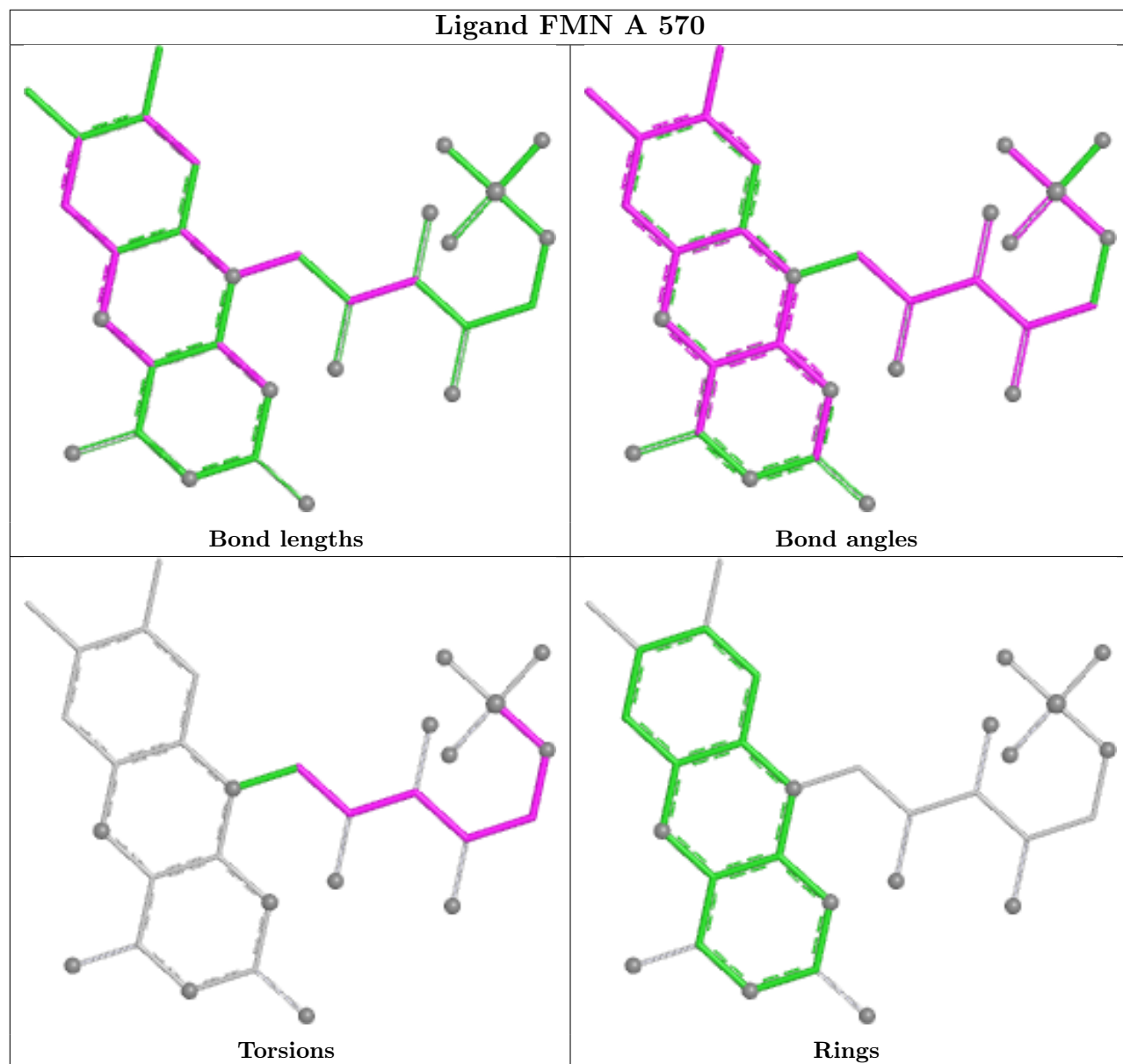
There are no ring outliers.

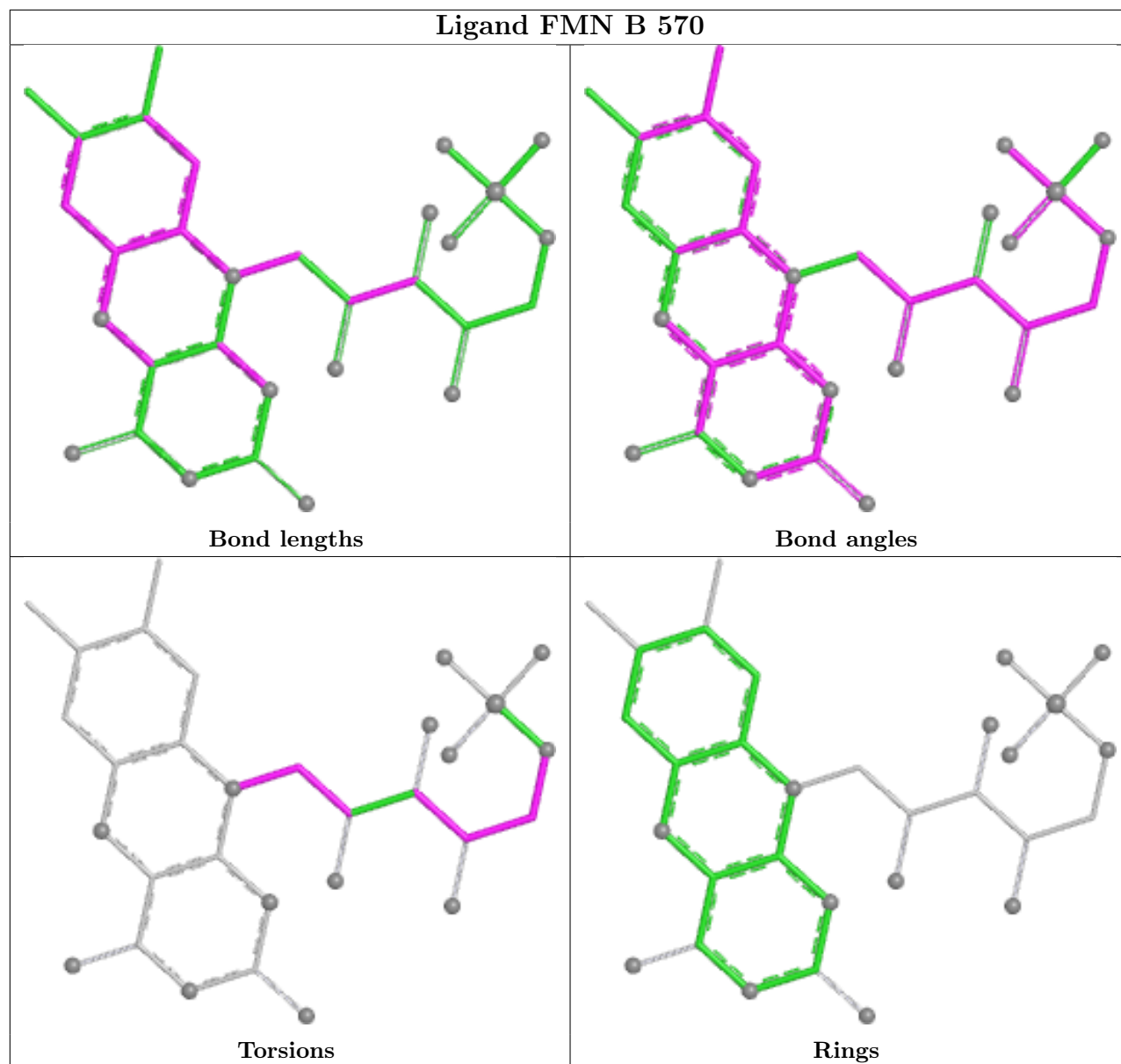
5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	580	PPY	2	0
4	A	580	PPY	1	0
2	A	560	HEM	3	0
3	A	570	FMN	4	0
3	B	570	FMN	7	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.







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.