



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:41 PM UTC

PDB ID : 1IO8 / pdb_00001io8
Title : Thermophilic cytochrome P450 (CYP119) from sulfolobus solfataricus: High resolution structural origin of its thermostability and functional properties
Authors : Park, S.-Y.; Yamane, K.; Adachi, S.; Shiro, Y.; Sligar, S.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2001-02-08
Resolution : 2.00 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)
Xtriage (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

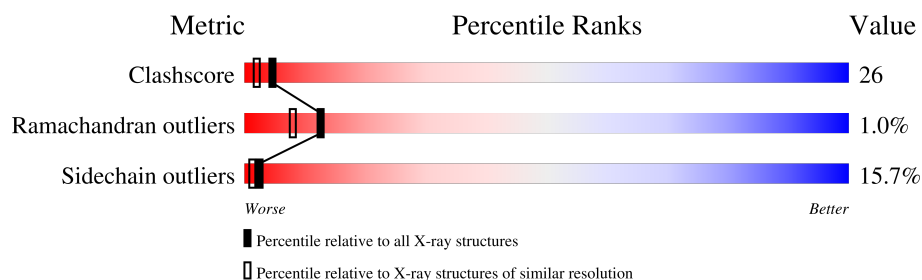
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	
1	B	368	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6334 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
			3007	1925	517	559	6			
1	B	359	Total	C	N	O	S	0	0	0
			2958	1893	509	550	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	LEU	PHE	engineered mutation	UNP Q55080
B	524	LEU	PHE	engineered mutation	UNP Q55080

- 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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	132	Total	O	0	0
			132	132		
3	B	151	Total	O	0	0
			151	151		

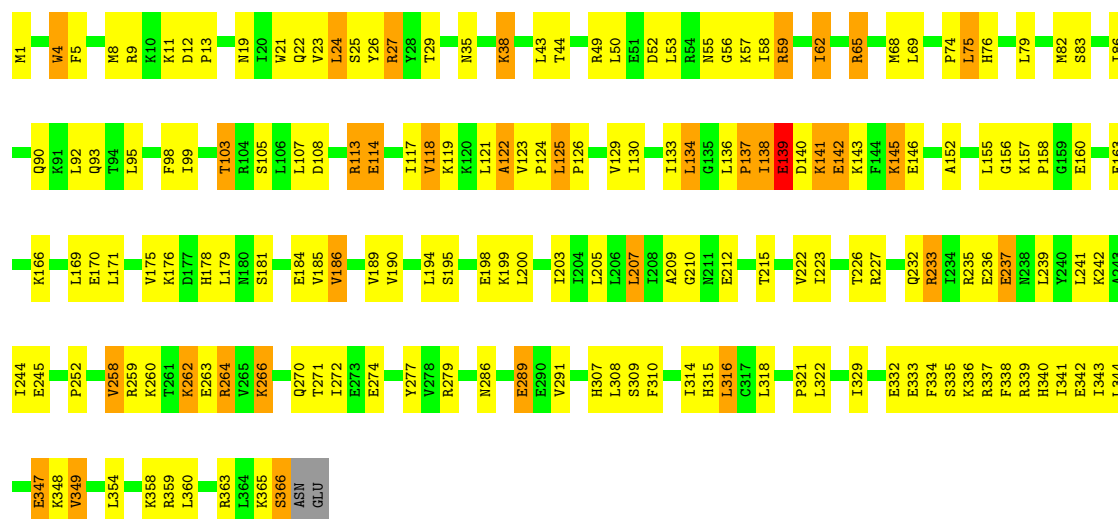
3 Residue-property plots

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.

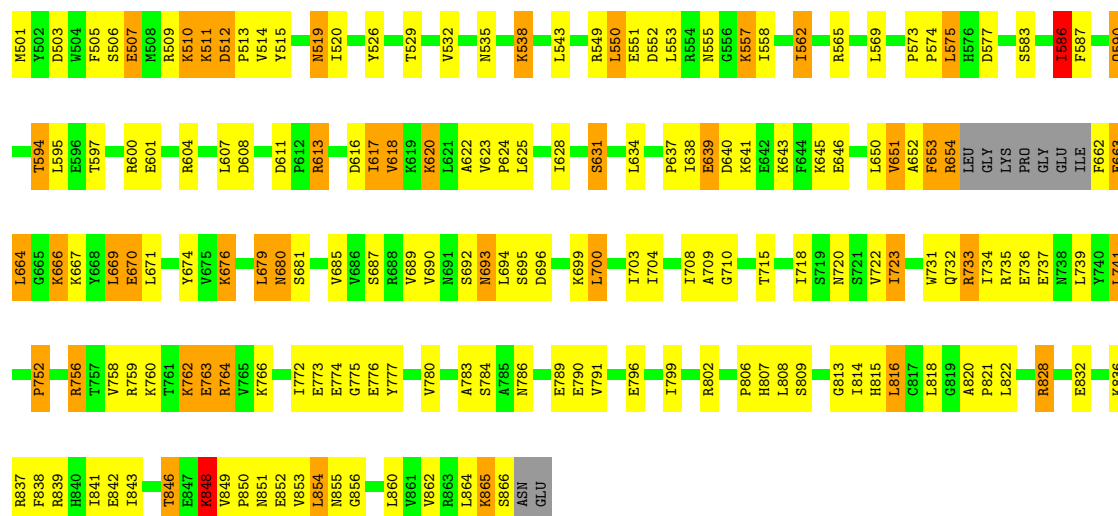
• Molecule 1: CYTOCHROME P450 CYP119

Chain A: 



• Molecule 1: CYTOCHROME P450 CYP119

Chain B: 



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, α , β , γ	85.52Å 85.52Å 221.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	94.5 (20.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.230 , 0.307	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6334	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.52	0/3070	0.99	12/4149 (0.3%)
1	B	0.53	0/3019	0.99	17/4079 (0.4%)
All	All	0.52	0/6089	0.99	29/8228 (0.4%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	618	VAL	N-CA-C	-8.06	102.96	110.53
1	A	4	TRP	N-CA-C	-7.01	103.64	111.28
1	A	252	PRO	N-CA-C	6.63	118.79	110.70
1	B	611	ASP	CA-C-N	6.57	126.81	119.32
1	B	611	ASP	C-N-CA	6.57	126.81	119.32
1	B	709	ALA	N-CA-C	6.45	120.73	112.34
1	A	118	VAL	N-CA-C	-6.19	104.72	110.53
1	B	671	LEU	N-CA-C	-5.98	104.67	111.07
1	B	848	LYS	N-CA-C	5.94	119.15	109.59
1	A	207	LEU	N-CA-C	5.76	117.64	111.36
1	A	56	GLY	N-CA-C	-5.66	107.51	115.32
1	A	62	ILE	CA-C-N	5.62	125.47	119.28
1	A	62	ILE	C-N-CA	5.62	125.47	119.28
1	B	752	PRO	N-CA-C	5.59	117.52	110.70
1	B	736	GLU	N-CA-C	5.53	117.31	111.28
1	B	708	ILE	N-CA-C	5.47	120.72	109.34
1	B	562	ILE	CA-C-N	5.45	125.53	119.32
1	B	562	ILE	C-N-CA	5.45	125.53	119.32
1	A	152	ALA	N-CA-C	5.41	117.87	111.33
1	B	715	THR	N-CA-C	-5.24	105.65	111.36
1	B	586	ILE	CB-CA-C	-5.23	105.19	112.04
1	A	262	LYS	N-CA-C	-5.21	106.77	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	LYS	N-CA-C	-5.21	105.28	111.69
1	A	122	ALA	N-CA-C	5.13	116.88	111.28
1	B	624	PRO	N-CA-C	5.10	120.24	113.40
1	B	512	ASP	N-CA-C	5.06	117.36	108.75
1	B	796	GLU	N-CA-C	-5.04	107.12	113.28
1	B	631	SER	N-CA-C	-5.02	105.88	111.36
1	A	156	GLY	N-CA-C	5.02	119.75	112.82

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	3007	0	3043	158	0
1	B	2958	0	2985	158	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
3	A	132	0	0	7	0
3	B	151	0	0	14	0
All	All	6334	0	6088	315	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 26.

All (315) 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:851:ASN:ND2	1:B:853:VAL:H	1.60	0.99
1:B:613:ARG:HH11	1:B:613:ARG:HB3	1.26	0.98
1:B:764:ARG:HH11	1:B:764:ARG:HB2	1.24	0.98
1:B:586:ILE:HD11	1:B:818:LEU:HD21	1.47	0.97
1:A:223:ILE:HD11	1:A:360:LEU:HD11	1.48	0.96
1:B:586:ILE:HG23	1:B:685:VAL:HG21	1.49	0.91
1:A:347:GLU:HB2	1:A:359:ARG:HB2	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:ASN:HD22	1:B:680:ASN:H	1.19	0.90
1:A:59:ARG:H	1:A:59:ARG:NE	1.70	0.88
1:A:58:ILE:HA	1:A:59:ARG:HH21	1.40	0.86
1:B:786:ASN:HD21	1:B:808:LEU:H	1.22	0.85
1:B:851:ASN:ND2	1:B:854:LEU:H	1.76	0.84
1:A:99:ILE:O	1:A:103:THR:HG23	1.77	0.82
1:B:652:ALA:HB3	1:B:654:ARG:HH21	1.42	0.82
1:B:763:GLU:HA	1:B:774:GLU:HB2	1.62	0.82
1:B:519:ASN:HD22	1:B:519:ASN:N	1.77	0.82
1:B:613:ARG:HB3	1:B:613:ARG:NH1	1.95	0.82
1:A:347:GLU:HG3	1:A:359:ARG:HH21	1.44	0.81
1:B:652:ALA:HB3	1:B:654:ARG:NH2	1.94	0.81
1:A:59:ARG:H	1:A:59:ARG:CZ	1.93	0.80
1:A:58:ILE:HA	1:A:59:ARG:NH2	1.96	0.79
1:B:849:VAL:HG12	1:B:856:GLY:O	1.83	0.79
1:A:136:LEU:HD12	1:A:207:LEU:HD13	1.67	0.76
1:B:828:ARG:O	1:B:832:GLU:HG3	1.84	0.76
1:A:55:ASN:HB3	1:A:57:LYS:HG2	1.67	0.75
1:B:503:ASP:OD2	1:B:506:SER:HB2	1.85	0.75
1:B:851:ASN:HD22	1:B:853:VAL:H	1.30	0.75
1:A:264:ARG:HB2	1:A:264:ARG:HH11	1.50	0.75
1:A:307:HIS:HD2	1:A:309:SER:H	1.32	0.74
1:A:166:LYS:O	1:A:170:GLU:HG3	1.87	0.74
1:B:843:ILE:HD12	1:B:860:LEU:HD21	1.70	0.73
1:B:764:ARG:HH11	1:B:764:ARG:CB	2.00	0.73
1:A:27:ARG:HG2	1:A:27:ARG:HH11	1.54	0.72
1:A:82:MET:CE	1:A:189:VAL:HA	2.19	0.72
1:A:344:LEU:HD21	1:A:363:ARG:HB2	1.72	0.72
1:A:349:VAL:HG21	3:A:482:HOH:O	1.88	0.72
1:A:123:VAL:HB	1:A:124:PRO:HD3	1.72	0.71
1:B:651:VAL:HG12	1:B:651:VAL:O	1.91	0.71
1:B:573:PRO:HB3	1:B:577:ASP:OD1	1.91	0.70
1:A:286:ASN:HD21	1:A:308:LEU:H	1.40	0.70
1:A:108:ASP:HA	1:A:337:ARG:NH2	2.06	0.69
1:A:59:ARG:NE	1:A:59:ARG:N	2.41	0.69
1:A:49:ARG:HG3	1:A:49:ARG:HH11	1.56	0.69
1:A:264:ARG:HH11	1:A:264:ARG:CB	2.07	0.68
1:B:616:ASP:O	1:B:620:LYS:HG2	1.92	0.68
1:B:543:LEU:HD22	1:B:777:TYR:HE2	1.57	0.68
1:B:628:ILE:HG12	1:B:638:ILE:HD11	1.74	0.68
1:A:82:MET:HE3	1:A:189:VAL:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:ARG:O	1:B:604:ARG:HG3	1.95	0.66
1:B:590:GLN:O	1:B:594:THR:HG23	1.95	0.66
1:A:113:ARG:NH1	1:A:113:ARG:HB3	2.11	0.66
1:B:848:LYS:NZ	1:B:855:ASN:HD22	1.93	0.65
1:A:74:PRO:HD2	3:A:468:HOH:O	1.96	0.65
1:B:676:LYS:HA	1:B:679:LEU:HD22	1.79	0.64
1:A:199:LYS:O	1:A:203:ILE:HG12	1.98	0.64
1:B:519:ASN:HD22	1:B:519:ASN:H	1.45	0.64
1:B:762:LYS:HD2	3:B:211:HOH:O	1.97	0.64
1:A:124:PRO:HB3	1:A:141:LYS:HE2	1.80	0.64
1:B:666:LYS:O	1:B:670:GLU:HG3	1.99	0.63
1:B:807:HIS:HD2	1:B:809:SER:H	1.46	0.63
1:B:586:ILE:HD11	1:B:818:LEU:CD2	2.27	0.63
1:B:851:ASN:HD22	1:B:853:VAL:N	1.97	0.63
1:A:95:LEU:HD11	1:A:133:ILE:HG12	1.80	0.62
1:A:138:ILE:C	1:A:140:ASP:H	2.06	0.62
1:A:142:GLU:O	1:A:146:GLU:HG3	2.00	0.62
1:A:27:ARG:HG2	1:A:27:ARG:NH1	2.14	0.62
1:A:86:ILE:HG21	1:A:185:VAL:HG13	1.82	0.62
1:B:839:ARG:HB3	1:B:866:SER:HA	1.81	0.62
1:B:510:LYS:HE2	1:B:511:LYS:HE2	1.80	0.62
1:A:58:ILE:HG23	1:A:59:ARG:NH2	2.15	0.61
1:B:510:LYS:HD3	1:B:511:LYS:HG2	1.81	0.61
1:A:49:ARG:HB3	1:A:58:ILE:HD13	1.82	0.61
1:B:507:GLU:OE1	1:B:511:LYS:HD2	2.00	0.61
1:B:692:SER:OG	1:B:694:LEU:HG	2.00	0.61
1:A:130:ILE:HG13	1:A:134:LEU:HD22	1.81	0.61
1:A:332:GLU:O	1:A:336:LYS:HG3	2.00	0.61
1:A:113:ARG:O	1:A:363:ARG:HG3	2.01	0.60
1:A:237:GLU:HB2	1:A:239:LEU:HG	1.82	0.60
1:B:618:VAL:HA	1:B:622:ALA:HB3	1.83	0.60
1:B:519:ASN:N	1:B:519:ASN:ND2	2.49	0.60
1:A:118:VAL:HG23	1:A:360:LEU:HB2	1.83	0.59
1:A:176:LYS:HA	1:A:179:LEU:CD1	2.32	0.59
1:A:264:ARG:O	1:A:264:ARG:HG3	2.03	0.59
1:A:117:ILE:HD11	1:A:222:VAL:HG11	1.85	0.58
1:B:641:LYS:HE2	3:B:192:HOH:O	2.02	0.58
1:A:83:SER:O	1:A:86:ILE:HG12	2.04	0.58
1:A:185:VAL:HG13	3:A:511:HOH:O	2.03	0.58
1:B:720:ASN:O	1:B:723:ILE:HG22	2.02	0.58
1:B:552:ASP:HA	1:B:555:ASN:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HA	1:A:122:ALA:HB3	1.85	0.58
1:A:13:PRO:CB	1:A:25:SER:HB3	2.34	0.57
1:A:289:GLU:CD	1:A:289:GLU:H	2.12	0.57
1:B:731:TRP:O	1:B:735:ARG:HG3	2.04	0.57
1:A:334:PHE:HZ	1:A:341:ILE:HD12	1.69	0.57
1:B:773:GLU:HB2	1:B:776:GLU:OE2	2.05	0.57
1:A:49:ARG:HB3	1:A:58:ILE:CD1	2.35	0.57
1:B:586:ILE:HD12	1:B:587:PHE:CE1	2.40	0.57
1:B:639:GLU:CD	1:B:639:GLU:H	2.13	0.57
1:A:233:ARG:O	1:A:237:GLU:HG3	2.05	0.56
1:A:44:THR:HB	1:A:65:ARG:HB3	1.87	0.56
1:A:163:GLU:HG2	3:A:448:HOH:O	2.05	0.56
1:B:696:ASP:HB2	3:B:143:HOH:O	2.05	0.56
1:B:693:ASN:N	1:B:693:ASN:HD22	2.04	0.55
1:A:43:LEU:CD2	1:A:260:LYS:HB2	2.36	0.55
1:A:25:SER:O	1:A:29:THR:HG23	2.07	0.55
1:A:347:GLU:CB	1:A:359:ARG:HB2	2.31	0.55
1:A:335:SER:HA	1:A:338:PHE:CE2	2.42	0.55
1:B:680:ASN:H	1:B:680:ASN:ND2	1.98	0.55
1:A:334:PHE:CZ	1:A:341:ILE:HD12	2.41	0.55
1:B:849:VAL:HG21	3:B:85:HOH:O	2.06	0.55
1:B:583:SER:O	1:B:586:ILE:HG13	2.07	0.55
1:B:764:ARG:HA	1:B:772:ILE:O	2.07	0.54
1:B:820:ALA:HB3	1:B:821:PRO:HD3	1.87	0.54
1:B:848:LYS:NZ	1:B:855:ASN:ND2	2.55	0.54
1:B:535:ASN:HB2	3:B:186:HOH:O	2.06	0.54
1:B:538:LYS:HE3	1:B:763:GLU:OE2	2.07	0.54
1:B:583:SER:O	1:B:586:ILE:CG1	2.56	0.54
1:A:226:THR:HG21	1:A:343:ILE:HG12	1.89	0.54
1:A:184:GLU:HG3	1:A:185:VAL:N	2.22	0.54
1:B:764:ARG:HG3	1:B:764:ARG:O	2.07	0.54
1:B:865:LYS:HG3	1:B:866:SER:H	1.73	0.53
1:A:233:ARG:HD2	1:A:237:GLU:CD	2.33	0.53
1:B:617:ILE:HD11	1:B:860:LEU:HD13	1.90	0.53
1:B:505:PHE:O	1:B:509:ARG:HG3	2.08	0.53
1:A:58:ILE:HA	1:A:59:ARG:CZ	2.38	0.53
1:B:848:LYS:HZ1	1:B:855:ASN:HD22	1.55	0.53
1:B:799:ILE:HD12	1:B:802:ARG:NH2	2.24	0.53
1:B:758:VAL:HG22	1:B:759:ARG:N	2.23	0.52
1:B:685:VAL:O	1:B:689:VAL:HG23	2.08	0.52
1:B:756:ARG:NH2	1:B:852:GLU:HB3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:ARG:HD2	1:B:604:ARG:NH2	2.24	0.52
1:A:22:GLN:HG3	3:A:525:HOH:O	2.09	0.52
1:A:35:ASN:ND2	1:A:38:LYS:HG3	2.25	0.52
1:B:733:ARG:HD3	1:B:737:GLU:CD	2.34	0.52
1:B:763:GLU:CA	1:B:774:GLU:HB2	2.38	0.52
1:B:773:GLU:O	1:B:776:GLU:HG3	2.10	0.52
1:A:212:GLU:OE2	1:A:354:LEU:HD13	2.10	0.52
1:A:245:GLU:OE2	1:A:307:HIS:HE1	1.91	0.52
1:A:113:ARG:HB3	1:A:113:ARG:CZ	2.38	0.51
1:B:505:PHE:HB3	1:B:509:ARG:NH1	2.25	0.51
1:B:832:GLU:O	1:B:836:LYS:HG3	2.09	0.51
1:A:241:LEU:C	1:A:241:LEU:HD23	2.34	0.51
1:B:849:VAL:HG13	1:B:849:VAL:O	2.10	0.51
1:A:13:PRO:HB2	1:A:25:SER:HB3	1.92	0.51
1:A:108:ASP:HA	1:A:337:ARG:HH21	1.74	0.51
1:A:171:LEU:O	1:A:175:VAL:HG23	2.11	0.51
1:B:550:LEU:HD11	1:B:575:LEU:HG	1.93	0.51
1:B:851:ASN:HD22	1:B:854:LEU:H	1.57	0.51
1:A:62:ILE:HD12	1:A:62:ILE:N	2.26	0.51
1:B:574:PRO:HD2	3:B:146:HOH:O	2.10	0.51
1:B:652:ALA:CB	1:B:654:ARG:HH21	2.17	0.51
1:A:307:HIS:CD2	1:A:309:SER:HB2	2.46	0.50
1:A:50:LEU:O	1:A:53:LEU:HB2	2.11	0.50
1:B:662:PHE:CG	1:B:663:GLU:N	2.80	0.50
1:B:815:HIS:O	1:B:816:LEU:C	2.54	0.50
1:A:13:PRO:HB3	1:A:25:SER:HB3	1.93	0.50
1:A:123:VAL:O	1:A:126:PRO:HD2	2.12	0.50
1:A:314:ILE:HG13	1:A:315:HIS:CD2	2.46	0.50
1:A:263:GLU:HA	1:A:274:GLU:HB2	1.92	0.50
1:B:600:ARG:HD3	3:B:132:HOH:O	2.12	0.50
1:A:175:VAL:O	1:A:179:LEU:HG	2.12	0.49
1:A:264:ARG:HH11	1:A:264:ARG:CG	2.25	0.49
1:A:344:LEU:HD11	1:A:363:ARG:HB2	1.94	0.49
1:B:865:LYS:HG3	1:B:866:SER:N	2.27	0.49
1:B:807:HIS:CD2	1:B:809:SER:H	2.28	0.49
1:A:35:ASN:HD21	1:A:38:LYS:HG3	1.78	0.49
1:B:763:GLU:CG	1:B:764:ARG:N	2.76	0.49
1:B:526:TYR:OH	1:B:806:PRO:HB2	2.13	0.49
1:B:608:ASP:OD1	1:B:837:ARG:NH2	2.46	0.49
1:B:680:ASN:HD22	1:B:680:ASN:N	1.96	0.49
1:A:49:ARG:HG3	1:A:49:ARG:NH1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:THR:HG22	3:B:88:HOH:O	2.12	0.48
1:A:139:GLU:H	1:A:139:GLU:HG2	1.45	0.48
1:B:552:ASP:C	1:B:558:ILE:HD12	2.38	0.48
1:B:653:PHE:HE2	3:B:225:HOH:O	1.95	0.48
1:A:74:PRO:O	1:A:75:LEU:C	2.55	0.48
1:A:176:LYS:HA	1:A:179:LEU:HD12	1.94	0.48
1:A:210:GLY:HA3	2:A:401:HEM:C2C	2.49	0.48
1:B:693:ASN:HD22	1:B:693:ASN:H	1.60	0.48
1:B:693:ASN:H	1:B:693:ASN:ND2	2.12	0.48
1:B:699:LYS:O	1:B:703:ILE:HG12	2.13	0.48
1:B:839:ARG:NH2	1:B:866:SER:HB3	2.29	0.48
1:B:555:ASN:HB3	1:B:557:LYS:HD3	1.95	0.48
1:A:195:SER:O	1:A:199:LYS:HG3	2.14	0.48
1:A:232:GLN:O	1:A:236:GLU:HG3	2.14	0.48
1:B:851:ASN:ND2	1:B:853:VAL:N	2.42	0.48
1:A:107:LEU:HD13	1:A:337:ARG:HG3	1.96	0.48
1:B:760:LYS:HD3	1:B:777:TYR:CE2	2.49	0.48
1:A:1:MET:HA	3:B:23:HOH:O	2.13	0.47
1:A:38:LYS:HE2	1:A:263:GLU:OE2	2.14	0.47
1:A:38:LYS:HE2	1:A:263:GLU:CD	2.40	0.47
1:A:205:LEU:HD12	1:A:209:ALA:HB2	1.96	0.47
1:B:583:SER:HB2	1:B:586:ILE:HG12	1.95	0.47
1:A:21:TRP:CD1	1:A:272:ILE:HG23	2.50	0.47
1:A:75:LEU:HD22	1:A:79:LEU:CD1	2.45	0.47
1:B:607:LEU:HD13	1:B:837:ARG:HG3	1.97	0.47
1:B:718:ILE:O	1:B:722:VAL:HG23	2.14	0.47
1:B:841:ILE:HG12	1:B:842:GLU:N	2.29	0.47
1:A:138:ILE:C	1:A:140:ASP:N	2.73	0.47
1:A:98:PHE:HE2	1:A:129:VAL:HA	1.80	0.47
1:A:92:LEU:HD11	1:A:321:PRO:HB2	1.97	0.47
1:A:315:HIS:O	1:A:316:LEU:C	2.57	0.46
1:A:58:ILE:HA	1:A:59:ARG:NE	2.30	0.46
1:A:83:SER:HB3	3:A:511:HOH:O	2.15	0.46
1:A:339:ARG:HG3	1:A:366:SER:C	2.41	0.46
1:A:86:ILE:CG2	1:A:185:VAL:HG13	2.44	0.46
1:A:129:VAL:O	1:A:133:ILE:HG13	2.15	0.46
1:A:347:GLU:HG3	1:A:359:ARG:NH2	2.22	0.46
1:A:235:ARG:HG2	1:A:235:ARG:HH11	1.80	0.46
1:B:731:TRP:CD2	1:B:838:PHE:HZ	2.34	0.46
1:B:838:PHE:CE1	1:B:841:ILE:HB	2.51	0.46
1:B:758:VAL:O	1:B:759:ARG:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:LEU:HD22	1:B:777:TYR:CE2	2.44	0.45
1:B:529:THR:HG23	1:B:780:VAL:HB	1.98	0.45
1:A:23:VAL:HG12	1:A:29:THR:HG23	1.98	0.45
1:A:24:LEU:HD22	1:A:24:LEU:N	2.32	0.45
1:A:338:PHE:CE1	1:A:341:ILE:HG22	2.52	0.45
1:B:597:THR:O	1:B:601:GLU:HB2	2.16	0.45
1:B:590:GLN:H	1:B:590:GLN:HE21	1.65	0.45
1:B:652:ALA:HB3	1:B:654:ARG:CZ	2.47	0.45
1:B:652:ALA:O	1:B:654:ARG:N	2.44	0.45
1:A:258:VAL:CG2	1:A:259:ARG:N	2.80	0.45
1:B:512:ASP:HB3	1:B:515:TYR:HB2	1.98	0.45
1:B:623:VAL:HG11	1:B:645:LYS:HD3	1.97	0.45
1:B:653:PHE:N	1:B:653:PHE:CD1	2.85	0.45
1:B:741:LEU:HD22	1:B:828:ARG:HD3	1.98	0.45
1:A:137:PRO:HG2	1:A:178:HIS:CD2	2.52	0.45
1:B:849:VAL:HG11	3:B:85:HOH:O	2.17	0.45
1:B:551:GLU:HB3	3:B:61:HOH:O	2.16	0.44
1:B:679:LEU:HD12	1:B:679:LEU:HA	1.79	0.44
1:A:92:LEU:CD1	1:A:321:PRO:HB2	2.47	0.44
1:A:176:LYS:HA	1:A:179:LEU:HD11	1.98	0.44
1:A:117:ILE:HD11	1:A:360:LEU:HD23	1.98	0.44
1:A:266:LYS:HA	1:A:270:GLN:O	2.18	0.44
1:B:505:PHE:CG	1:B:784:SER:HB2	2.53	0.44
1:A:76:HIS:HE2	2:A:401:HEM:CGD	2.31	0.44
1:A:136:LEU:CD1	1:A:207:LEU:HD13	2.42	0.44
1:A:179:LEU:O	1:A:190:VAL:HG21	2.17	0.44
1:A:186:VAL:HG22	3:A:455:HOH:O	2.18	0.44
1:B:505:PHE:HB3	1:B:509:ARG:HH12	1.82	0.44
1:B:789:GLU:H	1:B:789:GLU:CD	2.26	0.44
1:B:839:ARG:CB	1:B:866:SER:HA	2.45	0.44
1:A:58:ILE:HA	1:A:59:ARG:HE	1.83	0.44
1:A:195:SER:OG	1:A:198:GLU:OE2	2.34	0.44
1:B:532:VAL:HG11	1:B:780:VAL:HG11	2.00	0.44
1:B:543:LEU:HD11	1:B:758:VAL:HG13	2.00	0.44
1:B:674:TYR:C	1:B:674:TYR:CD2	2.96	0.43
1:B:848:LYS:HZ2	1:B:855:ASN:HD22	1.65	0.43
1:A:340:HIS:CE1	1:A:342:GLU:HB2	2.53	0.43
1:B:773:GLU:OE1	1:B:773:GLU:HA	2.18	0.43
1:B:695:SER:O	1:B:699:LYS:HG3	2.17	0.43
1:B:733:ARG:NH2	3:B:89:HOH:O	2.43	0.43
1:A:22:GLN:OE1	1:A:279:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:LEU:O	1:B:704:ILE:HG13	2.17	0.43
1:A:23:VAL:HG12	1:A:29:THR:CG2	2.49	0.43
1:A:194:LEU:HD13	1:A:198:GLU:HB3	2.01	0.43
1:A:95:LEU:HD11	1:A:133:ILE:CG1	2.49	0.43
1:B:646:GLU:OE2	1:B:667:LYS:HD3	2.19	0.43
1:A:108:ASP:OD1	1:A:337:ARG:NH2	2.52	0.43
1:B:693:ASN:N	1:B:693:ASN:ND2	2.66	0.43
1:B:700:LEU:HD12	1:B:700:LEU:HA	1.77	0.43
1:A:49:ARG:NH1	1:A:49:ARG:CG	2.82	0.43
1:A:68:MET:O	1:A:76:HIS:HD2	2.01	0.43
1:A:334:PHE:CE1	1:A:338:PHE:CE2	3.07	0.43
1:B:549:ARG:HH12	1:B:565:ARG:NH2	2.17	0.43
1:A:223:ILE:CD1	1:A:360:LEU:HD11	2.34	0.42
1:B:562:ILE:HG21	1:B:662:PHE:CE2	2.55	0.42
1:B:640:ASP:O	1:B:643:LYS:HB2	2.19	0.42
1:B:666:LYS:H	1:B:666:LYS:HG2	1.52	0.42
1:A:5:PHE:O	1:A:9:ARG:HG3	2.18	0.42
1:A:52:ASP:HA	1:A:55:ASN:HB2	2.00	0.42
1:A:55:ASN:CB	1:A:57:LYS:HG2	2.44	0.42
1:A:82:MET:HE2	1:A:189:VAL:HG22	2.00	0.42
1:B:851:ASN:HD21	1:B:853:VAL:H	1.59	0.42
1:B:550:LEU:O	1:B:553:LEU:HB2	2.19	0.42
1:B:664:LEU:HD21	1:B:669:LEU:HD22	2.00	0.42
1:B:848:LYS:O	1:B:850:PRO:HD3	2.19	0.42
1:A:122:ALA:HB1	1:A:215:THR:HG23	2.01	0.42
1:A:4:TRP:HB2	1:B:681:SER:O	2.20	0.42
1:A:142:GLU:OE1	1:A:145:LYS:HE2	2.19	0.42
1:A:124:PRO:HA	1:A:141:LYS:HZ1	1.84	0.42
1:A:264:ARG:CG	1:A:264:ARG:NH1	2.81	0.42
1:A:310:PHE:CE2	2:A:401:HEM:HBB2	2.55	0.42
1:B:664:LEU:CD2	1:B:669:LEU:HD22	2.50	0.42
1:B:813:GLY:O	1:B:816:LEU:HB2	2.19	0.42
1:A:118:VAL:HG23	1:A:360:LEU:CB	2.50	0.41
1:B:637:PRO:HD2	1:B:674:TYR:OH	2.20	0.41
1:A:260:LYS:NZ	1:A:277:TYR:CZ	2.83	0.41
1:B:662:PHE:CD2	1:B:663:GLU:N	2.83	0.41
1:B:758:VAL:CG2	1:B:759:ARG:N	2.82	0.41
1:B:814:ILE:HG12	3:B:279:HOH:O	2.21	0.41
1:B:620:LYS:HB3	1:B:620:LYS:HE2	1.55	0.41
1:A:79:LEU:CD2	1:A:194:LEU:HD11	2.50	0.41
1:B:710:GLY:HA3	2:B:901:HEM:C2C	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:ILE:HA	1:B:739:LEU:HB2	2.03	0.41
1:B:814:ILE:HG13	1:B:815:HIS:CD2	2.55	0.41
1:A:329:ILE:O	1:A:333:GLU:HG2	2.21	0.41
1:A:340:HIS:HE1	1:A:342:GLU:HB2	1.84	0.41
1:B:670:GLU:HG3	1:B:670:GLU:H	1.57	0.41
1:B:752:PRO:HG3	1:B:783:ALA:HA	2.02	0.41
1:B:774:GLU:HG3	1:B:775:GLY:N	2.36	0.41
1:A:334:PHE:CD1	1:A:338:PHE:HE2	2.39	0.41
1:A:344:LEU:HD21	1:A:363:ARG:CB	2.47	0.41
1:B:526:TYR:CD2	1:B:791:VAL:HG21	2.56	0.41
1:B:848:LYS:HZ2	1:B:855:ASN:ND2	2.17	0.41
1:A:125:LEU:HB3	1:A:126:PRO:HD3	2.03	0.40
1:A:130:ILE:HD12	1:A:130:ILE:HA	1.94	0.40
1:A:262:LYS:O	1:A:263:GLU:HB3	2.22	0.40
1:B:843:ILE:HD13	1:B:862:VAL:HG12	2.02	0.40
1:A:8:MET:O	1:A:12:ASP:N	2.50	0.40
1:A:22:GLN:HG2	1:A:279:ARG:HB3	2.03	0.40
1:A:26:TYR:CD2	1:A:291:VAL:HG21	2.57	0.40
1:A:49:ARG:O	1:A:50:LEU:C	2.63	0.40
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.90	0.40
1:A:108:ASP:HA	1:A:337:ARG:HH22	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	338 (93%)	22 (6%)	4 (1%)	11	7
1	B	355/368 (96%)	333 (94%)	19 (5%)	3 (1%)	16	11
All	All	719/736 (98%)	671 (93%)	41 (6%)	7 (1%)	12	8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	GLU
1	B	653	PHE
1	A	139	GLU
1	B	513	PRO
1	A	137	PRO
1	B	651	VAL
1	A	158	PRO

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	336/338 (99%)	286 (85%)	50 (15%)	3	1
1	B	331/338 (98%)	276 (83%)	55 (17%)	2	1
All	All	667/676 (99%)	562 (84%)	105 (16%)	2	1

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	19	ASN
1	A	24	LEU
1	A	27	ARG
1	A	38	LYS
1	A	59	ARG
1	A	65	ARG
1	A	69	LEU
1	A	75	LEU
1	A	90	GLN
1	A	93	GLN
1	A	103	THR
1	A	105	SER
1	A	113	ARG
1	A	114	GLU
1	A	119	LYS

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Mol	Chain	Res	Type
1	A	121	LEU
1	A	125	LEU
1	A	134	LEU
1	A	138	ILE
1	A	139	GLU
1	A	141	LYS
1	A	142	GLU
1	A	143	LYS
1	A	145	LYS
1	A	155	LEU
1	A	157	LYS
1	A	160	GLU
1	A	169	LEU
1	A	181	SER
1	A	186	VAL
1	A	200	LEU
1	A	227	ARG
1	A	233	ARG
1	A	237	GLU
1	A	242	LYS
1	A	244	ILE
1	A	258	VAL
1	A	264	ARG
1	A	266	LYS
1	A	271	THR
1	A	289	GLU
1	A	316	LEU
1	A	318	LEU
1	A	322	LEU
1	A	347	GLU
1	A	348	LYS
1	A	349	VAL
1	A	365	LYS
1	A	366	SER
1	B	501	MET
1	B	507	GLU
1	B	510	LYS
1	B	511	LYS
1	B	514	VAL
1	B	519	ASN
1	B	520	ILE
1	B	538	LYS

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Mol	Chain	Res	Type
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	594	THR
1	B	595	LEU
1	B	613	ARG
1	B	617	ILE
1	B	620	LYS
1	B	625	LEU
1	B	631	SER
1	B	634	LEU
1	B	639	GLU
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	670	GLU
1	B	676	LYS
1	B	679	LEU
1	B	680	ASN
1	B	687	SER
1	B	690	VAL
1	B	693	ASN
1	B	700	LEU
1	B	723	ILE
1	B	732	GLN
1	B	733	ARG
1	B	741	LEU
1	B	756	ARG
1	B	762	LYS
1	B	763	GLU
1	B	764	ARG
1	B	766	LYS
1	B	790	GLU
1	B	816	LEU
1	B	822	LEU
1	B	828	ARG

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Mol	Chain	Res	Type
1	B	846	THR
1	B	848	LYS
1	B	854	LEU
1	B	864	LEU
1	B	865	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	534	ASN
1	B	680	ASN
1	B	693	ASN
1	B	729	ASN
1	B	786	ASN
1	B	807	HIS
1	B	851	ASN
1	B	855	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	901	1,3	50,50,50	1.57	9 (18%)	67,82,82	1.18	5 (7%)
2	HEM	A	401	1,3	50,50,50	1.57	12 (24%)	67,82,82	1.15	6 (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
2	HEM	B	901	1,3	-	4/14/54/54	-
2	HEM	A	401	1,3	-	3/14/54/54	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	FE-NB	4.05	2.07	1.94
2	A	401	HEM	C4D-C3D	3.69	1.51	1.45
2	B	901	HEM	FE-ND	3.34	2.05	1.94
2	A	401	HEM	CAC-C3C	-2.92	1.39	1.47
2	B	901	HEM	CHD-C4C	2.91	1.44	1.38
2	A	401	HEM	CAB-C3B	-2.87	1.39	1.47
2	A	401	HEM	FE-ND	2.72	2.03	1.94
2	B	901	HEM	FE-NB	2.70	2.03	1.94
2	B	901	HEM	CAB-C3B	-2.66	1.40	1.47
2	A	401	HEM	C1B-C2B	2.59	1.49	1.44
2	B	901	HEM	FE-NA	2.59	2.03	1.95
2	A	401	HEM	CHD-C4C	2.56	1.43	1.38
2	A	401	HEM	CMB-C2B	2.50	1.55	1.50
2	B	901	HEM	CBC-CAC	2.34	1.41	1.30
2	B	901	HEM	CAC-C3C	-2.34	1.41	1.47
2	A	401	HEM	C1D-C2D	2.28	1.49	1.44
2	B	901	HEM	CHA-C4D	2.13	1.42	1.38
2	A	401	HEM	CBB-CAB	2.11	1.40	1.30
2	B	901	HEM	C1C-C2C	2.10	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	CBC-CAC	2.08	1.40	1.30
2	A	401	HEM	CHA-C4D	2.03	1.42	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	C3B-C2B-C1B	-3.69	103.64	106.41
2	B	901	HEM	CMC-C2C-C1C	3.47	130.84	124.73
2	B	901	HEM	CBD-CAD-C3D	-2.75	104.93	112.53
2	A	401	HEM	CMB-C2B-C1B	2.67	129.20	125.03
2	A	401	HEM	CMC-C2C-C1C	2.66	129.42	124.73
2	B	901	HEM	CMA-C3A-C4A	2.57	129.33	125.42
2	A	401	HEM	CMC-C2C-C3C	-2.46	122.47	128.43
2	A	401	HEM	C2B-C1B-NB	2.31	112.50	109.84
2	B	901	HEM	CMC-C2C-C3C	-2.16	123.21	128.43
2	B	901	HEM	C1A-C2A-C3A	2.08	110.09	106.87
2	A	401	HEM	CHB-C4A-C3A	-2.03	121.53	127.43

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	HEM	C2B-C3B-CAB-CBB
2	A	401	HEM	C4B-C3B-CAB-CBB
2	B	901	HEM	C2B-C3B-CAB-CBB
2	B	901	HEM	C2C-C3C-CAC-CBC
2	B	901	HEM	C4C-C3C-CAC-CBC
2	A	401	HEM	C4C-C3C-CAC-CBC
2	B	901	HEM	C4B-C3B-CAB-CBB

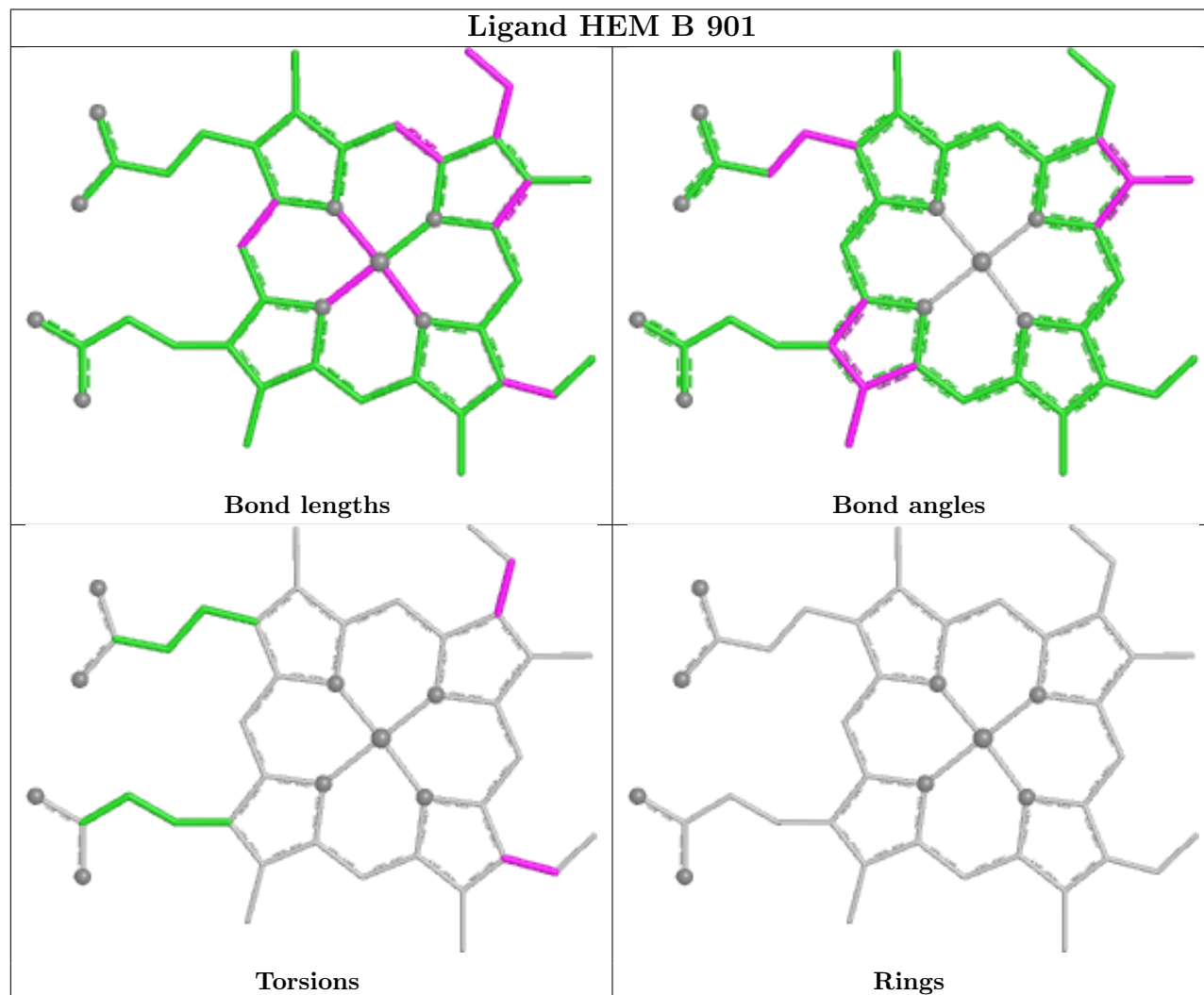
There are no ring outliers.

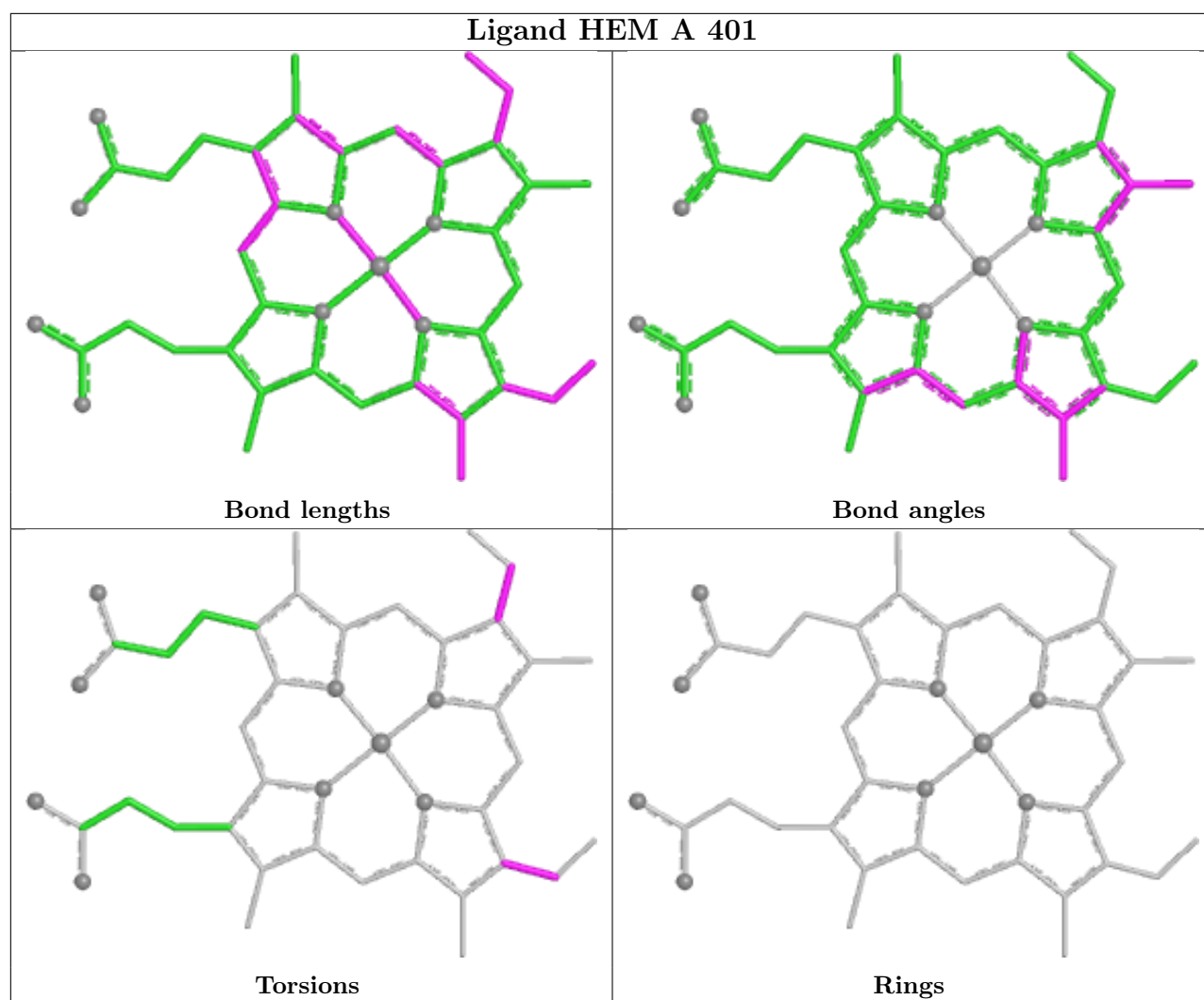
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	HEM	1	0
2	A	401	HEM	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.