



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 12:30 AM UTC

PDB ID : 8CAT / pdb_00008cat
Title : The NADPH binding site on beef liver catalase
Authors : Murthy, M.R.N.; Reid III, T.J.; Sicignano, A.; Tanaka, N.; Fita, I.; Rossmann, M.G.
Deposited on : 1984-11-15
Resolution : 2.50 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)
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

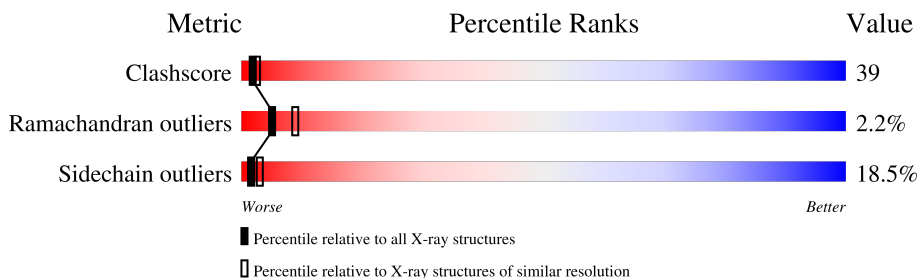
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	506	
1	B	506	

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	NDP	A	508	X	-	-	-
3	NDP	B	508	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8296 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 CATALASE.

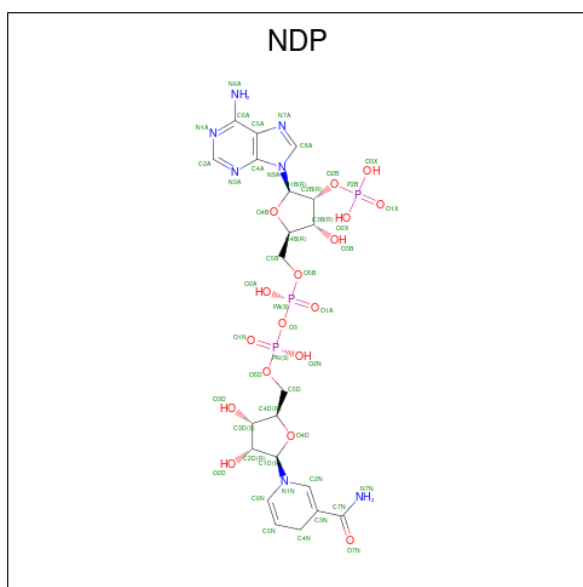
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	4008	2543	714	737	14	0	0	0
1	B	498	4008	2543	714	737	14	0	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	48	21	7	17	3	0	0
3	B	1	48	21	7	17	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	50	Total	O	0	0
			50	50		

4 Data and refinement statistics

Xtrriage (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	142.00Å 142.00Å 103.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.50 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.50-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8296	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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, NDP

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	1.98	98/4128 (2.4%)	2.84	444/5607 (7.9%)
1	B	2.05	110/4128 (2.7%)	2.95	505/5607 (9.0%)
All	All	2.01	208/8256 (2.5%)	2.90	949/11214 (8.5%)

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	4
1	B	0	2
All	All	0	6

The worst 5 of 208 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	GLU	N-CA	9.37	1.59	1.46
1	B	228	ALA	C-N	-9.04	1.25	1.33
1	B	426	GLY	N-CA	8.86	1.54	1.45
1	B	151	ILE	N-CA	8.80	1.57	1.46
1	A	122	ALA	N-CA	8.59	1.56	1.46

The worst 5 of 949 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	CD-NE-CZ	25.30	159.81	124.40
1	B	472	PHE	CA-CB-CG	19.95	133.75	113.80
1	A	179	ASP	CA-CB-CG	18.22	130.82	112.60
1	A	263	ASP	CA-CB-CG	15.93	128.53	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	ARG	CD-NE-CZ	15.40	145.96	124.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	ARG	Sidechain
1	A	362	ARG	Sidechain
1	A	430	ARG	Sidechain
1	A	71	ARG	Sidechain
1	B	105	ARG	Sidechain

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	4008	0	3833	344	3
1	B	4008	0	3833	309	2
2	A	43	0	30	16	0
2	B	43	0	30	11	0
3	A	48	0	24	0	0
3	B	48	0	24	3	0
4	A	48	0	0	4	1
4	B	50	0	0	5	0
All	All	8296	0	7774	629	3

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 39.

The worst 5 of 629 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:155:ARG:NH2	1:A:438:ASN:HD21	1.19	1.38
1:A:155:ARG:HH22	1:A:438:ASN:ND2	1.28	1.31
1:B:155:ARG:HH22	1:B:438:ASN:ND2	1.27	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ARG:NH2	1:B:438:ASN:HD21	1.34	1.26
1:A:367:PRO:HG2	1:A:390:PRO:HG2	1.19	1.14

All (3) 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)
1:A:419:GLU:OE2	1:B:430:ARG:NH1[6_556]	1.78	0.42
1:A:10:GLN:NE2	4:A:541:HOH:O[6_556]	1.86	0.34
1:A:183:ASP:OD1	1:B:407:SER:OG[6_556]	2.12	0.08

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	496/506 (98%)	418 (84%)	64 (13%)	14 (3%)	4 6
1	B	496/506 (98%)	425 (86%)	63 (13%)	8 (2%)	7 14
All	All	992/1012 (98%)	843 (85%)	127 (13%)	22 (2%)	5 9

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	LYS
1	A	267	ALA
1	A	373	PRO
1	A	440	THR
1	A	451	ASN

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	430/437 (98%)	346 (80%)	84 (20%)	1	2
1	B	430/437 (98%)	355 (83%)	75 (17%)	2	3
All	All	860/874 (98%)	701 (82%)	159 (18%)	1	3

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	223	ASN
1	B	405	PRO
1	B	242	LYS
1	B	318	ASN
1	B	448	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	480	ASN
1	B	429	GLN
1	B	148	ASN
1	B	420	HIS
1	B	396	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](#)

4 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	NDP	A	508	-	51,52,52	2.21	11 (21%)	71,80,80	2.55	16 (22%)
2	HEM	A	507	1	50,50,50	2.24	11 (22%)	67,82,82	3.31	21 (31%)
3	NDP	B	508	-	51,52,52	2.23	11 (21%)	71,80,80	2.55	16 (22%)
2	HEM	B	507	1	50,50,50	2.08	13 (26%)	67,82,82	3.04	20 (29%)

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	NDP	A	508	-	1/1/14/17	5/34/77/77	0/5/5/5
2	HEM	A	507	1	-	1/14/54/54	-
3	NDP	B	508	-	1/1/14/17	5/34/77/77	0/5/5/5
2	HEM	B	507	1	-	2/14/54/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	508	NDP	P2B-O2B	9.26	1.75	1.59
3	A	508	NDP	P2B-O2B	9.15	1.75	1.59
2	A	507	HEM	CHC-C1C	7.82	1.53	1.38
2	B	507	HEM	CHC-C1C	6.99	1.52	1.38
2	A	507	HEM	C4C-NC	5.72	1.50	1.39

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	507	HEM	CHC-C1C-NC	-20.70	101.92	124.45
2	B	507	HEM	CHC-C1C-NC	-17.82	105.05	124.45
3	B	508	NDP	C2B-C1B-N9A	12.15	133.75	113.75
3	A	508	NDP	C2B-C1B-N9A	12.12	133.69	113.75
3	A	508	NDP	O3B-C3B-C4B	9.53	138.46	111.08

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	508	NDP	C3B
3	B	508	NDP	C3B

5 of 13 torsion outliers are listed below:

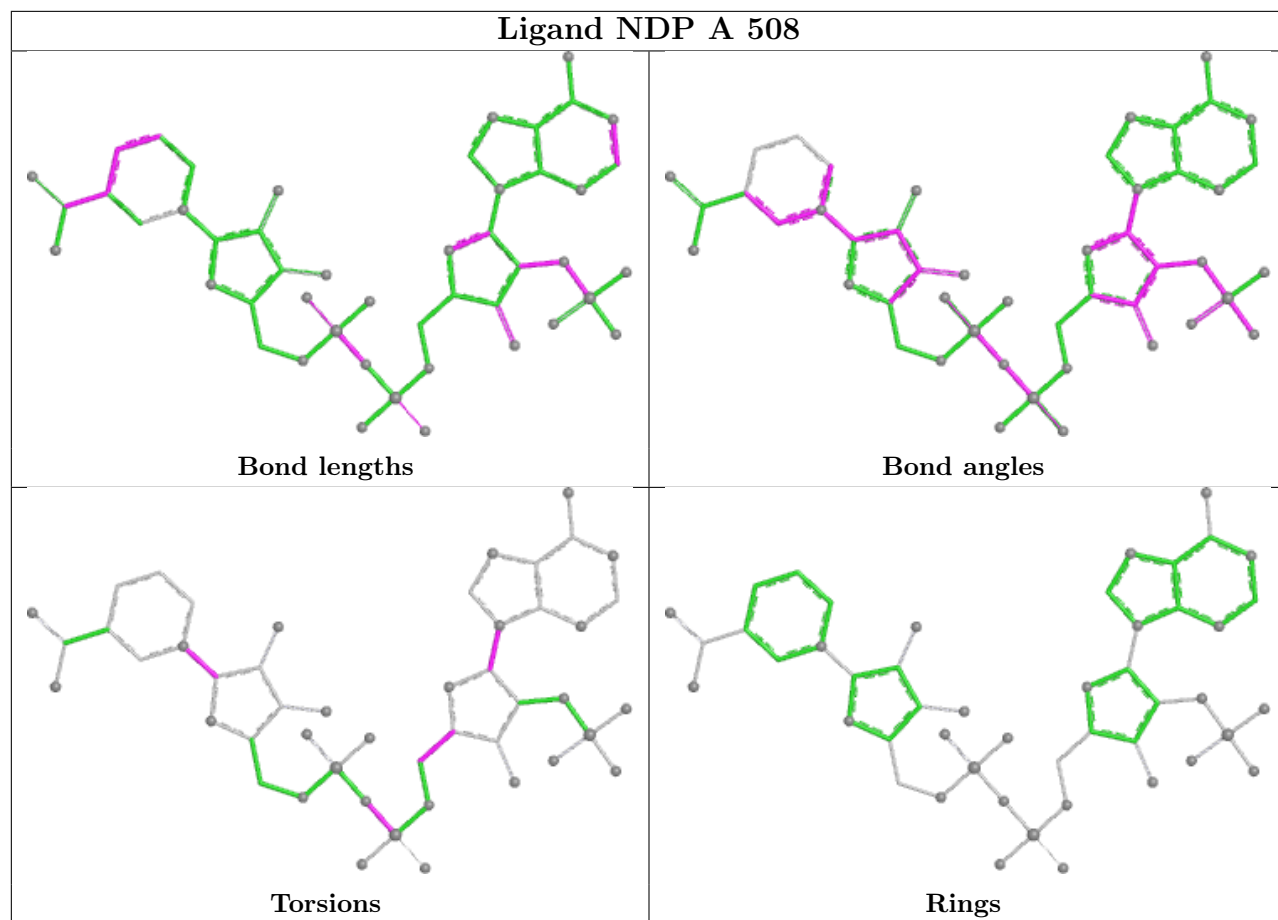
Mol	Chain	Res	Type	Atoms
2	B	507	HEM	C2C-C3C-CAC-CBC
2	B	507	HEM	C4C-C3C-CAC-CBC
3	A	508	NDP	O4B-C4B-C5B-O5B
3	B	508	NDP	O4B-C4B-C5B-O5B
3	A	508	NDP	C2B-C1B-N9A-C8A

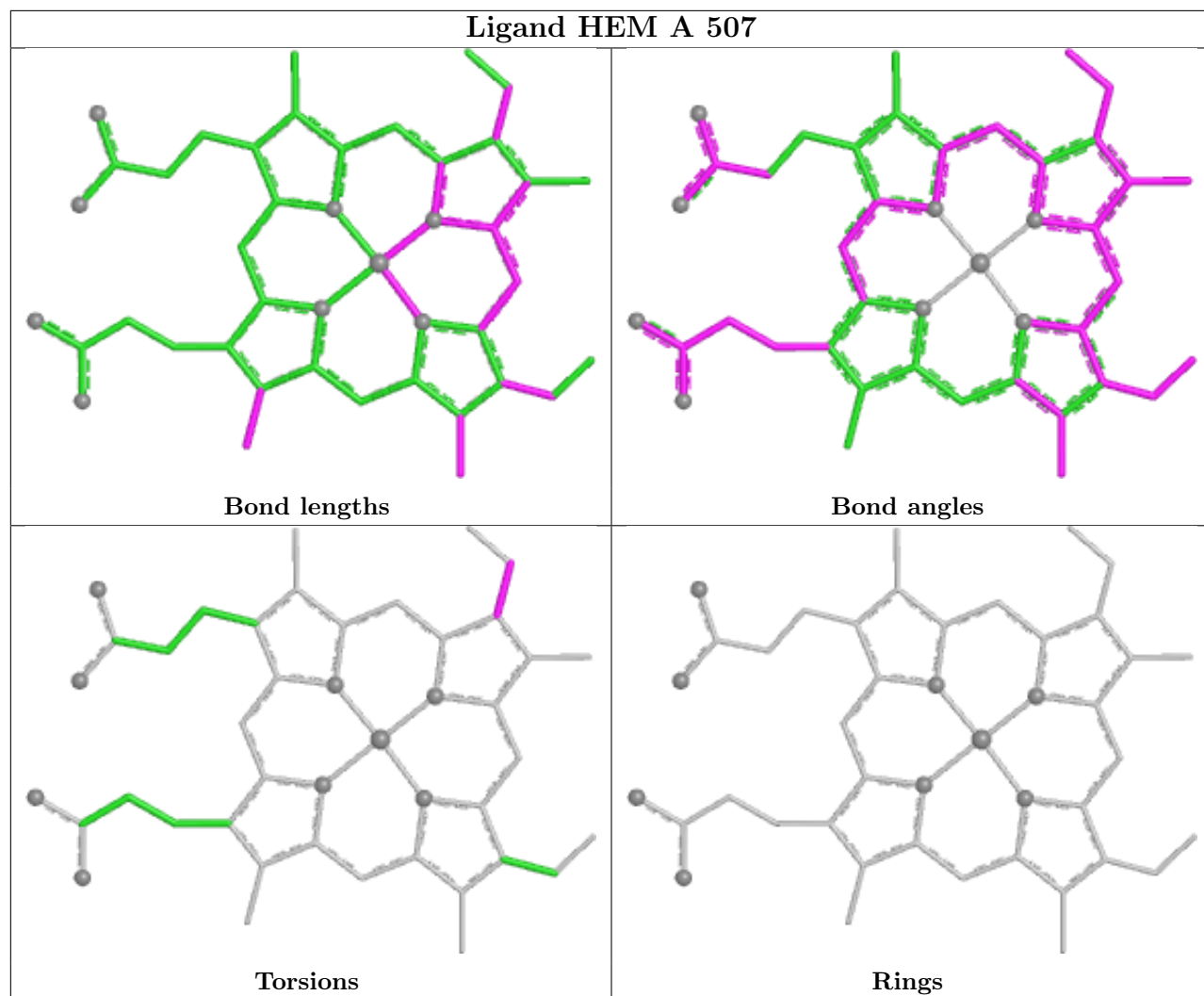
There are no ring outliers.

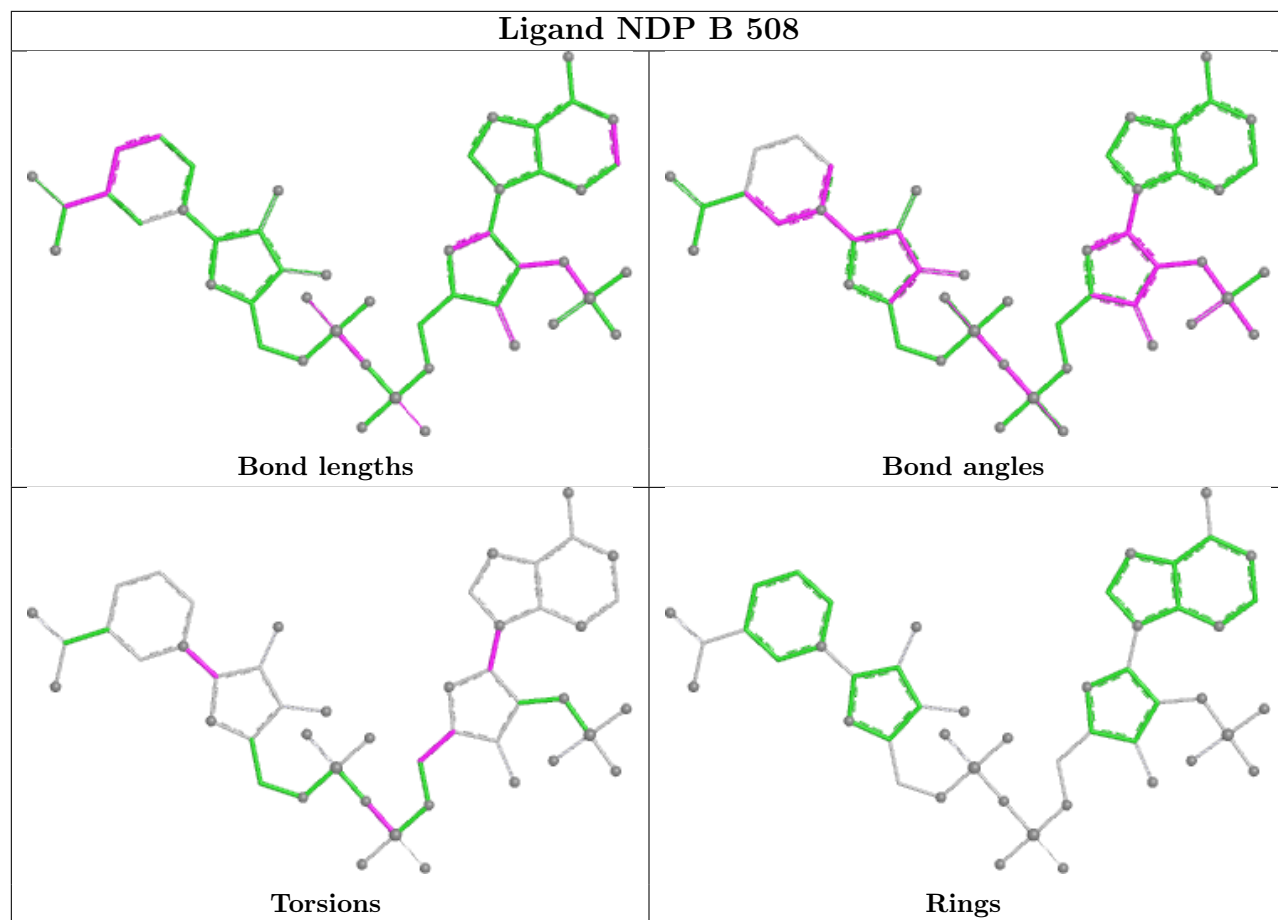
3 monomers are involved in 30 short contacts:

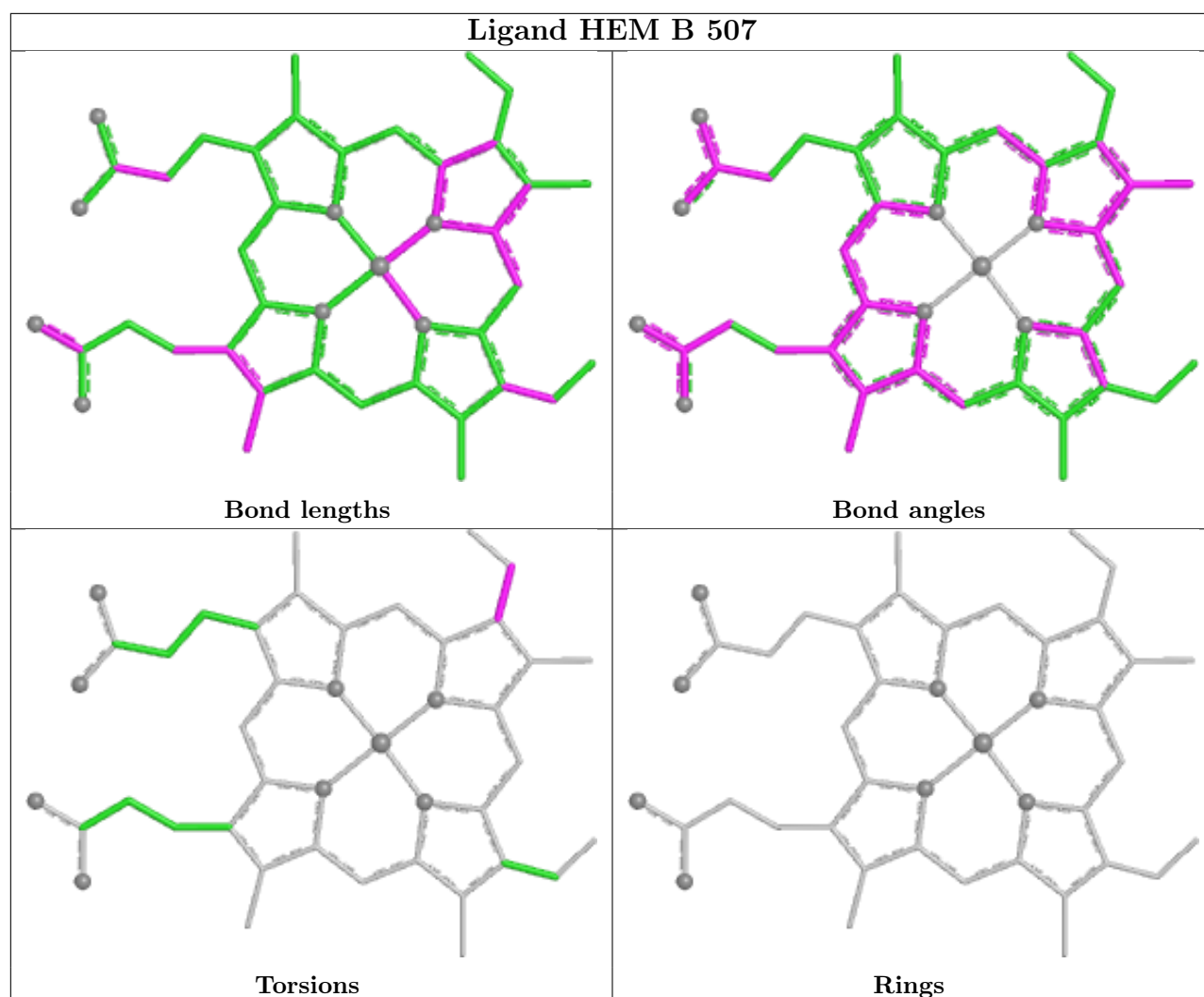
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	507	HEM	16	0
3	B	508	NDP	3	0
2	B	507	HEM	11	0

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.