Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 01:07 PM EST

PDB ID	:	8NSE
Title	:	BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE, NNA COMPLEX
Authors	:	Raman, C.S.; Li, H.; Martasek, P.; Masters, B.S.S.; Poulos, T.L.
Deposited on	:	1999-01-14
Resolution	:	2.25 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 (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:

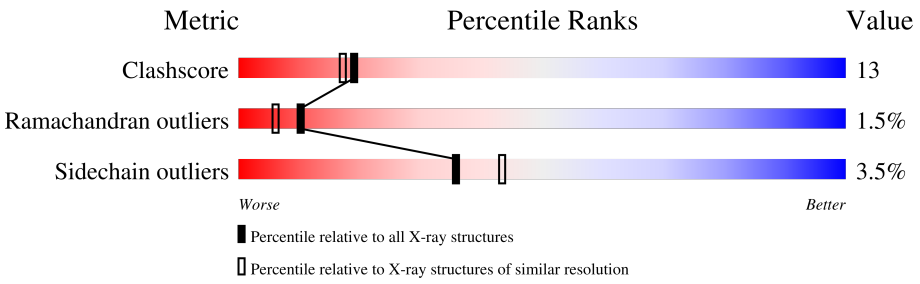
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.25 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	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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	444	69% 22% • 6%
1	B	444	66% 25% • 7%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6956 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 PROTEIN (NITRIC OXIDE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	416	3302	2099	584	603	16	0	0	0
1	B	414	3291	2092	582	601	16	0	0	0

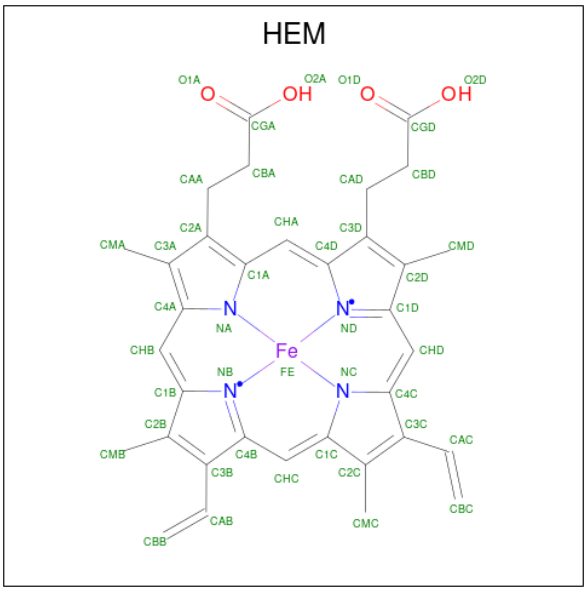
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

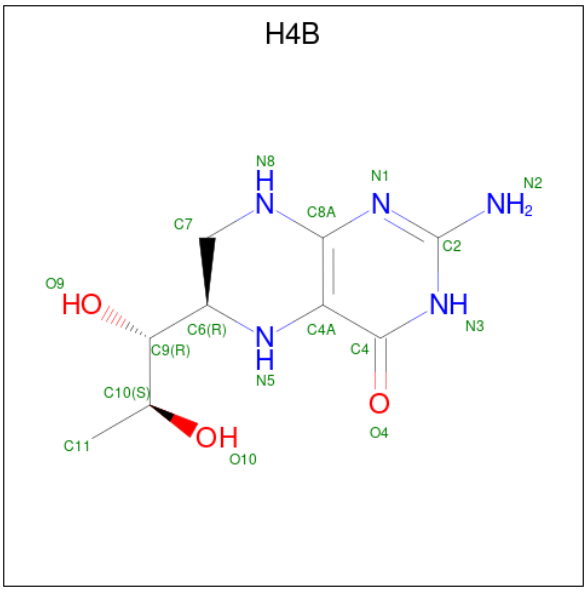
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

- Molecule 3 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		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



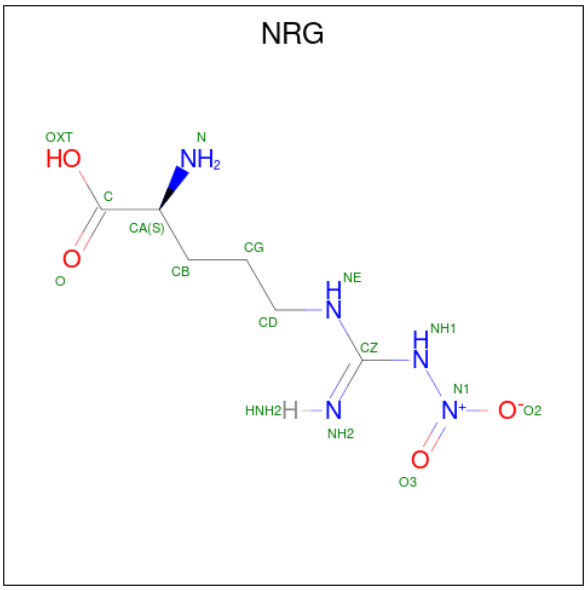
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	17	9	5	3	0	0

Continued on next page...

Continued from previous page...

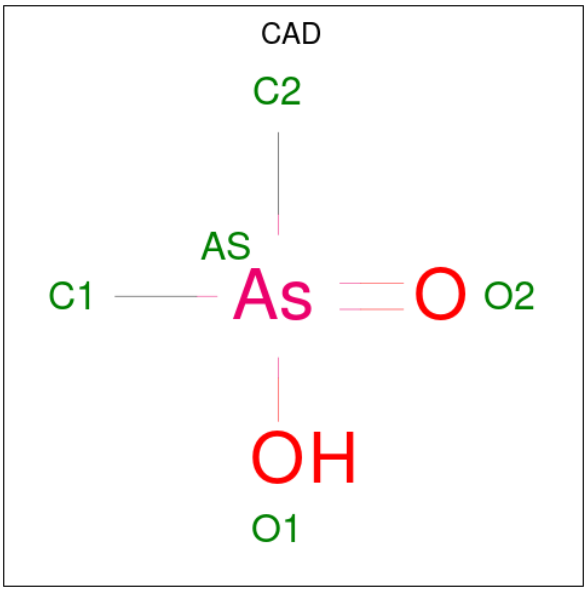
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	17	9	5	3	0	0

- Molecule 5 is N-OMEGA-NITRO-L-ARGININE (three-letter code: NRG) (formula: $C_6H_{13}N_5O_4$).



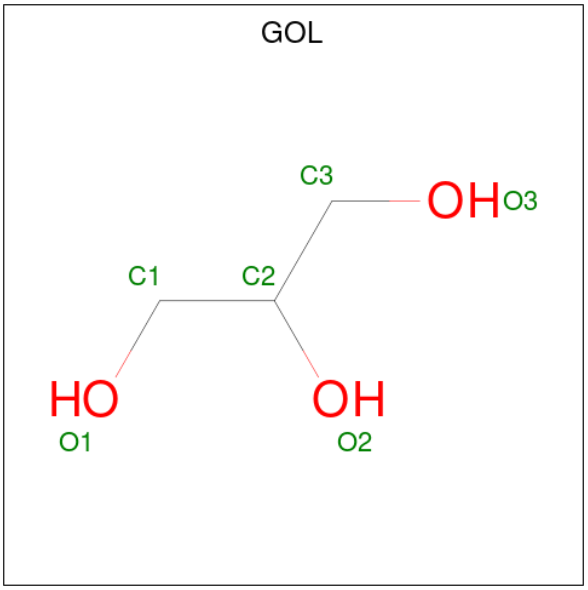
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	15	6	5	4	0	0
5	B	1	15	6	5	4	0	0

- Molecule 6 is CACODYLIC ACID (three-letter code: CAD) (formula: $C_2H_7AsO_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	As	C		
6	A	1	3	1	2	0	0
6	B	1	3	1	2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	6	3	3	0	0
7	B	1	6	3	3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	97	97	97	0	0
			Total	O		
8	B	97	97	97	0	0

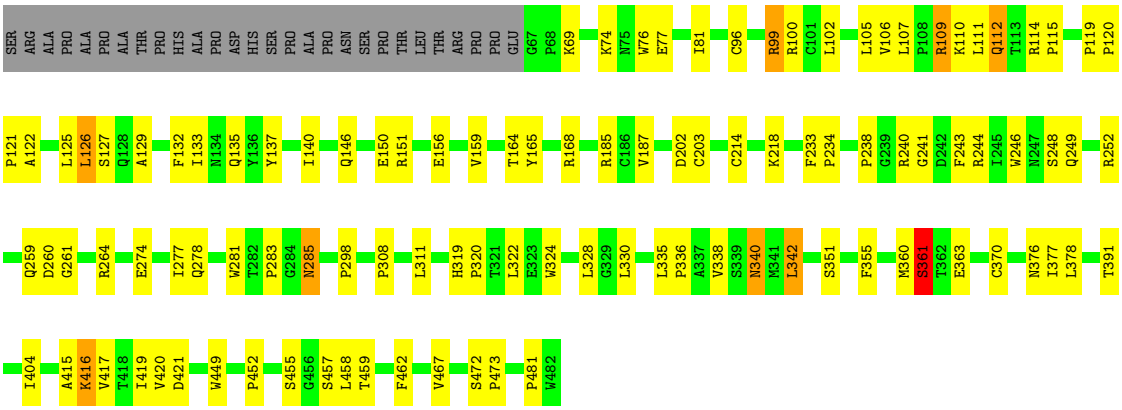
3 Residue-property plots (i)

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.

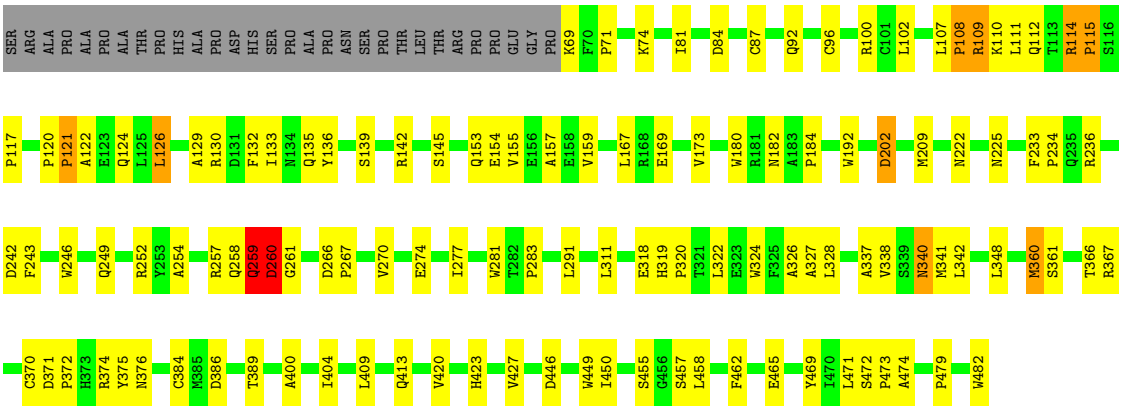
• Molecule 1: PROTEIN (NITRIC OXIDE SYNTHASE)

Chain A: 69% 22% • 6%



• Molecule 1: PROTEIN (NITRIC OXIDE SYNTHASE)

Chain B: 66% 25% • 7%



4 Data and refinement statistics (i)

Xtriage (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	58.31Å 105.78Å 156.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25	Depositor
% Data completeness (in resolution range)	84.4 (50.00-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6956	wwPDB-VP
Average B, all atoms (Å^2)	49.0	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: ZN, NRG, GOL, H4B, HEM, CAD

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	0.36	0/3397	0.62	0/4631
1	B	0.36	0/3385	0.63	1/4614 (0.0%)
All	All	0.36	0/6782	0.63	1/9245 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	360	MET	N-CA-C	-5.47	96.24	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3302	0	3215	80	0
1	B	3291	0	3205	94	0
2	A	1	0	0	0	0
3	A	43	0	30	2	0
3	B	43	0	30	1	0
4	A	17	0	15	1	0
4	B	17	0	15	1	0
5	A	15	0	11	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	15	0	11	0	0
6	A	3	0	0	0	0
6	B	3	0	0	1	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	A	97	0	0	2	0
8	B	97	0	0	0	0
All	All	6956	0	6548	173	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 13.

All (173) 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:126:LEU:HD11	1:A:156:GLU:HG2	1.46	0.95
1:B:136:TYR:O	1:B:139:SER:HB3	1.72	0.89
1:A:109:ARG:O	1:A:110:LYS:HD2	1.79	0.82
1:B:409:LEU:O	1:B:413:GLN:HG3	1.80	0.82
1:A:119:PRO:HG3	1:A:238:PRO:HG3	1.60	0.82
1:B:122:ALA:O	1:B:126:LEU:HB2	1.79	0.81
1:B:114:ARG:HA	1:B:114:ARG:HH11	1.53	0.73
1:A:472:SER:HA	1:A:473:PRO:O	1.89	0.72
1:A:99:ARG:HB2	1:A:99:ARG:HH11	1.54	0.72
1:B:340:ASN:HD22	1:B:340:ASN:H	1.38	0.72
1:B:126:LEU:O	1:B:130:ARG:HG3	1.90	0.71
1:A:361:SER:HB3	1:A:421:ASP:HA	1.73	0.69
1:B:130:ARG:HB3	1:B:130:ARG:NH1	2.09	0.67
1:B:120:PRO:HB2	1:B:124:GLN:OE1	1.94	0.67
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.60	0.67
1:A:102:LEU:HB3	1:A:105:LEU:HD22	1.76	0.67
1:A:126:LEU:CD1	1:A:156:GLU:HG2	2.25	0.67
1:B:249:GLN:HB2	1:B:252:ARG:CG	2.27	0.65
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.78	0.65
1:A:146:GLN:O	1:A:150:GLU:HG3	1.97	0.65
1:B:249:GLN:HB2	1:B:252:ARG:HG3	1.80	0.64
1:B:74:LYS:O	1:B:465:GLU:HG3	1.97	0.63
1:B:236:ARG:HD2	1:B:242:ASP:OD1	1.98	0.63
1:B:115:PRO:HA	1:B:236:ARG:HH12	1.63	0.62
1:B:108:PRO:HB3	1:B:111:LEU:HD13	1.80	0.62
1:B:257:ARG:NH2	1:B:270:VAL:HG11	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.30	0.61
1:A:119:PRO:HG3	1:A:238:PRO:CG	2.31	0.60
1:A:472:SER:HA	1:A:473:PRO:C	2.22	0.60
1:A:281:TRP:O	1:A:283:PRO:HD3	2.01	0.60
1:B:259:GLN:HG2	1:B:260:ASP:H	1.66	0.59
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.37	0.59
1:A:185:ARG:HD3	1:A:449:TRP:CD2	2.38	0.59
1:B:130:ARG:HB3	1:B:130:ARG:HH11	1.68	0.58
1:A:360:MET:HA	1:A:420:VAL:O	2.04	0.58
1:B:142:ARG:HH11	1:B:142:ARG:HG3	1.69	0.57
1:B:259:GLN:C	1:B:261:GLY:H	2.08	0.57
3:A:500:HEM:HBA2	5:A:705:NRG:HCG1	1.87	0.57
1:A:274:GLU:O	1:A:278:GLN:HG3	2.05	0.56
1:B:423:HIS:O	1:B:427:VAL:HG23	2.05	0.56
1:A:151:ARG:HD3	1:A:168:ARG:NH2	2.21	0.56
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.88	0.56
1:B:209:MET:HE1	1:B:243:PHE:HB3	1.88	0.55
1:B:270:VAL:O	1:B:274:GLU:HG2	2.07	0.55
1:A:378:LEU:HB2	8:A:955:HOH:O	2.06	0.54
1:B:449:TRP:HA	4:B:601:H4B:N1	2.23	0.54
1:B:472:SER:HA	1:B:473:PRO:C	2.28	0.54
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.43	0.54
1:A:109:ARG:HG2	1:A:109:ARG:NH1	2.22	0.53
1:A:449:TRP:HA	4:A:600:H4B:N1	2.24	0.53
1:B:259:GLN:O	1:B:261:GLY:N	2.42	0.53
1:B:115:PRO:O	1:B:117:PRO:HD3	2.09	0.52
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.91	0.52
1:A:415:ALA:O	1:A:417:VAL:HG23	2.09	0.52
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.44	0.52
1:B:108:PRO:O	1:B:109:ARG:HG3	2.10	0.52
1:A:340:ASN:H	1:A:340:ASN:HD22	1.56	0.51
1:A:137:TYR:HA	1:A:140:ILE:HG12	1.92	0.51
1:A:264:ARG:HH11	1:A:264:ARG:HG3	1.75	0.51
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.51	0.51
1:A:416:LYS:HE3	1:A:416:LYS:HA	1.92	0.51
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.46	0.51
1:A:202:ASP:OD1	1:A:203:CYS:N	2.44	0.51
1:B:254:ALA:HB2	1:B:291:LEU:CD2	2.41	0.51
1:B:455:SER:O	1:B:458:LEU:HB2	2.11	0.51
1:B:471:LEU:O	1:B:474:ALA:HB2	2.11	0.51
1:A:285:ASN:HD22	1:A:285:ASN:C	2.14	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ILE:HG12	1:B:283:PRO:HD3	1.93	0.50
1:A:120:PRO:HB2	1:A:125:LEU:HB2	1.94	0.50
1:B:457:SER:HA	1:B:462:PHE:CG	2.47	0.50
1:B:246:TRP:CH2	1:B:482:TRP:HB3	2.47	0.50
1:B:340:ASN:H	1:B:340:ASN:ND2	2.06	0.50
1:A:363:GLU:OE2	5:A:705:NRG:HCB2	2.13	0.49
1:B:324:TRP:O	1:B:327:ALA:HB3	2.12	0.49
1:B:341:MET:SD	3:B:500:HEM:HBD2	2.53	0.48
1:A:259:GLN:C	1:A:261:GLY:H	2.16	0.48
1:B:209:MET:CE	1:B:243:PHE:HB3	2.43	0.48
1:B:446:ASP:O	1:B:450:ILE:HG12	2.13	0.48
1:A:391:THR:HG23	1:A:391:THR:O	2.13	0.48
1:B:120:PRO:O	1:B:121:PRO:C	2.52	0.48
1:B:87:CYS:HB3	1:B:469:TYR:CD2	2.49	0.48
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.48	0.47
1:A:452:PRO:HG2	1:A:459:THR:HG21	1.96	0.47
1:B:259:GLN:C	1:B:261:GLY:N	2.67	0.47
1:B:400:ALA:O	1:B:404:ILE:HG13	2.14	0.47
1:A:240:ARG:HD2	1:A:241:GLY:O	2.14	0.47
1:B:108:PRO:O	1:B:109:ARG:CG	2.63	0.47
1:B:202:ASP:CG	1:B:202:ASP:O	2.52	0.47
1:B:342:LEU:C	1:B:342:LEU:HD23	2.35	0.47
1:A:338:VAL:HB	1:A:355:PHE:CZ	2.50	0.47
1:B:249:GLN:HB2	1:B:252:ARG:HD2	1.97	0.47
1:A:187:VAL:HG22	1:A:187:VAL:O	2.15	0.46
1:A:151:ARG:HD3	1:A:168:ARG:CZ	2.44	0.46
1:B:69:LYS:O	1:B:71:PRO:HD3	2.15	0.46
1:A:467:VAL:HG22	1:B:102:LEU:CD2	2.45	0.46
1:B:129:ALA:O	1:B:133:ILE:HG12	2.15	0.46
1:A:328:LEU:HB3	1:A:330:LEU:HG	1.98	0.46
1:B:74:LYS:HB2	1:B:81:ILE:HG12	1.96	0.46
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.46	0.46
1:A:96:CYS:HB3	1:B:96:CYS:HB3	1.98	0.46
1:A:126:LEU:HD23	1:A:159:VAL:HG11	1.98	0.46
1:A:249:GLN:HB2	1:A:252:ARG:HG2	1.98	0.46
1:A:248:SER:OG	1:A:252:ARG:HD2	2.15	0.45
1:B:169:GLU:O	1:B:173:VAL:HG23	2.16	0.45
1:A:129:ALA:O	1:A:133:ILE:HG12	2.16	0.45
1:A:377:ILE:HD11	1:A:404:ILE:HD13	1.99	0.45
1:A:244:ARG:NH2	1:A:481:PRO:HD3	2.31	0.45
1:A:340:ASN:HD22	1:A:340:ASN:N	2.13	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLN:O	1:B:260:ASP:N	2.49	0.45
1:B:87:CYS:HB3	1:B:469:TYR:CE2	2.52	0.45
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.97	0.45
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.98	0.44
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.53	0.44
1:A:234:PRO:HB2	1:A:243:PHE:CD1	2.52	0.44
1:B:108:PRO:HB2	1:B:109:ARG:H	1.45	0.44
1:B:132:PHE:O	1:B:135:GLN:HB2	2.18	0.44
1:B:71:PRO:HD2	1:B:84:ASP:O	2.17	0.44
1:B:366:THR:O	1:B:370:CYS:HB2	2.18	0.44
1:A:214:CYS:O	1:A:218:LYS:HG3	2.18	0.43
1:B:420:VAL:O	1:B:420:VAL:HG13	2.17	0.43
1:B:154:GLU:O	1:B:157:ALA:HB3	2.18	0.43
1:B:155:VAL:O	1:B:159:VAL:HG23	2.18	0.43
1:A:164:THR:HG23	1:A:165:TYR:N	2.34	0.43
1:B:384:CYS:C	1:B:386:ASP:H	2.22	0.43
1:A:99:ARG:HH11	1:A:99:ARG:CB	2.27	0.43
1:A:360:MET:HE2	3:A:500:HEM:CMA	2.49	0.43
1:B:108:PRO:HB2	1:B:111:LEU:H	1.83	0.43
1:A:285:ASN:C	1:A:285:ASN:ND2	2.72	0.43
1:A:335:LEU:HA	1:A:336:PRO:HD2	1.96	0.43
1:A:185:ARG:HD3	1:A:449:TRP:CE2	2.53	0.42
1:B:340:ASN:ND2	1:B:340:ASN:N	2.66	0.42
1:B:360:MET:HA	1:B:420:VAL:O	2.19	0.42
1:A:457:SER:HA	1:A:462:PHE:CG	2.54	0.42
1:B:110:LYS:HA	1:B:110:LYS:HD2	1.85	0.42
1:A:308:PRO:HB2	1:A:311:LEU:HG	2.01	0.42
1:B:367:ARG:O	1:B:371:ASP:HB2	2.20	0.42
1:A:74:LYS:HB2	1:A:81:ILE:HD13	2.01	0.42
1:A:121:PRO:O	1:A:122:ALA:C	2.57	0.42
1:B:182:ASN:O	1:B:184:PRO:HD3	2.19	0.42
1:A:246:TRP:CD1	1:A:481:PRO:HG3	2.54	0.42
1:A:69:LYS:O	1:A:69:LYS:HG2	2.20	0.42
1:A:111:LEU:HB2	8:A:983:HOH:O	2.20	0.42
1:A:74:LYS:HE2	1:A:76:TRP:CD2	2.55	0.42
5:A:705:NRG:O3	5:A:705:NRG:NH2	2.50	0.41
1:B:371:ASP:HB2	1:B:374:ARG:CG	2.50	0.41
1:B:318:GLU:HB3	1:B:326:ALA:HB2	2.02	0.41
1:A:132:PHE:O	1:A:135:GLN:HB2	2.20	0.41
1:B:109:ARG:HE	1:B:109:ARG:HB2	1.30	0.41
1:B:249:GLN:HB2	1:B:252:ARG:CD	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LEU:HD12	1:A:351:SER:HA	2.03	0.41
1:A:106:VAL:HG12	1:A:107:LEU:HG	2.02	0.41
1:B:259:GLN:HG2	1:B:260:ASP:OD2	2.19	0.41
1:A:74:LYS:HB2	1:A:81:ILE:CD1	2.50	0.41
1:B:130:ARG:HH11	1:B:130:ARG:CB	2.33	0.41
1:A:277:ILE:HD11	1:A:283:PRO:HB3	2.03	0.41
1:A:419:ILE:HG13	1:A:420:VAL:N	2.36	0.41
1:B:114:ARG:HH12	1:B:479:PRO:HG2	1.85	0.41
1:B:266:ASP:HA	1:B:267:PRO:HD3	1.96	0.41
1:B:375:TYR:O	1:B:376:ASN:C	2.59	0.41
1:A:233:PHE:HB3	1:A:234:PRO:HD2	2.03	0.41
1:A:164:THR:O	1:A:165:TYR:HB3	2.21	0.40
1:B:311:LEU:HD12	1:B:311:LEU:HA	1.89	0.40
1:B:340:ASN:HD22	1:B:340:ASN:N	2.02	0.40
1:A:112:GLN:HE21	1:A:112:GLN:HA	1.87	0.40
1:B:455:SER:HB3	1:B:458:LEU:HD22	2.04	0.40
1:B:281:TRP:CH2	1:B:283:PRO:HA	2.57	0.40
1:B:337:ALA:O	1:B:338:VAL:C	2.60	0.40
1:B:384:CYS:HA	6:B:950:CAD:C2	2.51	0.40
1:A:322:LEU:HD13	1:A:324:TRP:HZ2	1.87	0.40
1:B:107:LEU:HA	1:B:108:PRO:HD3	1.81	0.40
1:B:260:ASP:N	1:B:260:ASP:OD2	2.51	0.40
1:B:455:SER:HB3	1:B:458:LEU:CD2	2.51	0.40
1:B:361:SER:HB3	1:B:409:LEU:CD2	2.51	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	414/444 (93%)	374 (90%)	36 (9%)	4 (1%)	15 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	412/444 (93%)	378 (92%)	26 (6%)	8 (2%)	8 4
All	All	826/888 (93%)	752 (91%)	62 (8%)	12 (2%)	10 6

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	108	PRO
1	B	109	ARG
1	B	259	GLN
1	B	145	SER
1	B	260	ASP
1	A	115	PRO
1	B	115	PRO
1	B	328	LEU
1	A	260	ASP
1	A	361	SER
1	A	109	ARG
1	B	121	PRO

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	354/377 (94%)	342 (97%)	12 (3%)	37 45
1	B	353/377 (94%)	340 (96%)	13 (4%)	34 40
All	All	707/754 (94%)	682 (96%)	25 (4%)	36 43

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	100	ARG
1	A	112	GLN
1	A	114	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	126	LEU
1	A	127	SER
1	A	285	ASN
1	A	340	ASN
1	A	342	LEU
1	A	361	SER
1	A	376	ASN
1	A	416	LYS
1	B	92	GLN
1	B	100	ARG
1	B	112	GLN
1	B	114	ARG
1	B	126	LEU
1	B	153	GLN
1	B	202	ASP
1	B	222	ASN
1	B	225	ASN
1	B	259	GLN
1	B	260	ASP
1	B	340	ASN
1	B	389	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	124	GLN
1	A	153	GLN
1	A	191	GLN
1	A	259	GLN
1	A	278	GLN
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	B	146	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	235	GLN
1	B	278	GLN
1	B	340	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	405	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)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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	$\#\|Z\| > 2$
5	NRG	B	706	-	9,14,14	0.85	0	11,17,17	0.85	0
4	H4B	B	601	-	16,18,18	2.09	5 (31%)	11,26,26	4.39	8 (72%)
3	HEM	A	500	1	41,50,50	1.39	7 (17%)	45,82,82	1.41	5 (11%)
5	NRG	A	705	-	9,14,14	0.88	0	11,17,17	0.78	0
7	GOL	A	880	-	5,5,5	0.15	0	5,5,5	0.22	0
4	H4B	A	600	-	16,18,18	2.10	5 (31%)	11,26,26	4.16	9 (81%)
3	HEM	B	500	1	41,50,50	1.53	9 (21%)	45,82,82	1.32	3 (6%)
7	GOL	B	881	-	5,5,5	0.19	0	5,5,5	0.31	0
6	CAD	B	950	1	0,2,4	-	-	0,1,6	-	-
6	CAD	A	950	1	0,2,4	-	-	0,1,6	-	-

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
5	NRG	B	706	-	-	2/12/15/15	-
4	H4B	B	601	-	-	0/8/17/17	0/2/2/2
3	HEM	A	500	1	-	0/12/54/54	-
5	NRG	A	705	-	-	2/12/15/15	-
4	H4B	A	600	-	-	0/8/17/17	0/2/2/2
3	HEM	B	500	1	-	2/12/54/54	-
7	GOL	B	881	-	-	2/4/4/4	-
7	GOL	A	880	-	-	1/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	H4B	C4-N3	5.00	1.41	1.33
4	A	600	H4B	C4-N3	4.84	1.41	1.33
4	B	601	H4B	C4A-N5	4.36	1.46	1.38
4	A	600	H4B	C4A-N5	4.11	1.46	1.38
3	A	500	HEM	C3C-CAC	-3.94	1.39	1.47
4	A	600	H4B	C6-N5	3.89	1.53	1.45
3	B	500	HEM	C3C-C2C	-3.79	1.35	1.40
4	B	601	H4B	C6-N5	3.18	1.52	1.45
3	B	500	HEM	C3C-CAC	-3.10	1.41	1.47
3	B	500	HEM	C1A-NA	3.01	1.42	1.36
3	B	500	HEM	CHA-C4D	2.88	1.42	1.35
3	A	500	HEM	C3C-C2C	-2.70	1.36	1.40
3	A	500	HEM	CAB-C3B	-2.63	1.40	1.47
3	A	500	HEM	C4A-NA	2.62	1.41	1.36
4	A	600	H4B	C7-N8	2.45	1.48	1.44
4	B	601	H4B	C8A-N1	2.41	1.39	1.34
3	B	500	HEM	C4A-NA	2.39	1.41	1.36
3	A	500	HEM	CHA-C4D	2.31	1.40	1.35
3	B	500	HEM	CHB-C1B	2.31	1.40	1.35
3	A	500	HEM	C1A-NA	2.27	1.40	1.36
4	B	601	H4B	C4A-C8A	-2.23	1.37	1.41
3	B	500	HEM	C3B-C2B	-2.16	1.32	1.37
3	B	500	HEM	CAA-C2A	2.11	1.55	1.52
4	A	600	H4B	C8A-N1	2.08	1.38	1.34
3	A	500	HEM	CMD-C2D	2.04	1.55	1.50
3	B	500	HEM	CMD-C2D	2.03	1.55	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	H4B	C8A-C4A-C4	9.62	123.12	114.57
4	A	600	H4B	C8A-C4A-C4	8.74	122.34	114.57
4	A	600	H4B	C2-N3-C4	5.73	125.04	115.93
4	B	601	H4B	C2-N3-C4	5.57	124.79	115.93
3	B	500	HEM	CBA-CAA-C2A	-5.22	103.71	112.62
4	B	601	H4B	N1-C2-N3	-5.08	117.45	125.42
4	A	600	H4B	N1-C2-N3	-4.88	117.77	125.42
3	A	500	HEM	CMD-C2D-C1D	4.67	132.15	125.04
4	B	601	H4B	N2-C2-N1	3.77	123.12	117.25
4	A	600	H4B	C2-N1-C8A	3.62	122.66	114.54
4	B	601	H4B	C4A-C4-N3	-3.54	113.94	124.01
4	A	600	H4B	C4A-C4-N3	-3.52	114.01	124.01
4	A	600	H4B	N2-C2-N1	3.50	122.70	117.25
4	B	601	H4B	C2-N1-C8A	3.45	122.26	114.54
4	B	601	H4B	C4-C4A-N5	-3.23	116.42	119.12
3	B	500	HEM	C1B-NB-C4B	-2.87	102.11	105.07
4	B	601	H4B	C4A-N5-C6	-2.78	113.59	121.16
3	B	500	HEM	C3B-C2B-C1B	2.64	108.44	106.49
4	A	600	H4B	C4A-N5-C6	-2.55	114.21	121.16
4	A	600	H4B	C4-C4A-N5	-2.49	117.03	119.12
3	A	500	HEM	C2D-C1D-ND	2.32	112.67	109.88
3	A	500	HEM	CAB-C3B-C2B	-2.18	121.43	128.60
3	A	500	HEM	C1B-NB-C4B	-2.11	102.89	105.07
4	A	600	H4B	O9-C9-C6	2.05	113.89	108.98
3	A	500	HEM	C2B-C1B-NB	2.00	112.21	109.84

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	705	NRG	O3-N1-NH1-CZ
7	B	881	GOL	O1-C1-C2-C3
7	B	881	GOL	O1-C1-C2-O2
3	B	500	HEM	C2B-C3B-CAB-CBB
3	B	500	HEM	C4B-C3B-CAB-CBB
5	A	705	NRG	O-C-CA-N
5	B	706	NRG	O-C-CA-N
5	B	706	NRG	O3-N1-NH1-CZ
7	A	880	GOL	O1-C1-C2-O2

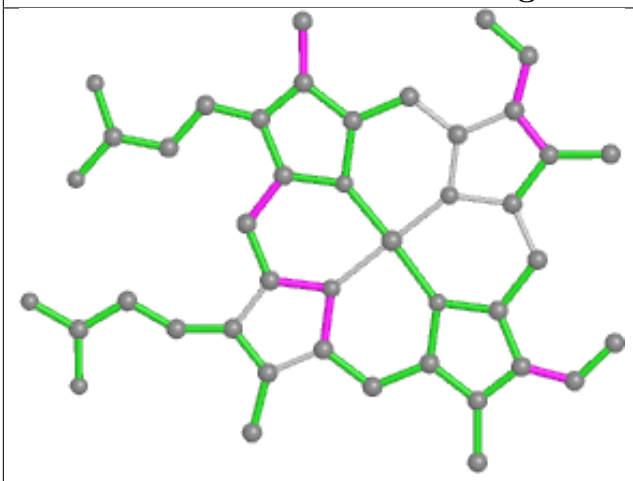
There are no ring outliers.

6 monomers are involved in 8 short contacts:

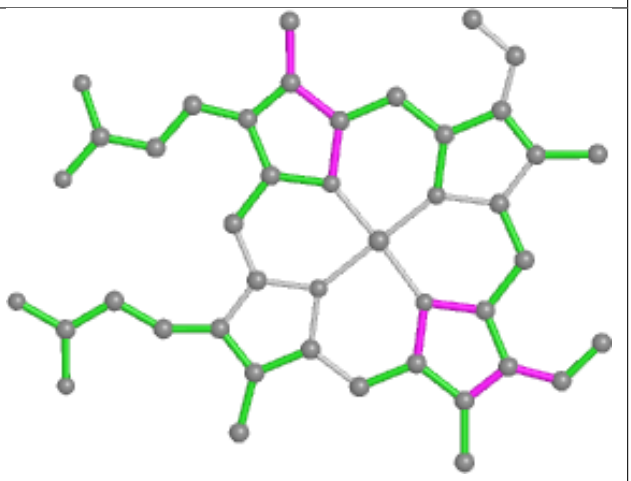
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	H4B	1	0
3	A	500	HEM	2	0
5	A	705	NRG	3	0
4	A	600	H4B	1	0
3	B	500	HEM	1	0
6	B	950	CAD	1	0

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 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.

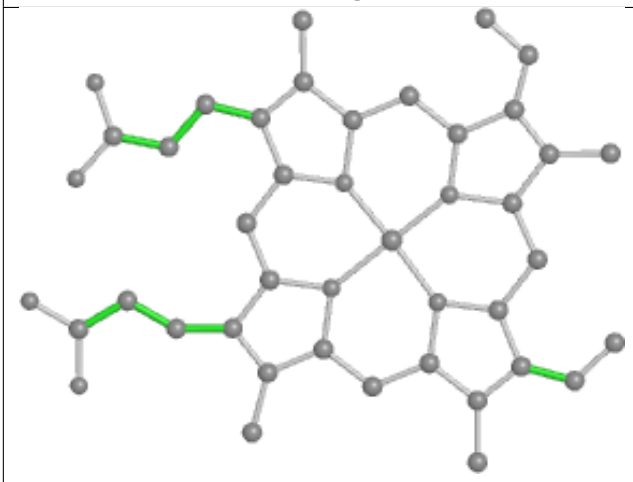
Ligand HEM A 500



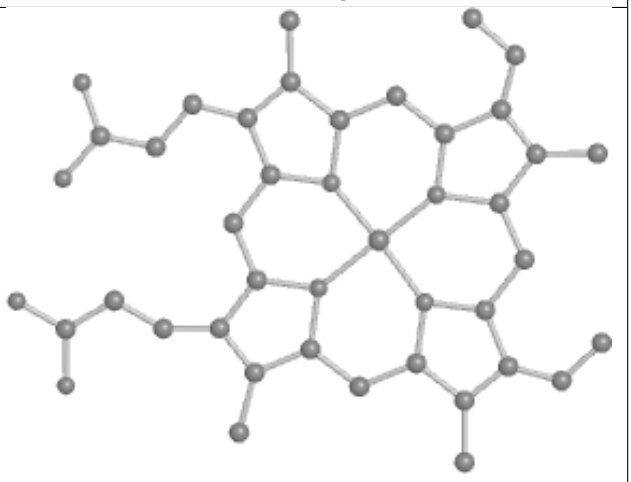
Bond lengths



Bond angles

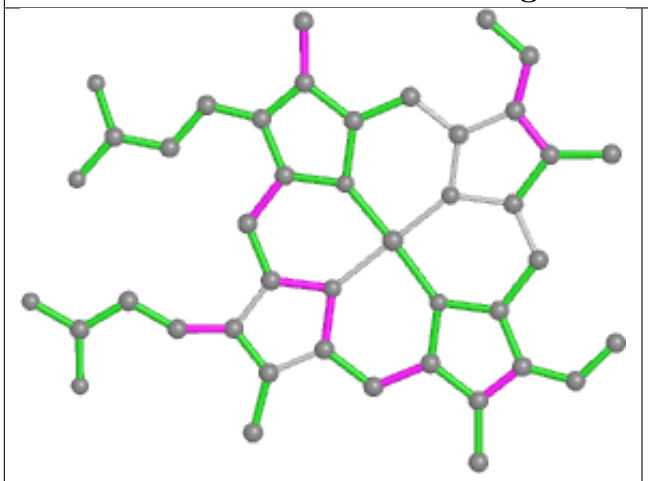


Torsions

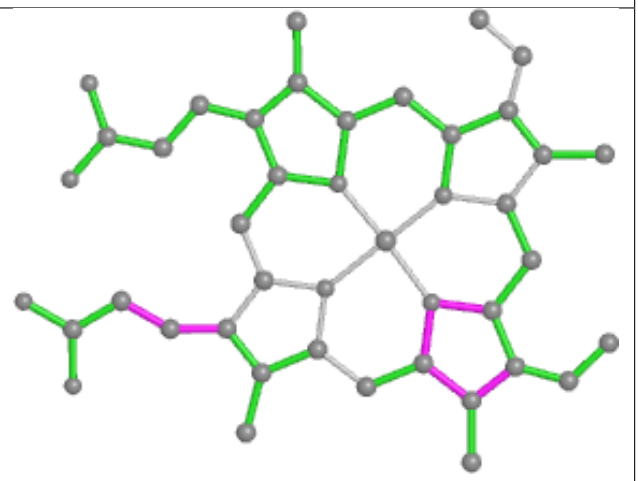


Rings

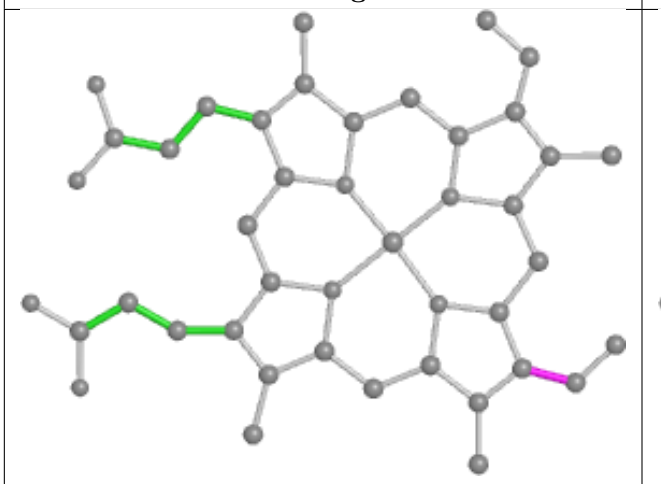
Ligand HEM B 500



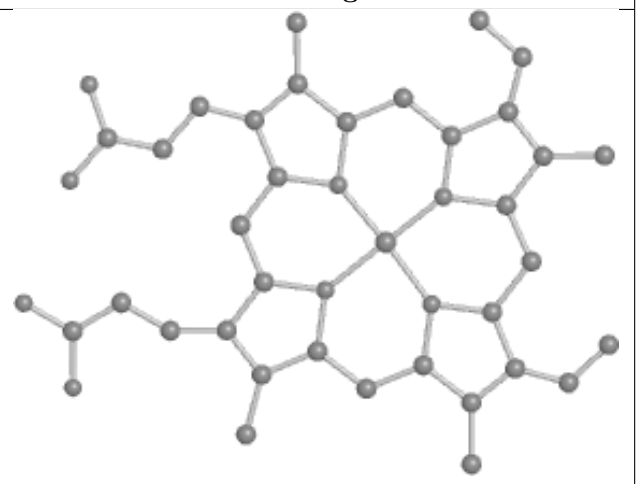
Bond lengths



Bond angles



Torsions



Rings

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.