



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:36 pm BST

PDB ID : 1IO9  
Title : THERMOPHILIC CYTOCHROME P450 (CYP119) FROM SULFOLOBUS SOLFATARICUS: HIGH RESOLUTION STRUCTURAL ORIGIN OF ITS THERMOSTABILITY AND FUNCTIONAL PROPERTIES  
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Deposited on : 2001-02-08  
Resolution : 2.05 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.

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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)
Xtriage (Phenix)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

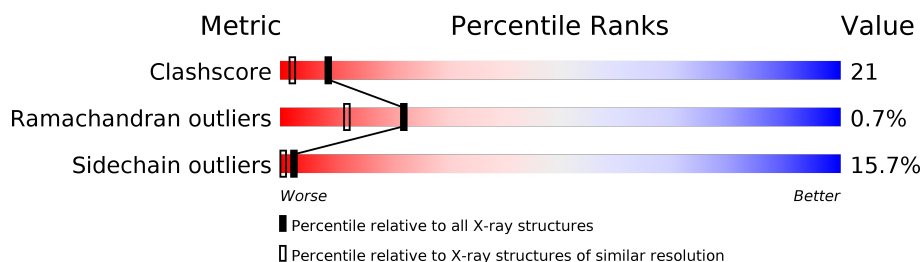
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	368	
1	B	368	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6127 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 CYTOCHROME P450 CYP119.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			3010	1928	517	559	6			
1	B	354	Total	C	N	O	S	0	0	0
			2914	1864	501	543	6			

- 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
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 water.

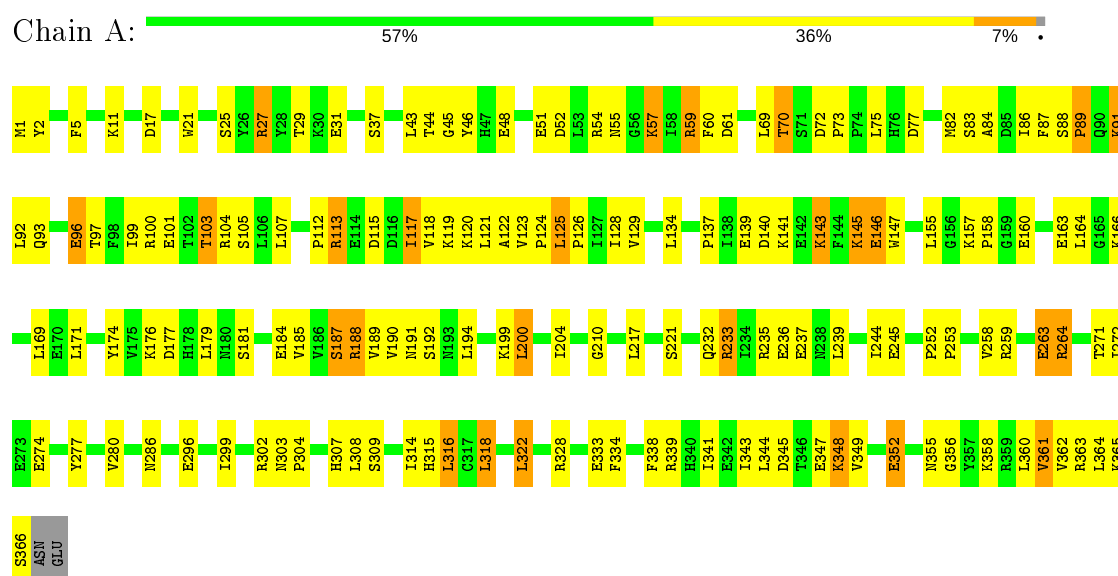
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total 61	O 61	0	0
3	B	56	Total 56	O 56	0	0

### 3 Residue-property plots

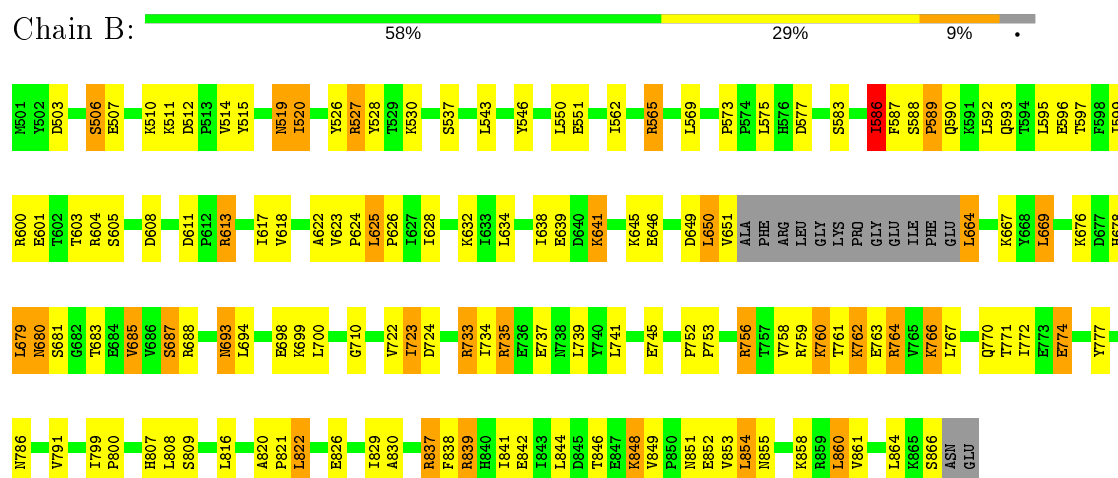
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: CYTOCHROME P450 CYP119



#### • Molecule 1: CYTOCHROME P450 CYP119



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.59 Å 87.59 Å 223.15 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.05	Depositor
% Data completeness (in resolution range)	93.2 (20.00-2.05)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.227 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6127	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	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: 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	0.40	0/3074	0.62	0/4154
1	B	0.40	0/2974	0.62	0/4019
All	All	0.40	0/6048	0.62	0/8173

There are no bond length outliers.

There are no bond angle outliers.

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	3010	0	3041	129	0
1	B	2914	0	2941	120	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
3	A	61	0	0	6	0
3	B	56	0	0	10	0
All	All	6127	0	6042	249	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 21.

All (249) 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:188:ARG:HH11	1:A:188:ARG:HB2	1.17	1.09
1:A:27:ARG:HG2	1:A:27:ARG:HH11	1.07	1.07
1:A:264:ARG:HB2	1:A:264:ARG:HH11	1.18	1.07
1:B:851:ASN:ND2	1:B:854:LEU:H	1.61	0.98
1:B:586:ILE:HG23	3:B:63:HOH:O	1.66	0.94
1:B:693:ASN:HD22	1:B:693:ASN:H	1.03	0.94
1:A:188:ARG:HB2	1:A:188:ARG:NH1	1.84	0.93
1:B:851:ASN:HD22	1:B:854:LEU:H	1.04	0.92
1:B:583:SER:HB2	1:B:586:ILE:HD11	1.51	0.92
1:B:839:ARG:HH21	1:B:866:SER:HB3	1.35	0.89
1:B:764:ARG:HB2	1:B:764:ARG:HH11	1.34	0.88
1:A:25:SER:O	1:A:29:THR:HG23	1.76	0.86
1:B:846:THR:HG23	3:B:58:HOH:O	1.75	0.85
1:A:27:ARG:HG2	1:A:27:ARG:NH1	1.81	0.85
1:B:617:ILE:HD11	1:B:860:LEU:HD13	1.59	0.84
1:B:586:ILE:HG21	1:B:685:VAL:HG22	1.59	0.84
1:B:586:ILE:HD13	1:B:685:VAL:HG13	1.60	0.83
1:B:723:ILE:HD13	1:B:860:LEU:HD11	1.61	0.82
1:A:113:ARG:HB3	1:A:113:ARG:NH1	1.93	0.82
1:B:693:ASN:ND2	1:B:693:ASN:H	1.72	0.82
1:B:735:ARG:HH21	1:B:735:ARG:HB2	1.43	0.81
1:A:344:LEU:HD21	1:A:363:ARG:HB3	1.62	0.81
1:A:113:ARG:CZ	1:A:113:ARG:HB3	2.11	0.80
1:A:88:SER:HB2	1:A:89:PRO:HD2	1.63	0.79
1:A:338:PHE:CE1	1:A:341:ILE:HB	2.18	0.78
1:A:99:ILE:O	1:A:103:THR:HG23	1.82	0.78
1:B:764:ARG:CB	1:B:764:ARG:HH11	1.96	0.78
1:B:839:ARG:HH21	1:B:866:SER:CB	1.96	0.77
1:B:618:VAL:HG23	1:B:860:LEU:HB2	1.67	0.77
1:B:562:ILE:O	1:B:565:ARG:HG3	1.85	0.77
1:A:286:ASN:HD21	1:A:308:LEU:H	1.31	0.76
1:A:83:SER:HB2	1:A:86:ILE:HD13	1.68	0.74
1:B:503:ASP:OD2	1:B:506:SER:HB2	1.88	0.74
1:B:851:ASN:HD22	1:B:854:LEU:N	1.85	0.74
1:B:514:VAL:HG22	1:B:770:GLN:HG3	1.68	0.73
1:A:264:ARG:NH1	1:A:264:ARG:HB2	2.01	0.72
1:B:786:ASN:HD21	1:B:808:LEU:H	1.35	0.71
1:B:680:ASN:H	1:B:680:ASN:HD22	1.39	0.70
1:B:848:LYS:NZ	1:B:855:ASN:HD22	1.89	0.70
1:A:339:ARG:HG3	1:A:366:SER:O	1.91	0.70
1:B:600:ARG:HD3	3:B:43:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:851:ASN:ND2	1:B:853:VAL:H	1.90	0.69
1:A:97:THR:O	1:A:101:GLU:HG3	1.93	0.68
1:A:117:ILE:HD11	1:A:360:LEU:HG	1.75	0.68
1:B:839:ARG:NH2	1:B:866:SER:HB3	2.08	0.67
1:B:613:ARG:HB3	1:B:613:ARG:HH11	1.59	0.67
1:A:88:SER:OG	1:A:91:LYS:HB2	1.94	0.67
1:B:676:LYS:HA	1:B:679:LEU:HD22	1.78	0.66
1:B:820:ALA:HB3	1:B:821:PRO:HD3	1.77	0.66
1:A:307:HIS:HD2	1:A:309:SER:H	1.43	0.65
1:B:807:HIS:HD2	1:B:809:SER:H	1.45	0.64
1:B:507:GLU:O	1:B:511:LYS:HG2	1.97	0.64
1:A:258:VAL:HG22	1:A:259:ARG:N	2.13	0.64
1:B:586:ILE:HG13	1:B:587:PHE:CD1	2.33	0.64
1:A:59:ARG:NH1	1:A:60:PHE:H	1.96	0.63
1:A:29:THR:HB	1:A:280:VAL:HG13	1.80	0.62
1:A:349:VAL:HG22	1:A:356:GLY:O	1.98	0.62
1:B:628:ILE:HG12	1:B:638:ILE:HD11	1.81	0.62
1:B:848:LYS:HZ1	1:B:855:ASN:HD22	1.46	0.62
1:A:59:ARG:H	1:A:59:ARG:NE	1.98	0.61
1:A:59:ARG:HH11	1:A:60:PHE:H	1.49	0.61
1:A:348:LYS:HZ1	1:A:355:ASN:ND2	1.99	0.61
1:A:123:VAL:HB	1:A:124:PRO:HD3	1.83	0.61
1:B:586:ILE:CD1	1:B:685:VAL:HG13	2.30	0.60
1:A:141:LYS:NZ	1:A:145:LYS:NZ	2.50	0.59
1:B:693:ASN:HD22	1:B:693:ASN:N	1.86	0.59
1:A:349:VAL:HG23	3:A:439:HOH:O	2.02	0.58
1:A:86:ILE:HG21	1:A:185:VAL:HG22	1.85	0.58
1:A:100:ARG:HD3	1:A:333:GLU:OE1	2.04	0.58
1:A:299:ILE:HD12	1:A:302:ARG:NH2	2.19	0.58
1:A:72:ASP:HA	3:A:421:HOH:O	2.03	0.57
1:A:140:ASP:OD2	1:A:174:TYR:HE1	1.87	0.57
1:A:88:SER:CB	1:A:89:PRO:HD2	2.33	0.57
1:A:245:GLU:OE2	1:A:307:HIS:HE1	1.87	0.57
1:A:21:TRP:CD1	1:A:272:ILE:HG23	2.41	0.56
1:A:59:ARG:H	1:A:59:ARG:CZ	2.19	0.56
1:B:586:ILE:HG13	1:B:587:PHE:CE1	2.40	0.56
1:B:608:ASP:OD1	1:B:837:ARG:NH2	2.39	0.56
1:A:338:PHE:HB2	1:A:364:LEU:HB3	1.88	0.56
1:B:618:VAL:HA	1:B:622:ALA:HB3	1.88	0.56
1:A:86:ILE:HD11	1:A:87:PHE:CE1	2.41	0.56
1:B:543:LEU:CD2	1:B:760:LYS:HB2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HA	1:A:122:ALA:HB3	1.89	0.55
1:A:339:ARG:HG3	1:A:366:SER:C	2.26	0.55
1:B:733:ARG:HD3	1:B:737:GLU:OE2	2.06	0.55
1:A:176:LYS:HA	1:A:179:LEU:CD1	2.37	0.55
1:A:143:LYS:HA	1:A:146:GLU:OE2	2.06	0.55
1:A:104:ARG:HA	1:A:107:LEU:HD12	1.89	0.55
1:A:345:ASP:HB3	1:A:361:VAL:CG2	2.36	0.55
1:B:519:ASN:H	1:B:519:ASN:ND2	2.05	0.55
1:B:745:GLU:OE2	1:B:807:HIS:HE1	1.90	0.54
1:A:264:ARG:HH11	1:A:264:ARG:CB	2.05	0.54
1:B:600:ARG:HG2	1:B:604:ARG:NH1	2.21	0.54
1:A:125:LEU:O	1:A:129:VAL:HG23	2.07	0.54
1:A:176:LYS:HA	1:A:179:LEU:HD11	1.88	0.54
1:B:597:THR:O	1:B:601:GLU:HG3	2.06	0.54
1:B:678:HIS:HD2	3:B:39:HOH:O	1.91	0.54
1:A:190:VAL:O	1:A:199:LYS:HE2	2.08	0.54
1:A:100:ARG:NE	3:A:419:HOH:O	2.26	0.54
1:B:822:LEU:O	1:B:826:GLU:HG3	2.08	0.54
1:A:348:LYS:HZ1	1:A:355:ASN:HD22	1.56	0.53
1:A:176:LYS:O	1:A:179:LEU:HD12	2.08	0.53
1:A:45:GLY:HA2	3:A:442:HOH:O	2.07	0.53
1:A:54:ARG:NH2	1:A:194:LEU:HD23	2.22	0.53
1:B:611:ASP:OD1	1:B:613:ARG:HG3	2.08	0.53
1:A:349:VAL:HG22	1:A:356:GLY:C	2.28	0.53
1:A:141:LYS:NZ	1:A:145:LYS:HZ3	2.06	0.53
1:A:263:GLU:HA	1:A:274:GLU:CG	2.39	0.53
1:B:735:ARG:CB	1:B:735:ARG:HH21	2.16	0.53
1:A:187:SER:O	1:A:191:ASN:ND2	2.42	0.53
1:B:519:ASN:H	1:B:519:ASN:HD22	1.57	0.53
1:B:639:GLU:CD	1:B:639:GLU:H	2.11	0.53
1:A:160:GLU:HG2	1:A:164:LEU:HG	1.91	0.52
1:B:664:LEU:HD21	1:B:669:LEU:HD22	1.92	0.52
1:B:723:ILE:CD1	1:B:860:LEU:HD11	2.37	0.51
1:B:758:VAL:HG22	1:B:759:ARG:N	2.25	0.51
1:A:82:MET:HE1	1:A:192:SER:HB3	1.93	0.51
1:B:600:ARG:NH1	3:B:43:HOH:O	2.43	0.51
1:A:99:ILE:O	1:A:103:THR:CG2	2.57	0.50
1:A:82:MET:HE1	1:A:189:VAL:HA	1.93	0.50
1:A:233:ARG:HD3	1:A:237:GLU:CD	2.31	0.50
1:B:512:ASP:HB3	1:B:515:TYR:HB2	1.92	0.50
1:A:82:MET:CE	1:A:189:VAL:HA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:848:LYS:NZ	1:B:855:ASN:ND2	2.58	0.50
1:B:526:TYR:CD2	1:B:791:VAL:HG21	2.47	0.50
1:A:263:GLU:HA	1:A:274:GLU:OE1	2.12	0.49
1:A:258:VAL:CG2	1:A:259:ARG:N	2.75	0.49
1:A:83:SER:HB2	1:A:86:ILE:CD1	2.40	0.49
1:A:244:ILE:CD1	1:A:328:ARG:HA	2.42	0.49
1:A:73:PRO:HB3	1:A:77:ASP:OD1	2.12	0.49
1:A:263:GLU:HA	1:A:274:GLU:CD	2.33	0.49
1:A:115:ASP:O	1:A:361:VAL:HA	2.13	0.49
1:B:676:LYS:HA	1:B:679:LEU:CD2	2.41	0.48
1:A:89:PRO:HA	3:A:454:HOH:O	2.13	0.48
1:B:764:ARG:HA	1:B:772:ILE:O	2.12	0.48
1:B:596:GLU:HB3	1:B:600:ARG:HH22	1.79	0.48
1:B:573:PRO:HB3	1:B:577:ASP:OD1	2.13	0.48
1:A:210:GLY:HA3	2:A:401:HEM:C2C	2.49	0.48
1:B:837:ARG:CG	1:B:837:ARG:HH11	2.26	0.48
1:B:613:ARG:HB3	1:B:613:ARG:NH1	2.27	0.48
1:B:512:ASP:CB	1:B:515:TYR:HB2	2.44	0.48
1:B:723:ILE:HG22	1:B:724:ASP:N	2.28	0.48
1:B:694:LEU:O	1:B:699:LYS:HE3	2.14	0.47
1:B:638:ILE:O	1:B:641:LYS:HG2	2.15	0.47
1:B:645:LYS:HE3	1:B:649:ASP:OD2	2.14	0.47
1:A:83:SER:O	1:A:86:ILE:HG12	2.14	0.47
1:B:623:VAL:HB	1:B:624:PRO:HD3	1.95	0.47
1:B:537:SER:O	1:B:762:LYS:HD2	2.14	0.47
1:B:723:ILE:HD11	1:B:860:LEU:HD21	1.97	0.47
1:B:851:ASN:HD22	1:B:853:VAL:H	1.61	0.47
1:A:334:PHE:CD1	1:A:338:PHE:CE2	3.02	0.47
1:A:137:PRO:HD2	1:A:174:TYR:OH	2.15	0.47
1:A:21:TRP:NE1	1:A:272:ILE:HG23	2.30	0.47
1:A:303:ASN:HA	1:A:304:PRO:C	2.35	0.46
1:A:51:GLU:O	1:A:55:ASN:HB2	2.14	0.46
1:B:650:LEU:HD11	1:B:667:LYS:HB3	1.96	0.46
1:A:86:ILE:CG2	1:A:185:VAL:HG22	2.45	0.46
1:A:93:GLN:O	1:A:96:GLU:HB2	2.15	0.46
1:B:587:PHE:HA	1:B:592:LEU:HD21	1.98	0.46
1:B:844:LEU:HD12	1:B:861:VAL:HG12	1.96	0.46
1:A:315:HIS:O	1:A:316:LEU:C	2.53	0.46
1:B:519:ASN:HD22	1:B:519:ASN:N	2.14	0.46
1:A:123:VAL:CB	1:A:124:PRO:HD3	2.45	0.46
1:A:217:LEU:HD22	2:A:401:HEM:HBB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:HD22	1:A:277:TYR:HE1	1.80	0.46
1:A:44:THR:HG23	1:A:70:THR:HG21	1.98	0.46
1:A:244:ILE:HD11	1:A:328:ARG:HA	1.98	0.46
1:A:339:ARG:NE	1:A:366:SER:O	2.49	0.46
1:B:600:ARG:HB2	1:B:600:ARG:CZ	2.46	0.46
1:A:118:VAL:HG23	1:A:360:LEU:HB3	1.97	0.46
1:A:125:LEU:HB3	1:A:126:PRO:HD3	1.96	0.45
1:A:200:LEU:O	1:A:204:ILE:HG13	2.16	0.45
1:A:100:ARG:CZ	1:A:100:ARG:HB2	2.47	0.45
1:A:140:ASP:OD2	1:A:174:TYR:CE1	2.68	0.45
1:B:510:LYS:HB3	1:B:511:LYS:HE2	1.98	0.45
1:B:588:SER:HB2	1:B:589:PRO:CD	2.47	0.45
1:B:527:ARG:NH2	1:B:528:TYR:CE2	2.85	0.45
1:B:617:ILE:CD1	1:B:722:VAL:HG11	2.47	0.45
1:B:763:GLU:HA	1:B:774:GLU:HB2	1.99	0.45
1:A:314:ILE:HG13	1:A:315:HIS:CD2	2.52	0.45
1:B:603:THR:HG21	1:B:830:ALA:HA	1.99	0.45
1:B:589:PRO:CA	3:B:62:HOH:O	2.64	0.45
1:B:625:LEU:HB3	1:B:626:PRO:HD3	1.98	0.45
1:A:59:ARG:NH1	1:A:60:PHE:O	2.50	0.44
1:B:618:VAL:CG2	1:B:860:LEU:HB2	2.42	0.44
1:B:683:THR:O	1:B:687:SER:HB2	2.18	0.44
1:A:87:PHE:CE1	1:A:318:LEU:HD13	2.53	0.44
1:A:343:ILE:HD13	1:A:362:VAL:HG12	1.99	0.44
1:B:741:LEU:HD23	3:B:83:HOH:O	2.18	0.44
1:A:141:LYS:HZ3	1:A:145:LYS:HZ2	1.65	0.44
1:A:252:PRO:HA	1:A:253:PRO:HD3	1.86	0.44
1:A:348:LYS:NZ	1:A:355:ASN:ND2	2.65	0.44
1:A:52:ASP:HB3	1:A:57:LYS:HB2	2.00	0.44
1:B:766:LYS:HG3	1:B:771:THR:OG1	2.17	0.44
1:B:543:LEU:HD23	1:B:760:LYS:HB2	2.00	0.44
1:B:838:PHE:CE1	1:B:841:ILE:HB	2.52	0.43
1:B:589:PRO:HA	3:B:62:HOH:O	2.19	0.43
1:B:651:VAL:O	1:B:651:VAL:HG12	2.19	0.43
1:A:118:VAL:HG23	1:A:360:LEU:CB	2.48	0.43
1:A:147:TRP:CE3	1:A:171:LEU:HD13	2.54	0.43
1:B:756:ARG:NH2	1:B:852:GLU:HB3	2.33	0.43
1:A:352:GLU:OE1	1:A:352:GLU:N	2.52	0.43
1:B:752:PRO:HA	1:B:753:PRO:HD3	1.89	0.43
1:B:710:GLY:HA3	2:B:901:HEM:C2C	2.54	0.43
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:ASN:N	1:B:693:ASN:ND2	2.48	0.42
1:A:163:GLU:HG2	3:A:441:HOH:O	2.20	0.42
1:B:837:ARG:CG	1:B:837:ARG:NH1	2.82	0.42
1:B:526:TYR:CG	1:B:791:VAL:HG21	2.55	0.42
1:A:92:LEU:HD13	1:A:322:LEU:HD23	2.01	0.42
1:B:737:GLU:HB3	1:B:739:LEU:HG	2.02	0.42
1:A:115:ASP:OD2	1:A:120:LYS:NZ	2.52	0.42
1:B:519:ASN:ND2	1:B:519:ASN:N	2.66	0.42
1:A:123:VAL:CG1	1:A:145:LYS:HD2	2.50	0.42
1:B:520:ILE:HG22	1:B:777:TYR:HB2	2.01	0.42
1:A:27:ARG:CG	1:A:27:ARG:HH11	1.96	0.42
1:A:27:ARG:CG	1:A:27:ARG:NH1	2.62	0.42
1:A:103:THR:O	1:A:107:LEU:HG	2.19	0.41
1:B:799:ILE:HA	1:B:800:PRO:HD2	1.83	0.41
1:B:650:LEU:HD11	1:B:667:LYS:CB	2.51	0.41
1:A:345:ASP:HB3	1:A:361:VAL:HG23	2.03	0.41
1:A:347:GLU:O	1:A:358:LYS:N	2.39	0.41
1:A:237:GLU:OE2	1:A:239:LEU:HD11	2.20	0.41
1:A:348:LYS:NZ	1:A:355:ASN:HD22	2.18	0.41
1:B:562:ILE:HB	1:B:565:ARG:CG	2.51	0.41
1:B:588:SER:CB	1:B:589:PRO:CD	2.98	0.41
1:A:124:PRO:O	1:A:128:ILE:HD12	2.19	0.41
1:A:232:GLN:HG2	1:A:236:GLU:OE1	2.19	0.41
1:B:664:LEU:HD21	1:B:669:LEU:CD2	2.50	0.41
1:B:733:ARG:O	1:B:737:GLU:HB2	2.20	0.41
1:A:339:ARG:CZ	1:A:366:SER:O	2.68	0.41
1:B:600:ARG:NH1	1:B:829:ILE:HG12	2.36	0.41
1:A:112:PRO:O	1:A:113:ARG:C	2.59	0.41
1:A:2:TYR:HA	1:A:5:PHE:CD2	2.56	0.41
1:B:595:LEU:O	1:B:599:ILE:HG13	2.20	0.41
1:B:618:VAL:HG23	1:B:860:LEU:CB	2.45	0.41
1:A:179:LEU:O	1:A:190:VAL:HG21	2.21	0.40
1:B:589:PRO:N	3:B:62:HOH:O	2.53	0.40
1:A:117:ILE:HG13	1:A:360:LEU:HB3	2.03	0.40
1:A:87:PHE:HD1	1:A:318:LEU:HD22	1.86	0.40
1:B:597:THR:HB	3:B:112:HOH:O	2.20	0.40
1:B:734:ILE:HA	1:B:739:LEU:HB2	2.02	0.40
1:A:334:PHE:O	1:A:338:PHE:HD2	2.04	0.40
1:A:345:ASP:HB3	1:A:361:VAL:HG21	2.03	0.40
1:B:600:ARG:NH1	1:B:600:ARG:HB2	2.36	0.40
1:A:60:PHE:CG	1:A:61:ASP:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:VAL:CG2	1:B:759:ARG:N	2.85	0.40
1:B:767:LEU:N	1:B:770:GLN:O	2.54	0.40
1:B:694:LEU:HD13	1:B:698:GLU:HB3	2.04	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	364/368 (99%)	336 (92%)	25 (7%)	3 (1%)	19	10
1	B	350/368 (95%)	328 (94%)	20 (6%)	2 (1%)	25	15
All	All	714/736 (97%)	664 (93%)	45 (6%)	5 (1%)	22	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ALA
1	A	89	PRO
1	A	158	PRO
1	B	586	ILE
1	B	589	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	336/338 (99%)	285 (85%)	51 (15%)	3	0
1	B	327/338 (97%)	274 (84%)	53 (16%)	2	0
All	All	663/676 (98%)	559 (84%)	104 (16%)	2	0

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	LYS
1	A	17	ASP
1	A	27	ARG
1	A	31	GLU
1	A	37	SER
1	A	46	TYR
1	A	48	GLU
1	A	57	LYS
1	A	59	ARG
1	A	69	LEU
1	A	70	THR
1	A	75	LEU
1	A	91	LYS
1	A	96	GLU
1	A	103	THR
1	A	105	SER
1	A	113	ARG
1	A	117	ILE
1	A	119	LYS
1	A	121	LEU
1	A	125	LEU
1	A	134	LEU
1	A	139	GLU
1	A	143	LYS
1	A	145	LYS
1	A	146	GLU
1	A	155	LEU
1	A	157	LYS
1	A	166	LYS
1	A	169	LEU
1	A	177	ASP
1	A	181	SER
1	A	184	GLU
1	A	187	SER

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Mol	Chain	Res	Type
1	A	188	ARG
1	A	200	LEU
1	A	221	SER
1	A	233	ARG
1	A	235	ARG
1	A	263	GLU
1	A	264	ARG
1	A	271	THR
1	A	296	GLU
1	A	316	LEU
1	A	318	LEU
1	A	322	LEU
1	A	348	LYS
1	A	352	GLU
1	A	361	VAL
1	A	365	LYS
1	B	506	SER
1	B	519	ASN
1	B	520	ILE
1	B	527	ARG
1	B	530	LYS
1	B	546	TYR
1	B	550	LEU
1	B	551	GLU
1	B	565	ARG
1	B	569	LEU
1	B	575	LEU
1	B	586	ILE
1	B	590	GLN
1	B	593	GLN
1	B	605	SER
1	B	613	ARG
1	B	625	LEU
1	B	632	LYS
1	B	634	LEU
1	B	641	LYS
1	B	646	GLU
1	B	650	LEU
1	B	664	LEU
1	B	669	LEU
1	B	679	LEU
1	B	680	ASN

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Mol	Chain	Res	Type
1	B	681	SER
1	B	685	VAL
1	B	687	SER
1	B	688	ARG
1	B	693	ASN
1	B	700	LEU
1	B	723	ILE
1	B	733	ARG
1	B	735	ARG
1	B	756	ARG
1	B	760	LYS
1	B	761	THR
1	B	762	LYS
1	B	764	ARG
1	B	766	LYS
1	B	774	GLU
1	B	816	LEU
1	B	822	LEU
1	B	837	ARG
1	B	839	ARG
1	B	842	GLU
1	B	848	LYS
1	B	849	VAL
1	B	854	LEU
1	B	858	LYS
1	B	860	LEU
1	B	864	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	232	GLN
1	A	238	ASN
1	A	286	ASN
1	A	307	HIS
1	A	355	ASN
1	B	519	ASN
1	B	693	ASN
1	B	729	ASN
1	B	786	ASN
1	B	803	ASN

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Mol	Chain	Res	Type
1	B	807	HIS
1	B	851	ASN
1	B	855	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	401	1,3	27,50,50	1.83	8 (29%)	17,82,82	1.81	3 (17%)
2	HEM	B	901	1,3	27,50,50	1.75	5 (18%)	17,82,82	1.55	3 (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	401	1,3	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	901	1,3	-	0/6/54/54	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	HEM	C3B-CAB	-4.76	1.38	1.47
2	A	401	HEM	C3C-CAC	-4.02	1.39	1.47
2	A	401	HEM	C3B-CAB	-3.74	1.40	1.47
2	B	901	HEM	C3C-CAC	-3.35	1.40	1.47
2	B	901	HEM	C1B-C2B	2.99	1.49	1.42
2	B	901	HEM	C1D-ND	2.97	1.42	1.36
2	A	401	HEM	C3B-C2B	-2.71	1.36	1.40
2	A	401	HEM	C4A-NA	2.70	1.41	1.36
2	A	401	HEM	C1C-C2C	2.46	1.48	1.42
2	B	901	HEM	C4A-NA	2.40	1.41	1.36
2	A	401	HEM	C4A-CHB	-2.17	1.35	1.41
2	A	401	HEM	C4D-C3D	2.14	1.47	1.42
2	A	401	HEM	C3C-C2C	-2.08	1.37	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	C4A-C3A-C2A	-5.40	103.24	107.00
2	B	901	HEM	CBD-CAD-C3D	-3.74	105.59	112.48
2	A	401	HEM	C1D-C2D-C3D	-3.11	104.83	107.00
2	B	901	HEM	C4C-C3C-C2C	-2.74	104.98	106.90
2	B	901	HEM	C1D-C2D-C3D	-2.72	105.10	107.00
2	A	401	HEM	CMD-C2D-C3D	2.33	129.34	124.94

There are no chirality outliers.

There are no torsion outliers.

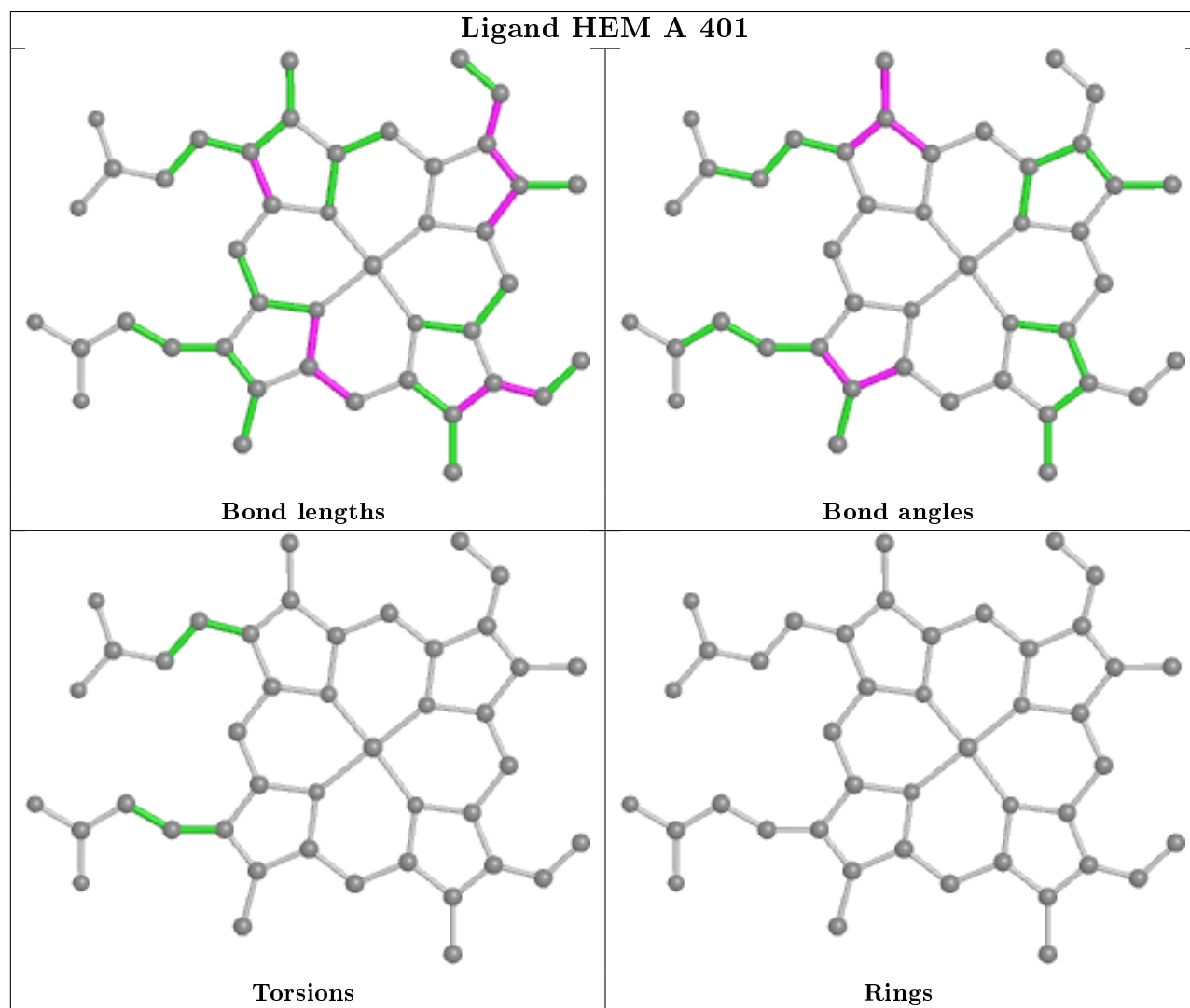
There are no ring outliers.

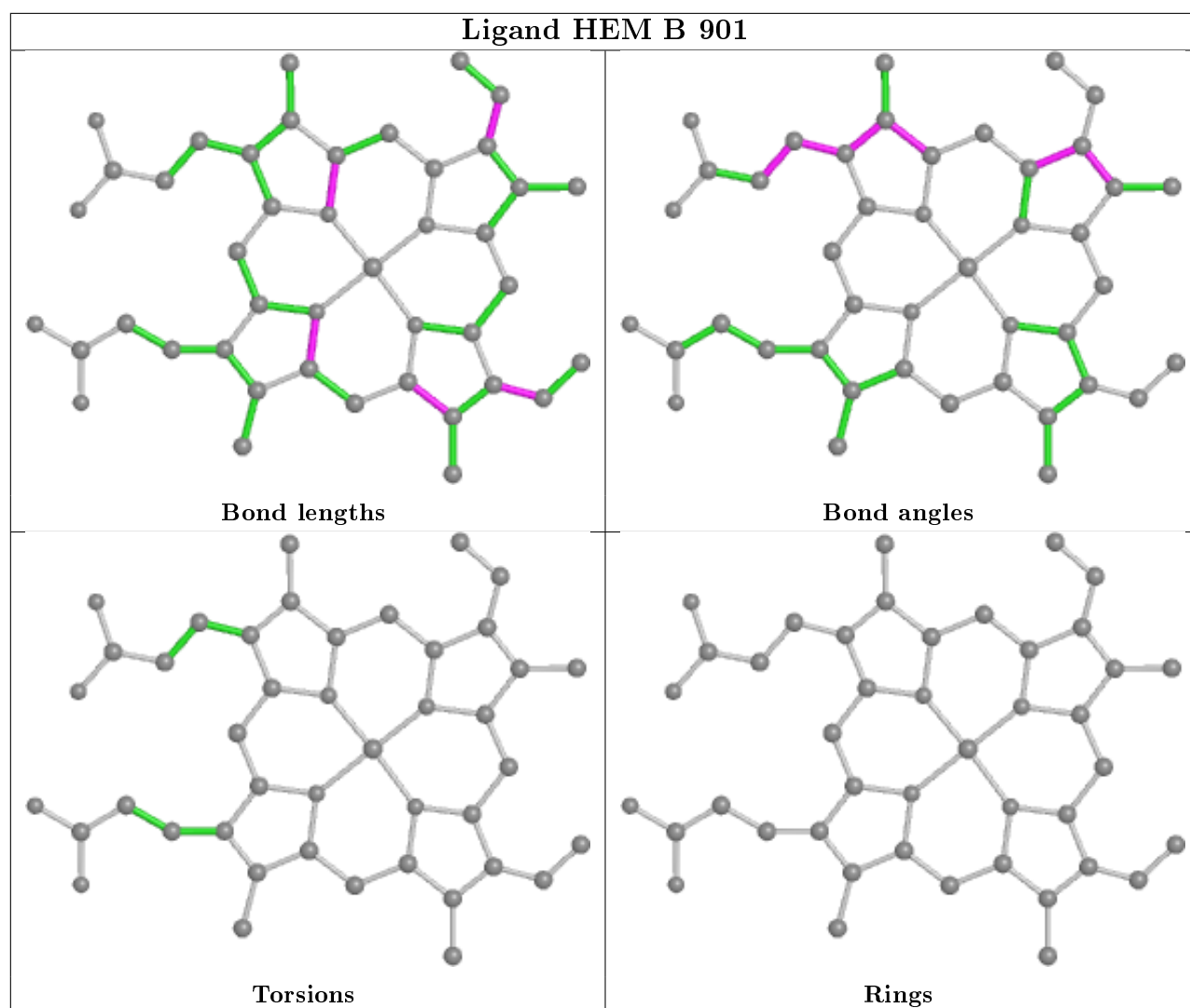
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	2	0
2	B	901	HEM	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 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.