wwPDB X-ray Structure Validation Summary Report (i)

Sep 18, 2023 – 02:14 PM EDT

PDB ID	:	7CAT
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 (i) 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 (1)) were used in the production of this report:

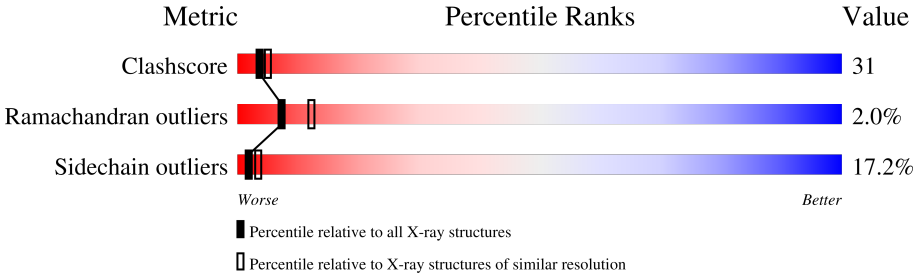
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	506	40% 38% 18% • •
1	B	506	39% 38% 19% • •

2 Entry composition (i)

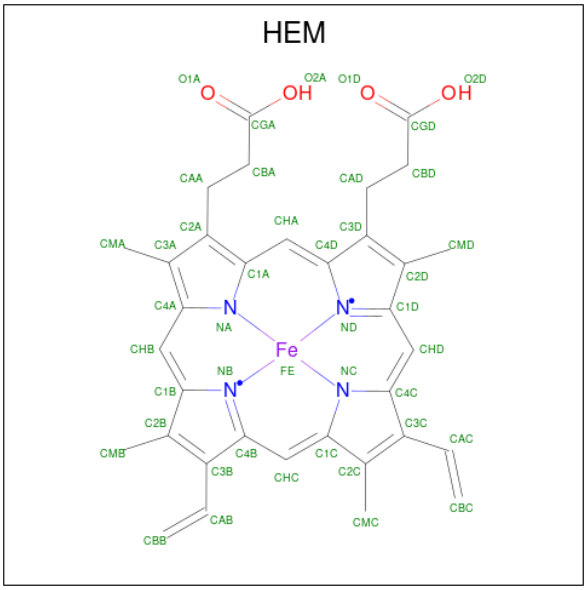
There are 4 unique types of molecules in this entry. The entry contains 8298 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

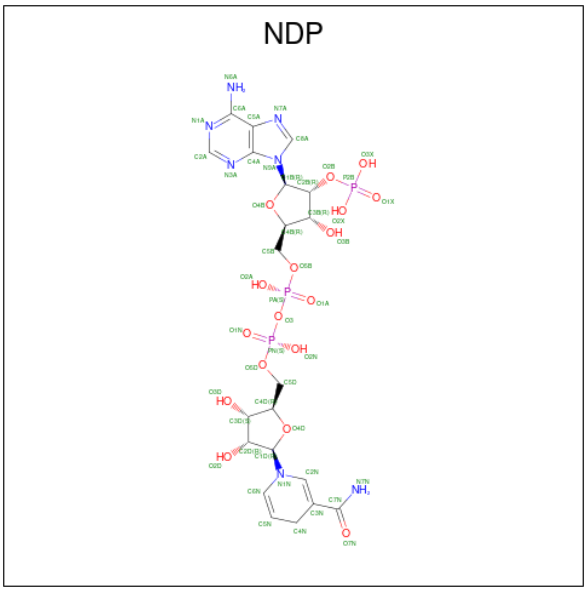
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	4008	2543	714	737	14	0	0	0
1	B	498	4008	2543	714	737	14	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: 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 (three-letter code: 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
			Total	C	N	O	P		
3	B	1	48	21	7	17	3	0	0

- Molecule 4 is water.

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

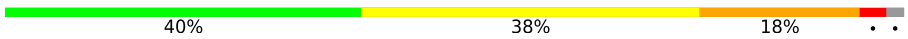
3 Residue-property plots (i)

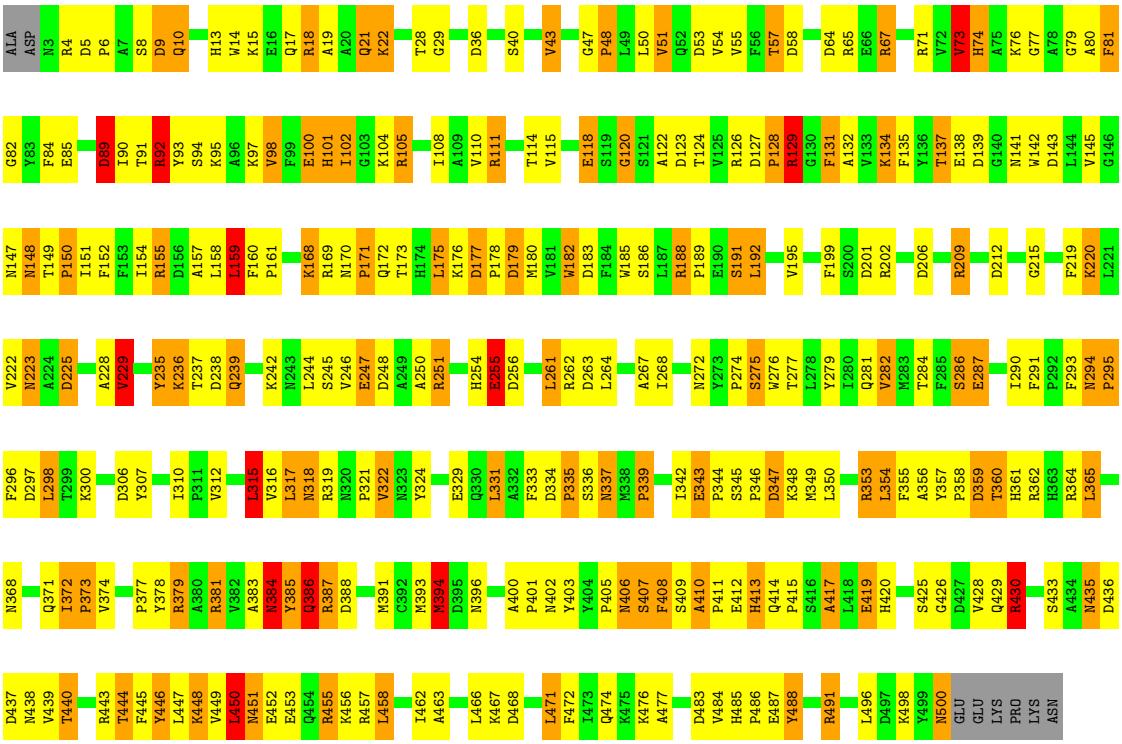
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

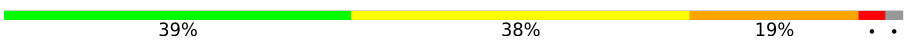
Chain A:

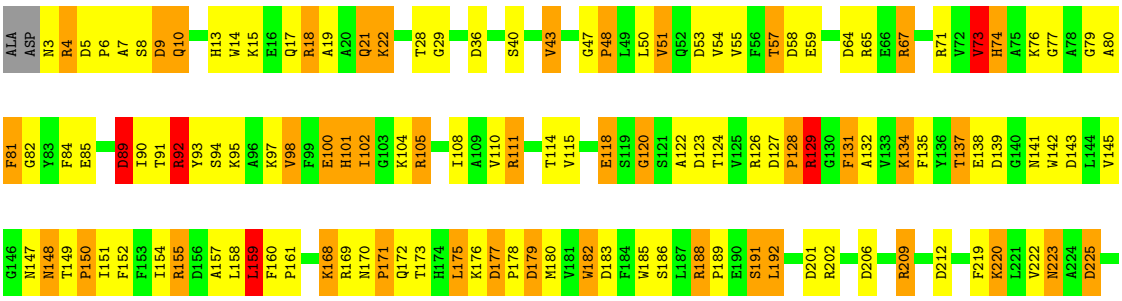


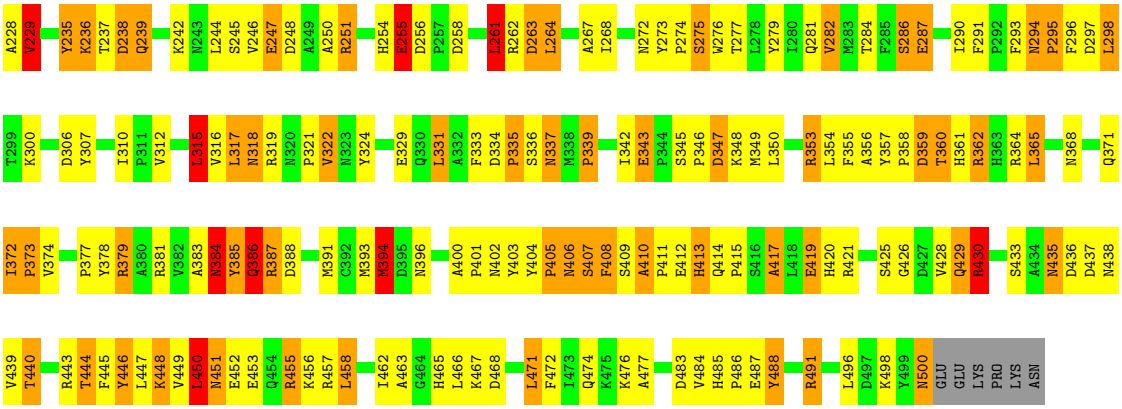


• Molecule 1: CATALASE

Chain B:






A228 V229 Y235 K236 T237 D238 Q239 K242 N243 L244 S245 V246 E247 D248 A249 A250 R251 H254 E255 D256 P257 D258 L261 R262 D263 L264 A267 I268 N272 Y273 P274 S275 W276 T277 L278 Y279 I280 Q281 V282 M283 T284 F285 S286 E287 I290 F291 P292 F293 N294 P295 F296 D297 L298
T299 K300 D306 Y307 I310 P311 V312 L315 V316 L317 N318 R319 N320 P321 V322 N323 Y324 E329 Q330 L331 A332 F333 D334 P335 S336 N337 M338 P339 I342 E343 P344 S345 P346 D347 K348 M349 L350 R353 L354 F355 A356 Y357 P358 D359 T360 H361 R362 H363 R364 L365 N368 Q371
I372 P373 V374 P377 Y378 R379 A380 R381 V382 A383 N384 Y385 Q386 R387 D388 M391 C392 M393 M394 D395 N396 A400 P401 N402 Y403 Y404 P405 M406 S407 F408 S409 A410 P411 E412 H413 Q414 P415 S416 A417 L418 E419 H420 R421 S425 G426 D427 V428 Q429 R430 S433 A434 N435 D436 D437 N438
V439 T440 R443 T444 F445 Y446 L447 K448 V449 L450 N451 E452 E453 Q454 R455 K456 R457 L458 I462 A463 G464 H465 L466 K467 D468 L471 F472 I473 Q474 K475 K476 A477 D483 V484 H485 P486 E487 Y488 R491 L496 D497 K498 Y499 N500 GLU GLU LYS PRO LYS ASN

4 Data and refinement statistics (i)

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	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.	Xtriage
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: NDP, HEM

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	1.45	15/4128 (0.4%)	2.14	148/5607 (2.6%)
1	B	1.45	16/4128 (0.4%)	2.14	147/5607 (2.6%)
All	All	1.45	31/8256 (0.4%)	2.14	295/11214 (2.6%)

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 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	SER	CB-OG	-7.37	1.32	1.42
1	A	336	SER	CB-OG	-7.28	1.32	1.42
1	A	364	ARG	NE-CZ	6.69	1.41	1.33
1	B	364	ARG	NE-CZ	6.67	1.41	1.33
1	A	171	PRO	N-CD	6.43	1.56	1.47

The worst 5 of 295 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	67	ARG	CD-NE-CZ	21.63	153.88	123.60
1	A	67	ARG	CD-NE-CZ	21.59	153.82	123.60
1	A	92	ARG	NE-CZ-NH1	18.39	129.49	120.30
1	B	92	ARG	NE-CZ-NH1	18.36	129.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	261	LEU	CA-CB-CG	16.87	154.11	115.30

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	3830	262	3
1	B	4008	0	3830	259	3
2	A	43	0	30	11	0
2	B	43	0	30	11	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	7772	502	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 31.

The worst 5 of 502 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: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	1.35	1.07

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%)	7 12
1	B	496/506 (98%)	434 (88%)	52 (10%)	10 (2%)	7 12
All	All	992/1012 (98%)	868 (88%)	104 (10%)	20 (2%)	7 12

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%)	356 (83%)	74 (17%)	2 3
1	B	430/437 (98%)	356 (83%)	74 (17%)	2 3
All	All	860/874 (98%)	712 (83%)	148 (17%)	2 3

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	294	ASN
1	B	458	LEU
1	B	318	ASN
1	B	386	GLN
1	A	337	ASN

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	474	GLN
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 monosaccharides 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	$\#\|Z\| > 2$
2	HEM	A	507	1	41,50,50	1.33	4 (9%)	45,82,82	1.53	8 (17%)
3	NDP	A	508	-	45,52,52	1.77	9 (20%)	53,80,80	1.58	7 (13%)
3	NDP	B	508	-	45,52,52	1.76	9 (20%)	53,80,80	1.57	7 (13%)
2	HEM	B	507	1	41,50,50	1.35	4 (9%)	45,82,82	1.53	8 (17%)

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	507	1	-	2/12/54/54	-
3	NDP	A	508	-	-	4/30/77/77	0/5/5/5
3	NDP	B	508	-	-	4/30/77/77	0/5/5/5
2	HEM	B	507	1	-	2/12/54/54	-

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	508	NDP	O4B-C1B	5.76	1.49	1.41
3	B	508	NDP	O4B-C1B	5.71	1.49	1.41
3	A	508	NDP	C4N-C3N	-4.44	1.41	1.49
3	B	508	NDP	C4N-C3N	-4.42	1.41	1.49
3	A	508	NDP	P2B-O2B	4.21	1.67	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	508	NDP	O2X-P2B-O2B	4.95	128.15	105.99
3	B	508	NDP	O2X-P2B-O2B	4.94	128.15	105.99
2	B	507	HEM	O2D-CGD-O1D	3.89	133.01	123.30
2	A	507	HEM	O2D-CGD-O1D	3.89	133.00	123.30
3	A	508	NDP	PN-O3-PA	3.80	145.88	132.83

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

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

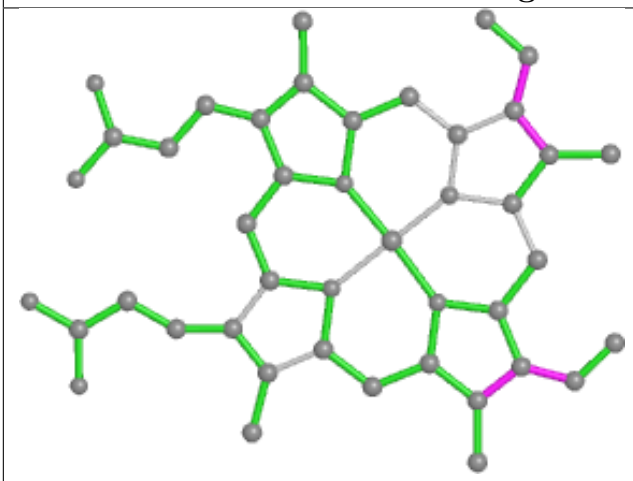
There are no ring outliers.

4 monomers are involved in 28 short contacts:

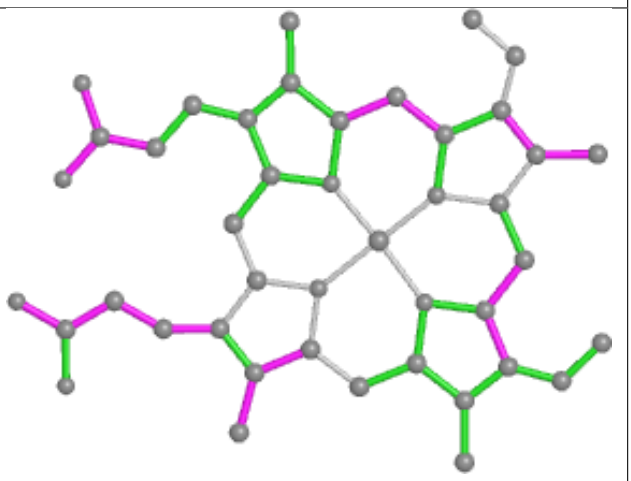
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	507	HEM	11	0
3	A	508	NDP	3	0
3	B	508	NDP	3	0
2	B	507	HEM	11	0

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 then 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.

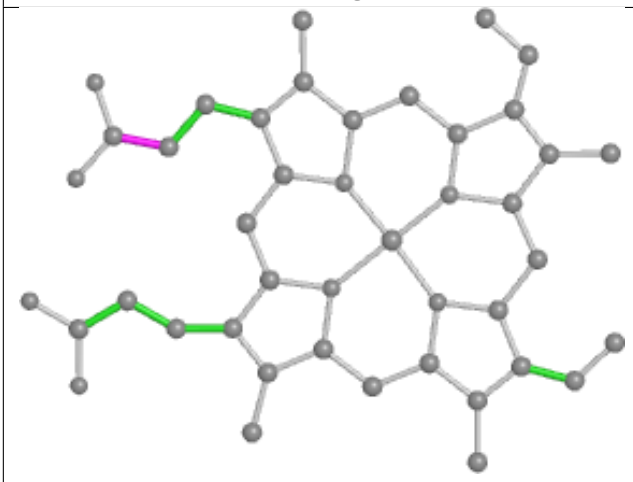
Ligand HEM A 507



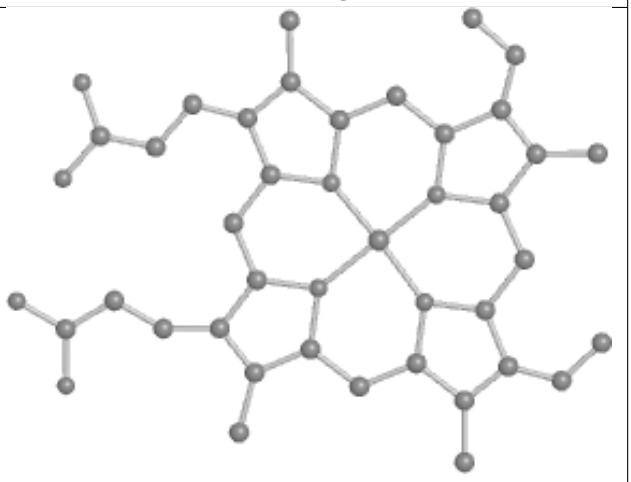
Bond lengths



Bond angles

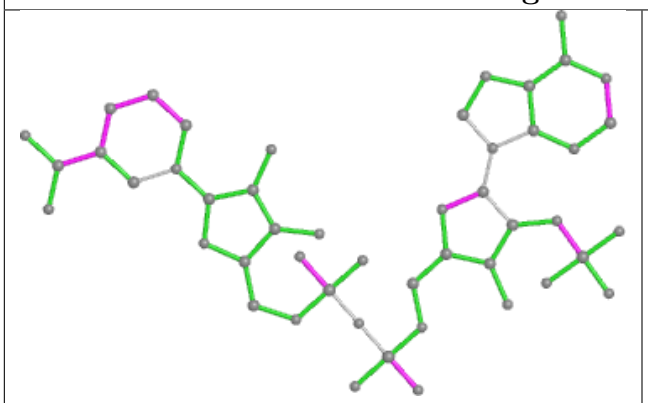


Torsions

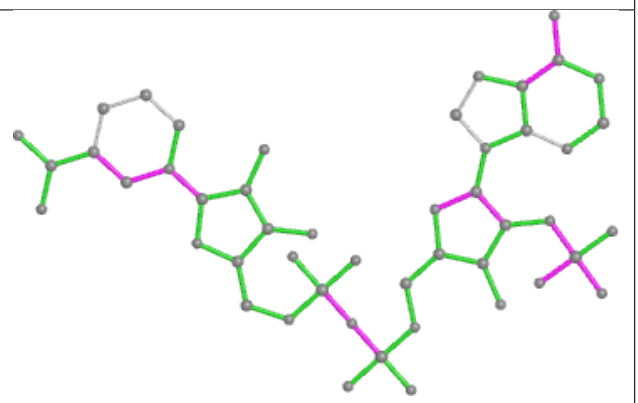


Rings

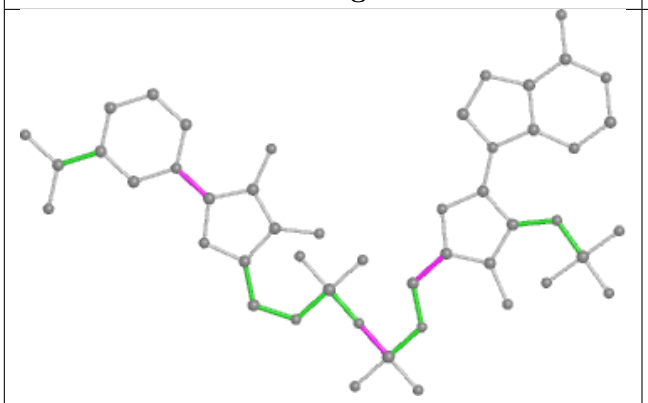
Ligand NDP A 508



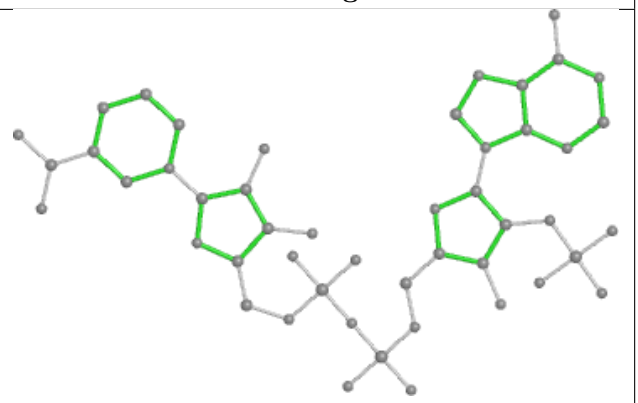
Bond lengths



Bond angles

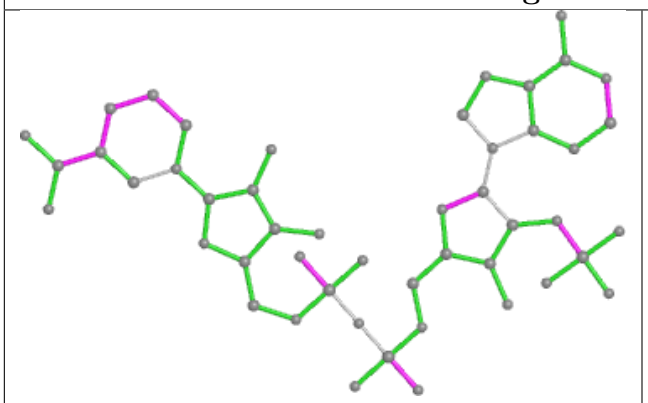


Torsions

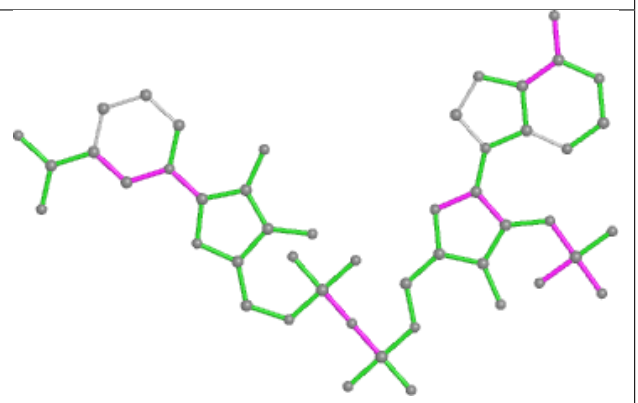


Rings

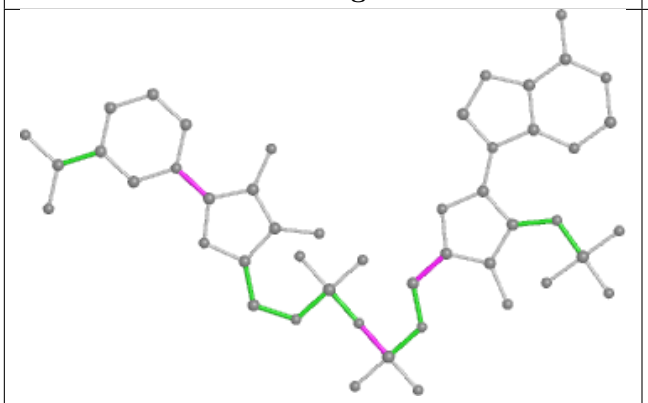
Ligand NDP B 508



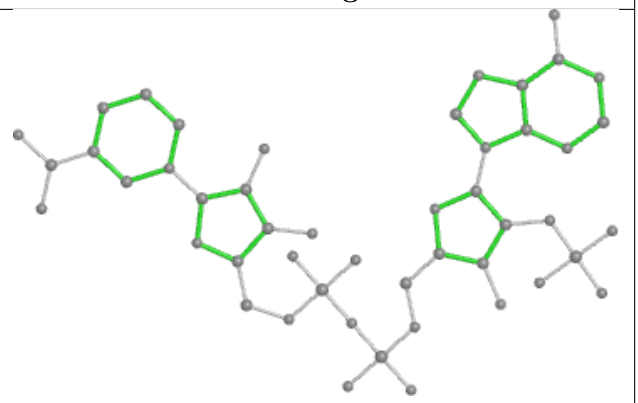
Bond lengths



Bond angles

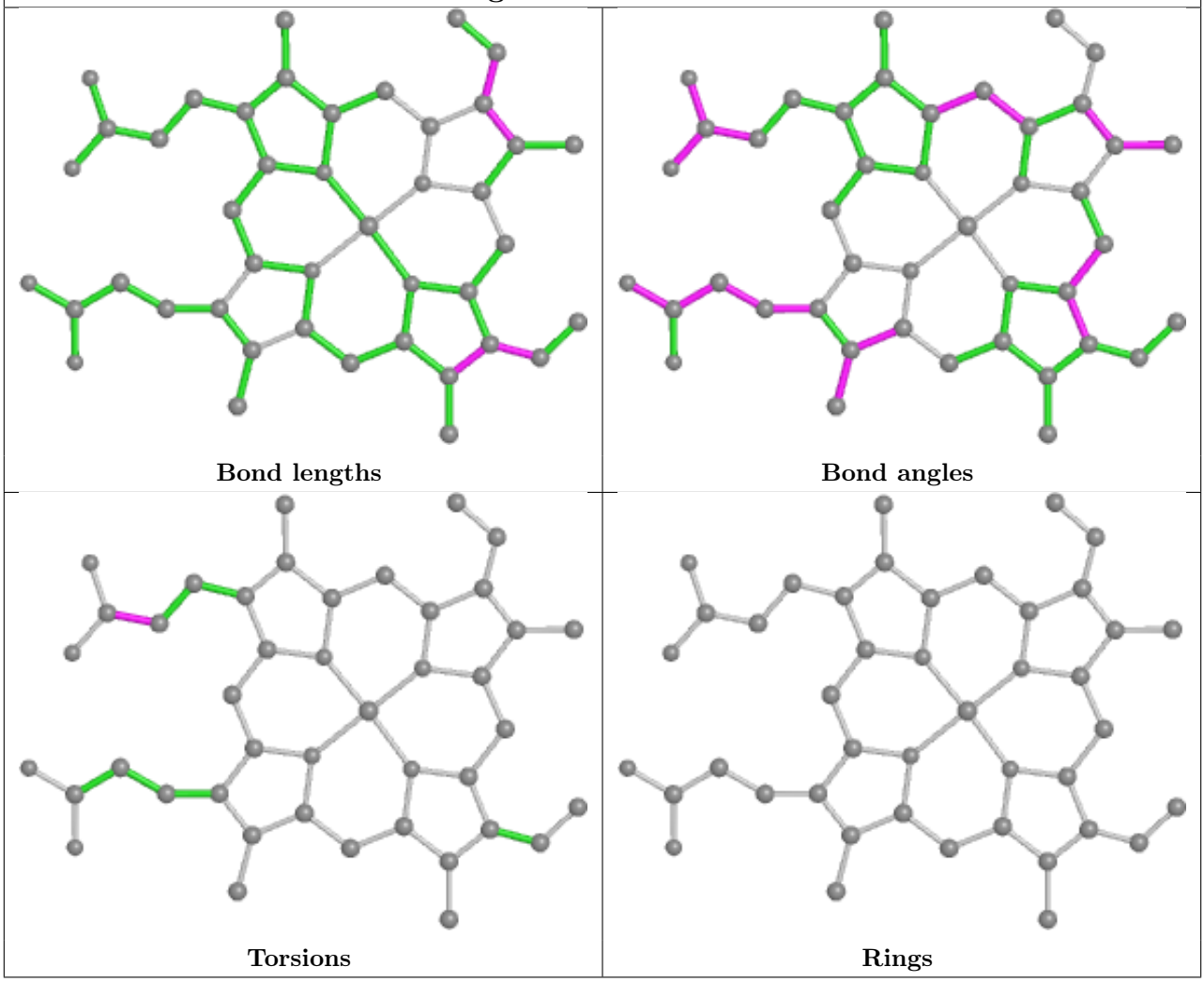


Torsions



Rings

Ligand HEM B 507



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.