



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2023 – 06:19 AM EST

PDB ID : 1I07
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 : 1.50 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 : 4.02b-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

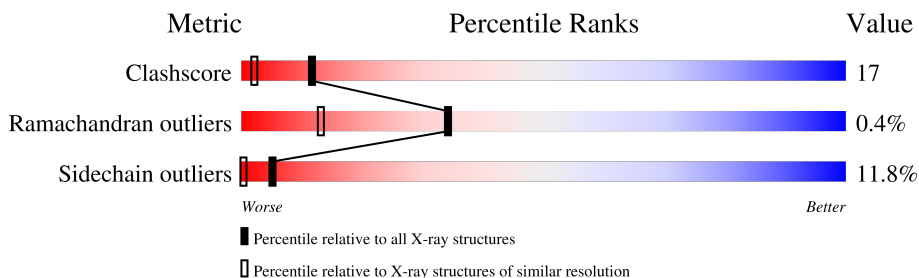
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	368	 64% 30% 5% •
1	B	368	 65% 26% 6% •

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	219	Total 219	O 219	0	0
3	B	257	Total 257	O 257	0	0

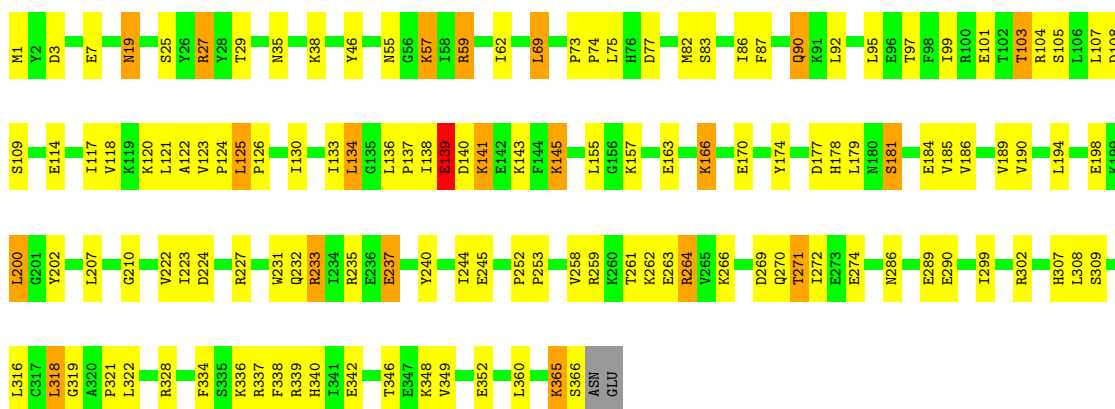
3 Residue-property plots [i](#)

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.

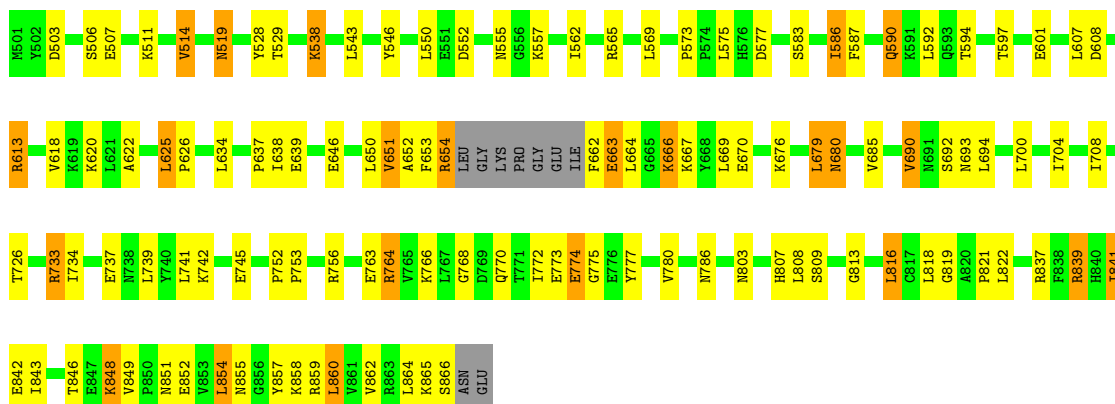
- Molecule 1: CYTOCHROME P450 CYP119

Chain A:  64% 30% 5%



- Molecule 1: CYTOCHROME P450 CYP119

Chain B:  65% 26% 6%



4 Data and refinement statistics

Xtrriage (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, α , β , γ	86.19Å 86.19Å 221.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 1.50	Depositor
% Data completeness (in resolution range)	91.2 (80.00-1.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.224 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6533	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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	0.61	0/4154
1	B	0.42	0/3023	0.65	0/4084
All	All	0.41	0/6097	0.63	0/8238

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	98	0
1	B	2961	0	2983	114	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
3	A	219	0	0	13	0
3	B	257	0	0	9	0
All	All	6533	0	6084	212	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 17.

All (212) 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:652:ALA:HB3	1:B:654:ARG:HH21	1.21	1.04
1:B:586:ILE:HG23	1:B:685:VAL:HG21	1.39	1.04
1:A:264:ARG:HB2	1:A:264:ARG:HH11	1.25	1.01
1:A:59:ARG:NE	1:A:59:ARG:H	1.63	0.96
1:B:851:ASN:HD22	1:B:854:LEU:H	1.08	0.95
1:B:764:ARG:HH11	1:B:764:ARG:CB	1.83	0.92
1:B:851:ASN:ND2	1:B:854:LEU:H	1.68	0.91
1:A:27:ARG:HG2	1:A:27:ARG:HH11	1.35	0.91
1:B:763:GLU:HA	1:B:774:GLU:HB2	1.49	0.90
1:A:266:LYS:HE3	1:A:271:THR:HG23	1.55	0.88
1:B:586:ILE:HD11	1:B:818:LEU:HD21	1.54	0.87
1:B:786:ASN:HD21	1:B:808:LEU:H	1.20	0.86
1:B:839:ARG:HB2	1:B:866:SER:HA	1.57	0.86
1:A:286:ASN:HD21	1:A:308:LEU:H	1.24	0.86
1:A:141:LYS:HZ1	1:A:145:LYS:HZ2	1.27	0.81
1:B:654:ARG:HB3	1:B:654:ARG:CZ	2.10	0.80
1:A:109:SER:OG	1:A:120:LYS:HD2	1.82	0.80
1:A:264:ARG:HH11	1:A:264:ARG:CB	1.94	0.79
1:B:583:SER:O	1:B:586:ILE:HG12	1.81	0.79
1:A:263:GLU:HA	1:A:274:GLU:HG3	1.64	0.79
1:B:652:ALA:HB3	1:B:654:ARG:NH2	1.96	0.78
1:B:680:ASN:H	1:B:680:ASN:HD22	1.28	0.78
1:B:586:ILE:CG2	1:B:685:VAL:HG21	2.12	0.78
1:A:223:ILE:HD11	1:A:360:LEU:HD11	1.64	0.77
1:B:652:ALA:CB	1:B:654:ARG:HH21	1.95	0.77
1:B:590:GLN:H	1:B:590:GLN:HE21	1.30	0.77
1:A:27:ARG:HG2	1:A:27:ARG:NH1	1.98	0.76
1:B:552:ASP:HA	1:B:555:ASN:HB2	1.67	0.76
1:B:846:THR:HG23	3:B:140:HOH:O	1.85	0.76
1:B:586:ILE:HD12	1:B:587:PHE:CE1	2.20	0.76
1:A:349:VAL:HG23	3:A:1461:HOH:O	1.86	0.76
1:B:586:ILE:HD11	1:B:818:LEU:CD2	2.15	0.76
1:B:763:GLU:CA	1:B:774:GLU:HB2	2.17	0.75
1:B:638:ILE:HD12	3:B:430:HOH:O	1.85	0.75
1:B:764:ARG:HH11	1:B:764:ARG:CG	2.01	0.74
1:B:597:THR:O	1:B:601:GLU:HG3	1.87	0.74
1:A:263:GLU:HA	1:A:274:GLU:CG	2.19	0.72
1:B:756:ARG:HH21	1:B:852:GLU:HB3	1.54	0.72
1:B:590:GLN:H	1:B:590:GLN:NE2	1.87	0.71
1:A:141:LYS:HZ1	1:A:145:LYS:NZ	1.89	0.69
1:A:163:GLU:HG2	3:A:1444:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:THR:HG22	1:A:360:LEU:HD12	1.73	0.69
1:B:733:ARG:HD3	1:B:737:GLU:OE2	1.93	0.69
1:A:82:MET:CE	1:A:189:VAL:HA	2.23	0.68
1:B:756:ARG:NH2	1:B:852:GLU:HB3	2.08	0.68
1:B:764:ARG:HH11	1:B:764:ARG:HB2	1.56	0.67
1:A:289:GLU:H	1:A:289:GLU:CD	1.98	0.67
1:A:97:THR:O	1:A:101:GLU:HG3	1.95	0.67
1:B:745:GLU:OE2	1:B:807:HIS:HE1	1.78	0.67
1:B:543:LEU:HD22	1:B:777:TYR:HE2	1.60	0.67
1:A:299:ILE:HD12	1:A:302:ARG:NH2	2.09	0.66
1:A:108:ASP:HA	1:A:337:ARG:HH22	1.60	0.66
1:B:807:HIS:HD2	1:B:809:SER:H	1.43	0.65
1:B:590:GLN:O	1:B:594:THR:HG23	1.98	0.64
1:B:733:ARG:HD3	1:B:737:GLU:CD	2.18	0.64
1:A:108:ASP:HA	1:A:337:ARG:NH2	2.13	0.63
1:A:141:LYS:NZ	1:A:145:LYS:NZ	2.47	0.63
1:B:662:PHE:CD2	1:B:663:GLU:N	2.65	0.63
1:B:666:LYS:O	1:B:670:GLU:HG3	2.00	0.62
1:A:25:SER:O	1:A:29:THR:HG23	2.00	0.61
1:A:136:LEU:HD12	1:A:207:LEU:HD13	1.82	0.61
1:A:99:ILE:O	1:A:103:THR:HG23	1.99	0.61
1:A:166:LYS:O	1:A:170:GLU:HG3	2.00	0.61
1:B:651:VAL:HG12	1:B:651:VAL:O	2.00	0.61
1:B:662:PHE:CG	1:B:663:GLU:N	2.69	0.61
1:B:851:ASN:HD22	1:B:854:LEU:N	1.89	0.61
1:B:680:ASN:HD22	1:B:680:ASN:N	1.93	0.60
1:A:263:GLU:HA	1:A:274:GLU:OE1	2.02	0.60
1:B:519:ASN:HD22	1:B:519:ASN:N	1.99	0.60
1:A:263:GLU:HA	1:A:274:GLU:CD	2.21	0.60
1:A:307:HIS:HD2	1:A:309:SER:H	1.50	0.60
1:B:704:ILE:HG23	1:B:708:ILE:HD12	1.84	0.59
1:B:639:GLU:H	1:B:639:GLU:CD	2.04	0.59
1:B:586:ILE:HG23	1:B:685:VAL:CG2	2.26	0.59
1:B:741:LEU:HD21	3:B:412:HOH:O	2.02	0.59
1:B:654:ARG:HB3	1:B:654:ARG:NH1	2.18	0.59
1:B:514:VAL:HG22	1:B:770:GLN:HG3	1.85	0.59
1:B:839:ARG:HH21	1:B:866:SER:HB3	1.67	0.58
1:A:107:LEU:HD13	1:A:337:ARG:HG3	1.84	0.58
1:B:529:THR:HG23	1:B:780:VAL:HB	1.85	0.58
1:B:608:ASP:OD1	1:B:837:ARG:NH2	2.37	0.58
1:B:680:ASN:H	1:B:680:ASN:ND2	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HD13	3:A:1494:HOH:O	2.04	0.57
1:A:1:MET:HA	3:B:15:HOH:O	2.03	0.57
1:A:179:LEU:HD22	1:A:190:VAL:HG22	1.84	0.57
1:A:245:GLU:OE2	1:A:307:HIS:HE1	1.86	0.57
1:A:349:VAL:HG21	3:A:1553:HOH:O	2.04	0.57
1:A:186:VAL:HG22	3:A:1497:HOH:O	2.05	0.57
1:A:263:GLU:CA	1:A:274:GLU:HG3	2.35	0.56
1:B:573:PRO:HB3	1:B:577:ASP:OD1	2.05	0.56
1:B:538:LYS:HE3	1:B:763:GLU:OE2	2.06	0.56
1:A:86:ILE:HD11	1:A:318:LEU:HD13	1.87	0.56
1:A:59:ARG:NE	1:A:59:ARG:N	2.44	0.55
1:B:646:GLU:OE2	1:B:667:LYS:HD3	2.06	0.55
1:B:764:ARG:HB2	1:B:764:ARG:NH1	2.21	0.55
1:B:839:ARG:CB	1:B:866:SER:HA	2.34	0.55
1:A:130:ILE:HG13	1:A:134:LEU:HD22	1.89	0.55
1:B:841:ILE:HD12	1:B:864:LEU:CD2	2.37	0.54
1:A:235:ARG:HG2	1:A:240:TYR:OH	2.07	0.53
1:A:124:PRO:HB3	1:A:141:LYS:HE2	1.90	0.53
1:B:519:ASN:N	1:B:519:ASN:ND2	2.56	0.52
1:B:839:ARG:NH2	1:B:866:SER:HB3	2.24	0.52
1:A:123:VAL:HB	1:A:124:PRO:HD3	1.91	0.52
1:B:653:PHE:CD1	1:B:653:PHE:N	2.77	0.52
1:A:74:PRO:HD2	3:A:1467:HOH:O	2.10	0.52
1:B:726:THR:HG21	1:B:843:ILE:HG12	1.92	0.51
1:A:59:ARG:H	1:A:59:ARG:CD	2.23	0.51
1:B:734:ILE:HA	1:B:739:LEU:HB2	1.92	0.51
1:B:841:ILE:HG13	1:B:842:GLU:N	2.27	0.50
1:A:185:VAL:HG13	3:A:1582:HOH:O	2.11	0.50
1:A:258:VAL:HG22	1:A:259:ARG:N	2.26	0.50
1:A:118:VAL:HG23	1:A:360:LEU:HB2	1.94	0.50
1:B:858:LYS:HD2	1:B:859:ARG:HG3	1.94	0.50
1:B:503:ASP:OD2	1:B:506:SER:HB2	2.12	0.50
1:B:843:ILE:HD12	1:B:860:LEU:HD21	1.93	0.49
1:A:69:LEU:HD21	2:A:1401:HEM:HBA1	1.94	0.49
1:A:244:ILE:CD1	1:A:328:ARG:HA	2.43	0.49
1:A:334:PHE:CD1	1:A:338:PHE:HE2	2.31	0.49
1:B:849:VAL:HG13	1:B:849:VAL:O	2.12	0.49
1:A:83:SER:O	1:A:86:ILE:HG12	2.12	0.49
1:A:224:ASP:OD2	1:A:227:ARG:NH2	2.44	0.49
1:B:786:ASN:ND2	1:B:808:LEU:H	1.99	0.49
1:A:178:HIS:HB3	3:A:1573:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:ARG:HH11	1:B:613:ARG:HB3	1.78	0.49
1:A:125:LEU:HB3	1:A:126:PRO:HD3	1.96	0.48
1:A:194:LEU:HD13	1:A:198:GLU:HB3	1.96	0.48
1:A:233:ARG:O	1:A:237:GLU:HG2	2.13	0.48
1:A:62:ILE:HD12	1:A:62:ILE:N	2.29	0.48
1:A:264:ARG:HH11	1:A:264:ARG:CG	2.26	0.48
1:B:848:LYS:NZ	1:B:855:ASN:HD22	2.12	0.47
1:A:35:ASN:HB2	3:A:1509:HOH:O	2.13	0.47
1:A:232:GLN:HB3	3:A:1453:HOH:O	2.13	0.47
1:B:625:LEU:HB3	1:B:626:PRO:HD3	1.94	0.47
1:A:184:GLU:HG3	1:A:185:VAL:N	2.29	0.47
1:B:590:GLN:HE21	1:B:590:GLN:N	2.07	0.47
1:B:543:LEU:HD22	1:B:777:TYR:CE2	2.46	0.47
1:B:590:GLN:NE2	1:B:590:GLN:N	2.60	0.47
1:A:19:ASN:N	1:A:19:ASN:OD1	2.46	0.47
1:A:179:LEU:HD22	1:A:190:VAL:CG2	2.45	0.47
1:B:613:ARG:HH11	1:B:613:ARG:CB	2.27	0.47
1:A:181:SER:HA	3:A:1605:HOH:O	2.15	0.47
1:B:601:GLU:HG2	3:B:352:HOH:O	2.15	0.47
1:A:118:VAL:HA	1:A:122:ALA:HB3	1.97	0.47
1:A:86:ILE:HD12	1:A:87:PHE:CZ	2.50	0.46
1:B:652:ALA:HB3	1:B:654:ARG:HE	1.81	0.46
1:A:73:PRO:HB3	1:A:77:ASP:OD1	2.16	0.46
1:A:138:ILE:C	1:A:140:ASP:H	2.19	0.46
1:A:137:PRO:HD2	1:A:174:TYR:OH	2.15	0.46
1:A:262:LYS:O	1:A:263:GLU:HB3	2.16	0.46
1:A:90:GLN:H	1:A:90:GLN:HG2	1.47	0.46
1:A:95:LEU:HD11	1:A:133:ILE:HD11	1.97	0.46
1:B:586:ILE:HD12	1:B:587:PHE:CZ	2.51	0.46
1:A:286:ASN:ND2	1:A:308:LEU:H	2.04	0.45
1:A:3:ASP:O	1:A:7:GLU:HG2	2.16	0.45
1:B:618:VAL:HA	1:B:622:ALA:HB3	1.99	0.45
1:B:733:ARG:HD3	1:B:737:GLU:OE1	2.17	0.45
1:B:764:ARG:HH11	1:B:764:ARG:HG2	1.80	0.45
1:B:846:THR:OG1	1:B:857:TYR:CD2	2.70	0.45
1:B:764:ARG:CG	1:B:764:ARG:NH1	2.68	0.45
1:A:339:ARG:HG3	1:A:365:LYS:O	2.17	0.45
1:B:637:PRO:HG2	3:B:469:HOH:O	2.17	0.44
1:A:258:VAL:CG2	1:A:259:ARG:N	2.80	0.44
1:B:848:LYS:NZ	1:B:855:ASN:ND2	2.65	0.44
1:A:231:TRP:HB2	3:A:1563:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:843:ILE:HD13	1:B:862:VAL:HG12	1.99	0.44
1:A:55:ASN:HB3	1:A:57:LYS:HG2	1.99	0.44
1:B:741:LEU:HD23	3:B:98:HOH:O	2.16	0.44
1:B:849:VAL:HG11	3:B:101:HOH:O	2.17	0.44
1:A:92:LEU:HD11	1:A:321:PRO:HB2	1.99	0.44
1:B:819:GLY:HA3	2:B:901:HEM:C3C	2.51	0.44
1:B:679:LEU:HG	1:B:690:VAL:CG2	2.47	0.44
1:B:764:ARG:HA	1:B:772:ILE:O	2.18	0.44
1:B:528:TYR:CZ	1:B:768:GLY:HA2	2.53	0.43
1:B:692:SER:OG	1:B:694:LEU:HG	2.18	0.43
1:A:59:ARG:H	1:A:59:ARG:CZ	2.25	0.43
1:B:774:GLU:HG3	1:B:775:GLY:N	2.33	0.43
1:A:99:ILE:O	1:A:103:THR:CG2	2.67	0.43
1:A:117:ILE:HD11	1:A:222:VAL:HG11	2.01	0.43
1:B:562:ILE:HB	1:B:565:ARG:CD	2.49	0.43
1:B:741:LEU:CD2	3:B:412:HOH:O	2.65	0.43
1:A:319:GLY:HA3	2:A:1401:HEM:C3C	2.54	0.42
1:B:813:GLY:O	1:B:816:LEU:HB2	2.19	0.42
1:B:742:LYS:HE3	1:B:803:ASN:HB2	2.00	0.42
1:A:252:PRO:HA	1:A:253:PRO:HD3	1.97	0.42
1:A:82:MET:HE1	1:A:189:VAL:HA	1.98	0.42
1:B:592:LEU:HD11	1:B:821:PRO:HB2	2.01	0.42
1:A:266:LYS:HG3	1:A:270:GLN:O	2.19	0.42
1:B:676:LYS:HA	1:B:679:LEU:HD22	2.02	0.42
1:A:235:ARG:NH1	1:A:336:LYS:HG2	2.34	0.42
1:A:262:LYS:HD2	1:A:262:LYS:HA	1.88	0.42
1:B:679:LEU:HD12	1:B:679:LEU:HA	1.90	0.42
1:A:338:PHE:CD1	1:A:338:PHE:C	2.93	0.42
1:A:186:VAL:CG2	3:A:1497:HOH:O	2.67	0.41
1:B:662:PHE:CE2	1:B:663:GLU:O	2.72	0.41
1:A:210:GLY:HA3	2:A:1401:HEM:C2C	2.56	0.41
1:A:261:THR:HG21	1:A:272:ILE:CG2	2.50	0.41
1:B:764:ARG:NH1	1:B:764:ARG:HG2	2.35	0.41
1:B:839:ARG:HH21	1:B:866:SER:CB	2.33	0.41
1:B:607:LEU:HD13	1:B:837:ARG:HG3	2.01	0.41
1:B:639:GLU:CD	1:B:639:GLU:N	2.73	0.41
1:B:839:ARG:HE	1:B:866:SER:HB3	1.85	0.41
1:A:264:ARG:CG	1:A:264:ARG:NH1	2.82	0.41
1:B:592:LEU:CD1	1:B:821:PRO:HB2	2.50	0.41
1:B:618:VAL:HG23	1:B:860:LEU:HB2	2.02	0.41
1:A:340:HIS:HE1	1:A:342:GLU:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:PRO:HA	1:B:753:PRO:HD3	1.93	0.41
1:B:848:LYS:HZ1	1:B:855:ASN:ND2	2.18	0.41
1:B:704:ILE:CG2	1:B:708:ILE:HD12	2.51	0.40
1:A:346:THR:CG2	1:A:360:LEU:HD12	2.48	0.40
1:A:139:GLU:H	1:A:139:GLU:HG2	1.50	0.40
1:B:583:SER:O	1:B:586:ILE:CG1	2.62	0.40
1:B:848:LYS:HZ1	1:B:855:ASN:HD22	1.70	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%)	350 (96%)	12 (3%)	2 (0%)	29	9
1	B	355/368 (96%)	340 (96%)	14 (4%)	1 (0%)	41	18
All	All	719/736 (98%)	690 (96%)	26 (4%)	3 (0%)	34	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	GLU
1	A	139	GLU
1	B	651	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/338 (99%)	297 (88%)	39 (12%)	5	0
1	B	331/338 (98%)	291 (88%)	40 (12%)	5	0
All	All	667/676 (99%)	588 (88%)	79 (12%)	5	0

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	27	ARG
1	A	38	LYS
1	A	46	TYR
1	A	57	LYS
1	A	59	ARG
1	A	69	LEU
1	A	75	LEU
1	A	90	GLN
1	A	103	THR
1	A	104	ARG
1	A	105	SER
1	A	121	LEU
1	A	125	LEU
1	A	134	LEU
1	A	139	GLU
1	A	141	LYS
1	A	143	LYS
1	A	145	LYS
1	A	155	LEU
1	A	157	LYS
1	A	166	LYS
1	A	177	ASP
1	A	181	SER
1	A	200	LEU
1	A	202	TYR
1	A	233	ARG
1	A	237	GLU
1	A	264	ARG
1	A	269	ASP
1	A	271	THR
1	A	290	GLU
1	A	316	LEU
1	A	318	LEU

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Mol	Chain	Res	Type
1	A	322	LEU
1	A	348	LYS
1	A	352	GLU
1	A	365	LYS
1	A	366	SER
1	B	507	GLU
1	B	511	LYS
1	B	514	VAL
1	B	519	ASN
1	B	538	LYS
1	B	546	TYR
1	B	550	LEU
1	B	557	LYS
1	B	569	LEU
1	B	575	LEU
1	B	586	ILE
1	B	590	GLN
1	B	613	ARG
1	B	620	LYS
1	B	625	LEU
1	B	634	LEU
1	B	650	LEU
1	B	654	ARG
1	B	663	GLU
1	B	664	LEU
1	B	666	LYS
1	B	669	LEU
1	B	679	LEU
1	B	680	ASN
1	B	690	VAL
1	B	693	ASN
1	B	700	LEU
1	B	733	ARG
1	B	764	ARG
1	B	766	LYS
1	B	773	GLU
1	B	774	GLU
1	B	816	LEU
1	B	822	LEU
1	B	839	ARG
1	B	841	ILE
1	B	848	LYS

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Mol	Chain	Res	Type
1	B	854	LEU
1	B	860	LEU
1	B	865	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	A	307	HIS
1	A	355	ASN
1	B	519	ASN
1	B	590	GLN
1	B	680	ASN
1	B	693	ASN
1	B	729	ASN
1	B	786	ASN
1	B	803	ASN
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 monosaccharides 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	1401	1,3	41,50,50	1.41	6 (14%)	45,82,82	0.98	3 (6%)
2	HEM	B	901	1,3	41,50,50	1.41	7 (17%)	45,82,82	1.00	2 (4%)

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	1401	1,3	-	1/12/54/54	-
2	HEM	B	901	1,3	-	0/12/54/54	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	HEM	C3C-CAC	-3.22	1.41	1.47
2	B	901	HEM	C3C-C2C	-3.19	1.35	1.40
2	A	1401	HEM	C3C-CAC	-3.12	1.41	1.47
2	A	1401	HEM	C1B-C2B	3.03	1.50	1.44
2	B	901	HEM	CBB-CAB	2.52	1.42	1.30
2	B	901	HEM	CHA-C4D	2.47	1.41	1.35
2	A	1401	HEM	CMB-C2B	2.38	1.55	1.50
2	A	1401	HEM	C4A-NA	2.30	1.40	1.36
2	B	901	HEM	CHB-C1B	2.29	1.40	1.35
2	B	901	HEM	C2C-C1C	2.28	1.47	1.42
2	B	901	HEM	C1A-NA	2.27	1.40	1.36
2	A	1401	HEM	CAB-C3B	-2.24	1.41	1.47
2	A	1401	HEM	CBB-CAB	2.22	1.41	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	HEM	C4C-CHD-C1D	2.90	126.38	122.56
2	A	1401	HEM	C3B-C2B-C1B	-2.41	104.70	106.49
2	A	1401	HEM	C4B-CHC-C1C	2.41	125.73	122.56
2	B	901	HEM	C4B-CHC-C1C	2.25	125.53	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	HEM	C4C-CHD-C1D	2.04	125.25	122.56

There are no chirality outliers.

All (1) torsion outliers are listed below:

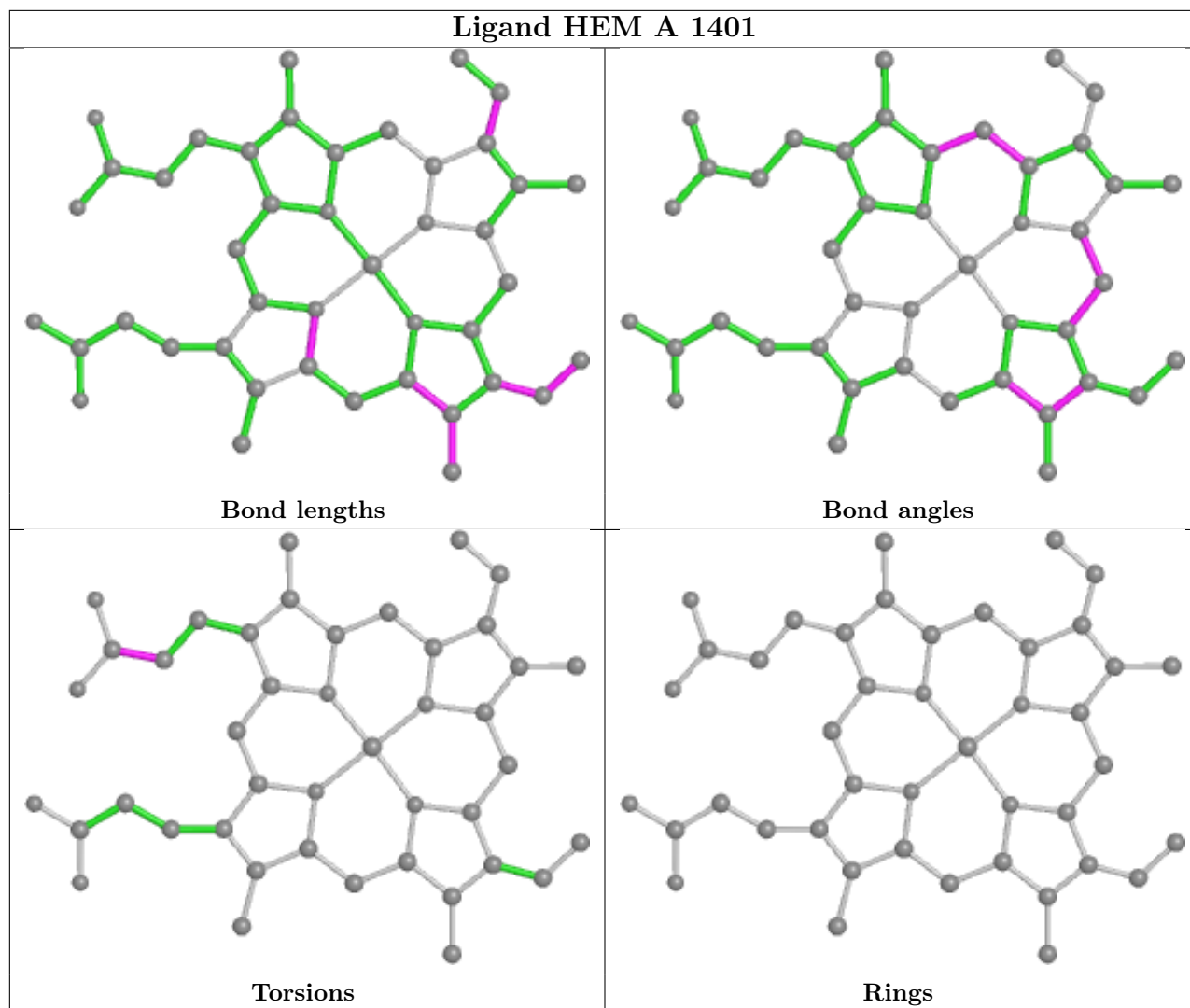
Mol	Chain	Res	Type	Atoms
2	A	1401	HEM	CAD-CBD-CGD-O2D

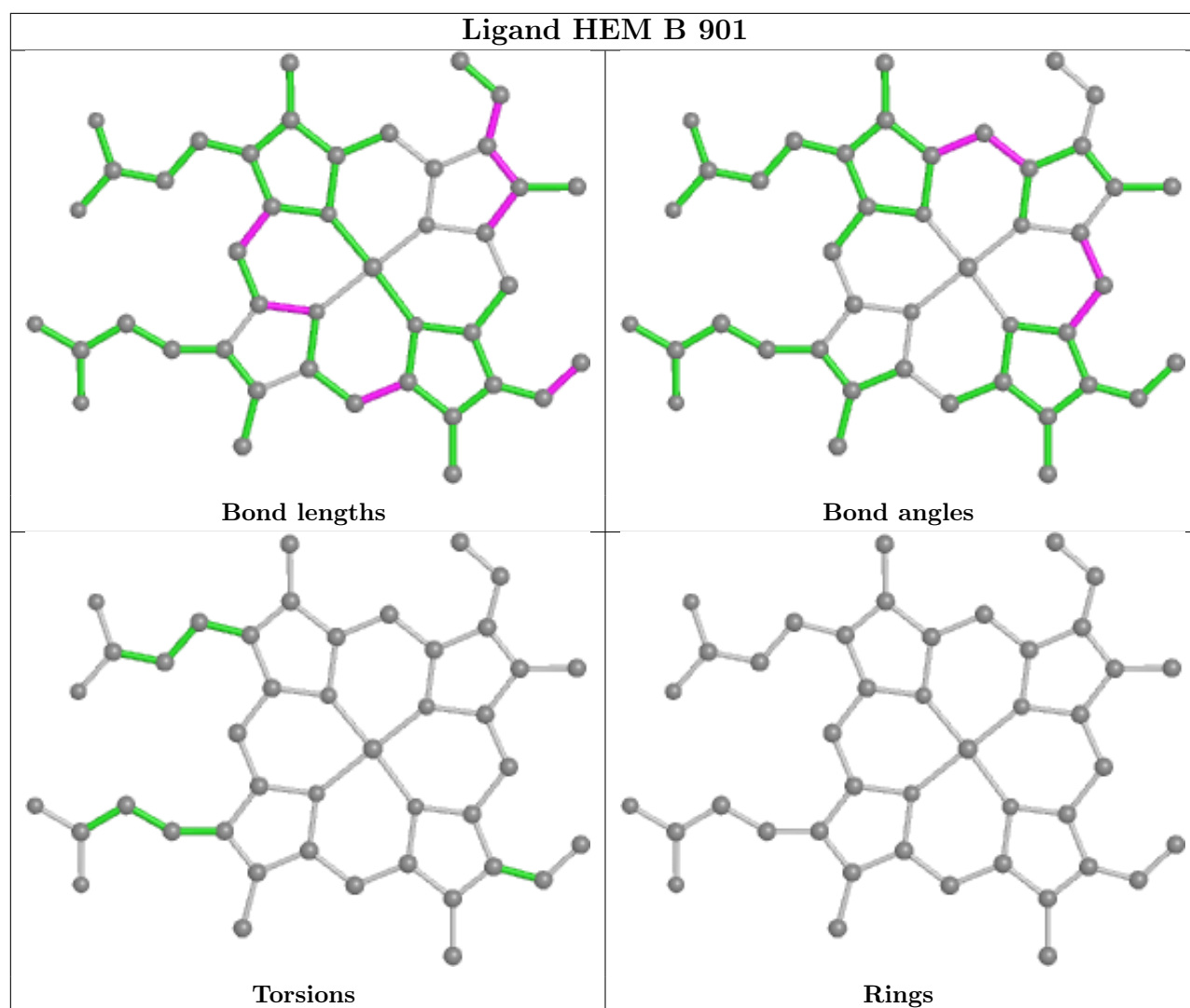
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	HEM	3	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.