



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:28 AM UTC

PDB ID : 1QOM / pdb_00001qom
Title : MURINE INDUCIBLE NITRIC OXIDE SYNTHASE OXYGENASE DIMER
(DELTA 65) WITH SWAPPED N-TERMINAL HOOK
Authors : Crane, B.R.; Rosenfeld, R.A.; Arvai, A.S.; Tainer, J.A.; Stuehr, D.J.; Getzoff, E.D.
Deposited on : 1999-11-15
Resolution : 2.70 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

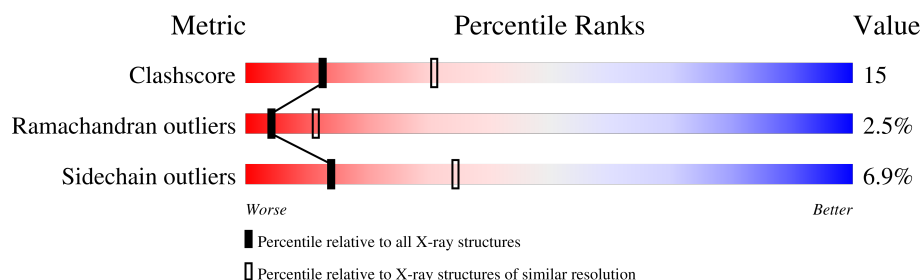
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	440	
1	B	440	

2 Entry composition [i](#)

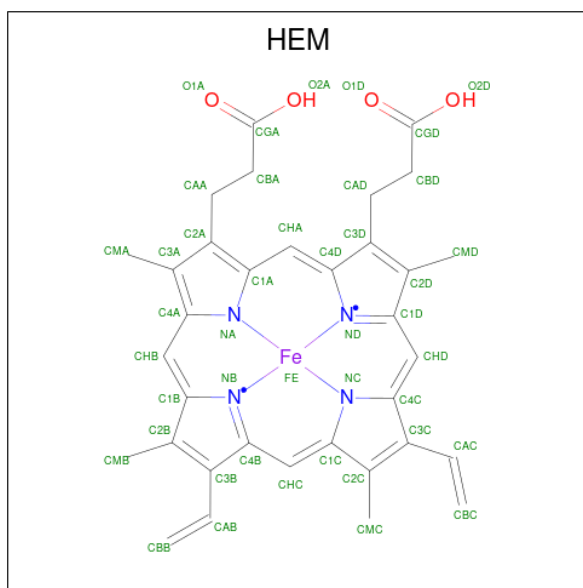
There are 4 unique types of molecules in this entry. The entry contains 7362 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NITRIC OXIDE SYNTHASE.

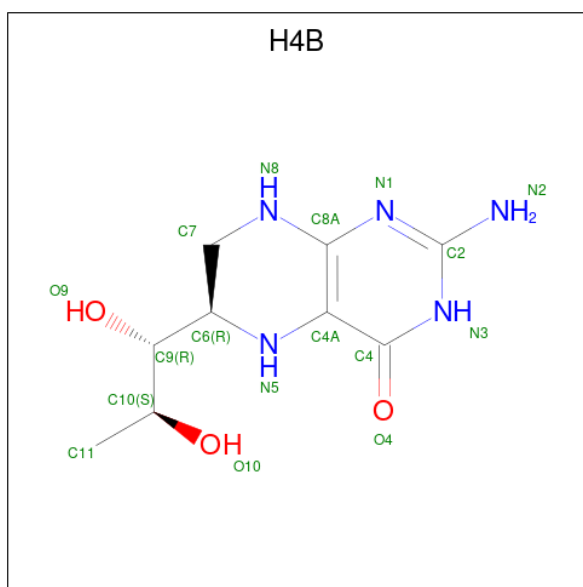
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3424	2194	590	619	21			
1	B	420	Total	C	N	O	S	0	0	0
			3424	2194	590	619	21			

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



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

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $C_9H_{15}N_5O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	191	Total	O	0	0
			191	191		
4	B	203	Total	O	0	0
			203	203		

4 Data and refinement statistics

Xtriage (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, α , β , γ	212.98Å 212.98Å 114.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	91.7 (20.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.236 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7362	wwPDB-VP
Average B, all atoms (Å ²)	75.0	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, 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	0.44	0/3524	1.03	22/4790 (0.5%)
1	B	0.44	0/3524	1.03	25/4790 (0.5%)
All	All	0.44	0/7048	1.03	47/9580 (0.5%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	LYS	N-CA-C	8.43	121.91	112.97
1	A	122	GLY	CA-C-N	8.39	130.32	119.84
1	A	122	GLY	C-N-CA	8.39	130.32	119.84
1	A	266	MET	CA-C-N	7.36	126.89	119.24
1	A	266	MET	C-N-CA	7.36	126.89	119.24
1	A	107	LYS	N-CA-C	7.23	121.41	112.59
1	B	467	THR	CA-C-N	6.96	126.21	118.97
1	B	467	THR	C-N-CA	6.96	126.21	118.97
1	B	348	ASN	N-CA-C	6.86	122.84	113.37
1	A	94	LEU	N-CA-C	6.76	119.51	111.33
1	A	488	GLU	CA-C-N	6.50	127.96	119.84
1	A	488	GLU	C-N-CA	6.50	127.96	119.84
1	B	378	CYS	N-CA-C	6.47	121.46	113.50
1	B	84	TRP	N-CA-C	6.45	120.25	112.38
1	B	114	MET	N-CA-C	6.40	118.05	111.14
1	A	459	VAL	CA-C-N	6.40	124.33	119.66
1	A	459	VAL	C-N-CA	6.40	124.33	119.66
1	B	316	PRO	CA-C-N	6.39	126.88	119.47
1	B	316	PRO	C-N-CA	6.39	126.88	119.47
1	A	378	CYS	N-CA-C	6.16	120.93	113.17
1	B	122	GLY	CA-C-N	6.15	127.53	119.84
1	B	122	GLY	C-N-CA	6.15	127.53	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	MET	N-CA-C	-6.04	98.57	108.41
1	B	266	MET	CA-C-N	6.03	125.24	118.97
1	B	266	MET	C-N-CA	6.03	125.24	118.97
1	B	188	TRP	N-CA-C	-5.91	104.75	111.14
1	B	488	GLU	CA-C-N	5.89	126.03	119.32
1	B	488	GLU	C-N-CA	5.89	126.03	119.32
1	B	466	ILE	N-CA-C	-5.83	105.42	113.00
1	B	147	SER	N-CA-C	5.79	117.46	111.03
1	A	197	ARG	N-CA-C	5.76	119.78	112.87
1	A	365	GLY	N-CA-C	-5.75	101.63	110.77
1	B	176	THR	N-CA-C	-5.73	102.96	110.53
1	A	485	TYR	N-CA-C	-5.64	103.25	110.53
1	B	104	CYS	N-CA-C	-5.62	105.92	112.89
1	B	148	PHE	N-CA-C	5.60	118.39	110.50
1	B	485	TYR	N-CA-C	-5.53	101.29	109.86
1	A	110	LEU	N-CA-C	-5.48	107.16	112.97
1	A	151	ALA	N-CA-C	5.46	118.00	110.35
1	A	348	ASN	N-CA-C	5.41	122.31	110.80
1	B	377	PHE	N-CA-C	5.27	118.17	111.69
1	A	467	THR	CA-C-N	5.20	124.82	119.05
1	A	467	THR	C-N-CA	5.20	124.82	119.05
1	A	466	ILE	N-CA-C	-5.10	106.08	113.07
1	A	217	MET	N-CA-C	-5.06	105.45	110.97
1	B	460	PRO	CA-C-N	5.01	125.68	120.12
1	B	460	PRO	C-N-CA	5.01	125.68	120.12

There are no chirality outliers.

There are no planarity outliers.

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	3424	0	3322	111	0
1	B	3424	0	3322	98	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	17	0	14	0	0
3	B	17	0	14	0	0
4	A	191	0	0	13	0
4	B	203	0	0	10	0
All	All	7362	0	6732	208	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 15.

All (208) 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:438:MET:HE3	1:B:469:VAL:HG12	1.51	0.92
1:A:105:LYS:HE2	1:A:106:SER:H	1.39	0.87
1:B:77:GLN:HE21	1:B:77:GLN:HA	1.41	0.85
1:A:438:MET:HE3	1:A:469:VAL:HG12	1.58	0.85
1:B:124:ARG:HH22	1:B:128:THR:HB	1.43	0.80
1:A:221:ILE:HG21	1:A:301:LEU:HD21	1.62	0.79
1:A:134:LEU:O	1:A:138:ILE:HG12	1.85	0.77
1:B:252:ARG:HD3	1:B:359:PRO:HB2	1.68	0.76
1:A:438:MET:HA	1:A:438:MET:HE2	1.70	0.74
1:A:252:ARG:NH2	1:A:489:PRO:HD3	2.03	0.73
1:A:105:LYS:CE	1:A:106:SER:H	2.02	0.73
1:B:105:LYS:HD2	1:B:106:SER:H	1.53	0.71
1:A:195:ILE:HG21	1:A:368:MET:HE3	1.71	0.71
1:A:344:PRO:HA	4:A:2126:HOH:O	1.91	0.70
1:A:410:THR:O	1:A:414:VAL:HG23	1.91	0.70
1:B:150:GLU:HB3	4:B:2032:HOH:O	1.92	0.69
1:A:132:GLU:O	1:A:135:PRO:HD2	1.92	0.68
1:B:105:LYS:CD	1:B:106:SER:H	2.07	0.68
1:A:258:LEU:HB2	1:A:345:ALA:HB3	1.74	0.68
1:B:467:THR:CG2	1:B:469:VAL:HG22	2.24	0.68
1:B:378:CYS:SG	1:B:386:LEU:HD23	2.34	0.67
1:A:163:VAL:O	1:A:167:ILE:HG13	1.95	0.66
1:A:105:LYS:HE2	1:A:105:LYS:HA	1.78	0.66
1:B:124:ARG:HH22	1:B:128:THR:CB	2.09	0.65
1:B:159:ARG:O	1:B:163:VAL:HG23	1.96	0.65
1:B:366:TRP:H	2:B:901:HEM:HAB	1.60	0.65
1:A:252:ARG:HD3	1:A:359:PRO:HB2	1.79	0.65
1:B:464:GLY:O	1:B:467:THR:HB	1.96	0.64
1:A:105:LYS:HE2	1:A:106:SER:N	2.11	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:THR:CG2	1:A:469:VAL:HG22	2.28	0.64
1:A:360:ALA:HA	4:A:2117:HOH:O	1.99	0.62
1:A:351:LEU:HD11	4:A:2039:HOH:O	1.99	0.62
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.34	0.61
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.36	0.61
1:A:116:PRO:HG2	1:A:119:LEU:HB2	1.82	0.60
1:B:360:ALA:HA	4:B:2135:HOH:O	2.01	0.59
1:B:128:THR:OG1	1:B:133:LEU:HB2	2.01	0.59
1:A:303:LEU:O	1:A:310:PRO:HA	2.03	0.58
1:B:298:VAL:HG21	1:B:320:VAL:HG11	1.83	0.58
1:A:217:MET:HE3	1:A:303:LEU:HB3	1.85	0.57
1:A:101:ASP:HA	1:A:106:SER:HA	1.86	0.57
1:B:101:ASP:HA	1:B:106:SER:HA	1.85	0.57
1:B:163:VAL:O	1:B:167:ILE:HG13	2.05	0.57
1:B:138:ILE:HG23	1:B:160:LEU:HD22	1.87	0.57
1:A:405:LYS:O	1:A:409:VAL:HG23	2.05	0.56
1:A:144:TYR:O	1:A:147:SER:HB3	2.06	0.56
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.41	0.56
1:A:148:PHE:HB2	4:A:2022:HOH:O	2.06	0.56
1:A:159:ARG:O	1:A:163:VAL:HG23	2.05	0.56
1:B:107:LYS:O	1:B:108:SER:HB2	2.05	0.56
1:B:252:ARG:HH11	1:B:252:ARG:HG3	1.71	0.56
1:B:144:TYR:CE1	1:B:179:GLU:HA	2.41	0.56
1:B:172:THR:OG1	1:B:356:LEU:HD21	2.06	0.56
1:A:304:GLN:O	1:A:304:GLN:HG3	2.04	0.56
1:B:134:LEU:O	1:B:138:ILE:HG13	2.06	0.55
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.88	0.55
1:B:251:PHE:O	1:B:360:ALA:HB2	2.05	0.55
1:B:239:THR:HG23	1:B:362:PRO:HG2	1.88	0.55
1:A:350:LEU:HD21	1:A:357:GLU:HB2	1.88	0.55
1:A:251:PHE:O	1:A:360:ALA:HB2	2.07	0.54
1:A:264:TYR:CE2	1:A:293:TYR:HA	2.42	0.54
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.36	0.54
1:A:293:TYR:CD2	1:B:267:PRO:HB3	2.43	0.54
1:A:384:ASN:HA	4:A:2134:HOH:O	2.08	0.54
1:B:350:LEU:HD21	1:B:357:GLU:HB2	1.90	0.54
1:A:84:TRP:NE1	1:A:114:MET:HG3	2.24	0.53
1:A:358:PHE:HB3	4:A:2123:HOH:O	2.09	0.53
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.43	0.53
1:A:341:TYR:HE2	4:A:2126:HOH:O	1.92	0.52
1:A:243:GLN:HB3	1:A:358:PHE:CE2	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:MET:HB3	1:A:267:PRO:HD2	1.92	0.52
1:A:308:GLN:HG3	4:A:2184:HOH:O	2.09	0.52
1:A:298:VAL:HG21	1:A:320:VAL:HG11	1.91	0.52
1:A:264:TYR:HE2	1:A:294:GLY:H	1.58	0.51
1:A:330:TYR:CD1	1:A:330:TYR:N	2.78	0.51
1:B:102:PHE:CE2	1:B:109:CYS:HB2	2.45	0.51
1:A:480:SER:HA	1:A:481:PRO:C	2.34	0.51
1:B:330:TYR:HD2	1:B:332:TRP:CZ2	2.28	0.51
1:A:80:ARG:NH2	4:A:2002:HOH:O	2.43	0.51
1:B:188:TRP:CZ3	1:B:200:TRP:HA	2.46	0.51
1:B:453:ALA:HB3	1:B:474:MET:HB2	1.92	0.51
1:A:154:GLU:H	1:A:154:GLU:CD	2.18	0.51
1:A:144:TYR:CE2	1:A:179:GLU:HA	2.45	0.51
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.92	0.51
1:B:102:PHE:HB3	1:B:105:LYS:O	2.11	0.51
1:B:137:ALA:O	1:B:141:ILE:HG13	2.11	0.50
1:B:138:ILE:HG23	1:B:160:LEU:CD2	2.42	0.50
1:B:252:ARG:NH2	1:B:489:PRO:HD3	2.25	0.50
1:B:286:ASP:C	1:B:288:GLY:H	2.19	0.50
1:B:385:ILE:O	1:B:389:VAL:HG23	2.12	0.50
1:B:480:SER:HA	1:B:481:PRO:C	2.37	0.50
1:A:77:GLN:O	1:A:96:HIS:HE1	1.93	0.50
1:B:78:TYR:C	1:B:78:TYR:CD1	2.90	0.50
1:A:343:LEU:HD11	1:A:364:ASN:HD22	1.77	0.50
1:B:209:ARG:O	1:B:242:PRO:HG3	2.11	0.50
1:B:239:THR:O	1:B:361:CYS:HA	2.12	0.49
1:B:116:PRO:HG2	1:B:119:LEU:HB2	1.93	0.49
1:B:102:PHE:HB2	1:B:106:SER:O	2.12	0.49
1:B:330:TYR:CD1	1:B:330:TYR:N	2.80	0.49
1:A:105:LYS:HE2	1:A:105:LYS:CA	2.43	0.49
1:B:148:PHE:HB2	4:B:2031:HOH:O	2.13	0.49
1:A:444:GLU:HG3	1:A:450:GLY:O	2.13	0.49
1:A:444:GLU:HG2	1:A:451:CYS:HB2	1.94	0.49
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.95	0.48
1:A:289:TRP:O	1:A:291:PRO:HD3	2.13	0.48
1:B:330:TYR:N	1:B:330:TYR:HD1	2.10	0.48
1:A:385:ILE:HD11	1:A:412:ILE:HD13	1.93	0.48
1:A:105:LYS:CD	1:A:106:SER:H	2.26	0.48
1:A:172:THR:HG23	1:A:173:TYR:N	2.28	0.48
1:A:248:LYS:HE3	1:A:494:ILE:HD12	1.95	0.48
1:A:438:MET:HE1	1:A:472:GLN:HG2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ILE:HG23	1:A:160:LEU:CD2	2.44	0.48
1:A:330:TYR:HB3	1:A:332:TRP:NE1	2.29	0.48
1:B:223:ARG:HD3	4:B:2071:HOH:O	2.13	0.47
1:A:368:MET:HE2	1:A:433:ALA:CB	2.44	0.47
1:B:128:THR:HA	1:B:129:PRO:HD2	1.80	0.47
1:B:177:LEU:O	1:B:181:ILE:HD13	2.15	0.47
1:A:289:TRP:CE2	1:A:300:PRO:HD3	2.49	0.47
1:A:343:LEU:HD11	1:A:364:ASN:ND2	2.29	0.47
1:B:441:MET:HE1	1:B:472:GLN:HG2	1.96	0.47
1:B:486:GLN:HB2	4:B:2019:HOH:O	2.15	0.47
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.15	0.47
1:A:78:TYR:CD1	1:A:78:TYR:C	2.93	0.47
1:B:127:PRO:HG3	1:B:246:ASP:HA	1.96	0.47
1:A:105:LYS:CE	1:A:105:LYS:HA	2.45	0.46
1:B:289:TRP:O	1:B:291:PRO:HD3	2.15	0.46
1:A:453:ALA:HB3	1:A:474:MET:HB3	1.96	0.46
1:B:258:LEU:HD12	1:B:258:LEU:HA	1.72	0.46
1:A:141:ILE:CD1	1:A:163:VAL:HG21	2.46	0.46
1:B:438:MET:HA	1:B:438:MET:HE2	1.98	0.46
1:A:368:MET:HE2	1:A:433:ALA:HB3	1.97	0.46
1:B:80:ARG:NH2	4:B:2001:HOH:O	2.47	0.46
1:A:261:TYR:CE2	1:A:296:PHE:HD1	2.34	0.46
1:B:260:ARG:HD2	4:B:2106:HOH:O	2.16	0.46
1:A:217:MET:CE	1:A:303:LEU:HB3	2.46	0.46
1:B:258:LEU:HB2	1:B:345:ALA:HB3	1.97	0.46
1:B:441:MET:HE1	1:B:472:GLN:CD	2.41	0.46
1:A:153:ILE:O	1:A:157:LEU:HD13	2.14	0.45
1:A:330:TYR:N	1:A:330:TYR:HD1	2.14	0.45
1:A:387:GLU:HG2	4:A:2053:HOH:O	2.17	0.45
1:A:438:MET:HG3	1:A:468:PRO:HB2	1.98	0.45
1:B:356:LEU:HD13	1:B:356:LEU:HA	1.71	0.45
1:A:153:ILE:O	1:A:156:HIS:HB3	2.16	0.45
1:A:263:GLY:O	1:A:278:LEU:HD23	2.17	0.45
1:A:262:ALA:HB2	1:A:299:LEU:CD2	2.47	0.45
1:B:249:HIS:HB3	1:B:306:ASP:OD1	2.17	0.44
1:B:302:VAL:C	1:B:303:LEU:HD23	2.42	0.44
1:B:99:THR:HG22	1:B:100:SER:N	2.32	0.44
1:B:285:ILE:CD1	1:B:291:PRO:HB3	2.46	0.44
1:B:372:ILE:HA	1:B:376:ASP:OD2	2.17	0.44
1:B:459:VAL:HG22	1:B:469:VAL:HG23	1.98	0.44
1:A:371:GLU:HB3	4:A:2128:HOH:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:LYS:NZ	4:B:2030:HOH:O	2.51	0.44
1:B:252:ARG:HG3	1:B:252:ARG:NH1	2.32	0.43
1:B:317:PRO:HD2	4:B:2121:HOH:O	2.18	0.43
1:B:417:LEU:O	1:B:421:GLN:HB2	2.19	0.43
1:A:482:PHE:HB3	1:A:484:TYR:CE1	2.53	0.43
1:A:257:GLN:HB2	1:A:345:ALA:O	2.18	0.43
1:B:167:ILE:HG23	1:B:171:GLY:O	2.17	0.43
1:B:252:ARG:CD	1:B:359:PRO:HB2	2.42	0.43
1:A:194:CYS:HB2	2:A:901:HEM:ND	2.33	0.43
1:A:389:VAL:O	1:A:393:MET:HG3	2.18	0.43
1:A:371:GLU:O	1:A:375:ARG:HB2	2.17	0.43
1:A:107:LYS:HB3	4:A:2008:HOH:O	2.19	0.43
1:A:227:TYR:CD1	1:A:227:TYR:C	2.96	0.43
1:A:105:LYS:CG	1:A:106:SER:N	2.81	0.43
1:A:417:LEU:O	1:A:421:GLN:HG3	2.18	0.43
1:B:77:GLN:HG3	1:B:78:TYR:N	2.34	0.43
1:B:105:LYS:CG	1:B:106:SER:N	2.82	0.43
1:B:305:ALA:O	1:B:306:ASP:C	2.62	0.43
1:A:252:ARG:HD2	1:A:359:PRO:O	2.19	0.42
1:B:107:LYS:O	1:B:108:SER:CB	2.67	0.42
1:A:330:TYR:HD2	1:A:332:TRP:CZ2	2.37	0.42
1:A:214:ALA:O	1:A:217:MET:HB2	2.19	0.42
1:B:136:HIS:O	1:B:139:GLU:HB3	2.19	0.42
1:B:371:GLU:O	1:B:375:ARG:HB2	2.19	0.42
1:A:217:MET:HG2	1:A:241:PHE:CE1	2.54	0.42
1:A:309:ASP:HB3	1:A:310:PRO:HD2	2.02	0.42
1:A:488:GLU:HA	1:A:489:PRO:HD2	1.73	0.42
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.93	0.42
1:B:141:ILE:HD11	1:B:163:VAL:HG11	2.01	0.42
1:B:153:ILE:O	1:B:156:HIS:HB3	2.20	0.42
1:A:316:PRO:HD2	1:A:319:LEU:HD12	2.00	0.41
1:B:121:ARG:HD3	1:B:121:ARG:HA	1.70	0.41
1:B:257:GLN:HB2	1:B:345:ALA:O	2.19	0.41
1:A:127:PRO:O	1:A:129:PRO:HD3	2.20	0.41
1:B:172:THR:OG1	1:B:173:TYR:N	2.52	0.41
1:A:258:LEU:HA	1:A:258:LEU:HD12	1.78	0.41
1:A:346:VAL:HB	1:A:363:PHE:CZ	2.55	0.41
1:A:153:ILE:H	1:A:153:ILE:HG13	1.47	0.41
1:A:217:MET:HE1	1:A:304:GLN:N	2.35	0.41
1:B:386:LEU:HB2	4:B:2153:HOH:O	2.20	0.41
1:A:351:LEU:O	1:A:357:GLU:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:GLN:HE21	1:B:77:GLN:CA	2.17	0.41
1:B:102:PHE:CD2	1:B:109:CYS:HB2	2.56	0.41
1:B:488:GLU:HA	1:B:489:PRO:HD2	1.80	0.41
1:A:186:MET:HE1	1:A:448:ARG:NH1	2.36	0.41
1:B:194:CYS:HB2	2:B:901:HEM:ND	2.36	0.40
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.52	0.40
1:A:143:GLN:HG2	1:A:182:PHE:HZ	1.87	0.40
1:A:350:LEU:HB2	1:A:486:GLN:CD	2.46	0.40
1:A:467:THR:HA	1:A:468:PRO:HD3	1.89	0.40
1:B:315:ILE:HA	1:B:316:PRO:HD3	1.98	0.40
1:A:217:MET:CB	1:A:303:LEU:HD23	2.51	0.40
1:A:333:PHE:HB3	4:A:2111:HOH:O	2.21	0.40
1:B:242:PRO:HB2	1:B:251:PHE:CE1	2.56	0.40
1:B:386:LEU:HD12	1:B:405:LYS:HG2	2.02	0.40
1:B:482:PHE:HB3	1:B:484:TYR:CE1	2.56	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	418/440 (95%)	365 (87%)	46 (11%)	7 (2%)	7	19
1	B	418/440 (95%)	363 (87%)	41 (10%)	14 (3%)	3	7
All	All	836/880 (95%)	728 (87%)	87 (10%)	21 (2%)	4	11

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	THR
1	A	103	THR
1	B	103	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	99	THR
1	B	108	SER
1	B	308	GLN
1	B	369	GLY
1	A	108	SER
1	A	293	TYR
1	B	306	ASP
1	B	149	LYS
1	B	268	ASP
1	B	384	ASN
1	A	123	PRO
1	A	369	GLY
1	B	197	ARG
1	B	200	TRP
1	B	348	ASN
1	A	84	TRP
1	B	102	PHE
1	B	106	SER

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	368/388 (95%)	341 (93%)	27 (7%)	13	32
1	B	368/388 (95%)	344 (94%)	24 (6%)	15	37
All	All	736/776 (95%)	685 (93%)	51 (7%)	14	34

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ILE
1	A	105	LYS
1	A	108	SER
1	A	110	LEU
1	A	114	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	119	LEU
1	A	129	PRO
1	A	150	GLU
1	A	153	ILE
1	A	154	GLU
1	A	157	LEU
1	A	161	GLU
1	A	170	THR
1	A	172	THR
1	A	180	LEU
1	A	213	THR
1	A	231	ASN
1	A	258	LEU
1	A	301	LEU
1	A	330	TYR
1	A	338	LEU
1	A	348	ASN
1	A	368	MET
1	A	400	LEU
1	A	467	THR
1	A	487	ILE
1	A	496	GLN
1	B	77	GLN
1	B	93	THR
1	B	103	THR
1	B	108	SER
1	B	119	LEU
1	B	128	THR
1	B	130	LEU
1	B	134	LEU
1	B	148	PHE
1	B	150	GLU
1	B	210	ASN
1	B	239	THR
1	B	258	LEU
1	B	330	TYR
1	B	348	ASN
1	B	356	LEU
1	B	386	LEU
1	B	400	LEU
1	B	421	GLN
1	B	436	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	441	MET
1	B	467	THR
1	B	475	LEU
1	B	495	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	96	HIS
1	A	115	ASN
1	A	156	HIS
1	A	231	ASN
1	A	233	ASN
1	A	243	GLN
1	A	257	GLN
1	A	348	ASN
1	A	364	ASN
1	A	440	HIS
1	A	443	ASN
1	A	471	HIS
1	A	486	GLN
1	B	77	GLN
1	B	91	HIS
1	B	95	HIS
1	B	96	HIS
1	B	199	GLN
1	B	219	GLN
1	B	231	ASN
1	B	233	ASN
1	B	348	ASN
1	B	364	ASN
1	B	384	ASN
1	B	421	GLN
1	B	431	HIS
1	B	486	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	H4B	B	902	-	17,18,18	2.76	3 (17%)	14,26,26	1.94	4 (28%)
3	H4B	A	902	-	17,18,18	2.65	4 (23%)	14,26,26	2.05	5 (35%)
2	HEM	A	901	1	50,50,50	1.29	4 (8%)	67,82,82	0.98	4 (5%)
2	HEM	B	901	1	50,50,50	1.34	6 (12%)	67,82,82	1.06	7 (10%)

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	H4B	B	902	-	-	2/8/17/17	0/2/2/2
3	H4B	A	902	-	-	2/8/17/17	0/2/2/2
2	HEM	A	901	1	-	6/14/54/54	-
2	HEM	B	901	1	-	4/14/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	H4B	C7-N8	-7.35	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	H4B	C7-C6	-7.32	1.45	1.52
3	A	902	H4B	C7-N8	-7.18	1.39	1.46
3	A	902	H4B	C7-C6	-6.82	1.45	1.52
2	A	901	HEM	FE-NB	3.32	2.05	1.94
2	B	901	HEM	C1A-NA	-3.09	1.33	1.39
2	B	901	HEM	CAB-C3B	-3.06	1.39	1.47
2	B	901	HEM	CAC-C3C	-3.03	1.39	1.47
2	A	901	HEM	CAB-C3B	-2.88	1.39	1.47
2	B	901	HEM	C4D-ND	-2.80	1.35	1.40
3	B	902	H4B	C4-N3	-2.75	1.33	1.38
3	A	902	H4B	C4-N3	-2.69	1.33	1.38
2	B	901	HEM	FE-NB	2.66	2.03	1.94
2	A	901	HEM	CAC-C3C	-2.58	1.40	1.47
2	B	901	HEM	C1C-NC	-2.36	1.35	1.39
3	A	902	H4B	C4A-C8A	2.15	1.42	1.38
2	A	901	HEM	C1B-NB	-2.13	1.36	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	H4B	C2-N1-C8A	4.14	120.67	113.36
3	A	902	H4B	O4-C4-C4A	-4.10	117.39	127.26
3	B	902	H4B	C2-N1-C8A	3.97	120.36	113.36
3	B	902	H4B	O4-C4-C4A	-3.80	118.11	127.26
2	B	901	HEM	C3B-C4B-NB	2.96	111.59	109.47
3	A	902	H4B	C4A-C4-N3	2.84	119.92	112.13
3	B	902	H4B	C4A-C4-N3	2.66	119.44	112.13
2	B	901	HEM	CMD-C2D-C1D	2.55	129.02	125.03
3	A	902	H4B	C2-N3-C4	-2.55	120.50	125.11
2	A	901	HEM	CMD-C2D-C1D	2.50	128.94	125.03
2	B	901	HEM	CAD-C3D-C2D	-2.44	123.29	127.87
2	A	901	HEM	C3B-C4B-NB	2.42	111.21	109.47
2	A	901	HEM	C4B-C3B-C2B	-2.39	105.09	107.28
3	B	902	H4B	C2-N3-C4	-2.30	120.94	125.11
2	B	901	HEM	C4C-C3C-C2C	-2.27	104.85	106.81
2	B	901	HEM	C4B-C3B-C2B	-2.18	105.28	107.28
2	B	901	HEM	CAD-C3D-C4D	2.14	128.43	124.70
2	A	901	HEM	CAD-C3D-C2D	-2.12	123.90	127.87
3	A	902	H4B	C4-C4A-N5	2.02	121.78	116.27
2	B	901	HEM	C1D-C2D-C3D	-2.00	104.87	106.98

There are no chirality outliers.

All (14) torsion outliers are listed below:

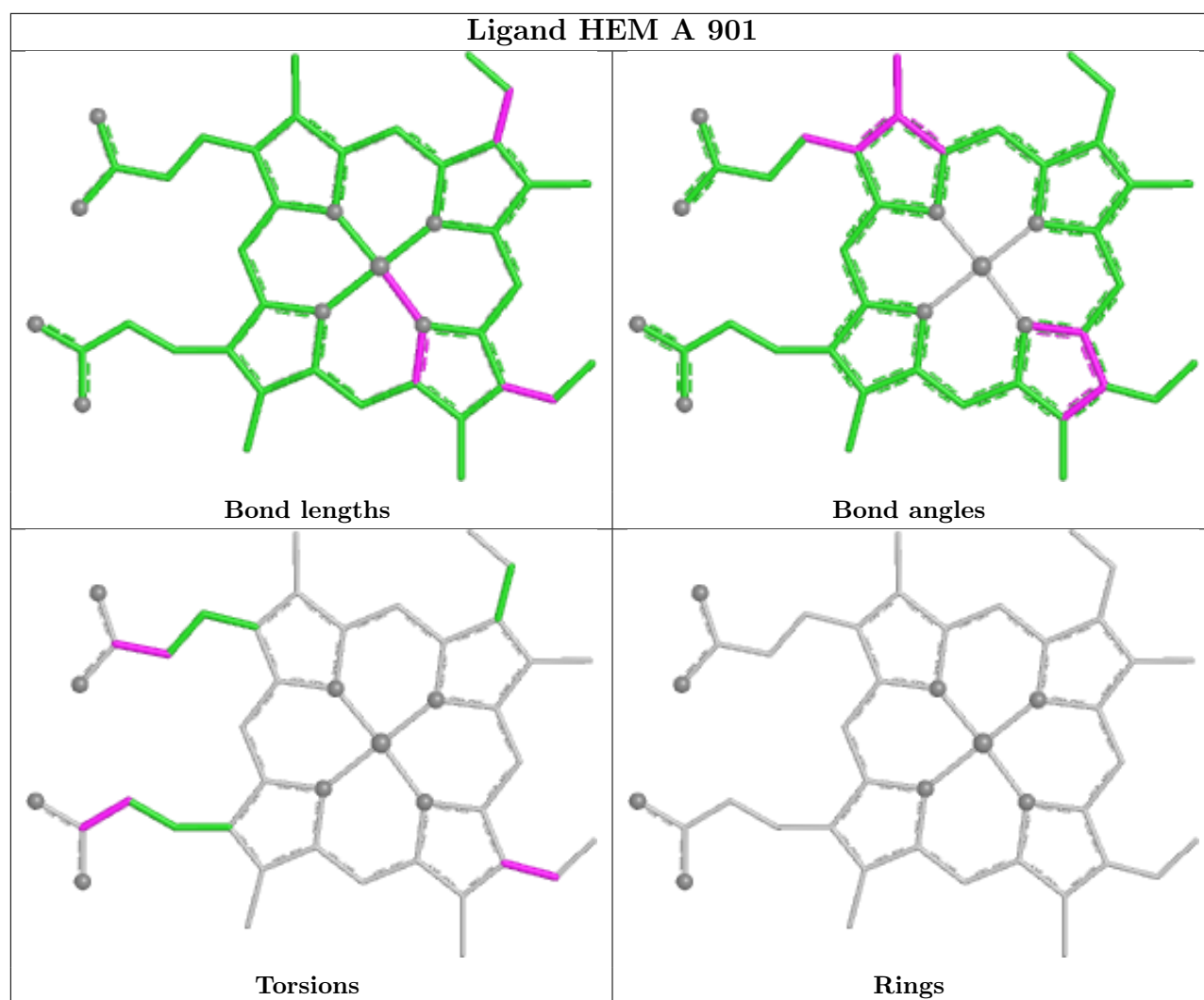
Mol	Chain	Res	Type	Atoms
3	A	902	H4B	C7-C6-C9-O9
3	B	902	H4B	C7-C6-C9-O9
2	B	901	HEM	C2B-C3B-CAB-CBB
3	A	902	H4B	C7-C6-C9-C10
2	B	901	HEM	C4B-C3B-CAB-CBB
3	B	902	H4B	C7-C6-C9-C10
2	A	901	HEM	C2B-C3B-CAB-CBB
2	A	901	HEM	C4B-C3B-CAB-CBB
2	A	901	HEM	CAD-CBD-CGD-O2D
2	A	901	HEM	CAA-CBA-CGA-O1A
2	B	901	HEM	CAA-CBA-CGA-O1A
2	A	901	HEM	CAA-CBA-CGA-O2A
2	B	901	HEM	CAA-CBA-CGA-O2A
2	A	901	HEM	CAD-CBD-CGD-O1D

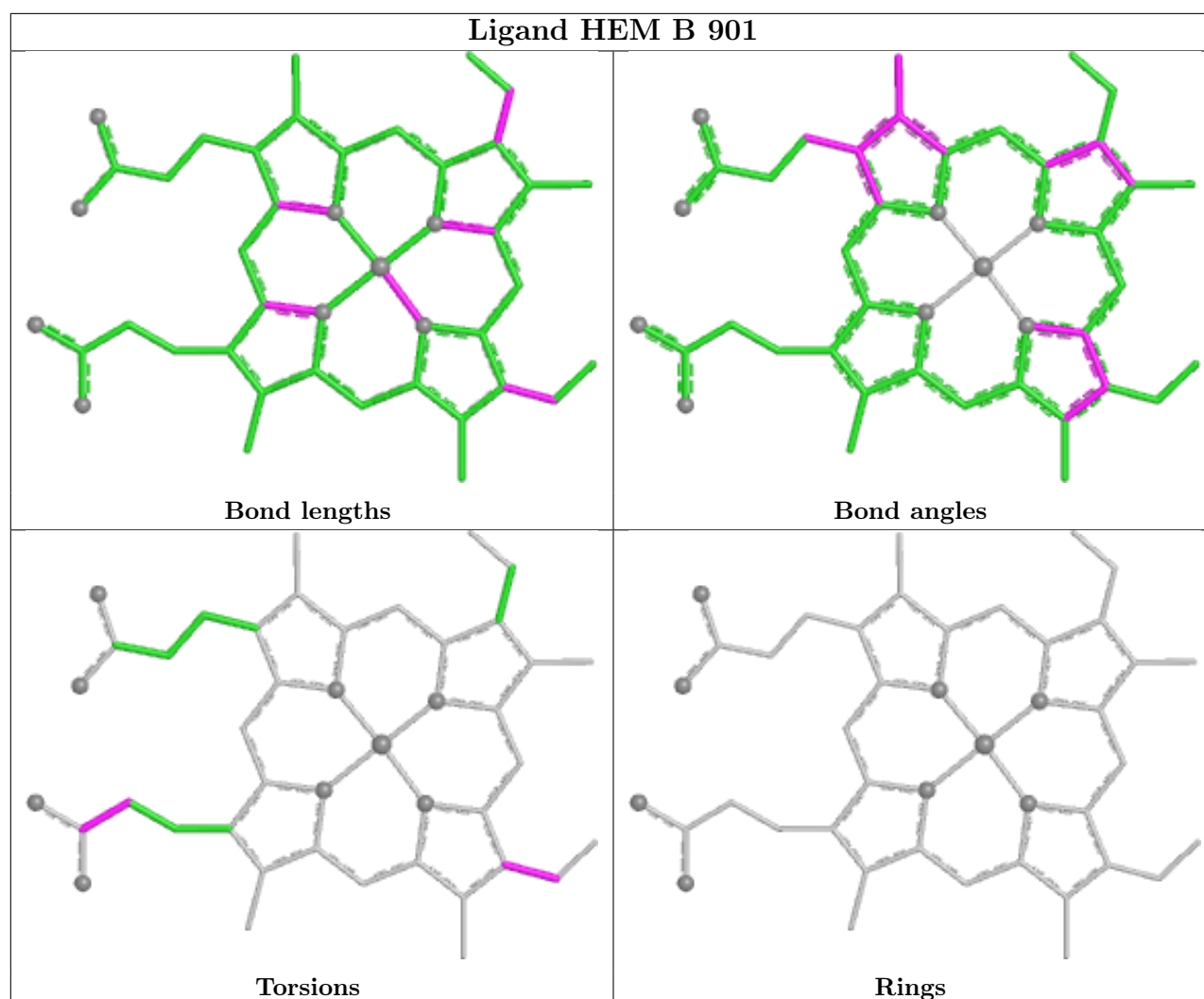
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	HEM	1	0
2	B	901	HEM	2	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.