



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 04:53 PM EST

PDB ID : 1M8H  
Title : inducible nitric oxide synthase with 6-nitroindazole bound  
Authors : Rosenfeld, R.J.; Garcin, E.D.; Panda, K.; Andersson, G.; Aberg, A.; Wallace, A.V.; Stuehr, D.J.; Tainer, J.A.; Getzoff, E.D.  
Deposited on : 2002-07-24  
Resolution : 2.85 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](mailto: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>.

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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)  
Xtrriage (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

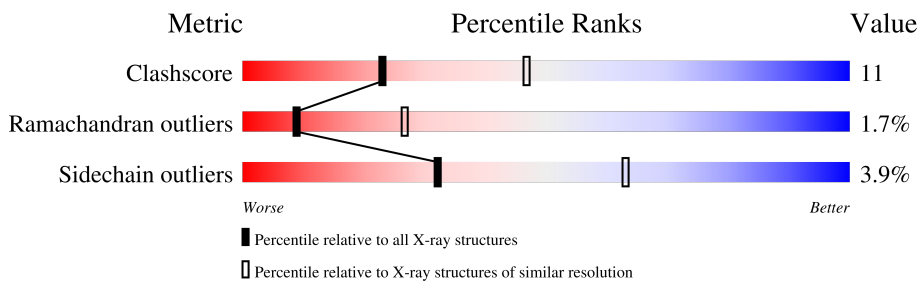
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)

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  $\geq 3$ , 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	434	
1	B	434	

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
4	H4B	A	902	X	-	-	-
4	H4B	B	903	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6954 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 inducible Nitric oxide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	413	3363	2157	580	606	20	0	0	0
1	B	412	3353	2152	578	603	20	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



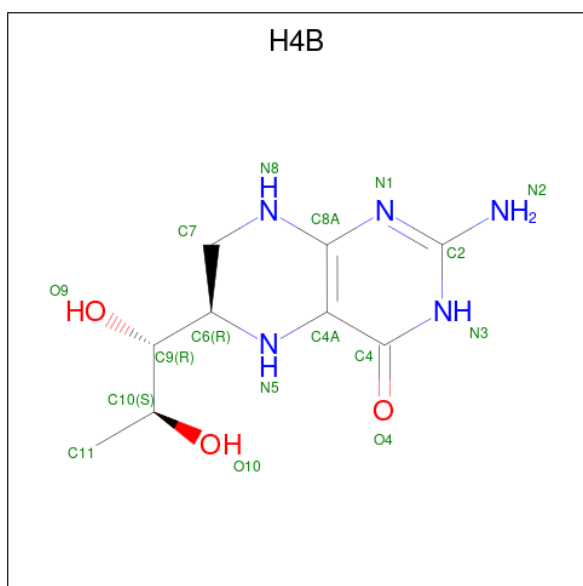
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

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



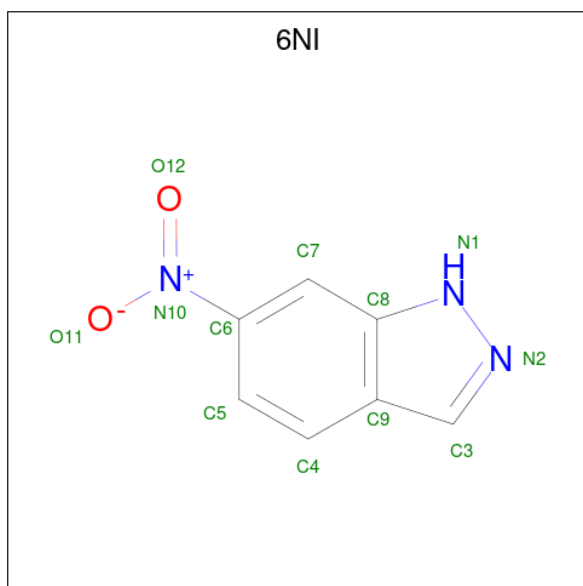
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
4	A	1	17	9	5	3	0	0

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

- Molecule 5 is 6-NITROINDAZOLE (three-letter code: 6NI) (formula: C<sub>7</sub>H<sub>5</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	12	7	3	2	0	0
5	B	1	12	7	3	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	50	Total O 50 50	0	0
6	B	39	Total O 39 39	0	0

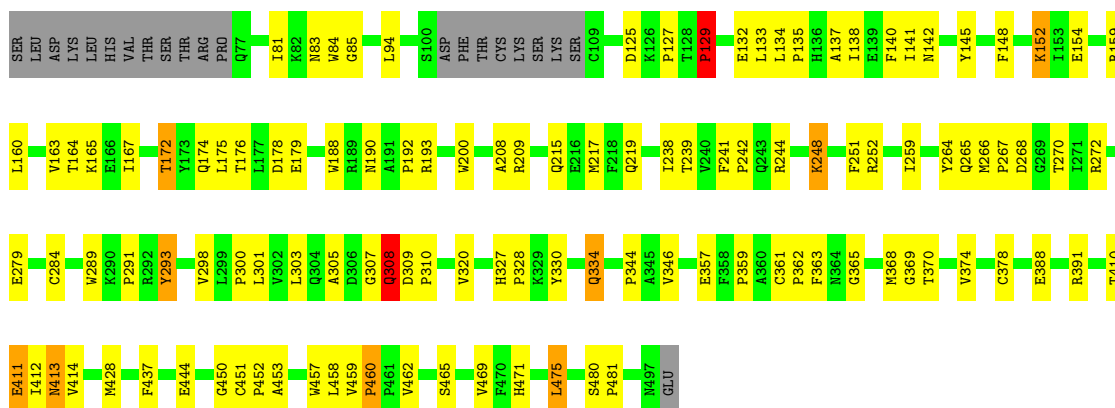
### 3 Residue-property plots [i](#)

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.

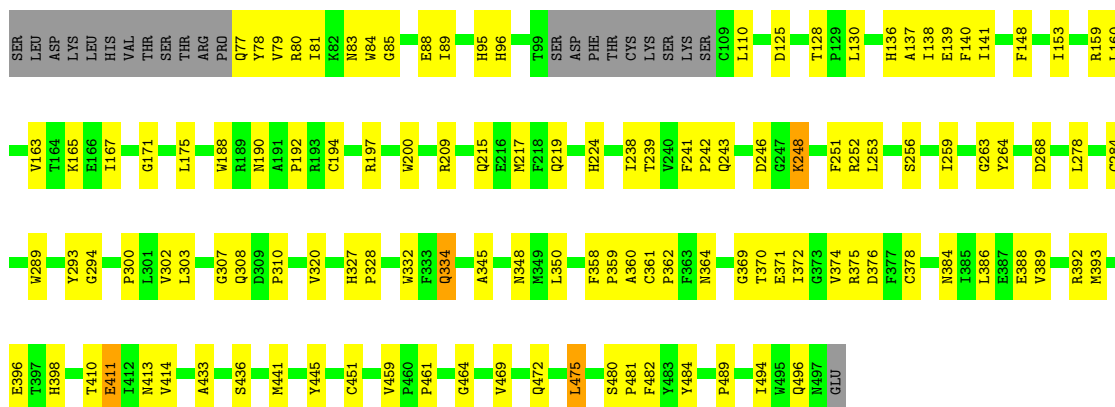
- Molecule 1: inducible Nitric oxide synthase

Chain A: 



- Molecule 1: inducible Nitric oxide synthase

Chain B: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	213.65Å 213.65Å 114.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.92 – 2.85	Depositor
% Data completeness (in resolution range)	88.5 (19.92-2.85)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.243 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6954	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	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: H4B, 6NI, HEM, SO4

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	0.42	0/3461	0.67	1/4706 (0.0%)
1	B	0.41	0/3451	0.65	0/4693
All	All	0.41	0/6912	0.66	1/9399 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	GLY	N-CA-C	-5.04	100.51	113.10

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	3363	0	3256	74	0
1	B	3353	0	3245	77	0
2	A	5	0	0	0	0
3	A	43	0	30	2	0
3	B	43	0	30	0	0
4	A	17	0	14	0	0
4	B	17	0	14	1	0
5	A	12	0	5	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	12	0	5	3	0
6	A	50	0	0	3	0
6	B	39	0	0	2	0
All	All	6954	0	6599	153	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 11.

All (153) 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:371:GLU:HG3	5:B:907:6NI:H31	1.50	0.93
1:B:371:GLU:HG3	5:B:907:6NI:C3	2.13	0.79
1:A:346:VAL:HB	1:A:363:PHE:CE1	2.18	0.78
1:A:334:GLN:HE21	1:A:334:GLN:H	1.32	0.74
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.23	0.74
1:B:334:GLN:HE21	1:B:334:GLN:H	1.36	0.73
1:A:410:THR:O	1:A:414:VAL:HG23	1.89	0.72
1:A:134:LEU:O	1:A:138:ILE:HG12	1.90	0.72
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.26	0.71
1:B:130:LEU:HD11	1:B:171:GLY:HA2	1.71	0.71
1:B:159:ARG:O	1:B:163:VAL:HG23	1.92	0.70
1:A:132:GLU:O	1:A:135:PRO:HD2	1.91	0.70
1:A:138:ILE:HG22	1:A:142:ASN:HD21	1.55	0.70
1:A:305:ALA:O	1:A:308:GLN:HB2	1.93	0.68
1:B:388:GLU:HB3	6:B:1082:HOH:O	1.95	0.66
1:A:127:PRO:O	1:A:129:PRO:HD3	1.95	0.66
1:B:163:VAL:O	1:B:167:ILE:HG13	1.95	0.66
1:A:138:ILE:HG22	1:A:142:ASN:ND2	2.10	0.66
1:A:137:ALA:O	1:A:141:ILE:HG12	1.95	0.65
1:A:217:MET:HE1	1:A:305:ALA:HB2	1.79	0.65
1:B:215:GLN:HE21	1:B:219:GLN:NE2	1.95	0.64
1:B:194:CYS:HB3	1:B:197:ARG:HD2	1.77	0.64
1:A:284:CYS:SG	1:A:300:PRO:HG2	2.38	0.64
1:B:217:MET:HE2	1:B:303:LEU:HB3	1.79	0.64
1:A:152:LYS:H	1:A:152:LYS:HD2	1.62	0.64
1:B:209:ARG:O	1:B:242:PRO:HG3	1.99	0.63
1:B:137:ALA:O	1:B:141:ILE:HG12	1.99	0.63
1:A:159:ARG:O	1:A:163:VAL:HG23	1.99	0.62
1:B:259:ILE:HD12	1:B:320:VAL:HG22	1.80	0.62
1:B:163:VAL:HG12	1:B:167:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:MET:CE	1:B:303:LEU:HB3	2.30	0.61
1:A:266:MET:HG3	1:A:267:PRO:HD2	1.81	0.59
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.36	0.59
1:B:361:CYS:SG	1:B:361:CYS:O	2.60	0.59
1:B:410:THR:O	1:B:414:VAL:HG23	2.02	0.59
1:A:134:LEU:HD11	1:A:164:THR:HG22	1.84	0.58
1:B:327:HIS:HE2	1:B:411:GLU:HG3	1.67	0.58
1:A:217:MET:CE	1:A:303:LEU:HB3	2.34	0.57
1:A:327:HIS:HE2	1:A:411:GLU:HG3	1.69	0.57
1:B:264:TYR:CE1	1:B:293:TYR:HA	2.39	0.57
1:B:215:GLN:HE21	1:B:219:GLN:HE21	1.53	0.56
1:B:371:GLU:CG	5:B:907:6NI:H31	2.30	0.56
1:A:140:PHE:HE2	1:A:175:LEU:HD22	1.70	0.56
1:B:138:ILE:HG23	1:B:160:LEU:HD21	1.88	0.56
1:A:217:MET:HE2	1:A:303:LEU:HB3	1.88	0.56
1:B:77:GLN:O	1:B:96:HIS:HE1	1.88	0.56
1:B:130:LEU:HD22	1:B:130:LEU:H	1.72	0.55
1:A:125:ASP:HB2	1:A:248:LYS:HE2	1.88	0.54
1:A:138:ILE:HG23	1:A:160:LEU:HD22	1.89	0.54
1:A:303:LEU:O	1:A:310:PRO:HA	2.08	0.54
1:A:480:SER:HA	1:A:481:PRO:C	2.27	0.54
1:A:238:ILE:HG13	1:A:362:PRO:O	2.07	0.54
1:A:327:HIS:CG	1:A:328:PRO:HD2	2.42	0.54
1:A:94:LEU:HB3	1:A:450:GLY:HA3	1.90	0.53
1:B:224:HIS:HE1	1:B:238:ILE:HA	1.73	0.53
1:A:145:TYR:HE2	1:A:159:ARG:HG2	1.73	0.53
1:B:284:CYS:SG	1:B:300:PRO:HG2	2.49	0.53
1:B:303:LEU:O	1:B:310:PRO:HA	2.09	0.53
1:A:284:CYS:SG	1:A:300:PRO:CG	2.97	0.53
1:B:480:SER:HA	1:B:481:PRO:C	2.30	0.52
1:B:239:THR:O	1:B:361:CYS:HA	2.09	0.52
1:A:327:HIS:NE2	1:A:411:GLU:HG3	2.24	0.52
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.75	0.52
1:B:389:VAL:O	1:B:393:MET:HB2	2.09	0.52
1:A:301:LEU:HB3	1:A:303:LEU:HD21	1.92	0.51
1:A:248:LYS:O	1:A:307:GLY:HA3	2.09	0.51
1:A:148:PHE:HB2	6:A:1002:HOH:O	2.10	0.51
1:A:217:MET:HG3	1:A:241:PHE:CZ	2.46	0.51
1:B:332:TRP:CE3	1:B:392:ARG:HD2	2.46	0.50
1:B:256:SER:HA	1:B:348:ASN:ND2	2.27	0.50
1:A:334:GLN:H	1:A:334:GLN:NE2	2.06	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:901:HEM:HMC2	3:A:901:HEM:HBC2	1.94	0.49
1:A:190:ASN:O	1:A:192:PRO:HD3	2.12	0.49
1:B:374:VAL:O	1:B:378:CYS:HB2	2.13	0.49
1:B:80:ARG:HD3	1:B:89:ILE:HG21	1.94	0.49
1:B:345:ALA:HB2	1:B:364:ASN:HB3	1.95	0.48
1:A:298:VAL:HG21	1:A:320:VAL:HG11	1.95	0.48
3:A:901:HEM:HBA2	5:A:906:6NI:H41	1.96	0.48
1:B:459:VAL:HG22	1:B:469:VAL:HG23	1.94	0.48
1:B:378:CYS:SG	1:B:386:LEU:HD13	2.53	0.48
1:A:215:GLN:HE21	1:A:219:GLN:HE21	1.60	0.47
1:B:238:ILE:HG13	1:B:362:PRO:O	2.15	0.47
1:A:83:ASN:O	1:A:85:GLY:N	2.48	0.47
1:B:327:HIS:CG	1:B:328:PRO:HD2	2.50	0.47
1:B:148:PHE:H	1:B:148:PHE:HD2	1.63	0.46
1:A:133:LEU:HD21	1:A:172:THR:HA	1.98	0.46
1:B:445:TYR:HE1	1:B:451:CYS:HB3	1.81	0.46
1:A:266:MET:HB2	1:A:270:THR:O	2.14	0.46
1:A:465:SER:O	1:A:471:HIS:HE1	1.98	0.46
1:A:272:ARG:HG3	1:A:272:ARG:NH1	2.30	0.46
1:A:370:THR:HA	1:A:413:ASN:HD21	1.80	0.46
1:B:138:ILE:HG23	1:B:160:LEU:CD2	2.45	0.46
1:B:248:LYS:O	1:B:307:GLY:HA3	2.14	0.46
1:B:327:HIS:NE2	1:B:411:GLU:HG3	2.30	0.46
1:B:372:ILE:HA	1:B:376:ASP:OD2	2.16	0.46
1:A:437:PHE:CE2	1:A:458:LEU:HD13	2.51	0.46
1:B:190:ASN:O	1:B:192:PRO:HD3	2.16	0.46
1:B:441:MET:CE	1:B:472:GLN:HG2	2.45	0.46
1:A:259:ILE:HD12	1:A:320:VAL:HG22	1.97	0.46
1:B:264:TYR:HE1	1:B:294:GLY:H	1.64	0.46
1:B:125:ASP:HB2	1:B:248:LYS:HE2	1.96	0.46
1:B:246:ASP:OD2	1:B:248:LYS:HD3	2.16	0.46
1:A:363:PHE:HE1	5:A:906:6NI:O11	1.99	0.45
1:B:140:PHE:HE2	1:B:175:LEU:HD22	1.81	0.45
1:A:374:VAL:HG11	1:A:462:VAL:HG13	1.98	0.45
1:B:334:GLN:H	1:B:334:GLN:NE2	2.08	0.45
1:B:348:ASN:HB2	6:B:1092:HOH:O	2.16	0.45
1:A:174:GLN:HA	6:A:1042:HOH:O	2.16	0.45
1:B:136:HIS:O	1:B:139:GLU:HB3	2.16	0.45
1:B:188:TRP:CZ3	1:B:200:TRP:HA	2.52	0.45
1:A:252:ARG:HD3	1:A:359:PRO:HB3	1.99	0.45
1:B:375:ARG:HH12	4:B:903:H4B:C4	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ILE:HD11	1:A:475:LEU:CD1	2.48	0.44
1:A:163:VAL:O	1:A:167:ILE:HG13	2.17	0.44
1:A:209:ARG:O	1:A:242:PRO:HG3	2.17	0.44
1:A:244:ARG:HD2	1:A:357:GLU:OE2	2.17	0.44
1:A:264:TYR:CE1	1:A:293:TYR:HA	2.52	0.44
1:B:482:PHE:HB3	1:B:484:TYR:CE1	2.53	0.44
1:B:263:GLY:O	1:B:278:LEU:HD23	2.17	0.44
1:B:83:ASN:O	1:B:85:GLY:N	2.51	0.44
1:A:172:THR:HG22	6:A:1043:HOH:O	2.18	0.44
1:A:239:THR:O	1:A:361:CYS:HA	2.17	0.43
1:B:252:ARG:HH21	1:B:489:PRO:HD3	1.83	0.43
1:A:459:VAL:HG22	1:A:469:VAL:HG12	2.00	0.43
1:B:252:ARG:HD3	1:B:359:PRO:HB3	2.00	0.43
1:B:350:LEU:HA	1:B:358:PHE:O	2.18	0.43
1:A:208:ALA:O	1:A:242:PRO:HD3	2.19	0.43
1:A:378:CYS:SG	1:A:412:ILE:HD12	2.59	0.43
1:B:494:ILE:O	1:B:494:ILE:HG13	2.19	0.42
1:B:81:ILE:HD11	1:B:475:LEU:CD1	2.50	0.42
1:A:242:PRO:HB2	1:A:251:PHE:CE1	2.55	0.42
1:B:79:VAL:HG23	1:B:95:HIS:CE1	2.55	0.42
1:A:368:MET:HA	1:A:428:MET:O	2.19	0.42
1:A:451:CYS:HA	1:A:452:PRO:HD2	1.87	0.42
1:B:396:GLU:HB2	1:B:398:HIS:CE1	2.55	0.42
1:B:217:MET:HG3	1:B:241:PHE:CE2	2.55	0.41
1:B:302:VAL:C	1:B:303:LEU:HD23	2.40	0.41
1:A:266:MET:CE	1:A:272:ARG:HD2	2.50	0.41
1:B:251:PHE:O	1:B:360:ALA:HB2	2.20	0.41
1:B:167:ILE:O	1:B:171:GLY:HA2	2.20	0.41
1:A:330:TYR:N	1:A:330:TYR:CD2	2.86	0.41
1:A:453:ALA:HB1	1:A:458:LEU:HD12	2.03	0.41
1:A:444:GLU:HB3	1:A:451:CYS:HB2	2.02	0.41
1:A:459:VAL:HA	1:A:460:PRO:HD3	1.93	0.41
1:A:134:LEU:HB3	1:A:135:PRO:HD3	2.02	0.40
1:B:433:ALA:O	1:B:436:SER:HB3	2.20	0.40
1:B:253:LEU:HD12	1:B:360:ALA:HB1	2.03	0.40
1:A:289:TRP:O	1:A:291:PRO:HD3	2.22	0.40
1:B:153:ILE:H	1:B:153:ILE:HG12	1.66	0.40
1:B:289:TRP:CE2	1:B:300:PRO:HD3	2.57	0.40
1:A:176:THR:OG1	1:A:179:GLU:HG3	2.21	0.40
1:A:193:ARG:HB3	1:A:457:TRP:CE3	2.56	0.40
1:B:370:THR:HB	1:B:461:PRO:HG2	2.03	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	409/434 (94%)	352 (86%)	51 (12%)	6 (2%)	10	30
1	B	408/434 (94%)	361 (88%)	39 (10%)	8 (2%)	7	23
All	All	817/868 (94%)	713 (87%)	90 (11%)	14 (2%)	9	27

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	TRP
1	B	496	GLN
1	A	293	TYR
1	A	308	GLN
1	B	84	TRP
1	B	110	LEU
1	B	308	GLN
1	B	369	GLY
1	B	268	ASP
1	A	129	PRO
1	A	369	GLY
1	B	384	ASN
1	A	344	PRO
1	B	464	GLY

### 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	359/382 (94%)	340 (95%)	19 (5%)	22	50
1	B	357/382 (94%)	348 (98%)	9 (2%)	47	76
All	All	716/764 (94%)	688 (96%)	28 (4%)	32	63

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	PRO
1	A	152	LYS
1	A	154	GLU
1	A	165	LYS
1	A	172	THR
1	A	178	ASP
1	A	248	LYS
1	A	265	GLN
1	A	268	ASP
1	A	279	GLU
1	A	308	GLN
1	A	309	ASP
1	A	334	GLN
1	A	388	GLU
1	A	391	ARG
1	A	411	GLU
1	A	413	ASN
1	A	460	PRO
1	A	475	LEU
1	B	78	TYR
1	B	88	GLU
1	B	128	THR
1	B	165	LYS
1	B	248	LYS
1	B	334	GLN
1	B	411	GLU
1	B	413	ASN
1	B	475	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	215	GLN

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Mol	Chain	Res	Type
1	A	265	GLN
1	A	308	GLN
1	A	334	GLN
1	A	442	GLN
1	A	471	HIS
1	A	493	HIS
1	B	91	HIS
1	B	96	HIS
1	B	142	ASN
1	B	143	GLN
1	B	156	HIS
1	B	219	GLN
1	B	334	GLN
1	B	442	GLN
1	B	493	HIS

### 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](#)

7 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	HEM	B	901	1	41,50,50	1.61	5 (12%)	45,82,82	1.63	9 (20%)
3	HEM	A	901	1	41,50,50	1.66	8 (19%)	45,82,82	1.67	9 (20%)
2	SO4	A	3003	-	4,4,4	0.28	0	6,6,6	0.08	0
5	6NI	A	906	-	10,13,13	3.14	4 (40%)	12,18,18	1.41	1 (8%)
4	H4B	B	903	-	16,18,18	3.82	4 (25%)	11,26,26	2.19	6 (54%)
4	H4B	A	902	-	16,18,18	3.32	4 (25%)	11,26,26	2.19	6 (54%)
5	6NI	B	907	-	10,13,13	3.15	5 (50%)	12,18,18	1.41	1 (8%)

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	HEM	B	901	1	-	4/12/54/54	-
3	HEM	A	901	1	-	3/12/54/54	-
5	6NI	A	906	-	-	0/2/4/4	0/2/2/2
4	H4B	B	903	-	1/1/3/5	2/8/17/17	0/2/2/2
4	H4B	A	902	-	1/1/3/5	2/8/17/17	0/2/2/2
5	6NI	B	907	-	-	2/2/4/4	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	903	H4B	C7-C6	-13.23	1.39	1.52
4	A	902	H4B	C7-C6	-10.98	1.41	1.52
5	A	906	6NI	O12-N10	8.38	1.37	1.22
5	B	907	6NI	O12-N10	7.94	1.36	1.22
4	A	902	H4B	C6-N5	-6.13	1.33	1.45
4	B	903	H4B	C6-N5	-6.11	1.33	1.45
3	A	901	HEM	C3C-CAC	-5.14	1.37	1.47
3	B	901	HEM	C3C-CAC	-4.99	1.37	1.47
3	A	901	HEM	C4D-ND	-4.34	1.32	1.40
5	B	907	6NI	C6-N10	-4.09	1.35	1.45
4	B	903	H4B	C7-N8	-3.87	1.38	1.44
3	B	901	HEM	C4D-ND	-3.69	1.33	1.40
4	A	902	H4B	C7-N8	-3.51	1.38	1.44
5	A	906	6NI	C6-N10	-3.39	1.37	1.45
3	A	901	HEM	C2C-C1C	2.91	1.49	1.42
3	B	901	HEM	CAB-C3B	-2.76	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	907	6NI	C4-C5	2.49	1.41	1.36
5	B	907	6NI	C7-C6	2.44	1.42	1.36
3	A	901	HEM	FE-NB	2.26	2.08	1.96
5	A	906	6NI	C7-C6	2.17	1.41	1.36
3	A	901	HEM	C1B-C2B	-2.15	1.40	1.44
4	B	903	H4B	C4A-N5	-2.13	1.33	1.38
3	B	901	HEM	C4B-NB	-2.12	1.34	1.38
4	A	902	H4B	C4A-N5	-2.11	1.33	1.38
3	A	901	HEM	C1D-C2D	2.08	1.48	1.44
3	A	901	HEM	C3B-C4B	2.08	1.49	1.44
5	A	906	6NI	C4-C5	2.05	1.40	1.36
3	A	901	HEM	C1A-CHA	-2.04	1.35	1.41
3	B	901	HEM	C3D-C2D	-2.02	1.32	1.36
5	B	907	6NI	C5-C6	2.02	1.42	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	HEM	CBA-CAA-C2A	-5.64	103.00	112.62
5	A	906	6NI	C7-C8-N1	4.02	137.03	130.51
3	B	901	HEM	CMD-C2D-C1D	4.00	131.13	125.04
5	B	907	6NI	C7-C8-N1	3.99	136.99	130.51
3	B	901	HEM	C4B-CHC-C1C	3.94	127.75	122.56
3	B	901	HEM	CMC-C2C-C3C	3.69	131.57	124.68
3	A	901	HEM	C4B-CHC-C1C	3.40	127.04	122.56
3	A	901	HEM	CMD-C2D-C1D	3.33	130.10	125.04
4	B	903	H4B	C4-C4A-N5	3.27	121.87	119.12
4	A	902	H4B	C8A-C4A-C4	3.24	117.45	114.57
4	B	903	H4B	O9-C9-C6	2.98	116.10	108.98
4	A	902	H4B	C2-N3-C4	2.98	120.66	115.93
3	B	901	HEM	CAB-C3B-C2B	-2.95	118.88	128.60
3	B	901	HEM	C2C-C3C-C4C	-2.95	104.84	106.90
3	A	901	HEM	C4C-CHD-C1D	2.85	126.32	122.56
3	B	901	HEM	C4C-CHD-C1D	2.82	126.28	122.56
4	A	902	H4B	C4-C4A-N5	2.80	121.47	119.12
4	A	902	H4B	O9-C9-C6	2.74	115.54	108.98
4	B	903	H4B	C8A-C4A-C4	2.70	116.97	114.57
4	A	902	H4B	C2-N1-C8A	2.67	120.53	114.54
4	B	903	H4B	C2-N3-C4	2.65	120.14	115.93
4	B	903	H4B	N1-C2-N3	-2.55	121.42	125.42
3	A	901	HEM	C2C-C3C-C4C	-2.52	105.14	106.90
3	B	901	HEM	C3D-C4D-ND	2.46	112.91	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	HEM	CBA-CAA-C2A	-2.44	108.45	112.62
3	A	901	HEM	CMC-C2C-C3C	2.39	129.15	124.68
3	A	901	HEM	C1D-C2D-C3D	-2.33	104.50	106.96
3	A	901	HEM	C4B-C3B-C2B	-2.32	105.27	107.11
4	A	902	H4B	N1-C2-N3	-2.29	121.83	125.42
3	B	901	HEM	CAB-C3B-C4B	2.14	134.45	124.47
4	B	903	H4B	C2-N1-C8A	2.08	119.21	114.54
3	A	901	HEM	C2B-C1B-NB	2.07	112.29	109.84

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	902	H4B	C6
4	B	903	H4B	C6

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	H4B	C7-C6-C9-O9
4	A	902	H4B	C7-C6-C9-C10
4	B	903	H4B	C7-C6-C9-O9
4	B	903	H4B	C7-C6-C9-C10
5	B	907	6NI	C7-C6-N10-O12
5	B	907	6NI	C5-C6-N10-O12
3	A	901	HEM	CAA-CBA-CGA-O1A
3	B	901	HEM	CAA-CBA-CGA-O1A
3	A	901	HEM	CAA-CBA-CGA-O2A
3	B	901	HEM	CAD-CBD-CGD-O1D
3	B	901	HEM	CAA-CBA-CGA-O2A
3	B	901	HEM	CAD-CBD-CGD-O2D
3	A	901	HEM	CAD-CBD-CGD-O2D

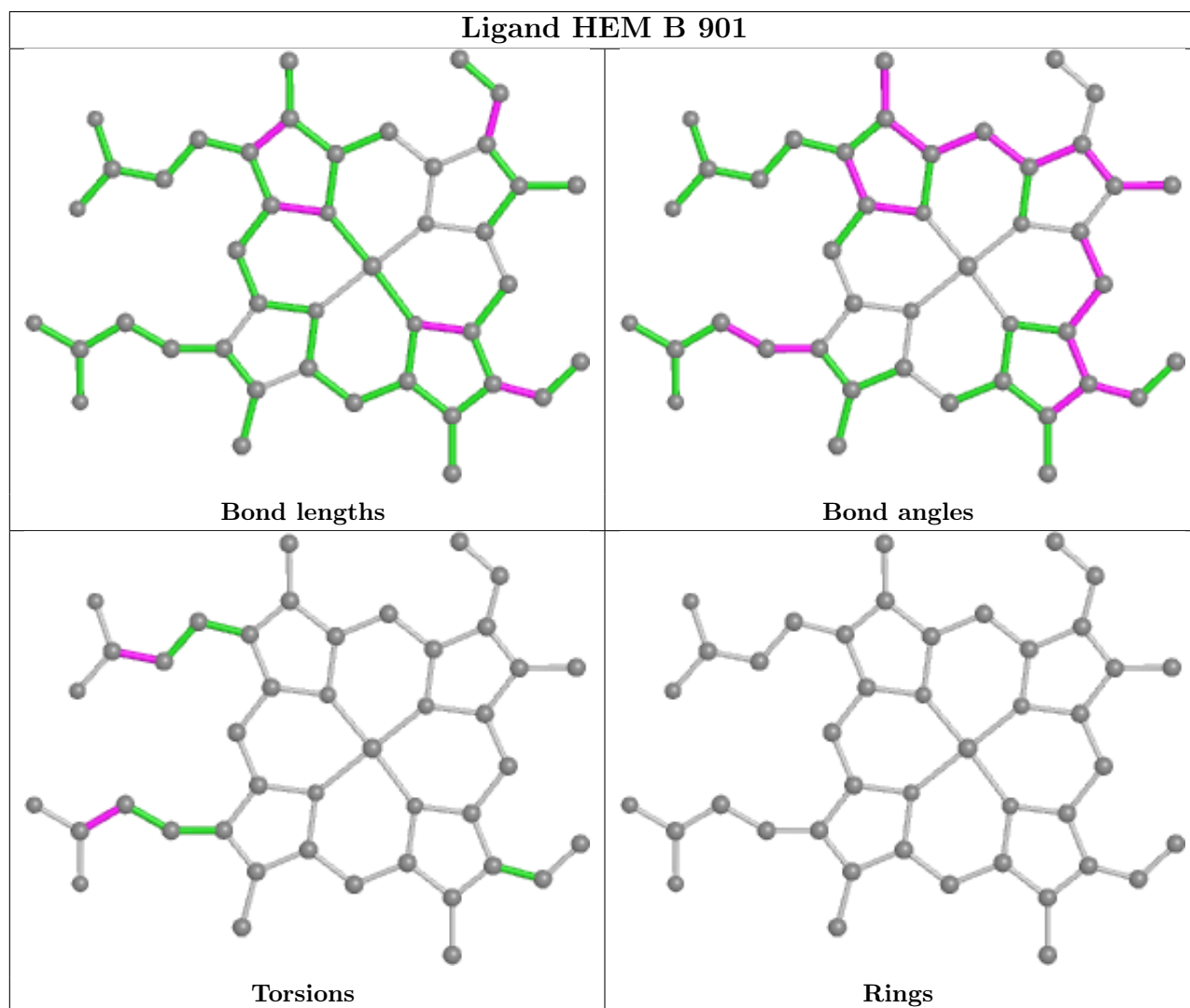
There are no ring outliers.

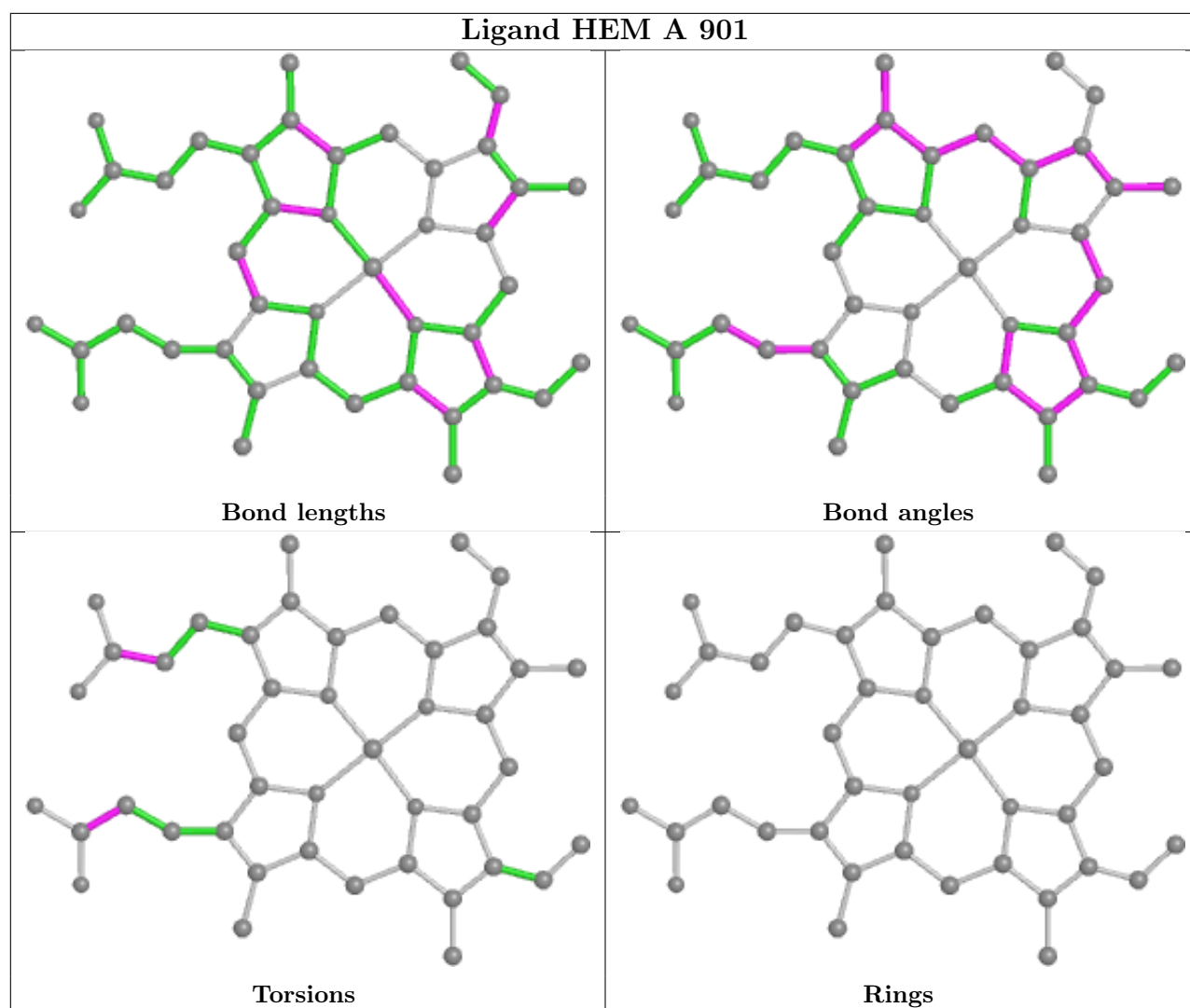
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	HEM	2	0
5	A	906	6NI	2	0
4	B	903	H4B	1	0
5	B	907	6NI	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

### 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.