



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:46 AM UTC

PDB ID : 2HPD / pdb_00002hpd
Title : CRYSTAL STRUCTURE OF HEMOPROTEIN DOMAIN OF P450BM-3, A
PROTOTYPE FOR MICROSOMAL P450'S
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Deisenhofer, J.
Deposited on : 1993-09-16
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

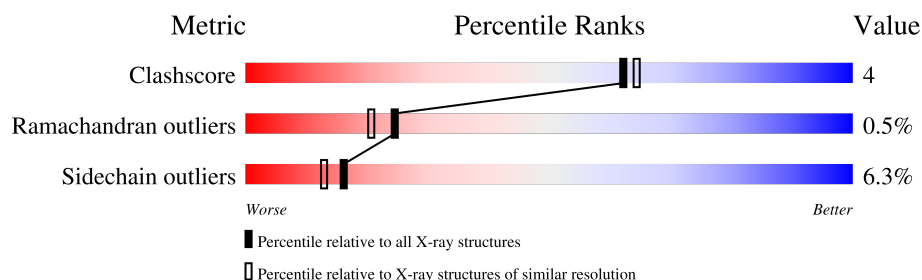
1 Overall quality at a glance

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	471	
1	B	471	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7897 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 BM-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3678	2349	625	687	17			
1	B	457	Total	C	N	O	S	0	0	0
			3678	2349	625	687	17			

- 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 water.

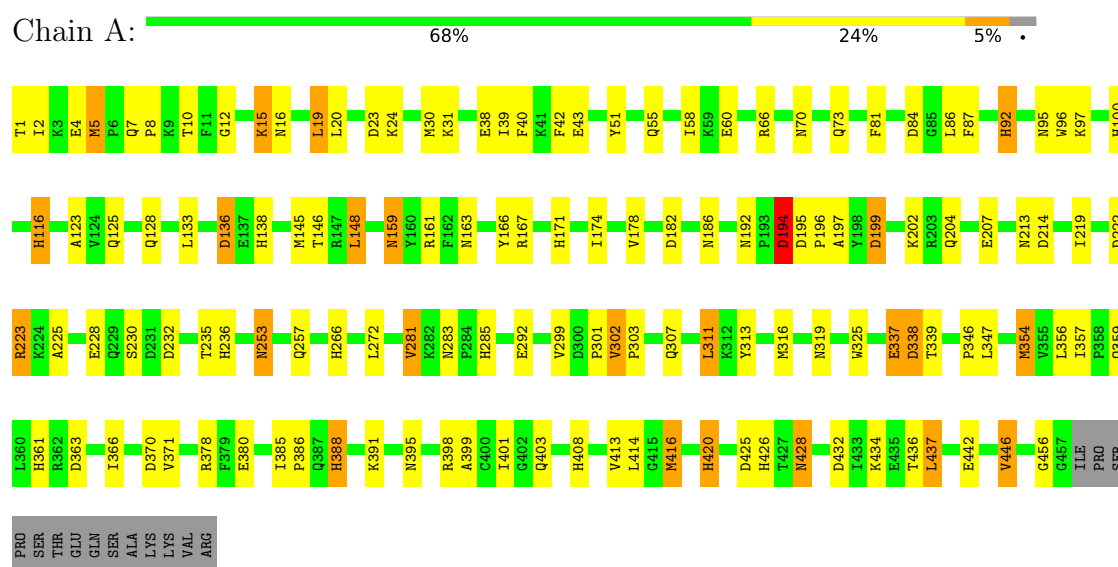
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	233	Total 233	O 233	0	0
3	B	222	Total 222	O 222	0	0

3 Residue-property plots

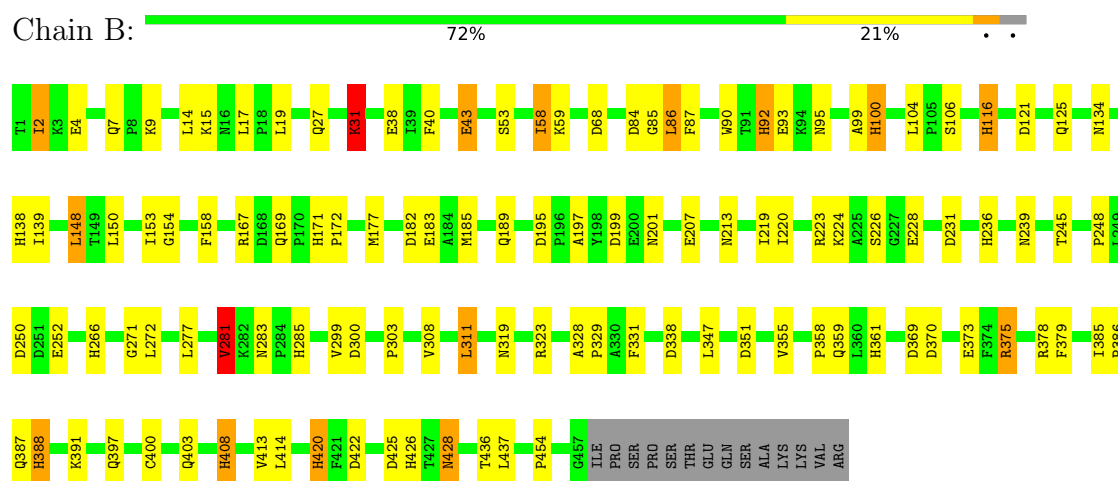
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 BM-3



• Molecule 1: CYTOCHROME P450 BM-3



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.40Å 154.00Å 62.20Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7897	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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	1.16	20/3763 (0.5%)	1.89	93/5087 (1.8%)
1	B	1.17	17/3763 (0.5%)	1.85	77/5087 (1.5%)
All	All	1.17	37/7526 (0.5%)	1.87	170/10174 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	HIS	CD2-NE2	-7.55	1.29	1.37
1	A	408	HIS	CD2-NE2	-7.39	1.29	1.37
1	B	361	HIS	CD2-NE2	-7.26	1.29	1.37
1	B	388	HIS	CD2-NE2	-7.21	1.29	1.37
1	A	100	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	116	HIS	CD2-NE2	-6.78	1.30	1.37
1	B	116	HIS	CD2-NE2	-6.72	1.30	1.37
1	B	361	HIS	CG-ND1	-6.56	1.31	1.38
1	B	420	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	388	HIS	CD2-NE2	-6.36	1.30	1.37
1	B	408	HIS	CD2-NE2	-6.33	1.30	1.37
1	B	138	HIS	CD2-NE2	-6.31	1.30	1.37
1	A	420	HIS	CD2-NE2	-6.28	1.30	1.37
1	A	236	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	266	HIS	CD2-NE2	-6.14	1.31	1.37
1	B	358	PRO	CA-CB	-6.12	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	357	ILE	CA-CB	6.06	1.58	1.53
1	A	285	HIS	CD2-NE2	-6.03	1.31	1.37
1	B	266	HIS	CD2-NE2	-6.01	1.31	1.37
1	B	92	HIS	CD2-NE2	-5.89	1.31	1.37
1	A	420	HIS	CG-ND1	-5.82	1.31	1.38
1	B	266	HIS	CG-ND1	-5.79	1.31	1.38
1	B	426	HIS	CD2-NE2	-5.73	1.31	1.37
1	A	138	HIS	CD2-NE2	-5.71	1.31	1.37
1	B	171	HIS	CD2-NE2	-5.70	1.31	1.37
1	A	92	HIS	CD2-NE2	-5.66	1.31	1.37
1	B	17	LEU	CA-CB	-5.61	1.46	1.53
1	B	100	HIS	CD2-NE2	-5.58	1.31	1.37
1	A	100	HIS	CG-ND1	-5.48	1.32	1.38
1	B	236	HIS	CD2-NE2	-5.38	1.31	1.37
1	A	171	HIS	CG-ND1	-5.34	1.32	1.38
1	A	161	ARG	CA-CB	-5.34	1.46	1.53
1	A	361	HIS	CD2-NE2	-5.23	1.32	1.37
1	B	285	HIS	CD2-NE2	-5.22	1.32	1.37
1	A	401	ILE	CA-CB	5.08	1.60	1.54
1	A	2	ILE	CA-CB	5.07	1.61	1.54

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	GLU	N-CA-C	14.03	128.95	111.69
1	A	38	GLU	N-CA-C	9.87	124.71	112.87
1	A	428	ASN	CA-CB-CG	-9.55	103.05	112.60
1	A	95	ASN	OD1-CG-ND2	-9.26	113.34	122.60
1	A	223	ARG	NE-CZ-NH2	-9.09	111.02	119.20
1	A	266	HIS	CB-CG-CD2	-8.65	119.96	131.20
1	B	231	ASP	CA-CB-CG	8.41	121.01	112.60
1	A	40	PHE	CA-CB-CG	8.39	122.19	113.80
1	A	356	LEU	CA-C-N	7.99	125.27	120.24
1	A	356	LEU	C-N-CA	7.99	125.27	120.24
1	A	222	ASP	CA-CB-CG	7.95	120.55	112.60
1	B	331	PHE	CA-CB-CG	7.95	121.75	113.80
1	B	266	HIS	N-CA-C	7.67	119.42	111.14
1	A	307	GLN	OE1-CD-NE2	-7.63	114.97	122.60
1	A	171	HIS	CB-CG-CD2	-7.55	121.38	131.20
1	B	95	ASN	OD1-CG-ND2	-7.36	115.24	122.60
1	A	136	ASP	CA-CB-CG	7.34	119.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	ASP	CA-CB-CG	7.33	119.93	112.60
1	A	23	ASP	CA-CB-CG	7.27	119.87	112.60
1	A	87	PHE	CA-CB-CG	7.27	121.07	113.80
1	B	370	ASP	CA-CB-CG	7.16	119.76	112.60
1	B	38	GLU	N-CA-C	7.05	121.33	112.87
1	B	373	GLU	O-C-N	-7.04	114.70	123.01
1	B	239	ASN	CA-CB-CG	7.01	119.61	112.60
1	A	192	ASN	CA-CB-CG	7.01	119.61	112.60
1	A	223	ARG	CG-CD-NE	-7.00	96.60	112.00
1	B	239	ASN	OD1-CG-ND2	-6.93	115.67	122.60
1	B	171	HIS	CB-CG-CD2	-6.83	122.32	131.20
1	B	139	ILE	N-CA-CB	-6.79	102.84	110.99
1	A	363	ASP	CA-CB-CG	6.79	119.39	112.60
1	B	84	ASP	CA-CB-CG	6.79	119.39	112.60
1	B	351	ASP	CA-CB-CG	6.77	119.37	112.60
1	A	125	GLN	OE1-CD-NE2	-6.76	115.84	122.60
1	A	338	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	204	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	A	253	ASN	OD1-CG-ND2	-6.66	115.94	122.60
1	A	416	MET	CG-SD-CE	-6.62	86.33	100.90
1	B	422	ASP	N-CA-C	-6.62	99.42	109.95
1	B	338	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	437	LEU	N-CA-C	-6.60	104.17	111.82
1	A	138	HIS	CB-CG-CD2	-6.58	122.64	131.20
1	B	420	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	A	403	GLN	OE1-CD-NE2	-6.55	116.05	122.60
1	A	125	GLN	CG-CD-NE2	6.51	126.16	116.40
1	B	15	LYS	CB-CA-C	-6.48	109.08	116.54
1	A	366	ILE	N-CA-C	-6.46	106.67	111.90
1	B	87	PHE	CA-CB-CG	6.41	120.21	113.80
1	A	236	HIS	CB-CG-CD2	-6.37	122.91	131.20
1	A	92	HIS	CA-CB-CG	6.37	120.17	113.80
1	A	84	ASP	CA-CB-CG	6.35	118.95	112.60
1	B	93	GLU	N-CA-C	-6.34	99.37	109.76
1	A	95	ASN	CB-CG-ND2	6.34	125.91	116.40
1	A	432	ASP	CA-CB-CG	6.31	118.91	112.60
1	B	328	ALA	N-CA-C	-6.28	96.00	109.01
1	B	213	ASN	OD1-CG-ND2	-6.25	116.34	122.60
1	A	213	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	B	388	HIS	CB-CG-CD2	-6.20	123.14	131.20
1	B	43	GLU	CA-CB-CG	6.19	126.49	114.10
1	B	426	HIS	CB-CG-CD2	-6.19	123.15	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	LYS	O-C-N	-6.19	115.79	121.42
1	B	226	SER	N-CA-C	6.15	118.95	111.82
1	B	85	GLY	N-CA-C	-6.14	103.11	112.51
1	B	199	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	159	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	A	302	VAL	CA-C-N	6.04	126.36	119.83
1	A	302	VAL	C-N-CA	6.04	126.36	119.83
1	B	281	VAL	N-CA-CB	-6.01	99.89	110.77
1	A	204	GLN	CG-CD-NE2	6.00	125.40	116.40
1	B	323	ARG	NE-CZ-NH1	5.99	127.49	121.50
1	B	223	ARG	CG-CD-NE	-5.95	98.90	112.00
1	B	86	LEU	N-CA-CB	-5.93	100.24	110.32
1	B	154	GLY	O-C-N	-5.92	116.50	122.19
1	A	199	ASP	CA-CB-CG	5.92	118.52	112.60
1	B	379	PHE	CA-CB-CG	-5.89	107.91	113.80
1	B	40	PHE	CA-CB-CG	5.89	119.69	113.80
1	B	182	ASP	CA-CB-CG	-5.89	106.71	112.60
1	A	432	ASP	N-CA-C	-5.89	98.69	108.34
1	A	436	THR	N-CA-C	-5.89	98.26	110.80
1	B	436	THR	N-CA-C	-5.87	98.29	110.80
1	B	138	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	A	266	HIS	CB-CG-ND1	5.87	131.50	122.70
1	A	128	GLN	OE1-CD-NE2	-5.86	116.75	122.60
1	B	403	GLN	N-CA-C	5.85	117.66	111.28
1	B	228	GLU	CB-CG-CD	5.81	122.48	112.60
1	A	398	ARG	NE-CZ-NH1	5.81	127.31	121.50
1	A	1	THR	N-CA-CB	-5.73	101.76	111.50
1	A	398	ARG	O-C-N	-5.73	114.80	122.19
1	B	428	ASN	CA-CB-CG	-5.72	106.88	112.60
1	B	2	ILE	N-CA-C	-5.72	97.44	109.34
1	B	90	TRP	O-C-N	-5.72	116.11	122.86
1	A	171	HIS	CB-CG-ND1	5.71	131.27	122.70
1	B	300	ASP	CA-C-N	5.70	125.17	119.24
1	B	300	ASP	C-N-CA	5.70	125.17	119.24
1	A	7	GLN	CB-CA-C	5.69	117.05	109.65
1	B	14	LEU	N-CA-C	-5.69	106.30	113.18
1	A	354	MET	CG-SD-CE	-5.68	88.40	100.90
1	B	171	HIS	CA-C-N	5.65	126.90	119.84
1	B	171	HIS	C-N-CA	5.65	126.90	119.84
1	A	145	MET	CA-C-O	-5.62	113.51	119.97
1	B	153	ILE	N-CA-C	-5.62	105.37	110.82
1	A	283	ASN	OD1-CG-ND2	-5.60	117.00	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	GLU	N-CA-C	-5.58	100.58	109.96
1	B	319	ASN	N-CA-C	5.58	117.36	111.28
1	A	223	ARG	NE-CZ-NH1	5.55	127.06	121.50
1	A	236	HIS	CB-CG-ND1	5.55	131.02	122.70
1	A	96	TRP	CG-CD2-CE3	5.54	139.44	133.90
1	A	399	ALA	N-CA-C	-5.53	102.71	110.35
1	B	252	GLU	O-C-N	-5.53	115.85	122.15
1	A	378	ARG	NE-CZ-NH2	-5.53	114.23	119.20
1	A	186	ASN	CB-CG-ND2	5.51	124.66	116.40
1	B	169	GLN	CA-C-N	5.51	126.28	120.11
1	B	169	GLN	C-N-CA	5.51	126.28	120.11
1	B	15	LYS	CA-CB-CG	5.50	125.11	114.10
1	B	195	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	219	ILE	CB-CA-C	-5.48	104.87	111.88
1	A	446	VAL	N-CA-CB	-5.47	103.31	112.06
1	A	232	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	239	ASN	CB-CG-ND2	5.42	124.53	116.40
1	A	182	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	166	TYR	N-CA-C	-5.40	106.06	113.30
1	B	139	ILE	N-CA-C	5.38	116.05	108.36
1	B	121	ASP	CA-C-O	-5.37	115.18	120.82
1	A	4	GLU	CA-C-O	-5.34	114.31	120.24
1	B	359	GLN	N-CA-C	-5.34	105.12	111.69
1	A	133	LEU	O-C-N	-5.32	116.95	122.96
1	A	214	ASP	CA-C-O	-5.31	114.92	120.55
1	A	197	ALA	N-CA-C	5.31	119.24	112.34
1	B	139	ILE	O-C-N	-5.30	117.14	123.03
1	A	319	ASN	O-C-N	-5.28	116.53	122.12
1	A	55	GLN	CA-C-N	5.26	127.28	120.44
1	A	55	GLN	C-N-CA	5.26	127.28	120.44
1	A	116	HIS	CB-CG-ND1	5.26	130.58	122.70
1	A	426	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	B	171	HIS	CB-CG-ND1	5.25	130.57	122.70
1	A	337	GLU	CB-CG-CD	5.24	121.50	112.60
1	A	15	LYS	CB-CG-CD	-5.23	99.27	111.30
1	B	283	ASN	CA-C-N	5.22	125.03	119.28
1	B	283	ASN	C-N-CA	5.22	125.03	119.28
1	B	373	GLU	CA-CB-CG	5.22	124.55	114.10
1	A	194	ASP	CA-C-O	-5.22	113.05	120.51
1	A	395	ASN	N-CA-C	5.21	117.74	109.50
1	A	225	ALA	CA-C-O	-5.21	115.33	120.70
1	A	325	TRP	CG-CD2-CE3	5.21	139.10	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	B	397	GLN	CG-CD-NE2	5.17	124.16	116.40
1	B	271	GLY	N-CA-C	-5.17	106.47	113.24
1	A	311	LEU	CA-C-N	5.17	127.15	120.44
1	A	311	LEU	C-N-CA	5.17	127.15	120.44
1	A	370	ASP	CA-C-N	5.15	128.61	120.47
1	A	370	ASP	C-N-CA	5.15	128.61	120.47
1	A	426	HIS	CB-CG-ND1	5.14	130.41	122.70
1	A	116	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	B	134	ASN	N-CA-C	-5.13	103.62	110.55
1	A	7	GLN	CA-CB-CG	5.11	124.32	114.10
1	A	73	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	70	ASN	O-C-N	-5.09	117.24	123.19
1	B	201	ASN	CA-CB-CG	-5.09	107.51	112.60
1	B	236	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	A	58	ILE	CA-C-O	-5.07	115.48	120.85
1	A	159	ASN	CB-CG-ND2	5.06	123.99	116.40
1	A	325	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	A	81	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	346	PRO	CB-CA-C	5.05	117.58	111.46
1	B	207	GLU	CB-CG-CD	5.04	121.17	112.60
1	B	58	ILE	CA-C-N	5.04	127.03	120.28
1	B	58	ILE	C-N-CA	5.04	127.03	120.28
1	A	146	THR	CA-CB-OG1	-5.01	102.09	109.60
1	B	31	LYS	CA-CB-CG	5.01	124.12	114.10
1	B	53	SER	CA-C-N	-5.01	114.39	122.81
1	B	53	SER	C-N-CA	-5.01	114.39	122.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	ASP	Peptide

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	3678	0	3651	33	0
1	B	3678	0	3651	26	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
3	A	233	0	0	3	0
3	B	222	0	0	2	0
All	All	7897	0	7362	61	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 4.

All (61) 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:123:ALA:HB1	1:A:416:MET:HE1	1.53	0.88
1:A:301:PRO:HB3	1:A:456:GLY:H	1.57	0.69
1:A:123:ALA:CB	1:A:416:MET:HE1	2.26	0.62
1:B:420:HIS:HE1	3:B:2182:HOH:O	1.81	0.62
1:B:400:CYS:HB2	2:B:472:HEM:NA	2.15	0.61
1:B:281:VAL:HG13	1:B:425:ASP:HB2	1.82	0.61
1:A:223:ARG:HH21	1:A:235:THR:HG23	1.68	0.59
1:A:15:LYS:HD3	1:A:43:GLU:HG2	1.84	0.58
1:B:92:HIS:HD2	3:B:2333:HOH:O	1.86	0.57
1:A:116:HIS:HE1	1:A:303:PRO:O	1.87	0.57
1:A:199:ASP:HA	1:A:202:LYS:HB3	1.86	0.56
1:A:20:LEU:HG	1:A:42:PHE:CZ	2.41	0.56
1:A:39:ILE:HA	1:A:51:TYR:O	2.06	0.56
1:A:230:SER:H	1:A:235:THR:HG21	1.71	0.56
1:A:97:LYS:HB3	3:A:1217:HOH:O	2.07	0.55
1:B:388:HIS:HD2	1:B:391:LYS:NZ	2.04	0.55
1:B:9:LYS:H	1:B:9:LYS:HD3	1.72	0.54
1:A:194:ASP:HA	1:A:202:LYS:NZ	2.23	0.54
1:A:8:PRO:HB2	1:A:19:LEU:HD21	1.90	0.53
1:A:60:GLU:HG2	1:A:66:ARG:HH12	1.73	0.52
1:B:375:ARG:HB2	1:B:378:ARG:NH1	2.25	0.52
1:A:174:ILE:O	1:A:178:VAL:HG23	2.10	0.51
1:A:194:ASP:HA	1:A:202:LYS:HZ1	1.76	0.50
1:A:281:VAL:HG13	1:A:425:ASP:HB2	1.93	0.49
1:A:30:MET:HG2	1:A:359:GLN:HE21	1.76	0.49
1:B:308:VAL:HA	1:B:311:LEU:HD22	1.93	0.49
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.95	0.48
1:A:388:HIS:HA	1:A:391:LYS:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:GLN:O	1:B:31:LYS:HD2	2.12	0.48
1:B:7:GLN:NE2	1:B:43:GLU:HG2	2.29	0.48
1:B:58:ILE:HD13	1:B:355:VAL:HG13	1.98	0.46
1:B:400:CYS:HB2	2:B:472:HEM:C1A	2.50	0.46
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.98	0.45
1:A:416:MET:HB2	1:A:416:MET:HE3	1.74	0.45
1:B:150:LEU:HD21	1:B:177:MET:HE1	1.99	0.45
1:B:158:PHE:HD2	1:B:219:ILE:HG21	1.82	0.44
1:B:388:HIS:HD2	1:B:391:LYS:HZ2	1.66	0.44
1:A:437:LEU:HD23	3:A:1165:HOH:O	2.17	0.44
1:A:223:ARG:NH2	1:A:235:THR:HG23	2.33	0.43
1:A:420:HIS:HE1	3:A:1182:HOH:O	2.01	0.43
1:B:116:HIS:HD2	1:B:408:HIS:NE2	2.17	0.43
1:A:434:LYS:HB2	1:A:442:GLU:HB2	2.00	0.43
1:B:185:MET:SD	1:B:437:LEU:HD13	2.58	0.43
1:B:7:GLN:HE22	1:B:43:GLU:HG2	1.83	0.43
1:A:92:HIS:H	1:A:92:HIS:CD2	2.36	0.43
1:A:163:ASN:O	1:A:167:ARG:HG3	2.19	0.43
1:B:220:ILE:O	1:B:224:LYS:HG3	2.18	0.42
1:A:16:ASN:O	1:A:19:LEU:HB2	2.19	0.42
1:A:253:ASN:O	1:A:257:GLN:HG2	2.20	0.42
2:A:472:HEM:HBC2	2:A:472:HEM:HMC2	2.01	0.42
1:B:116:HIS:HE1	1:B:303:PRO:O	2.03	0.42
1:B:385:ILE:HA	1:B:386:PRO:HD3	1.89	0.42
1:A:123:ALA:HB1	1:A:416:MET:CE	2.38	0.41
1:A:385:ILE:HA	1:A:386:PRO:HD2	1.88	0.41
1:A:313:TYR:HA	1:A:316:MET:HE3	2.01	0.41
1:A:60:GLU:HG2	1:A:66:ARG:NH1	2.34	0.41
2:A:472:HEM:HHH	2:A:472:HEM:HAC	1.84	0.41
1:B:277:LEU:O	1:B:281:VAL:HB	2.21	0.41
1:B:86:LEU:HD13	1:B:99:ALA:HB3	2.03	0.40
1:B:59:LYS:HE2	1:B:59:LYS:HB3	1.91	0.40
1:B:100:HIS:O	1:B:104:LEU:HB2	2.21	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	455/471 (97%)	434 (95%)	17 (4%)	4 (1%)	14	9
1	B	455/471 (97%)	435 (96%)	19 (4%)	1 (0%)	43	42
All	All	910/942 (97%)	869 (96%)	36 (4%)	5 (0%)	24	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	GLY
1	A	196	PRO
1	A	194	ASP
1	A	5	MET
1	B	197	ALA

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	399/412 (97%)	373 (94%)	26 (6%)	15	12
1	B	399/412 (97%)	375 (94%)	24 (6%)	17	14
All	All	798/824 (97%)	748 (94%)	50 (6%)	16	13

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET

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Mol	Chain	Res	Type
1	A	10	THR
1	A	19	LEU
1	A	31	LYS
1	A	86	LEU
1	A	136	ASP
1	A	148	LEU
1	A	159	ASN
1	A	207	GLU
1	A	228	GLU
1	A	272	LEU
1	A	281	VAL
1	A	292	GLU
1	A	299	VAL
1	A	302	VAL
1	A	311	LEU
1	A	337	GLU
1	A	338	ASP
1	A	339	THR
1	A	347	LEU
1	A	354	MET
1	A	371	VAL
1	A	380	GLU
1	A	414	LEU
1	A	428	ASN
1	A	446	VAL
1	B	2	ILE
1	B	19	LEU
1	B	31	LYS
1	B	106	SER
1	B	148	LEU
1	B	167	ARG
1	B	172	PRO
1	B	183	GLU
1	B	189	GLN
1	B	245	THR
1	B	248	PRO
1	B	250	ASP
1	B	272	LEU
1	B	281	VAL
1	B	299	VAL
1	B	311	LEU
1	B	329	PRO

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Mol	Chain	Res	Type
1	B	347	LEU
1	B	369	ASP
1	B	375	ARG
1	B	387	GLN
1	B	414	LEU
1	B	428	ASN
1	B	454	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	92	HIS
1	A	116	HIS
1	A	125	GLN
1	A	128	GLN
1	A	138	HIS
1	A	159	ASN
1	A	163	ASN
1	A	201	ASN
1	A	381	ASN
1	A	387	GLN
1	A	388	HIS
1	A	404	GLN
1	A	420	HIS
1	A	426	HIS
1	B	7	GLN
1	B	116	HIS
1	B	125	GLN
1	B	128	GLN
1	B	189	GLN
1	B	229	GLN
1	B	239	ASN
1	B	388	HIS
1	B	420	HIS
1	B	426	HIS

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](#)

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	472	1,3	50,50,50	1.35	10 (20%)	67,82,82	1.13	4 (5%)
2	HEM	A	472	1,3	50,50,50	1.39	8 (16%)	67,82,82	1.29	8 (11%)

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	472	1,3	-	4/14/54/54	-
2	HEM	A	472	1,3	-	2/14/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	472	HEM	FE-NB	3.20	2.04	1.94
2	A	472	HEM	CBC-CAC	3.18	1.45	1.30
2	B	472	HEM	CAB-C3B	-3.18	1.38	1.47
2	A	472	HEM	CBB-CAB	3.11	1.45	1.30
2	B	472	HEM	CBC-CAC	2.99	1.44	1.30
2	A	472	HEM	C3C-C4C	-2.95	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	472	HEM	CAC-C3C	-2.93	1.39	1.47
2	A	472	HEM	CAB-C3B	-2.84	1.39	1.47
2	B	472	HEM	O2D-CGD	-2.74	1.21	1.30
2	A	472	HEM	CAC-C3C	-2.67	1.40	1.47
2	B	472	HEM	O2A-CGA	-2.63	1.22	1.30
2	B	472	HEM	CBB-CAB	2.55	1.42	1.30
2	A	472	HEM	O2A-CGA	-2.39	1.22	1.30
2	B	472	HEM	CMC-C2C	2.28	1.55	1.50
2	A	472	HEM	CMC-C2C	2.27	1.55	1.50
2	B	472	HEM	CMB-C2B	2.06	1.55	1.50
2	B	472	HEM	C1B-C2B	2.04	1.48	1.44
2	A	472	HEM	FE-ND	2.00	2.01	1.94

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	472	HEM	C3B-C4B-NB	3.54	112.01	109.47
2	A	472	HEM	C2B-C1B-NB	2.90	113.17	109.84
2	A	472	HEM	C4A-C3A-C2A	-2.84	103.57	106.82
2	A	472	HEM	C3B-C2B-C1B	-2.73	104.36	106.41
2	B	472	HEM	C3C-C2C-C1C	-2.63	104.55	107.05
2	B	472	HEM	C3B-C2B-C1B	-2.61	104.45	106.41
2	A	472	HEM	C3B-C4B-NB	2.50	111.27	109.47
2	A	472	HEM	CHD-C1D-ND	-2.37	121.88	124.42
2	B	472	HEM	C2B-C1B-NB	2.33	112.51	109.84
2	A	472	HEM	C1A-C2A-C3A	2.30	110.43	106.87
2	A	472	HEM	O2A-CGA-CBA	2.23	121.05	114.00
2	A	472	HEM	C3C-C2C-C1C	-2.08	105.08	107.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

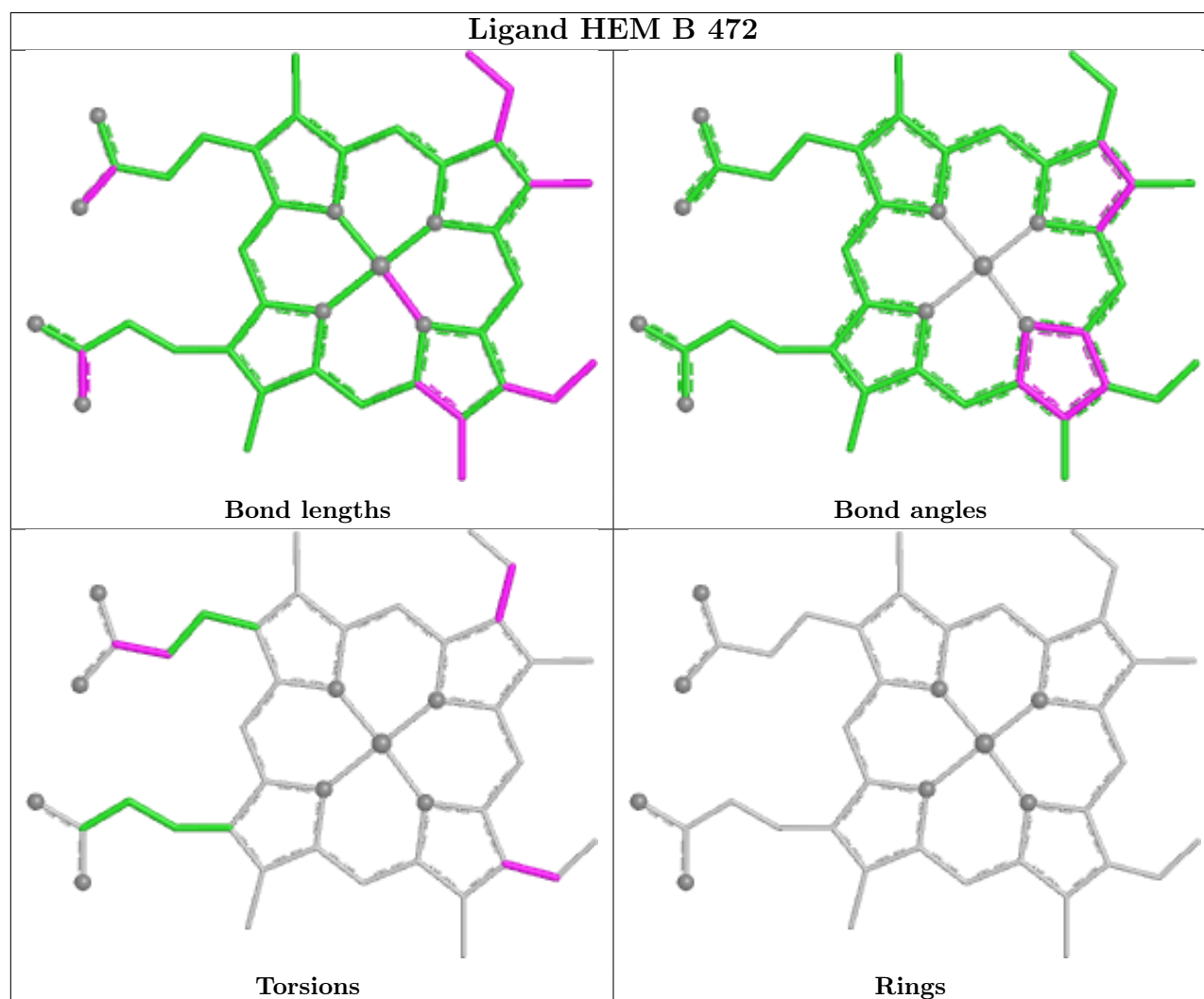
Mol	Chain	Res	Type	Atoms
2	B	472	HEM	C2B-C3B-CAB-CBB
2	B	472	HEM	C2C-C3C-CAC-CBC
2	A	472	HEM	CAD-CBD-CGD-O1D
2	B	472	HEM	CAD-CBD-CGD-O1D
2	A	472	HEM	CAD-CBD-CGD-O2D
2	B	472	HEM	CAD-CBD-CGD-O2D

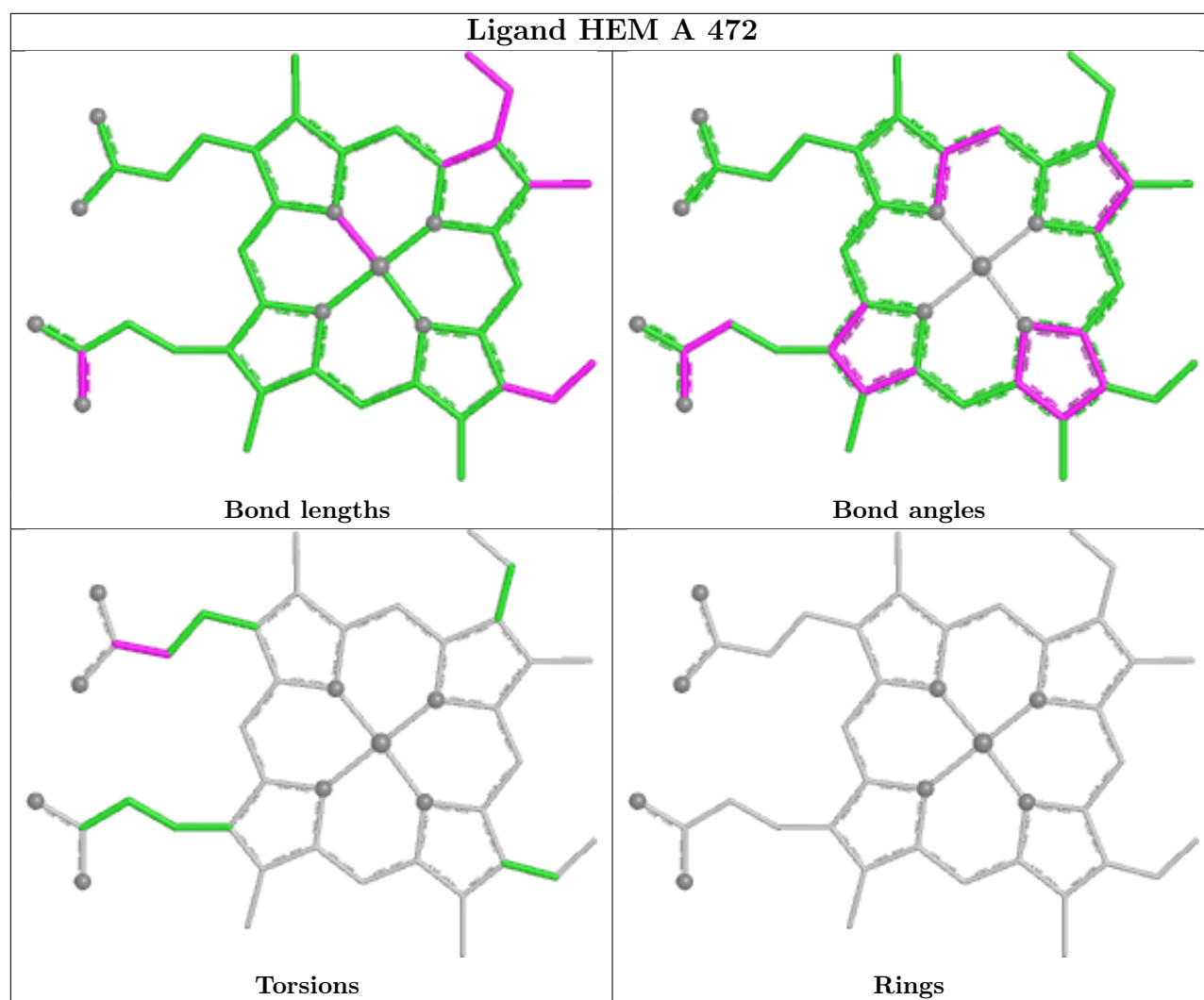
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	472	HEM	2	0
2	A	472	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.