



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:28 AM UTC

PDB ID : 7CAT / pdb_00007cat
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

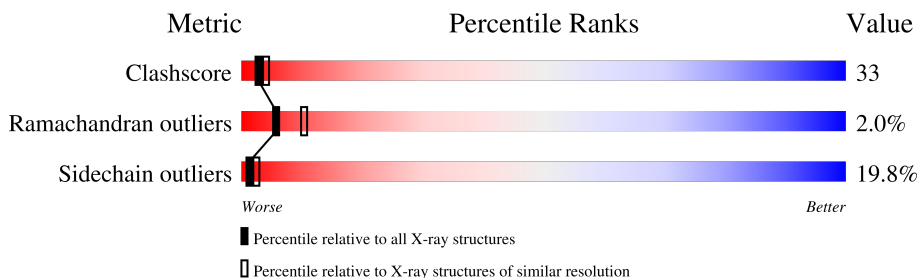
1 Overall quality at a glance

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.

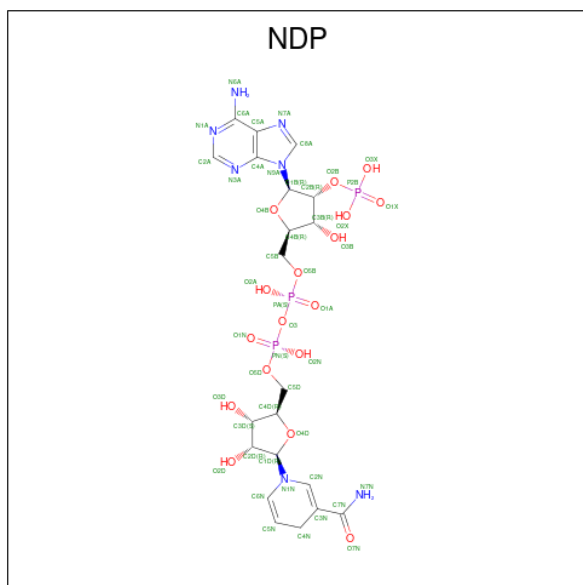


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	 26% 39% 29% 6% •
1	B	506	 25% 39% 29% 6% •



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	50	Total	O	0	0
			50	50		
4	B	50	Total	O	0	0
			50	50		

P128	P129	P130	P131	P132	P133	P134	P135	P136	P137	P138	P139	P140	P141	P142	P143	P144	P145	P146	P147	P148	P149	P150	P151	P152	P153	P154	P155	P156	P157	P158	P159	P160	P161	P162	P163	P164	P165	P166	P167	P168	P169	P170	P171	P172	P173	P174	P175	P176	P177	P178	P179	P180	P181	P182	P183	P184	P185	P186	P187	P188	P189
E190	S191	L192	H193	Q194	V195	F199	G203	I204	E138	P205	D139	G140	N141	H208	R209	D143	L144	V145	G146	N147	M148	T149	P150	I151	F152	F153	I154	R155	D156	A157	L158	L159	F160	P161	I162	I163	I164	H165	I166	K168	R169	N170	P171	Q172	T173	H174	L175	K176	D177	P178	D179	M180	V181	W182	D183	F184	W185	S186	L187	R188	P189
D263	L264	F265	N266	A267	I268	A269	T270	Y273	P274	S275	P205	K276	T277	L278	Y279	I280	Q281	V282	K283	L284	F285	T286	S287	E288	E289	I290	F291	N292	A293	D294	P295	F296	D297	L298	T299	K300	P303	H304	G305	D306	Y307	I310	F311	V312	D248	G313	K314	L315	V316	L317	N318	R319	N320	P321	V322	N323	Y324	L261	R262		
V328	E329	Q330	L331	A332	F333	D334	P335	S336	N337	M338	P339	F340	G341	I342	E343	P344	S345	P346	D347	K348	M349	L350	R353	L354	F355	A356	Y357	P358	D359	T360	H361	R362	H363	R364	L365	G366	P367	N368	Y369	L370	Q371	L372	P373	V374	N375	G376	P377	Y378	R379	A383	N384	Y385	Q386	R387	D388	G389					
P390	N391	C392	N393	N394	Q397	A400	P401	M402	G403	Y404	P405	M406	S407	F408	Q470	S409	A410	P411	E412	H413	Q414	P415	S416	A417	L418	E419	H420	R421	T422	S425	G426	D427	V428	Q429	R430	F431	N432	S433	Y434	D435	M436	L437	M438	V439	T440	D441	V442	R443	T444	F445	Y446	L447	K448	V449	L450	N451	E452				
E453	Q454	K455	K456	R457	L458	N461	I462	A463	G464	H465	L466	K467	D468	A469	Q470	L471	F472	I473	Q474	K475	K476	A477	S482	D483	V484	H485	P486	E487	Y488	G489	S490	R491	I492	L496	D497	K498	Y499	N500	GLU	GLU	LYS	PRO	LYS	ASN																	

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}	0.212 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8298	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	1.87	65/4128 (1.6%)	2.67	372/5607 (6.6%)
1	B	1.87	64/4128 (1.6%)	2.67	373/5607 (6.7%)
All	All	1.87	129/8256 (1.6%)	2.67	745/11214 (6.6%)

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	1
1	B	0	1
All	All	0	2

The worst 5 of 129 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	GLY	N-CA	9.43	1.54	1.45
1	B	426	GLY	N-CA	9.36	1.54	1.45
1	B	151	ILE	N-CA	8.24	1.56	1.46
1	A	151	ILE	N-CA	8.21	1.56	1.46
1	A	364	ARG	NE-CZ	7.90	1.41	1.33

The worst 5 of 745 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	CD-NE-CZ	21.05	153.88	124.40
1	A	67	ARG	CD-NE-CZ	21.02	153.82	124.40
1	A	472	PHE	CA-CB-CG	17.55	131.35	113.80
1	B	472	PHE	CA-CB-CG	17.51	131.31	113.80

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	139	ASP	CA-CB-CG	15.76	128.36	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	430	ARG	Sidechain
1	B	430	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	275	3
1	B	4008	0	3833	265	3
2	A	43	0	30	11	0
2	B	43	0	30	12	0
3	A	48	0	26	3	0
3	B	48	0	26	3	0
4	A	50	0	0	4	1
4	B	50	0	0	3	1
All	All	8298	0	7778	522	4

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 33.

The worst 5 of 522 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (\AA)	Clash overlap (\AA)
1:B:155:ARG:NH2	1:B:438:ASN:HD21	1.22	1.35
1:A:155:ARG:NH2	1:A:438:ASN:HD21	1.22	1.34
1:A:155:ARG:HH22	1:A:438:ASN:ND2	1.22	1.33
1:B:155:ARG:HH22	1:B:438:ASN:ND2	1.22	1.32
1:A:177:ASP:HB3	1:A:180:MET:HE2	1.14	1.08

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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]	1.98	0.22
1:A:430:ARG:NH1	1:B:419:GLU:OE2[6_556]	1.98	0.22
1:B:10:GLN:NE2	4:B:551:HOH:O[6_556]	2.13	0.07
1:A:10:GLN:NE2	4:A:543:HOH:O[6_556]	2.14	0.06

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%)	434 (88%)	52 (10%)	10 (2%)	6	10
1	B	496/506 (98%)	434 (88%)	52 (10%)	10 (2%)	6	10
All	All	992/1012 (98%)	868 (88%)	104 (10%)	20 (2%)	6	10

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ALA
1	B	267	ALA
1	A	54	VAL
1	A	440	THR
1	B	54	VAL

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%)	345 (80%)	85 (20%)	1	2
1	B	430/437 (98%)	345 (80%)	85 (20%)	1	2
All	All	860/874 (98%)	690 (80%)	170 (20%)	1	2

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	159	LEU
1	B	354	LEU
1	B	223	ASN
1	B	263	ASP
1	B	405	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	438	ASN
1	B	406	ASN
1	B	21	GLN
1	B	402	ASN
1	B	438	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	B	508	-	51,52,52	1.76	10 (19%)	71,80,80	1.80	10 (14%)
2	HEM	A	507	1	50,50,50	1.21	6 (12%)	67,82,82	1.27	8 (11%)
2	HEM	B	507	1	50,50,50	1.22	6 (12%)	67,82,82	1.26	8 (11%)
3	NDP	A	508	-	51,52,52	1.76	10 (19%)	71,80,80	1.81	10 (14%)

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	B	508	-	-	6/34/77/77	0/5/5/5
2	HEM	A	507	1	-	4/14/54/54	-
2	HEM	B	507	1	-	4/14/54/54	-
3	NDP	A	508	-	-	6/34/77/77	0/5/5/5

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	508	NDP	PN-O3	-5.97	1.53	1.59
3	A	508	NDP	PN-O3	-5.94	1.53	1.59
3	A	508	NDP	C4N-C3N	-4.65	1.41	1.50
3	B	508	NDP	C4N-C3N	-4.63	1.41	1.50
3	A	508	NDP	P2B-O2B	4.41	1.67	1.59

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	NDP	C2B-C1B-N9A	7.92	126.79	113.75
3	B	508	NDP	C2B-C1B-N9A	7.91	126.77	113.75
3	A	508	NDP	O2X-P2B-O2B	5.72	128.15	105.85
3	B	508	NDP	O2X-P2B-O2B	5.72	128.15	105.85
3	B	508	NDP	O2N-PN-O3	4.59	119.67	107.27

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

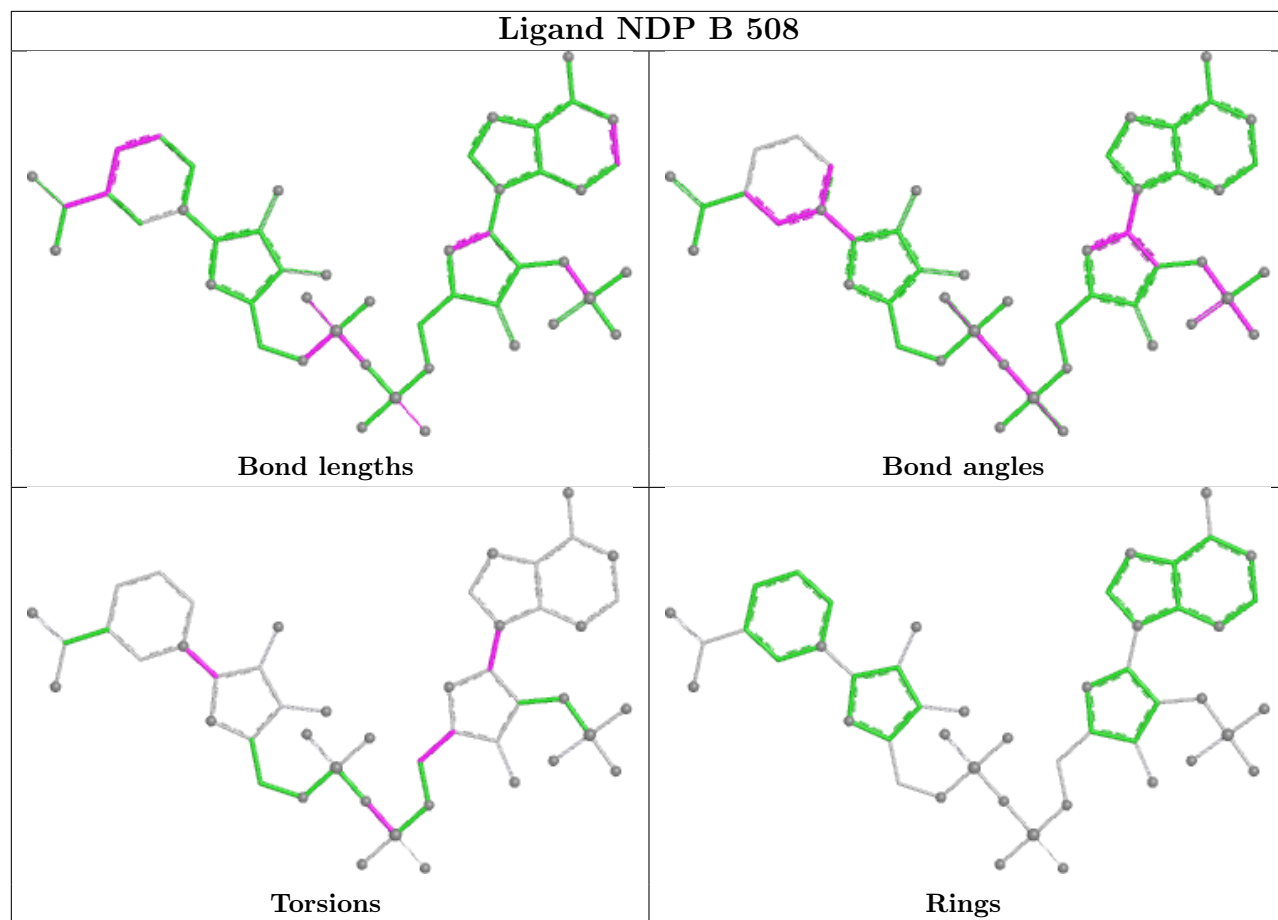
Mol	Chain	Res	Type	Atoms
2	A	507	HEM	C2C-C3C-CAC-CBC
2	B	507	HEM	C2C-C3C-CAC-CBC
2	A	507	HEM	C4C-C3C-CAC-CBC
2	B	507	HEM	C4C-C3C-CAC-CBC
3	A	508	NDP	O4B-C4B-C5B-O5B

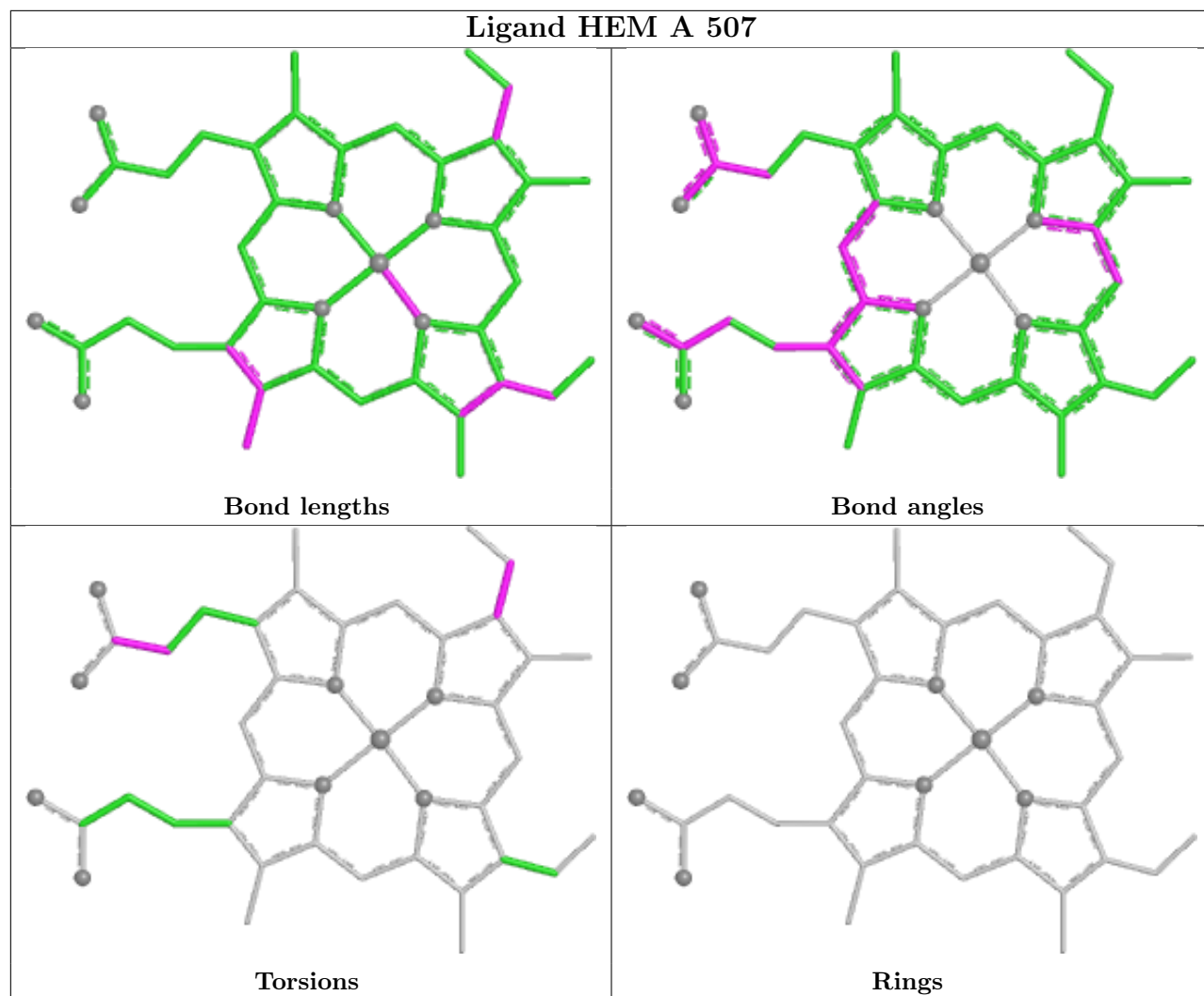
There are no ring outliers.

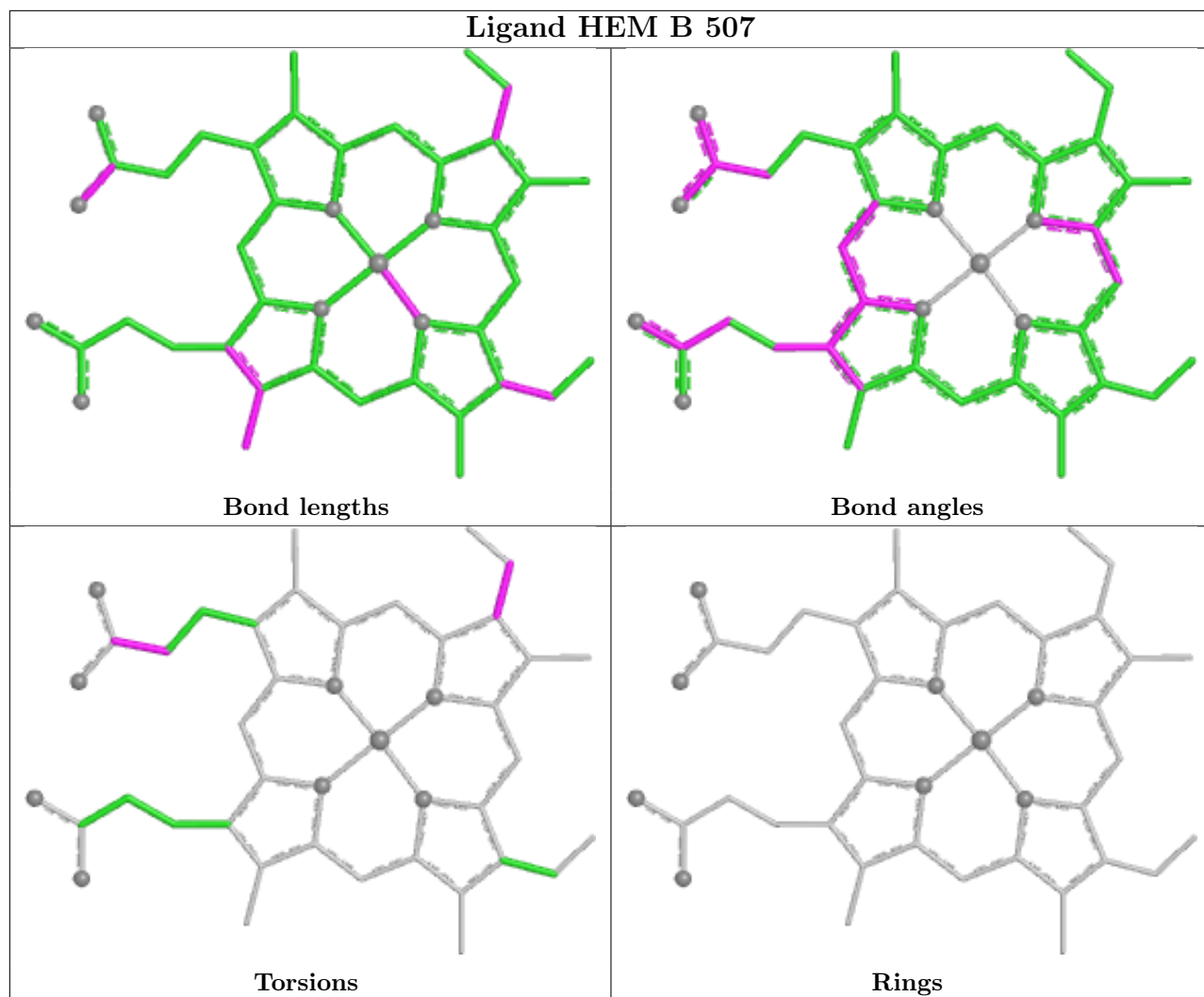
4 monomers are involved in 29 short contacts:

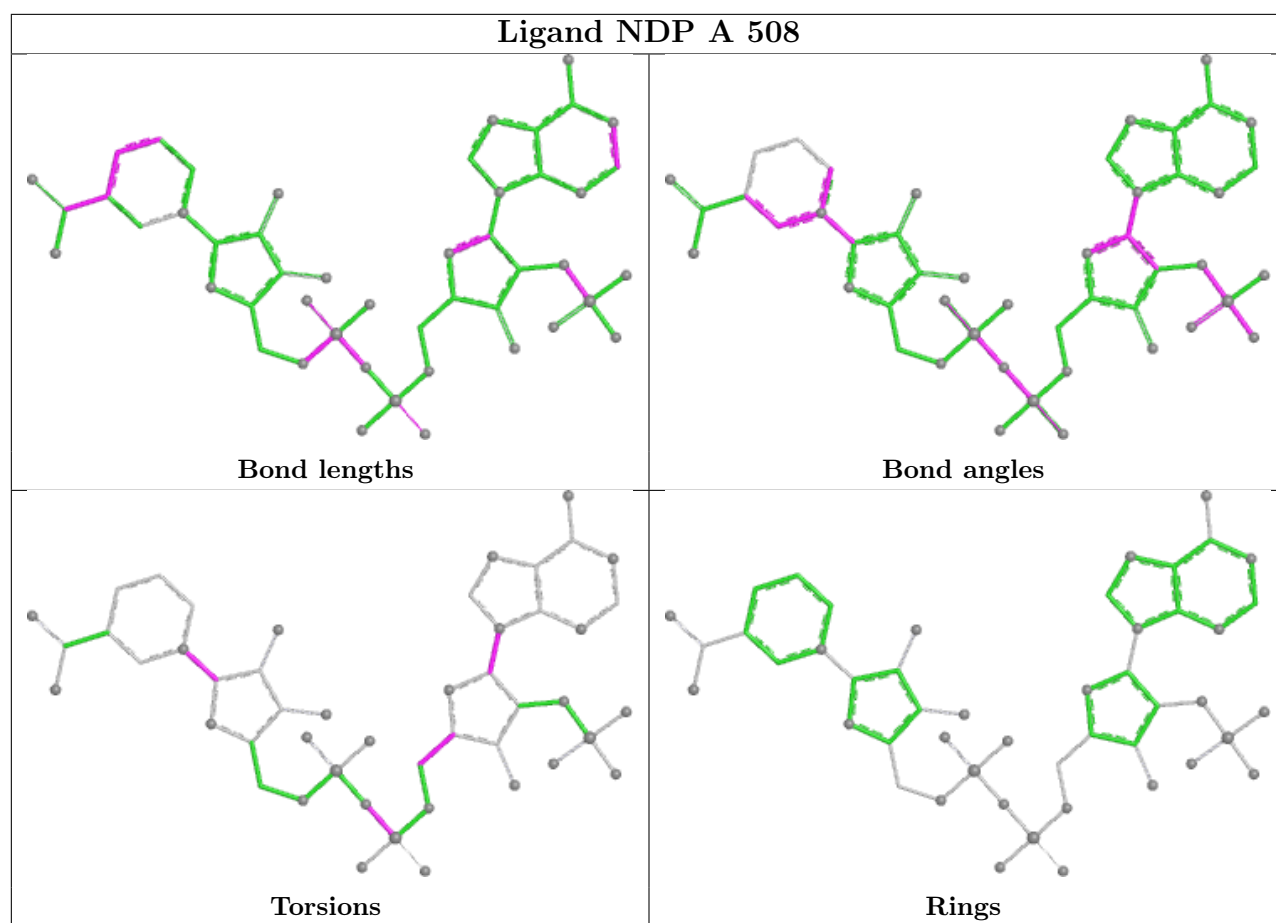
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	508	NDP	3	0
2	A	507	HEM	11	0
2	B	507	HEM	12	0
3	A	508	NDP	3	0

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.