



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:16 PM UTC

PDB ID : 1EA1 / pdb_00001ea1
Title : Cytochrome P450 14 alpha-sterol demethylase (CYP51) from Mycobacterium tuberculosis in complex with fluconazole
Authors : Podust, L.M.; Poulos, T.L.; Waterman, M.R.
Deposited on : 2000-11-02
Resolution : 2.21 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

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)
Xtrriage (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 2.21 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.

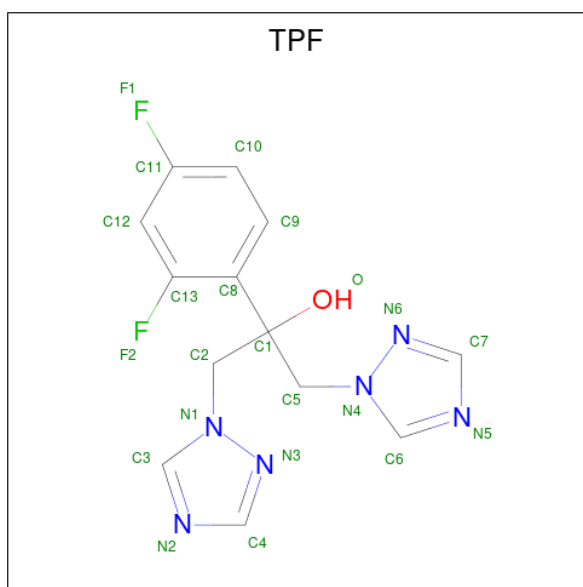


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)

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	455	



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	22	13	2	6	1	0	0

- Molecule 4 is water.

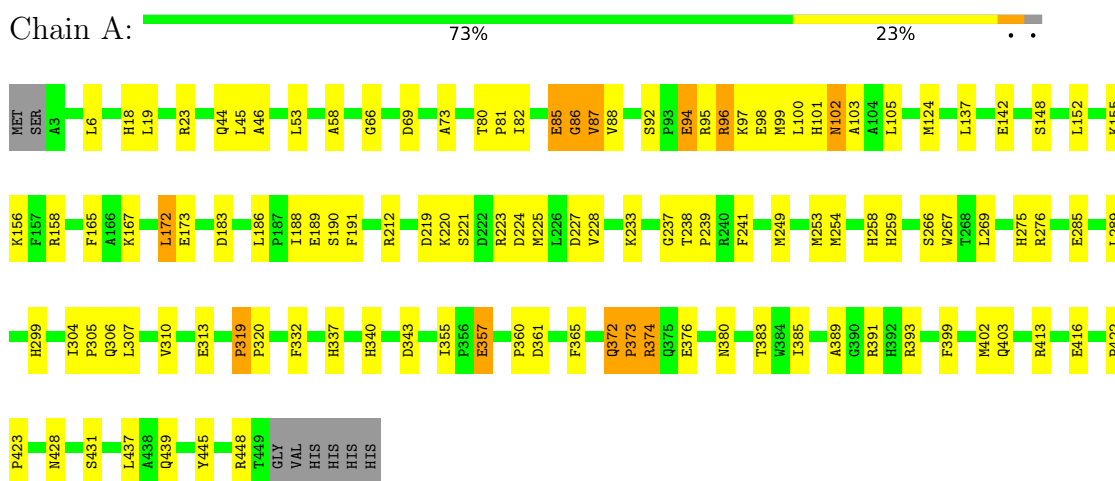
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	175	Total	O	0	0
			175	175		

3 Residue-property plots

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: CYTOCHROME P450 51-LIKE RV0764C



4 Data and refinement statistics

Xtrriage (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	46.19Å 84.26Å 109.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.00 – 2.21	Depositor
% Data completeness (in resolution range)	89.3 (38.00-2.21)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3749	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: HEM, TPF

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	0.40	0/3591	0.94	16/4863 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	PRO	CA-C-N	7.14	127.46	119.32
1	A	319	PRO	C-N-CA	7.14	127.46	119.32
1	A	304	ILE	CA-C-N	6.34	127.77	119.84
1	A	304	ILE	C-N-CA	6.34	127.77	119.84
1	A	94	GLU	N-CA-C	-6.17	105.73	113.20
1	A	259	HIS	N-CA-C	5.80	118.38	111.71
1	A	299	HIS	N-CA-C	5.52	118.22	111.82
1	A	385	ILE	N-CA-C	5.38	120.51	108.88
1	A	73	ALA	N-CA-C	5.38	117.84	111.33
1	A	374	ARG	N-CA-C	5.34	120.18	111.37
1	A	102	ASN	N-CA-C	-5.32	106.62	113.01
1	A	376	GLU	N-CA-C	5.08	118.57	112.38
1	A	355	ILE	CA-C-N	5.04	125.07	119.32
1	A	355	ILE	C-N-CA	5.04	125.07	119.32
1	A	361	ASP	CA-C-N	5.04	124.70	119.56
1	A	361	ASP	C-N-CA	5.04	124.70	119.56

There are no chirality outliers.

There are no planarity outliers.

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	3509	0	3384	81	0
2	A	43	0	30	1	0
3	A	22	0	12	0	0
4	A	175	0	0	4	0
All	All	3749	0	3426	81	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 12.

All (81) 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:82:ILE:HG13	1:A:172:LEU:HD22	1.50	0.94
1:A:95:ARG:HG2	1:A:96:ARG:HD3	1.53	0.88
1:A:87:VAL:HG13	1:A:249:MET:HG3	1.63	0.80
1:A:66:GLY:HA2	1:A:391:ARG:HH12	1.51	0.74
1:A:95:ARG:HA	1:A:99:MET:HE3	1.74	0.68
1:A:275:HIS:HB2	4:A:2094:HOH:O	1.93	0.67
1:A:80:THR:HB	1:A:81:PRO:HD3	1.75	0.67
1:A:102:ASN:HB2	1:A:105:LEU:HD11	1.77	0.66
1:A:393:ARG:HH11	1:A:393:ARG:HG3	1.60	0.66
1:A:124:MET:HE1	1:A:142:GLU:CD	2.21	0.66
1:A:158:ARG:HD3	1:A:158:ARG:C	2.20	0.66
1:A:267:TRP:HE1	1:A:428:ASN:HD21	1.44	0.65
1:A:372:GLN:HB2	1:A:373:PRO:HD3	1.78	0.64
1:A:124:MET:HE1	1:A:142:GLU:OE1	1.98	0.64
1:A:219:ASP:C	1:A:221:SER:H	2.05	0.64
1:A:95:ARG:C	1:A:97:LYS:H	2.07	0.63
1:A:285:GLU:OE2	1:A:305:PRO:HG2	2.02	0.60
1:A:95:ARG:O	1:A:95:ARG:HD3	2.04	0.58
1:A:66:GLY:HA2	1:A:391:ARG:NH1	2.19	0.57
1:A:428:ASN:HD22	1:A:437:LEU:HA	1.69	0.57
1:A:88:VAL:HG13	1:A:241:PHE:CE1	2.42	0.55
1:A:320:PRO:HG2	2:A:460:HEM:HMB3	1.89	0.55
1:A:155:LYS:HB3	4:A:2061:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:HD21	4:A:2109:HOH:O	2.09	0.52
1:A:188:ILE:HD12	1:A:191:PHE:CE2	2.44	0.52
1:A:95:ARG:O	1:A:97:LYS:N	2.40	0.52
1:A:389:ALA:HA	1:A:393:ARG:HD3	1.91	0.52
1:A:137:LEU:HD23	1:A:439:GLN:CD	2.35	0.51
1:A:223:ARG:HA	1:A:227:ASP:OD2	2.12	0.49
1:A:105:LEU:HD12	1:A:105:LEU:C	2.38	0.49
1:A:148:SER:O	1:A:152:LEU:HB2	2.12	0.49
1:A:267:TRP:HE1	1:A:428:ASN:ND2	2.10	0.49
1:A:69:ASP:HB3	1:A:332:PHE:CZ	2.48	0.48
1:A:233:LYS:HD2	1:A:237:GLY:O	2.15	0.47
1:A:380:ASN:HB3	1:A:383:THR:OG1	2.15	0.47
1:A:102:ASN:HA	1:A:105:LEU:HG	1.97	0.47
1:A:95:ARG:C	1:A:97:LYS:N	2.73	0.46
1:A:6:LEU:HD12	1:A:337:HIS:HB3	1.97	0.46
1:A:85:GLU:O	1:A:86:GLY:C	2.59	0.46
1:A:310:VAL:HG13	1:A:365:PHE:HZ	1.80	0.46
1:A:219:ASP:C	1:A:221:SER:N	2.72	0.46
1:A:183:ASP:HB3	1:A:186:LEU:HG	1.98	0.46
1:A:6:LEU:N	1:A:6:LEU:HD22	2.32	0.45
1:A:53:LEU:HB3	1:A:58:ALA:HB1	1.97	0.45
1:A:137:LEU:HD23	1:A:439:GLN:HG3	1.99	0.45
1:A:313:GLU:HA	1:A:313:GLU:OE1	2.15	0.45
1:A:238:THR:HG23	1:A:239:PRO:HD2	1.98	0.45
1:A:88:VAL:HB	1:A:249:MET:SD	2.58	0.44
1:A:188:ILE:HG22	1:A:190:SER:H	1.82	0.44
1:A:225:MET:HE1	1:A:253:MET:HE1	1.99	0.44
1:A:94:GLU:HB3	1:A:98:GLU:CB	2.48	0.44
1:A:402:MET:C	1:A:402:MET:SD	3.01	0.43
1:A:173:GLU:OE2	1:A:258:HIS:ND1	2.46	0.43
1:A:266:SER:HB3	1:A:437:LEU:HD22	2.00	0.43
1:A:101:HIS:C	1:A:103:ALA:N	2.75	0.42
1:A:422:PRO:HA	1:A:423:PRO:HD3	1.87	0.42
1:A:413:ARG:HA	1:A:448:ARG:HH11	1.84	0.42
1:A:285:GLU:OE1	1:A:306:GLN:HB2	2.19	0.42
1:A:373:PRO:HB2	1:A:374:ARG:H	1.60	0.42
1:A:19:LEU:C	1:A:19:LEU:HD23	2.45	0.42
1:A:23:ARG:O	1:A:431:SER:HA	2.20	0.42
1:A:18:HIS:HB2	1:A:44:GLN:O	2.20	0.41
1:A:319:PRO:HA	1:A:320:PRO:HD3	1.79	0.41
1:A:45:LEU:O	1:A:46:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLU:O	1:A:289:LEU:HB2	2.20	0.41
1:A:137:LEU:HD23	1:A:439:GLN:CG	2.49	0.41
1:A:88:VAL:HG23	1:A:249:MET:HB2	2.02	0.41
1:A:101:HIS:C	1:A:103:ALA:H	2.27	0.41
1:A:156:LYS:HB3	1:A:224:ASP:OD2	2.21	0.41
1:A:224:ASP:O	1:A:228:VAL:HG23	2.20	0.41
1:A:340:HIS:O	1:A:343:ASP:HB2	2.20	0.41
1:A:100:LEU:O	1:A:101:HIS:C	2.64	0.41
1:A:96:ARG:HD2	1:A:96:ARG:N	2.36	0.41
1:A:416:GLU:O	1:A:445:TYR:HA	2.21	0.41
1:A:156:LYS:HG2	1:A:212:ARG:NH2	2.35	0.41
1:A:445:TYR:CD1	1:A:445:TYR:C	2.99	0.40
1:A:165:PHE:CZ	1:A:254:MET:HE1	2.56	0.40
1:A:399:PHE:HE1	1:A:403:GLN:NE2	2.19	0.40
1:A:393:ARG:HG3	1:A:393:ARG:NH1	2.32	0.40
1:A:167:LYS:HD3	1:A:167:LYS:HA	1.95	0.40
1:A:357:GLU:HB2	4:A:2132:HOH:O	2.20	0.40

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	445/455 (98%)	416 (94%)	22 (5%)	7 (2%)	7 5

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	PRO
1	A	86	GLY
1	A	87	VAL
1	A	92	SER

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Mol	Chain	Res	Type
1	A	96	ARG
1	A	220	LYS
1	A	372	GLN

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	358/378 (95%)	350 (98%)	8 (2%)	45 59

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	GLU
1	A	172	LEU
1	A	189	GLU
1	A	269	LEU
1	A	276	ARG
1	A	307	LEU
1	A	357	GLU
1	A	360	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	59	ASN
1	A	109	GLN
1	A	199	ASN
1	A	210	ASN
1	A	303	GLN
1	A	337	HIS
1	A	403	GLN
1	A	428	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](#)

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](#)

2 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	HEM	A	460	1,3	50,50,50	1.69	11 (22%)	67,82,82	0.85	3 (4%)
3	TPF	A	470	2	24,24,24	2.02	9 (37%)	34,34,34	1.82	13 (38%)

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	HEM	A	460	1,3	-	4/14/54/54	-
3	TPF	A	470	2	-	0/16/16/16	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	460	HEM	CBC-CAC	5.04	1.54	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	470	TPF	C8-C13	5.00	1.45	1.39
2	A	460	HEM	CBB-CAB	4.90	1.53	1.30
3	A	470	TPF	C1-C8	4.11	1.58	1.53
3	A	470	TPF	N1-N3	3.18	1.42	1.36
2	A	460	HEM	CAC-C3C	3.11	1.55	1.47
2	A	460	HEM	CAB-C3B	2.97	1.55	1.47
2	A	460	HEM	FE-NA	2.93	2.04	1.95
3	A	470	TPF	C9-C8	2.88	1.43	1.39
2	A	460	HEM	FE-NB	2.78	2.03	1.94
3	A	470	TPF	C12-C13	2.73	1.42	1.37
3	A	470	TPF	C10-C11	2.60	1.42	1.37
2	A	460	HEM	CMC-C2C	2.58	1.56	1.50
3	A	470	TPF	N4-N6	2.44	1.40	1.36
3	A	470	TPF	C12-C11	2.38	1.41	1.37
2	A	460	HEM	O2A-CGA	-2.26	1.23	1.30
2	A	460	HEM	FE-NC	2.19	2.02	1.95
2	A	460	HEM	CMD-C2D	2.18	1.55	1.50
2	A	460	HEM	O1A-CGA	2.11	1.29	1.22
3	A	470	TPF	C10-C9	2.01	1.42	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	470	TPF	C2-N1-N3	3.67	126.59	121.25
3	A	470	TPF	C13-C12-C11	3.51	120.41	116.67
3	A	470	TPF	C12-C13-C8	-3.25	120.34	123.88
3	A	470	TPF	C5-N4-N6	2.89	125.46	121.25
3	A	470	TPF	C6-N5-C7	2.66	110.03	102.85
3	A	470	TPF	C10-C11-C12	-2.60	119.80	123.23
3	A	470	TPF	C3-N2-C4	2.59	109.85	102.85
3	A	470	TPF	C3-N1-N3	-2.57	105.84	109.39
2	A	460	HEM	CBB-CAB-C3B	-2.51	114.98	127.53
2	A	460	HEM	CBC-CAC-C3C	-2.47	115.17	127.53
2	A	460	HEM	O1A-CGA-CBA	-2.22	116.06	123.09
3	A	470	TPF	C9-C10-C11	2.20	120.64	118.38
3	A	470	TPF	N3-C4-N2	-2.14	108.79	114.90
3	A	470	TPF	C6-N4-N6	-2.12	106.46	109.39
3	A	470	TPF	N6-C7-N5	-2.09	108.93	114.90
3	A	470	TPF	F2-C13-C8	2.02	121.24	119.01

There are no chirality outliers.

All (4) torsion outliers are listed below:

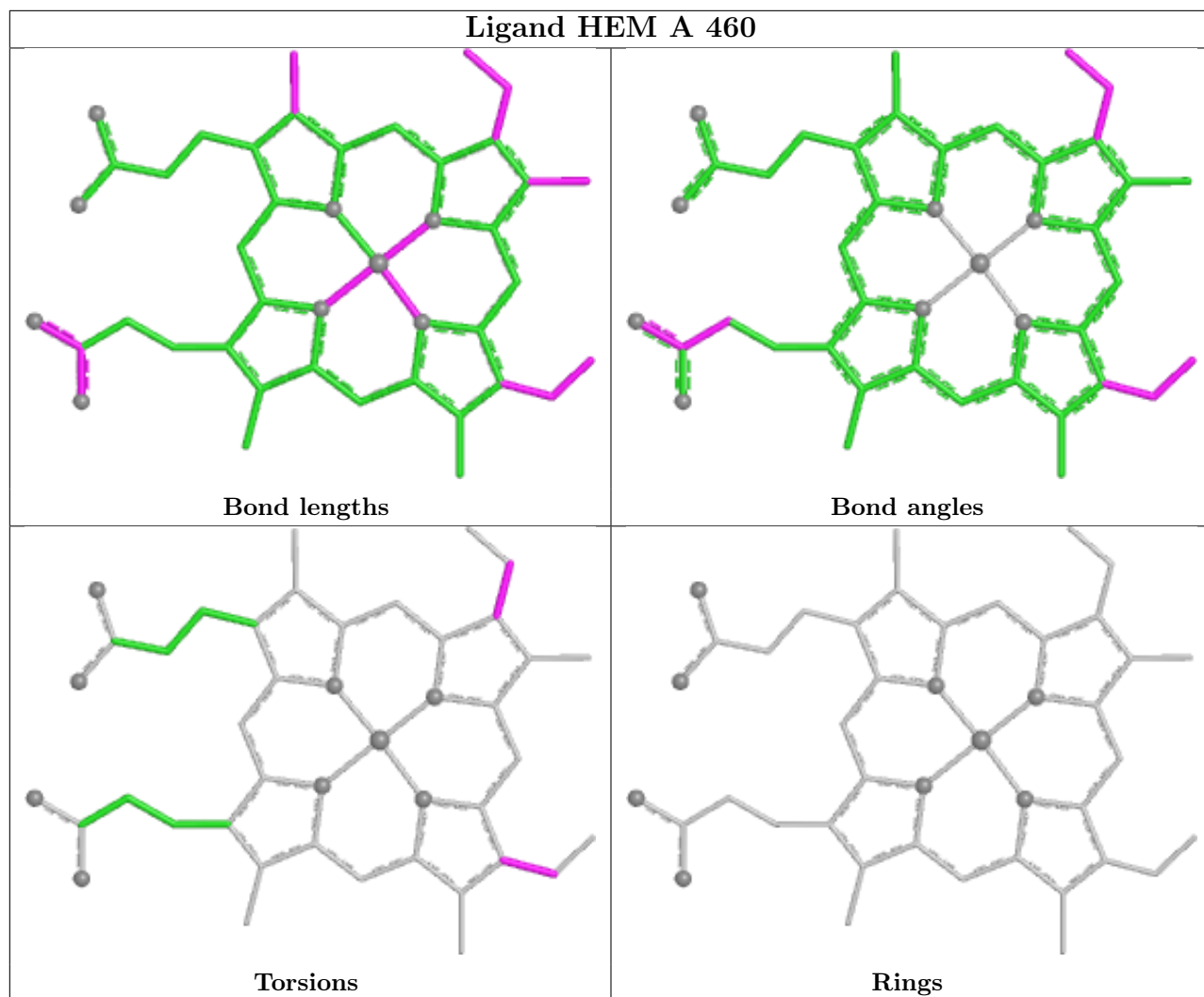
Mol	Chain	Res	Type	Atoms
2	A	460	HEM	C2B-C3B-CAB-CBB
2	A	460	HEM	C2C-C3C-CAC-CBC
2	A	460	HEM	C4B-C3B-CAB-CBB
2	A	460	HEM	C4C-C3C-CAC-CBC

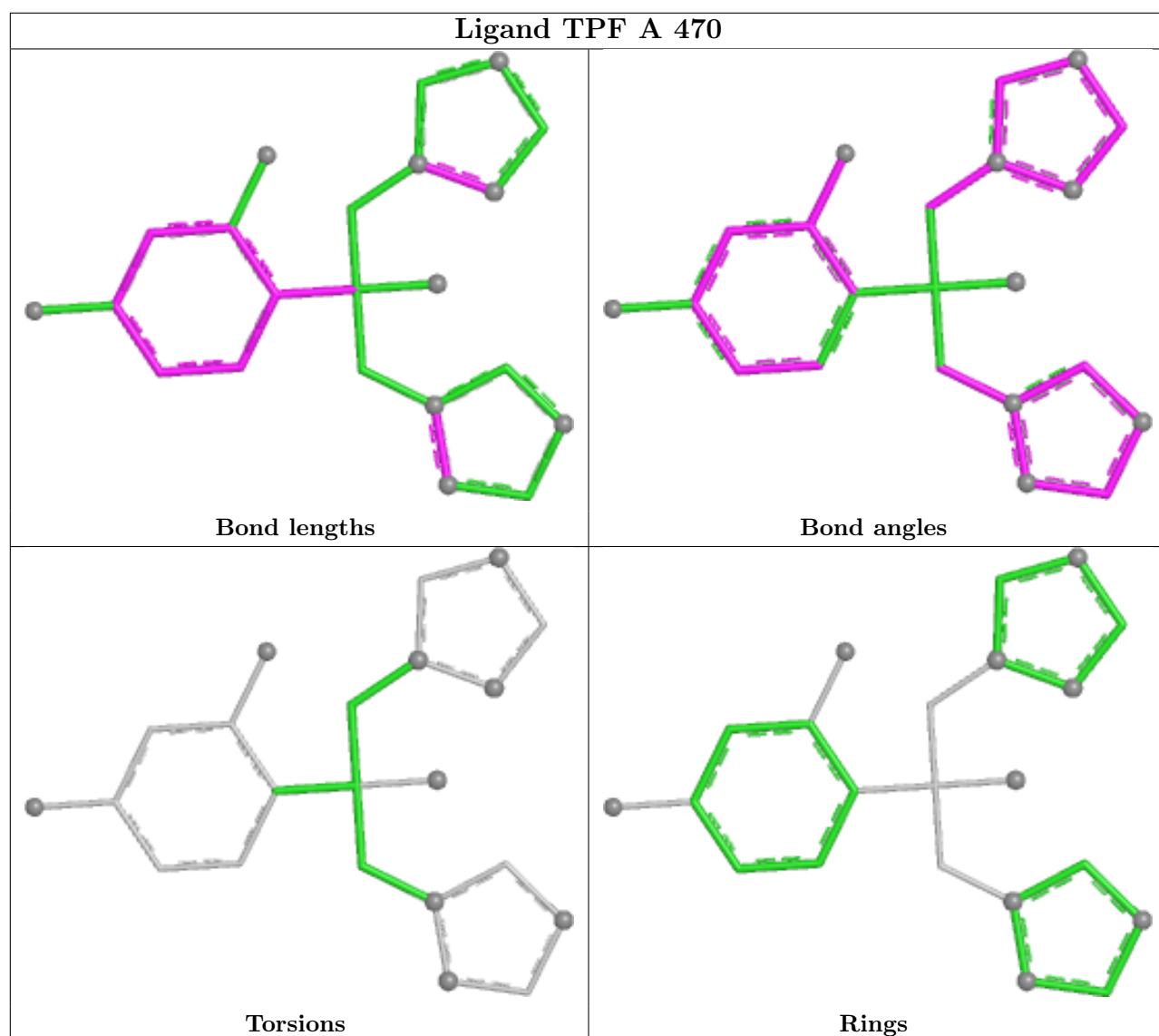
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	460	HEM	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 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 was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.