



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 08:36 am BST

PDB ID : 8CAT
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : 2.11

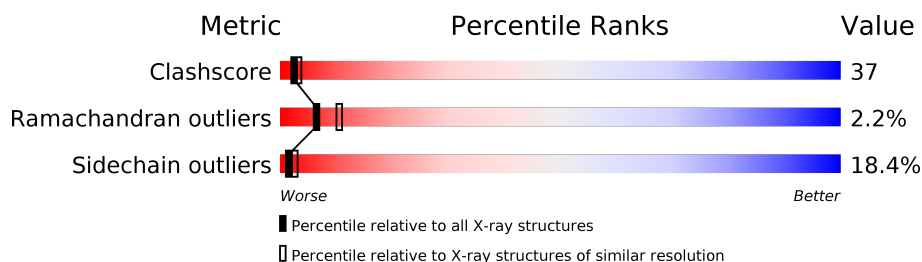
1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 on 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](#)

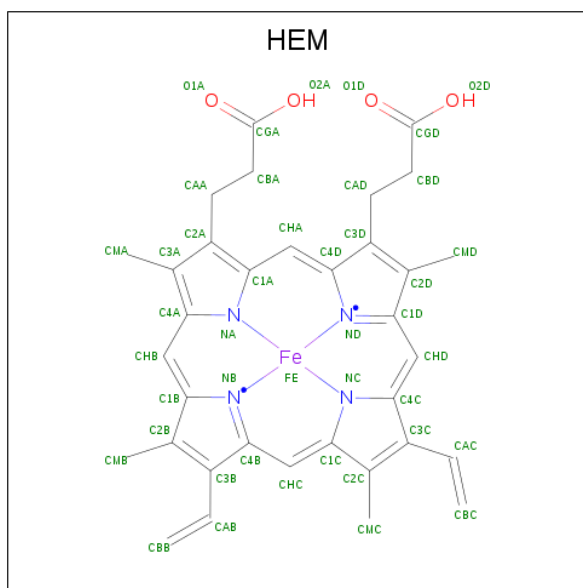
There are 4 unique types of molecules in this entry. The entry contains 8296 atoms, of which 0 are hydrogens and 0 are deuteriums.

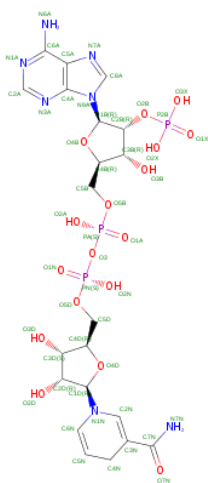
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CATALASE.

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

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





- Molecule 4 is water.

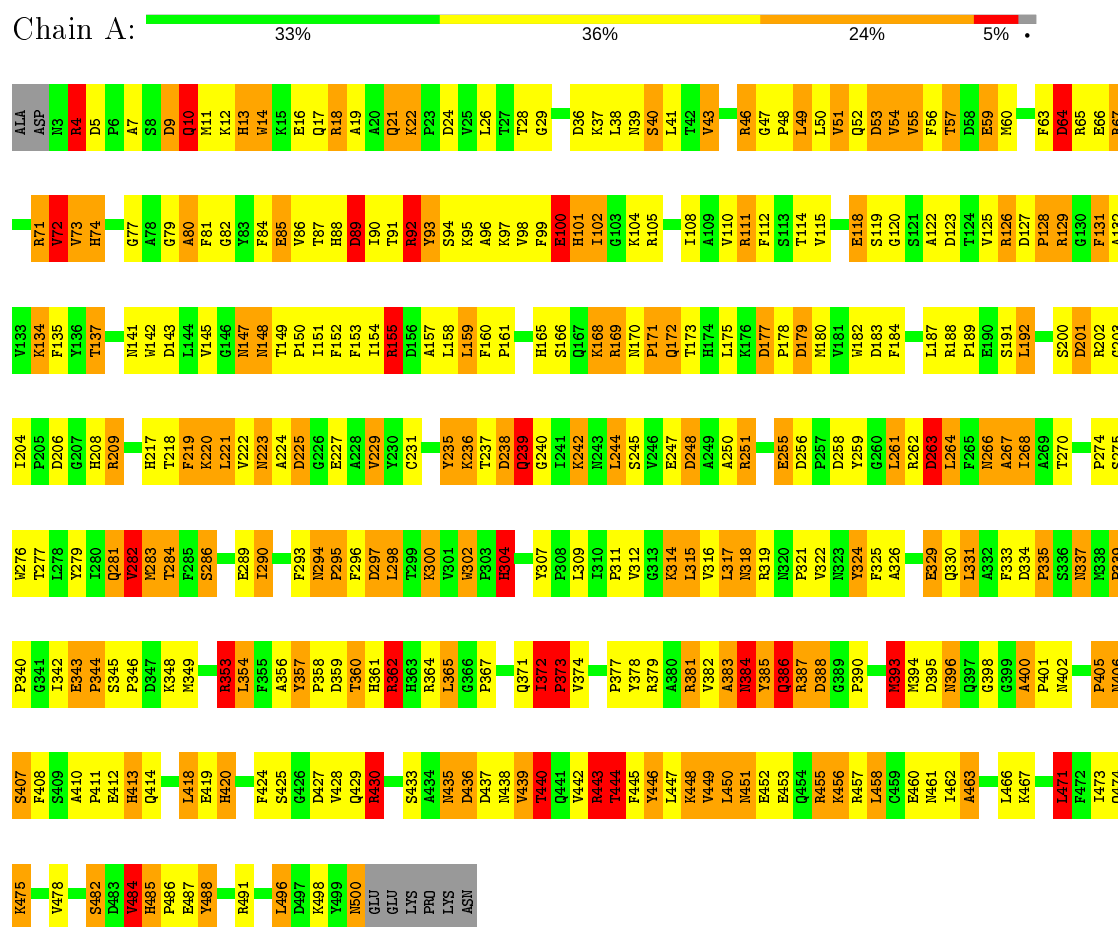


3 Residue-property plots

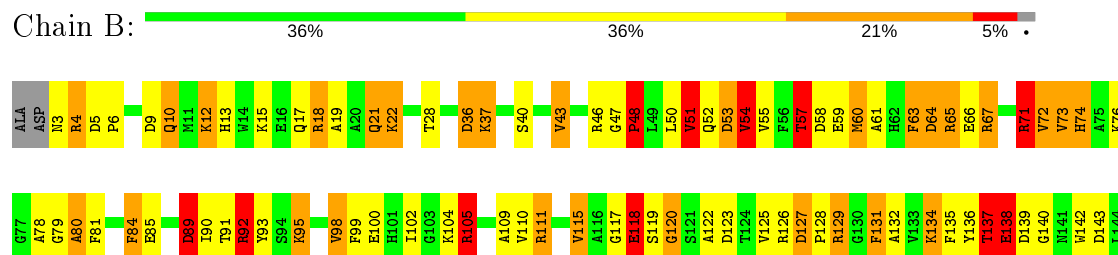
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: CATALASE



• Molecule 1: CATALASE



LYS	D437	L365	F293	V145
PRO	M438		M294	G146
LYS	V439	L370	P295	N147
ASN	T440	Q371	F296	N148
	Q441	I372	D297	T149
	V442	P373	L298	P150
	R443	V374	T299	I151
	T444	N375	K300	F152
	P445		V301	F153
	Y446	Y378	W302	I154
	L447	Y379	W303	R155
	V449	A380	H304	D156
	K448	R381	G305	A157
	L450	Y382	D306	L158
	M451	A383	Y307	L159
	E452	N384	P308	F160
	E453	Y385	L309	P161
	Q454	Q386	I310	S162
	R455	R387	P311	S162
	K456	D388	V312	F163
	R457		G313	
	L458	C392	K314	K168
	C459	M393	I315	R169
	E460	M394	V316	N170
	M461	D395	L317	P171
	L462	N396	N318	Q172
			R319	T173
			N320	H174
	L466	A400	P321	L175
	K467	P401	V322	K176
	D468	N402		D177
	A469	Y403		P178
	Q470	Y404	L331	D179
	L471	P405	A332	M180
	F472	N406	F333	V181
		S407	D334	D183
	K475	F408	P335	
	K476	S409	S336	L187
	A477	A410	N337	R188
	V478	P411	K338	P189
	K479	E412	P339	E190
		H413		S191
	D483	Q414	E343	L192
	V484	P415		H193
	H485	S416	D347	Q194
	P486	A417	K348	V195
	E487		M349	
	Y488	H420	L350	L198
		R421	Q351	
	R491		G352	D201
	Y492	S425	R353	R202
	Q493	G426	L354	
	A494	D427	F355	D206
	L495	V428	A356	
	L496	Q429		R209
	D497	R430	D359	
	K498	F431	T360	D212
	Y499	N432	H361	G213
	M500		R362	T218
	GLU	N435	H363	
	GLU	D436	R364	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.00 Å 142.00 Å 103.70 Å 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.	Xtriage
Total number of atoms	8296	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.53	22/4128 (0.5%)	2.37	195/5607 (3.5%)
1	B	1.57	20/4128 (0.5%)	2.42	229/5607 (4.1%)
All	All	1.55	42/8256 (0.5%)	2.39	424/11214 (3.8%)

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 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ARG	CD-NE	-6.86	1.34	1.46
1	A	343	GLU	N-CA	6.53	1.59	1.46
1	A	166	SER	CB-OG	6.43	1.50	1.42
1	B	100	GLU	CD-OE2	-6.36	1.18	1.25
1	B	119	SER	CB-OG	-6.30	1.34	1.42

The worst 5 of 424 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	CD-NE-CZ	25.86	159.81	123.60
1	B	92	ARG	NE-CZ-NH1	23.28	131.94	120.30
1	B	126	ARG	NE-CZ-NH2	21.12	130.86	120.30
1	B	261	LEU	CA-CB-CG	20.39	162.19	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ARG	NE-CZ-NH2	-20.36	110.12	120.30

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

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	3830	329	3
1	B	4008	0	3825	293	2
2	A	43	0	30	15	0
2	B	43	0	30	9	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	7763	596	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 37.

The worst 5 of 596 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	1.40
1:B:155:ARG:HH22	1:B:438:ASN:ND2	1.28	1.30
1:A:155:ARG:HH22	1:A:438:ASN:ND2	1.28	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	1.24
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%)	5	7
1	B	496/506 (98%)	425 (86%)	63 (13%)	8 (2%)	9	17
All	All	992/1012 (98%)	843 (85%)	127 (13%)	22 (2%)	6	10

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 ⓘ

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%)	351 (82%)	79 (18%)	1	2
1	B	430/437 (98%)	351 (82%)	79 (18%)	1	2
All	All	860/874 (98%)	702 (82%)	158 (18%)	1	2

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	458	LEU
1	B	51	VAL
1	B	414	GLN
1	A	475	LYS
1	B	10	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	GLN
1	B	21	GLN
1	B	420	HIS
1	A	438	ASN
1	A	485	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	-	45,52,52	2.54	11 (24%)	53,80,80	2.20	12 (22%)
2	HEM	B	507	1	27,50,50	1.71	6 (22%)	17,82,82	2.35	8 (47%)
2	HEM	A	507	1	27,50,50	1.86	9 (33%)	17,82,82	3.18	8 (47%)
3	NDP	A	508	-	45,52,52	2.52	11 (24%)	53,80,80	2.20	12 (22%)

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	-	1/1/14/17	3/30/77/77	0/5/5/5
2	HEM	B	507	1	-	0/6/54/54	-
2	HEM	A	507	1	-	0/6/54/54	-
3	NDP	A	508	-	1/1/14/17	3/30/77/77	0/5/5/5

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	508	NDP	O4B-C1B	9.69	1.54	1.41
3	A	508	NDP	O4B-C1B	9.65	1.54	1.41
3	B	508	NDP	P2B-O2B	8.71	1.75	1.59
3	A	508	NDP	P2B-O2B	8.61	1.75	1.59
3	B	508	NDP	O3B-C3B	-5.10	1.31	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	NDP	O3B-C3B-C4B	9.48	138.46	111.05
3	B	508	NDP	O3B-C3B-C4B	9.46	138.41	111.05
2	A	507	HEM	CAA-CBA-CGA	9.27	128.23	112.67
2	B	507	HEM	CMC-C2C-C3C	6.43	136.71	124.68
3	A	508	NDP	O4B-C1B-C2B	-6.36	95.55	106.59

All (2) chirality outliers are listed below:

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

5 of 6 torsion outliers are listed below:

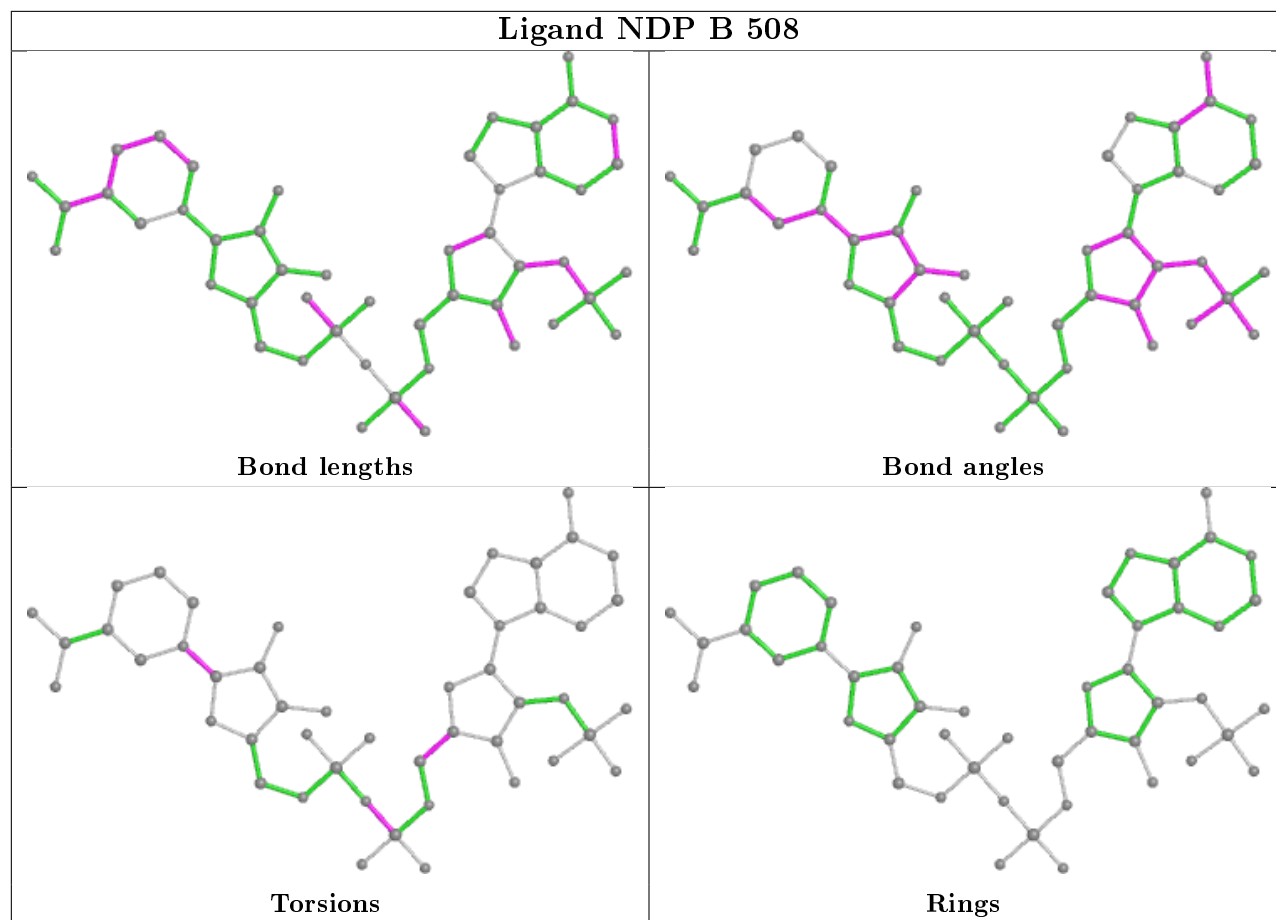
Mol	Chain	Res	Type	Atoms
3	B	508	NDP	O4B-C4B-C5B-O5B
3	A	508	NDP	O4B-C4B-C5B-O5B
3	B	508	NDP	PN-O3-PA-O2A
3	A	508	NDP	PN-O3-PA-O2A
3	B	508	NDP	O4D-C1D-N1N-C6N

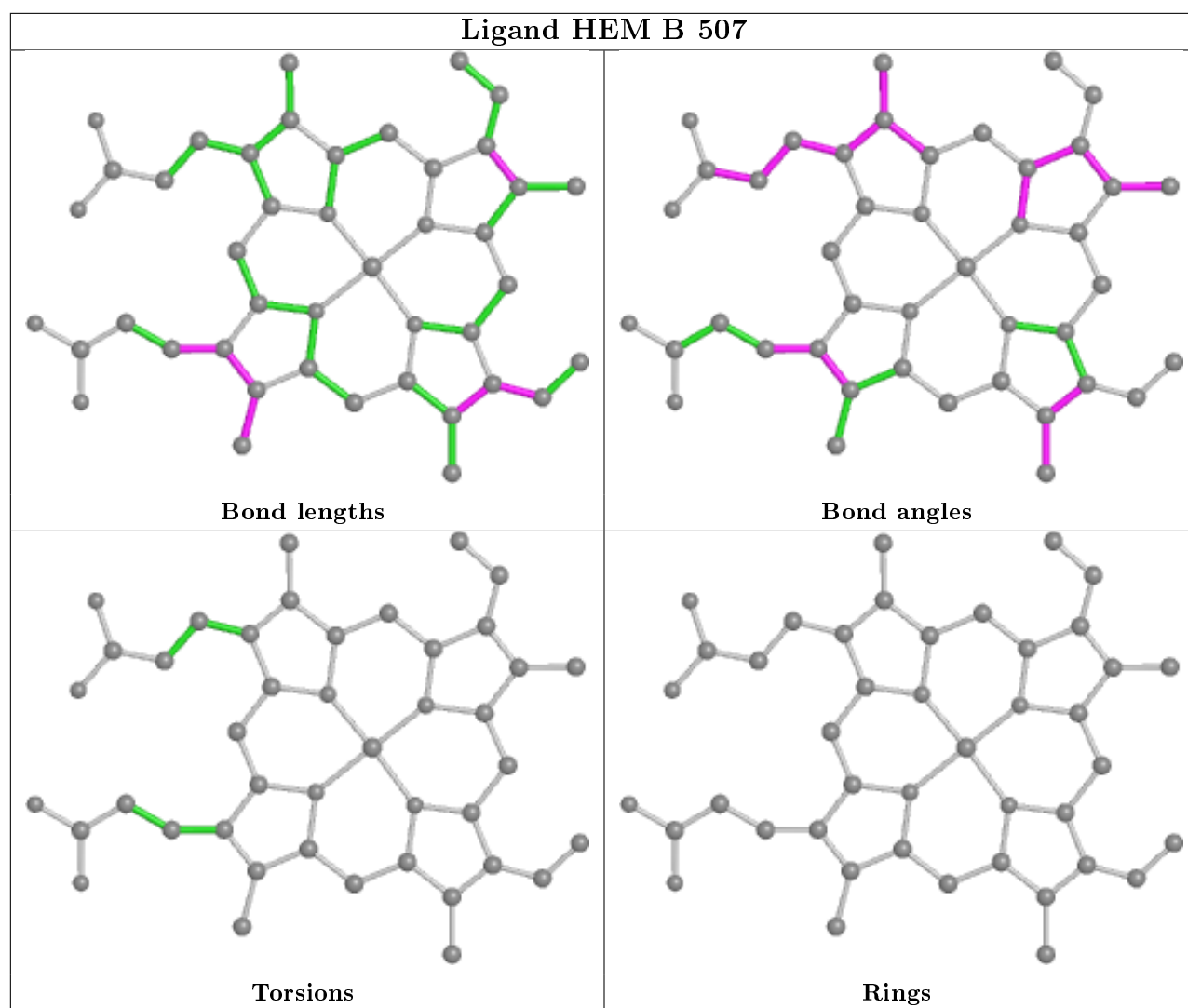
There are no ring outliers.

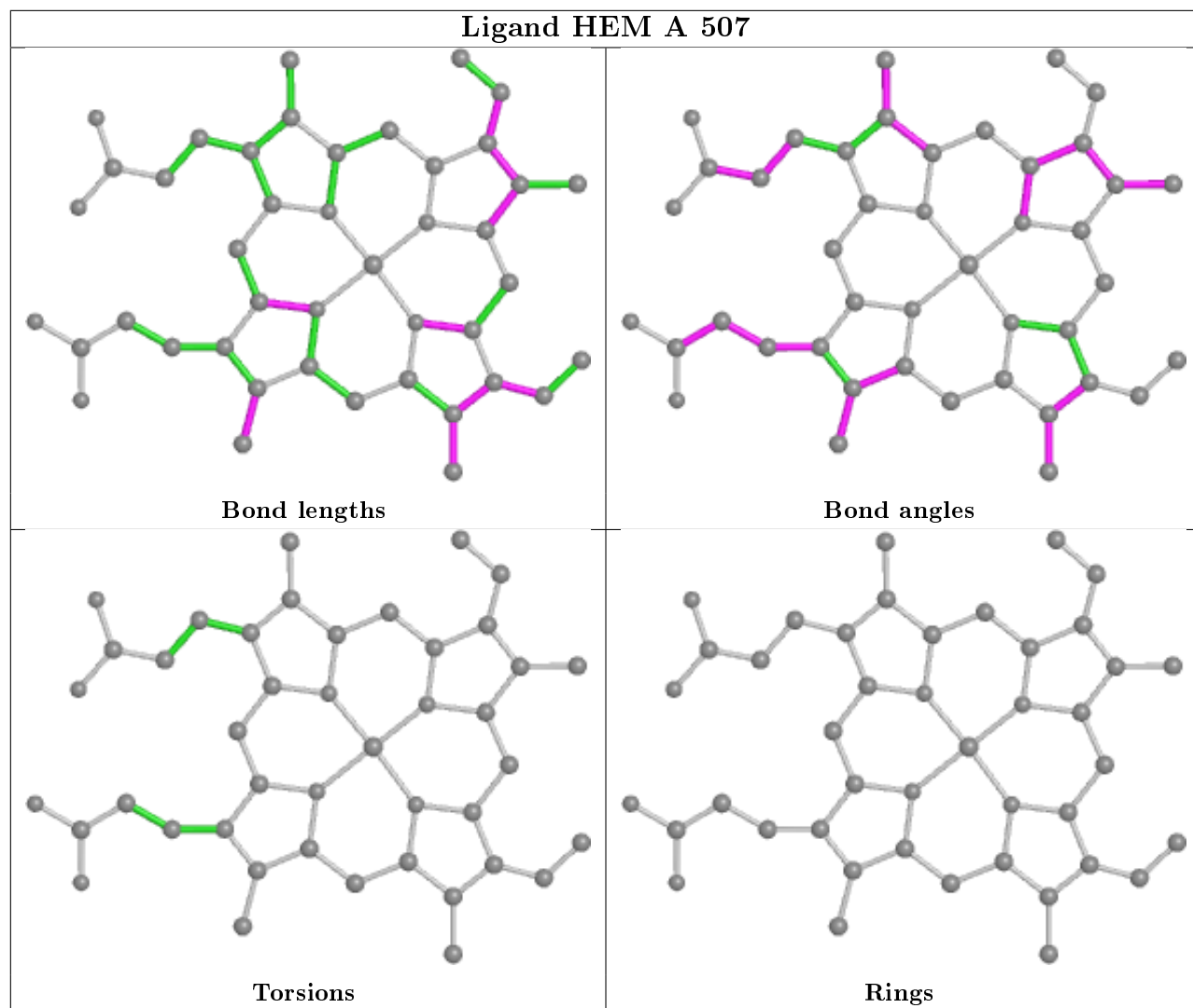
3 monomers are involved in 27 short contacts:

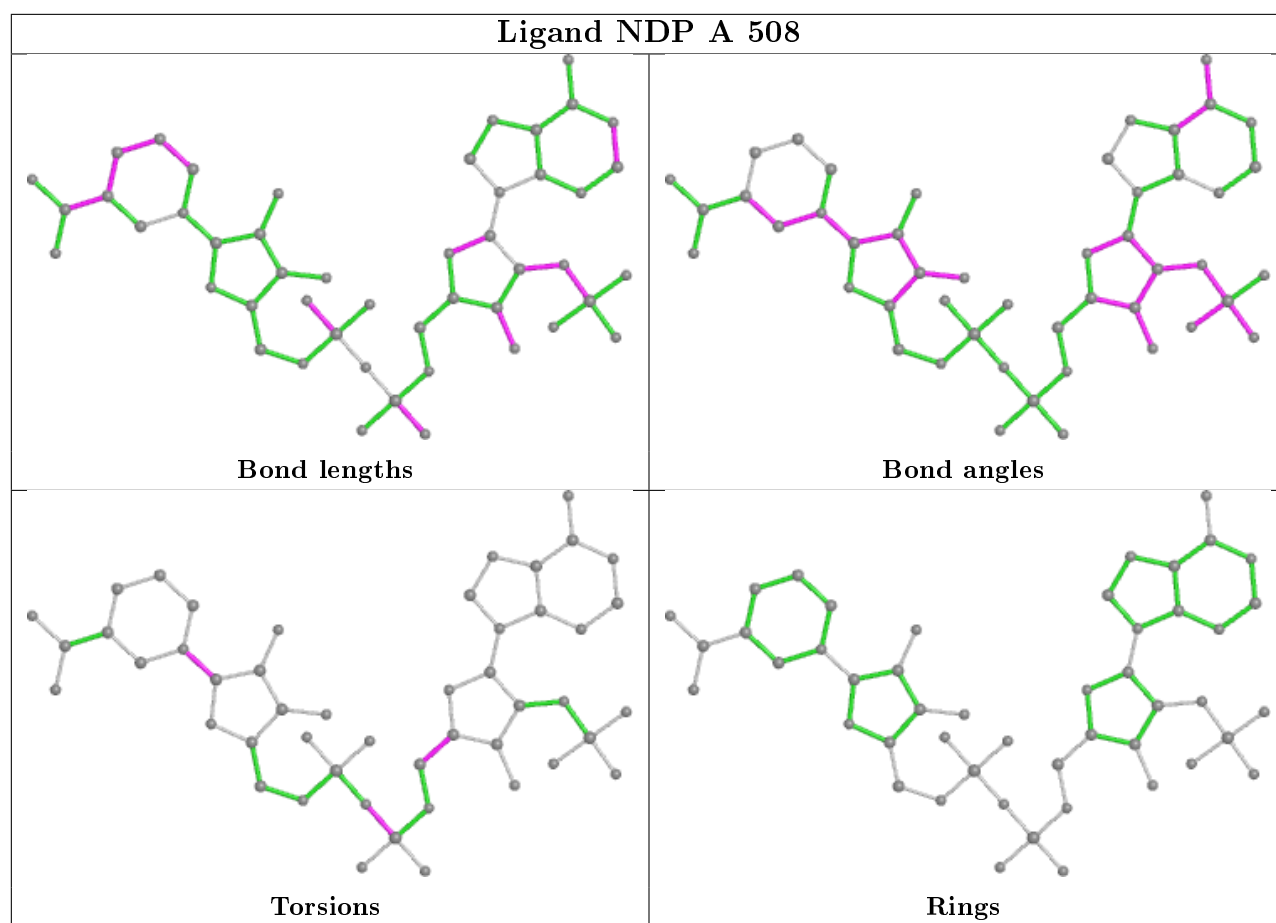
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	508	NDP	3	0
2	B	507	HEM	9	0
2	A	507	HEM	15	0

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.