



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:10 PM UTC

PDB ID : 1MBD / pdb_00001mbd
Title : X-ray structure of sperm whale deoxymoglobin refined at 1.4Å resolution
Authors : Phillips, S.E.V.
Deposited on : 1981-08-27
Resolution : 1.40 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

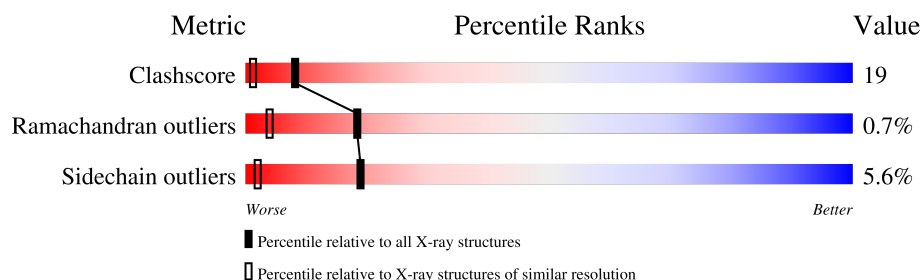
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)

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	153	25% 48% 20% 7%

2 Entry composition [i](#)

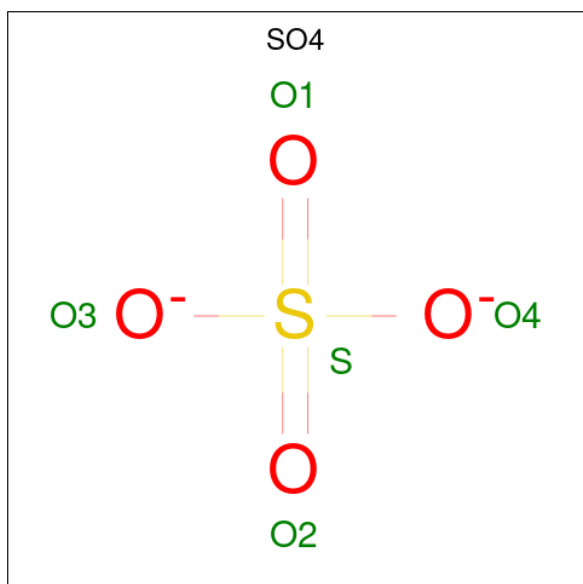
There are 4 unique types of molecules in this entry. The entry contains 1666 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MYOGLOBIN.

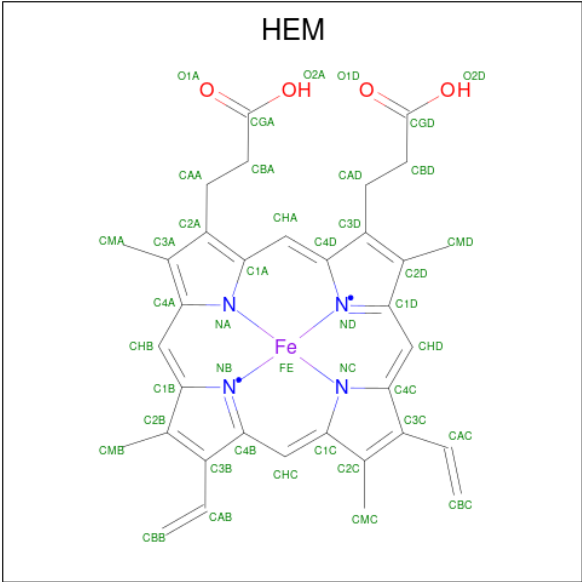
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	4	0
			1230	795	216	217	2			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 4 is water.

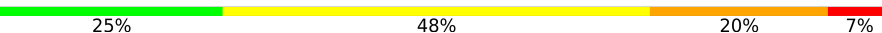
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	388	Total	O	0	0
			388	388		

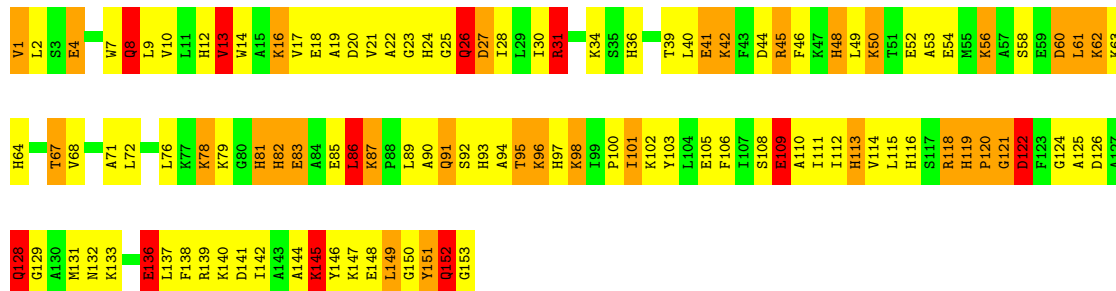
3 Residue-property plots [i](#)

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: MYOGLOBIN

Chain A: 



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	64.66Å 31.12Å 35.06Å 90.00° 105.78° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CONSTRAINED RECIPROCAL-SPACE LEAST-SQUARES	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1666	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: SO4, 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	3.11	121/1281 (9.4%)	3.43	185/1721 (10.7%)

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	16

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	HIS	CE1-NE2	21.36	1.53	1.32
1	A	93	HIS	ND1-CE1	16.82	1.49	1.32
1	A	81	HIS	CE1-NE2	16.25	1.48	1.32
1	A	12	HIS	ND1-CE1	14.62	1.47	1.32
1	A	81	HIS	ND1-CE1	13.73	1.46	1.32
1	A	12	HIS	CE1-NE2	13.37	1.46	1.32
1	A	81	HIS	CG-ND1	12.88	1.52	1.38
1	A	116	HIS	CD2-NE2	12.10	1.51	1.37
1	A	91	GLN	C-N	11.58	1.50	1.34
1	A	86[A]	LEU	CA-C	-10.92	1.37	1.52
1	A	86[B]	LEU	CA-C	-10.92	1.37	1.52
1	A	68	VAL	CA-C	-10.60	1.39	1.52
1	A	81	HIS	CG-CD2	10.48	1.47	1.35
1	A	81	HIS	CD2-NE2	9.95	1.48	1.37
1	A	98	LYS	C-N	-9.88	1.22	1.33
1	A	113	HIS	ND1-CE1	9.62	1.42	1.32
1	A	82	HIS	ND1-CE1	8.32	1.40	1.32
1	A	120	PRO	C-N	-8.22	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	ALA	N-CA	8.18	1.56	1.46
1	A	150	GLY	C-N	8.11	1.44	1.33
1	A	121	GLY	C-N	-8.10	1.21	1.33
1	A	116	HIS	ND1-CE1	8.01	1.40	1.32
1	A	81	HIS	N-CA	7.96	1.56	1.46
1	A	25	GLY	N-CA	7.70	1.55	1.45
1	A	12	HIS	CD2-NE2	7.69	1.46	1.37
1	A	16	LYS	C-N	7.59	1.43	1.34
1	A	9	LEU	CA-CB	-7.56	1.41	1.53
1	A	17	VAL	CA-CB	7.39	1.63	1.54
1	A	152	GLN	N-CA	7.37	1.55	1.46
1	A	118	ARG	NE-CZ	7.35	1.41	1.33
1	A	27	ASP	CA-C	7.22	1.62	1.52
1	A	41	GLU	C-N	7.20	1.43	1.33
1	A	83	GLU	C-N	-7.18	1.24	1.33
1	A	78	LYS	N-CA	7.09	1.55	1.46
1	A	18	GLU	CA-C	6.95	1.62	1.52
1	A	24	HIS	CE1-NE2	6.92	1.39	1.32
1	A	144	ALA	CA-CB	-6.88	1.42	1.53
1	A	31	ARG	CD-NE	6.77	1.55	1.46
1	A	14	TRP	NE1-CE2	-6.75	1.30	1.37
1	A	20	ASP	CA-C	6.72	1.61	1.53
1	A	23	GLY	N-CA	-6.69	1.37	1.45
1	A	28	ILE	N-CA	6.68	1.54	1.46
1	A	119	HIS	ND1-CE1	6.66	1.39	1.32
1	A	24	HIS	CG-ND1	6.62	1.45	1.38
1	A	22	ALA	CA-C	-6.62	1.44	1.52
1	A	12	HIS	N-CA	6.62	1.54	1.46
1	A	60	ASP	N-CA	6.59	1.54	1.46
1	A	124	GLY	N-CA	6.58	1.53	1.44
1	A	62	LYS	CA-CB	6.56	1.64	1.53
1	A	108	SER	CA-CB	-6.49	1.43	1.53
1	A	116	HIS	CG-ND1	6.46	1.45	1.38
1	A	86[A]	LEU	N-CA	-6.45	1.37	1.46
1	A	86[B]	LEU	N-CA	-6.45	1.37	1.46
1	A	64	HIS	ND1-CE1	6.39	1.39	1.32
1	A	64	HIS	CD2-NE2	6.39	1.44	1.37
1	A	136	GLU	N-CA	6.34	1.54	1.46
1	A	103	TYR	N-CA	6.28	1.54	1.46
1	A	118	ARG	CD-NE	-6.27	1.37	1.46
1	A	12	HIS	CG-ND1	6.26	1.45	1.38
1	A	68	VAL	N-CA	6.25	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	LEU	N-CA	6.25	1.53	1.46
1	A	82	HIS	CG-CD2	6.23	1.42	1.35
1	A	76	LEU	CA-CB	6.23	1.63	1.53
1	A	125	ALA	C-N	-6.19	1.26	1.33
1	A	4	GLU	C-O	6.18	1.31	1.24
1	A	108	SER	N-CA	-6.12	1.39	1.46
1	A	93	HIS	C-N	6.09	1.42	1.33
1	A	86[A]	LEU	CB-CG	-6.08	1.41	1.53
1	A	86[B]	LEU	CB-CG	-6.08	1.41	1.53
1	A	19	ALA	N-CA	6.05	1.54	1.46
1	A	91	GLN	N-CA	-6.04	1.39	1.46
1	A	113	HIS	CD2-NE2	-6.03	1.31	1.37
1	A	145	LYS	C-O	6.02	1.31	1.24
1	A	110	ALA	N-CA	6.02	1.53	1.46
1	A	53	ALA	CA-C	-5.98	1.45	1.52
1	A	42	LYS	C-N	5.94	1.43	1.33
1	A	112	ILE	CA-CB	5.94	1.61	1.54
1	A	27	ASP	N-CA	-5.85	1.39	1.46
1	A	112	ILE	C-O	5.84	1.31	1.24
1	A	145	LYS	N-CA	-5.83	1.39	1.46
1	A	24	HIS	CD2-NE2	5.82	1.44	1.37
1	A	13[A]	VAL	CA-CB	-5.80	1.46	1.54
1	A	13[B]	VAL	CA-CB	-5.80	1.46	1.54
1	A	24	HIS	C-N	-5.80	1.26	1.33
1	A	136	GLU	C-O	5.73	1.30	1.24
1	A	96	LYS	CG-CD	5.69	1.69	1.52
1	A	21	VAL	N-CA	5.58	1.53	1.46
1	A	121	GLY	N-CA	5.57	1.54	1.45
1	A	76	LEU	N-CA	-5.54	1.39	1.46
1	A	28	ILE	CA-CB	-5.50	1.48	1.54
1	A	48	HIS	CE1-NE2	-5.49	1.27	1.32
1	A	7	TRP	CA-CB	-5.48	1.44	1.53
1	A	137	LEU	N-CA	5.47	1.53	1.46
1	A	93	HIS	CA-C	5.46	1.60	1.52
1	A	16	LYS	CA-CB	-5.46	1.44	1.53
1	A	115	LEU	CB-CG	-5.44	1.42	1.53
1	A	114	VAL	C-O	5.41	1.30	1.24
1	A	144	ALA	C-O	5.39	1.30	1.24
1	A	45	ARG	CZ-NH2	5.38	1.40	1.33
1	A	82	HIS	CA-C	-5.37	1.46	1.53
1	A	45	ARG	CZ-NH1	5.36	1.40	1.32
1	A	45	ARG	CB-CG	-5.33	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	GLN	CD-NE2	-5.33	1.22	1.33
1	A	71	ALA	N-CA	5.31	1.52	1.46
1	A	133	LYS	CA-CB	-5.29	1.45	1.53
1	A	146	TYR	CA-C	5.28	1.59	1.52
1	A	10	VAL	CA-CB	5.27	1.60	1.54
1	A	118	ARG	N-CA	-5.27	1.39	1.46
1	A	67	THR	CA-C	5.24	1.59	1.52
1	A	114	VAL	CA-C	-5.24	1.46	1.52
1	A	129	GLY	C-N	-5.22	1.27	1.33
1	A	105	GLU	CA-CB	5.21	1.61	1.53
1	A	138	PHE	CA-CB	5.20	1.61	1.53
1	A	142	ILE	CA-CB	5.17	1.61	1.54
1	A	129	GLY	N-CA	5.16	1.52	1.45
1	A	131	MET	CA-C	5.11	1.59	1.52
1	A	95	THR	C-N	5.09	1.40	1.33
1	A	41	GLU	CD-OE2	-5.09	1.15	1.25
1	A	82	HIS	CE1-NE2	5.06	1.37	1.32
1	A	8	GLN	N-CA	5.06	1.52	1.46
1	A	148	GLU	N-CA	-5.05	1.40	1.46

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	GLN	OE1-CD-NE2	-32.40	90.20	122.60
1	A	118	ARG	NE-CZ-NH2	-28.12	93.89	119.20
1	A	64	HIS	ND1-CE1-NE2	15.78	124.18	108.40
1	A	1	VAL	N-CA-CB	-14.48	86.89	111.50
1	A	91	GLN	CA-C-O	14.13	135.66	120.82
1	A	8	GLN	OE1-CD-NE2	-13.34	109.26	122.60
1	A	116	HIS	CB-CG-CD2	-13.26	113.96	131.20
1	A	91	GLN	O-C-N	-12.66	109.03	122.07
1	A	87	LYS	O-C-N	-12.61	108.86	120.71
1	A	64	HIS	CE1-NE2-CD2	-12.14	96.86	109.00
1	A	86[A]	LEU	CA-C-O	11.98	133.93	119.79
1	A	86[B]	LEU	CA-C-O	11.98	133.93	119.79
1	A	113	HIS	ND1-CG-CD2	11.94	118.04	106.10
1	A	86[A]	LEU	CD1-CG-CD2	-11.55	85.38	110.80
1	A	86[B]	LEU	CD1-CG-CD2	-11.55	85.38	110.80
1	A	64	HIS	ND1-CG-CD2	11.38	117.48	106.10
1	A	113	HIS	ND1-CE1-NE2	11.32	119.72	108.40
1	A	118	ARG	CD-NE-CZ	11.10	139.94	124.40
1	A	81	HIS	ND1-CE1-NE2	10.88	119.28	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	GLU	O-C-N	10.29	135.76	122.39
1	A	97	HIS	CE1-NE2-CD2	-10.23	98.77	109.00
1	A	97	HIS	ND1-CE1-NE2	10.18	118.58	108.40
1	A	118	ARG	NH1-CZ-NH2	9.98	132.28	119.30
1	A	101	ILE	O-C-N	-9.86	112.31	121.87
1	A	144	ALA	O-C-N	-9.75	111.03	122.15
1	A	113	HIS	CG-ND1-CE1	-9.74	92.75	109.30
1	A	116	HIS	ND1-CG-CD2	9.65	115.75	106.10
1	A	31	ARG	NE-CZ-NH1	-9.62	111.88	121.50
1	A	4	GLU	CG-CD-OE2	-9.56	96.40	118.40
1	A	145	LYS	CB-CG-CD	9.51	133.16	111.30
1	A	106	PHE	CA-CB-CG	9.31	123.11	113.80
1	A	86[A]	LEU	O-C-N	-9.29	109.88	122.33
1	A	86[B]	LEU	O-C-N	-9.29	109.88	122.33
1	A	122	ASP	N-CA-CB	9.20	124.50	110.80
1	A	45	ARG	N-CA-CB	-9.15	96.09	110.28
1	A	91	GLN	OE1-CD-NE2	-9.09	113.52	122.60
1	A	118	ARG	CA-C-O	9.03	130.36	119.97
1	A	36	HIS	ND1-CE1-NE2	8.90	117.30	108.40
1	A	64	HIS	CG-ND1-CE1	-8.74	94.44	109.30
1	A	68	VAL	O-C-N	-8.69	113.25	121.94
1	A	152	GLN	OE1-CD-NE2	-8.69	113.92	122.60
1	A	139	ARG	NE-CZ-NH2	8.54	126.89	119.20
1	A	87	LYS	CB-CG-CD	-8.54	91.66	111.30
1	A	97	HIS	CA-C-O	8.42	129.72	119.79
1	A	118	ARG	O-C-N	-8.36	111.99	122.27
1	A	45	ARG	NH1-CZ-NH2	-8.22	108.61	119.30
1	A	64	HIS	CB-CG-CD2	-8.17	120.58	131.20
1	A	129	GLY	O-C-N	-8.13	114.38	122.19
1	A	81	HIS	CE1-NE2-CD2	-8.11	100.89	109.00
1	A	93	HIS	ND1-CG-CD2	8.11	114.21	106.10
1	A	128	GLN	CG-CD-OE1	-8.11	104.59	120.80
1	A	128	GLN	OE1-CD-NE2	8.07	130.67	122.60
1	A	87	LYS	CA-CB-CG	-8.06	97.98	114.10
1	A	81	HIS	CA-CB-CG	-7.99	105.81	113.80
1	A	109	GLU	CB-CG-CD	7.85	125.94	112.60
1	A	39	THR	N-CA-C	7.81	120.69	111.71
1	A	126	ASP	N-CA-CB	7.80	121.29	109.91
1	A	97	HIS	CG-CD2-NE2	7.77	114.97	107.20
1	A	76	LEU	N-CA-C	7.76	119.73	111.28
1	A	79	LYS	O-C-N	7.75	131.88	122.58
1	A	4	GLU	CG-CD-OE1	7.74	136.21	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	CD-NE-CZ	7.66	135.13	124.40
1	A	17	VAL	O-C-N	7.66	129.39	121.89
1	A	125	ALA	CA-C-N	7.65	130.75	120.65
1	A	125	ALA	C-N-CA	7.65	130.75	120.65
1	A	41	GLU	CB-CG-CD	-7.55	99.76	112.60
1	A	12	HIS	ND1-CG-CD2	7.54	113.64	106.10
1	A	128	GLN	CG-CD-NE2	-7.49	105.17	116.40
1	A	121	GLY	N-CA-C	7.47	122.89	114.67
1	A	87	LYS	CA-C-O	7.46	125.58	118.34
1	A	118	ARG	N-CA-C	7.45	120.46	111.82
1	A	42	LYS	N-CA-C	7.37	121.38	112.38
1	A	63	LYS	CB-CG-CD	-7.37	94.35	111.30
1	A	131	MET	O-C-N	7.35	129.65	122.07
1	A	4	GLU	CB-CA-C	7.28	122.46	110.81
1	A	42	LYS	CA-C-O	7.23	128.23	119.49
1	A	129	GLY	N-CA-C	-7.21	103.77	112.49
1	A	96	LYS	CA-C-O	7.14	130.12	120.13
1	A	8	GLN	O-C-N	-7.09	114.06	122.15
1	A	46	PHE	CA-CB-CG	-7.06	106.74	113.80
1	A	41	GLU	CA-C-O	7.04	128.21	119.05
1	A	30	ILE	O-C-N	7.02	128.79	121.91
1	A	133	LYS	O-C-N	-7.01	114.84	122.07
1	A	144	ALA	CA-C-O	6.94	127.77	120.42
1	A	9	LEU	CA-C-N	6.93	129.29	120.56
1	A	9	LEU	C-N-CA	6.93	129.29	120.56
1	A	144	ALA	N-CA-C	-6.91	103.83	111.36
1	A	136	GLU	N-CA-C	-6.90	103.84	111.36
1	A	31	ARG	CG-CD-NE	-6.87	96.89	112.00
1	A	72	LEU	O-C-N	-6.87	115.00	122.07
1	A	8	GLN	N-CA-C	-6.83	103.91	111.36
1	A	45	ARG	NE-CZ-NH2	6.82	125.34	119.20
1	A	7	TRP	N-CA-CB	6.78	120.09	110.12
1	A	12	HIS	CB-CG-CD2	-6.77	122.40	131.20
1	A	45	ARG	O-C-N	-6.72	114.00	122.27
1	A	109	GLU	CA-C-O	-6.72	113.77	120.82
1	A	101	ILE	CA-C-O	6.62	127.84	120.95
1	A	58	SER	CA-C-O	6.62	128.17	120.49
1	A	83	GLU	CG-CD-OE1	6.61	133.61	118.40
1	A	41	GLU	O-C-N	-6.57	113.39	122.46
1	A	81	HIS	CG-ND1-CE1	-6.56	98.15	109.30
1	A	122	ASP	CA-CB-CG	-6.53	106.07	112.60
1	A	67	THR	N-CA-C	-6.47	103.12	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	HIS	ND1-CE1-NE2	6.43	114.83	108.40
1	A	9	LEU	O-C-N	-6.43	115.41	122.09
1	A	4	GLU	CB-CG-CD	-6.42	101.68	112.60
1	A	109	GLU	OE1-CD-OE2	-6.38	107.60	122.90
1	A	46	PHE	O-C-N	-6.33	114.92	122.27
1	A	26	GLN	CG-CD-NE2	6.33	125.89	116.40
1	A	45	ARG	CA-C-O	6.32	127.24	119.97
1	A	100	PRO	CA-C-O	6.30	129.83	121.95
1	A	81	HIS	ND1-CG-CD2	6.28	112.38	106.10
1	A	48	HIS	O-C-N	-6.28	113.80	122.46
1	A	120	PRO	O-C-N	-6.25	114.60	122.17
1	A	139	ARG	NE-CZ-NH1	-6.24	115.26	121.50
1	A	61	LEU	CA-C-O	6.22	127.15	120.55
1	A	149	LEU	O-C-N	-6.20	113.91	122.46
1	A	12	HIS	CE1-NE2-CD2	-6.15	102.85	109.00
1	A	60	ASP	N-CA-C	-6.14	104.58	111.28
1	A	114	VAL	O-C-N	-6.13	115.53	121.90
1	A	83	GLU	CB-CG-CD	-6.09	102.24	112.60
1	A	118	ARG	NE-CZ-NH1	6.09	127.59	121.50
1	A	78	LYS	CG-CD-CE	-6.05	97.39	111.30
1	A	132	ASN	CB-CG-ND2	-6.02	107.37	116.40
1	A	87	LYS	CB-CA-C	-6.00	100.58	112.05
1	A	124	GLY	CA-C-O	-6.00	116.03	122.76
1	A	132	ASN	CA-CB-CG	-5.98	106.62	112.60
1	A	100	PRO	O-C-N	-5.95	115.71	122.91
1	A	24	HIS	O-C-N	5.94	128.41	122.12
1	A	93	HIS	O-C-N	5.93	130.28	122.33
1	A	147	LYS	CD-CE-NZ	-5.92	92.94	111.90
1	A	94	ALA	O-C-N	5.91	129.91	122.23
1	A	109	GLU	CG-CD-OE2	5.76	131.65	118.40
1	A	25	GLY	CA-C-O	5.76	126.68	120.75
1	A	111	ILE	CA-C-O	5.76	127.27	121.17
1	A	133	LYS	CB-CG-CD	-5.74	98.10	111.30
1	A	90	ALA	O-C-N	-5.74	115.22	122.27
1	A	129	GLY	CA-C-N	5.68	127.83	120.44
1	A	129	GLY	C-N-CA	5.68	127.83	120.44
1	A	79	LYS	CA-C-O	-5.68	115.00	121.65
1	A	22	ALA	O-C-N	-5.67	115.68	122.15
1	A	64	HIS	CA-CB-CG	-5.66	108.14	113.80
1	A	91	GLN	N-CA-CB	5.66	118.22	110.01
1	A	115	LEU	CB-CG-CD1	5.60	127.51	110.70
1	A	18	GLU	CA-C-O	-5.59	112.73	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	GLN	CG-CD-NE2	-5.58	108.02	116.40
1	A	111	ILE	O-C-N	-5.57	116.45	121.91
1	A	115	LEU	CD1-CG-CD2	-5.57	98.56	110.80
1	A	7	TRP	CE2-CD2-CE3	-5.55	113.25	118.80
1	A	132	ASN	CA-C-N	5.55	127.66	120.44
1	A	132	ASN	C-N-CA	5.55	127.66	120.44
1	A	116	HIS	N-CA-C	-5.51	105.19	111.14
1	A	133	LYS	N-CA-CB	5.49	117.97	110.01
1	A	56	LYS	O-C-N	5.49	128.64	122.22
1	A	152	GLN	N-CA-C	5.49	122.48	110.80
1	A	92	SER	CA-C-O	5.47	126.26	119.97
1	A	39	THR	CA-CB-CG2	5.46	119.78	110.50
1	A	101	ILE	N-CA-CB	5.44	117.93	110.54
1	A	12	HIS	N-CA-C	-5.40	105.31	111.14
1	A	126	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	108	SER	CA-C-O	5.34	126.43	120.82
1	A	50	LYS	N-CA-C	-5.31	106.74	113.43
1	A	128	GLN	O-C-N	5.31	127.75	122.12
1	A	93	HIS	CA-C-N	-5.26	111.58	120.58
1	A	93	HIS	C-N-CA	-5.26	111.58	120.58
1	A	7	TRP	CG-CD2-CE3	5.25	139.16	133.90
1	A	128	GLN	CB-CA-C	-5.24	102.09	110.79
1	A	124	GLY	O-C-N	5.23	126.79	122.71
1	A	60	ASP	CA-C-O	-5.19	115.05	120.55
1	A	52	GLU	OE1-CD-OE2	5.15	135.26	122.90
1	A	23	GLY	CA-C-N	-5.13	113.40	120.28
1	A	23	GLY	C-N-CA	-5.13	113.40	120.28
1	A	90	ALA	N-CA-CB	-5.13	102.33	110.28
1	A	41	GLU	CA-CB-CG	5.12	124.34	114.10
1	A	106	PHE	CD1-CG-CD2	5.12	126.28	118.60
1	A	110	ALA	O-C-N	-5.11	116.70	122.12
1	A	90	ALA	CA-C-O	5.11	125.85	119.97
1	A	139	ARG	CA-C-O	-5.09	115.15	120.55
1	A	94	ALA	N-CA-CB	-5.07	102.65	110.20
1	A	17	VAL	CA-C-O	-5.05	115.80	121.05
1	A	116	HIS	CB-CG-ND1	5.05	130.27	122.70
1	A	102	LYS	CA-C-N	-5.04	112.64	120.31
1	A	102	LYS	C-N-CA	-5.04	112.64	120.31
1	A	119	HIS	N-CA-CB	5.02	119.31	110.37
1	A	82	HIS	CA-C-O	5.00	126.81	120.65

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	GLU	Sidechain
1	A	118	ARG	Sidechain
1	A	122	ASP	Sidechain
1	A	128	GLN	Sidechain
1	A	136	GLU	Sidechain
1	A	151[A]	TYR	Sidechain
1	A	151[B]	TYR	Sidechain
1	A	26	GLN	Sidechain
1	A	31	ARG	Sidechain
1	A	4	GLU	Sidechain
1	A	42	LYS	Mainchain
1	A	45	ARG	Sidechain
1	A	48	HIS	Mainchain
1	A	54	GLU	Sidechain
1	A	67	THR	Mainchain
1	A	8	GLN	Sidechain

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	1230	0	1258	49	22
2	A	5	0	0	0	0
3	A	43	0	30	1	0
4	A	388	0	0	31	57
All	All	1666	0	1288	50	58

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 19.

All (50) 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:61:LEU:HG	4:A:528:HOH:O	1.16	1.32
1:A:26:GLN:CD	4:A:328:HOH:O	1.86	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LYS:NZ	1:A:151[B]:TYR:HE1	1.48	1.11
1:A:91:GLN:O	4:A:321:HOH:O	1.66	1.11
1:A:86[B]:LEU:CD1	1:A:86[B]:LEU:CD2	2.31	1.08
1:A:34:LYS:HE3	4:A:332:HOH:O	1.53	1.08
1:A:122:ASP:CG	4:A:350:HOH:O	2.08	0.95
1:A:140:LYS:HE3	4:A:525:HOH:O	1.64	0.94
1:A:98:LYS:NZ	1:A:151[B]:TYR:CE1	2.35	0.94
1:A:91:GLN:NE2	4:A:276:HOH:O	2.07	0.86
1:A:34:LYS:NZ	4:A:286:HOH:O	2.10	0.85
1:A:153:GLY:N	4:A:539:HOH:O	2.10	0.83
1:A:8:GLN:OE1	4:A:541:HOH:O	1.98	0.82
1:A:34:LYS:HD3	4:A:287:HOH:O	1.81	0.78
1:A:83:GLU:OE2	4:A:248:HOH:O	2.05	0.74
1:A:153:GLY:CA	4:A:539:HOH:O	2.36	0.73
1:A:109:GLU:OE1	4:A:543:HOH:O	2.08	0.72
1:A:98:LYS:HZ3	1:A:151[B]:TYR:HE1	1.38	0.71
1:A:153:GLY:HA3	4:A:539:HOH:O	1.90	0.71
1:A:86[B]:LEU:CD1	1:A:86[B]:LEU:HD22	2.21	0.70
1:A:56:LYS:NZ	4:A:490:HOH:O	2.26	0.68
1:A:26:GLN:NE2	4:A:328:HOH:O	2.13	0.66
1:A:113:HIS:ND1	4:A:508:HOH:O	2.29	0.64
1:A:26:GLN:OE1	1:A:62:LYS:HD2	1.99	0.62
1:A:86[B]:LEU:HD22	1:A:86[B]:LEU:HD13	1.83	0.60
1:A:60:ASP:OD1	4:A:296:HOH:O	2.17	0.60
1:A:145:LYS:HE3	4:A:365:HOH:O	2.02	0.60
1:A:121:GLY:C	4:A:350:HOH:O	2.47	0.58
1:A:141:ASP:O	1:A:145:LYS:HE2	2.03	0.57
1:A:83:GLU:H	1:A:83:GLU:CD	2.14	0.55
1:A:81:HIS:HD2	4:A:307:HOH:O	1.92	0.51
3:A:155:HEM:HBC2	3:A:155:HEM:HMC2	1.92	0.51
1:A:91:GLN:C	4:A:321:HOH:O	2.34	0.50
1:A:83:GLU:HG3	4:A:248:HOH:O	2.12	0.49
1:A:109:GLU:HG3	4:A:355:HOH:O	2.13	0.49
1:A:31:ARG:NH2	4:A:338:HOH:O	2.43	0.48
1:A:82:HIS:CD2	1:A:86[B]:LEU:HD22	2.49	0.48
1:A:78:LYS:HE3	1:A:85:GLU:OE2	2.15	0.47
1:A:83:GLU:OE1	4:A:196:HOH:O	2.20	0.47
1:A:13[A]:VAL:HG12	1:A:122:ASP:O	2.16	0.46
1:A:13[B]:VAL:HG22	1:A:122:ASP:O	2.16	0.46
1:A:95:THR:OG1	4:A:321:HOH:O	1.91	0.45
1:A:149:LEU:HD11	4:A:230:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LYS:CE	4:A:525:HOH:O	2.40	0.45
1:A:98:LYS:HZ1	1:A:151[B]:TYR:HE1	1.55	0.42
1:A:101:ILE:HG12	1:A:152:GLN:HE22	1.83	0.42
1:A:128:GLN:OE1	4:A:225:HOH:O	2.22	0.42
1:A:119:HIS:N	1:A:120:PRO:CD	2.83	0.42

All (58) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:436:HOH:O	4:A:439:HOH:O[1_554]	0.05	2.15
4:A:538:HOH:O	4:A:542:HOH:O[2_555]	0.28	1.92
1:A:153:GLY:C	4:A:353:HOH:O[2_555]	0.33	1.87
4:A:193:HOH:O	4:A:296:HOH:O[2_645]	0.53	1.67
4:A:157:HOH:O	4:A:295:HOH:O[2_556]	0.82	1.38
1:A:153:GLY:OXT	4:A:540:HOH:O[2_555]	1.01	1.19
4:A:447:HOH:O	4:A:505:HOH:O[2_656]	1.06	1.14
1:A:153:GLY:O	4:A:353:HOH:O[2_555]	1.07	1.13
1:A:27:ASP:OD1	4:A:377:HOH:O[2_646]	1.09	1.11
4:A:437:HOH:O	4:A:502:HOH:O[2_556]	1.11	1.09
4:A:224:HOH:O	4:A:524:HOH:O[1_565]	1.26	0.94
1:A:153:GLY:OXT	4:A:353:HOH:O[2_555]	1.34	0.86
4:A:318:HOH:O	4:A:529:HOH:O[1_556]	1.38	0.82
4:A:169:HOH:O	4:A:520:HOH:O[1_564]	1.41	0.79
4:A:191:HOH:O	4:A:368:HOH:O[1_554]	1.43	0.77
4:A:180:HOH:O	4:A:467:HOH:O[2_556]	1.44	0.76
4:A:269:HOH:O	4:A:477:HOH:O[2_656]	1.52	0.68
1:A:1:VAL:C	4:A:384:HOH:O[2_546]	1.56	0.64
4:A:324:HOH:O	4:A:359:HOH:O[1_554]	1.56	0.64
4:A:220:HOH:O	4:A:426:HOH:O[1_554]	1.58	0.62
4:A:333:HOH:O	4:A:493:HOH:O[2_655]	1.59	0.61
4:A:180:HOH:O	4:A:526:HOH:O[2_556]	1.60	0.60
1:A:91:GLN:OE1	1:A:153:GLY:O[2_555]	1.63	0.57
4:A:224:HOH:O	4:A:489:HOH:O[2_656]	1.64	0.56
1:A:136:GLU:OE2	4:A:539:HOH:O[2_545]	1.66	0.54
4:A:465:HOH:O	4:A:505:HOH:O[2_656]	1.66	0.54
1:A:41:GLU:OE1	4:A:362:HOH:O[1_554]	1.72	0.48
4:A:302:HOH:O	4:A:381:HOH:O[2_646]	1.72	0.48
4:A:276:HOH:O	4:A:316:HOH:O[1_565]	1.75	0.45
1:A:153:GLY:CA	4:A:353:HOH:O[2_555]	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:221:HOH:O	4:A:397:HOH:O[1_554]	1.80	0.40
4:A:315:HOH:O	4:A:347:HOH:O[2_545]	1.81	0.39
4:A:244:HOH:O	4:A:417:HOH:O[2_646]	1.82	0.38
1:A:1:VAL:O	4:A:384:HOH:O[2_546]	1.83	0.37
1:A:2:LEU:N	4:A:384:HOH:O[2_546]	1.86	0.34
4:A:217:HOH:O	4:A:468:HOH:O[2_656]	1.86	0.34
1:A:50:LYS:CE	4:A:434:HOH:O[1_554]	1.90	0.30
4:A:320:HOH:O	4:A:451:HOH:O[2_646]	1.90	0.30
4:A:180:HOH:O	4:A:453:HOH:O[2_556]	1.94	0.26
4:A:210:HOH:O	4:A:428:HOH:O[2_646]	1.98	0.22
4:A:170:HOH:O	4:A:336:HOH:O[2_556]	1.99	0.21
1:A:16:LYS:NZ	4:A:280:HOH:O[2_646]	2.00	0.20
1:A:27:ASP:CG	4:A:377:HOH:O[2_646]	2.00	0.20
4:A:170:HOH:O	4:A:526:HOH:O[2_556]	2.01	0.19
4:A:377:HOH:O	4:A:491:HOH:O[2_656]	2.01	0.19
1:A:40:LEU:CD2	4:A:433:HOH:O[1_554]	2.02	0.18
1:A:136:GLU:CD	4:A:539:HOH:O[2_545]	2.05	0.15
4:A:344:HOH:O	4:A:370:HOH:O[1_545]	2.06	0.14
1:A:136:GLU:OE1	4:A:539:HOH:O[2_545]	2.09	0.11
4:A:159:HOH:O	4:A:530:HOH:O[1_545]	2.12	0.08
1:A:44:ASP:OD1	4:A:368:HOH:O[1_554]	2.14	0.06
4:A:311:HOH:O	4:A:415:HOH:O[2_646]	2.14	0.06
4:A:324:HOH:O	4:A:460:HOH:O[1_554]	2.14	0.06
1:A:50:LYS:NZ	4:A:411:HOH:O[1_554]	2.15	0.05
1:A:153:GLY:C	4:A:540:HOH:O[2_555]	2.16	0.04
1:A:96:LYS:NZ	4:A:338:HOH:O[1_565]	2.17	0.03
4:A:207:HOH:O	4:A:476:HOH:O[2_655]	2.17	0.03
4:A:436:HOH:O	4:A:451:HOH:O[1_554]	2.19	0.01

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	155/153 (101%)	150 (97%)	4 (3%)	1 (1%)	21 5

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	GLN

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	129/125 (103%)	119 (92%)	10 (8%)	11 0

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13[A]	VAL
1	A	13[B]	VAL
1	A	86[A]	LEU
1	A	86[B]	LEU
1	A	87	LYS
1	A	89[A]	LEU
1	A	89[B]	LEU
1	A	109	GLU
1	A	145	LYS
1	A	152	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	116	HIS
1	A	152	GLN

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	$\# Z > 2$
3	HEM	A	155	1	50,50,50	1.96	15 (30%)	67,82,82	2.01	17 (25%)
2	SO4	A	154	-	4,4,4	0.55	0	6,6,6	0.81	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	155	1	-	4/14/54/54	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	HEM	FE-ND	4.70	2.09	1.94
3	A	155	HEM	C1A-NA	4.22	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	HEM	C4A-C3A	3.83	1.52	1.43
3	A	155	HEM	CHA-C4D	-3.77	1.30	1.38
3	A	155	HEM	C1D-ND	-3.50	1.32	1.38
3	A	155	HEM	O2D-CGD	-3.29	1.19	1.30
3	A	155	HEM	C3C-C2C	3.06	1.43	1.37
3	A	155	HEM	CMB-C2B	2.83	1.56	1.50
3	A	155	HEM	C4A-NA	2.76	1.44	1.39
3	A	155	HEM	FE-NC	2.55	2.03	1.95
3	A	155	HEM	CMA-C3A	2.34	1.55	1.50
3	A	155	HEM	CBA-CGA	2.25	1.55	1.50
3	A	155	HEM	C4D-ND	-2.16	1.36	1.40
3	A	155	HEM	CHD-C1D	2.06	1.43	1.39
3	A	155	HEM	C1D-C2D	2.00	1.48	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	155	HEM	C4C-C3C-C2C	-6.88	100.84	106.81
3	A	155	HEM	C2A-C1A-NA	-5.08	104.51	110.15
3	A	155	HEM	C1D-C2D-C3D	-4.87	101.86	106.98
3	A	155	HEM	C3B-C4B-NB	4.39	112.62	109.47
3	A	155	HEM	C1A-C2A-C3A	4.13	113.26	106.87
3	A	155	HEM	C2D-C1D-ND	4.10	114.65	109.90
3	A	155	HEM	O2A-CGA-O1A	2.57	129.93	123.33
3	A	155	HEM	CHC-C4B-NB	2.38	126.98	124.42
3	A	155	HEM	CHC-C4B-C3B	-2.34	120.40	125.07
3	A	155	HEM	CHD-C1D-C2D	-2.34	121.33	125.03
3	A	155	HEM	O2A-CGA-CBA	-2.31	106.70	114.00
3	A	155	HEM	C4A-NA-C1A	2.28	109.53	105.82
3	A	155	HEM	C3C-C2C-C1C	2.27	109.19	107.05
3	A	155	HEM	C3A-C4A-NA	-2.23	106.57	110.14
3	A	155	HEM	CMA-C3A-C2A	2.22	130.32	125.62
3	A	155	HEM	CHA-C1A-C2A	2.11	129.93	125.30
3	A	155	HEM	CHB-C4A-NA	2.10	127.67	123.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	155	HEM	CAD-CBD-CGD-O1D
3	A	155	HEM	CAD-CBD-CGD-O2D
3	A	155	HEM	CAA-CBA-CGA-O1A

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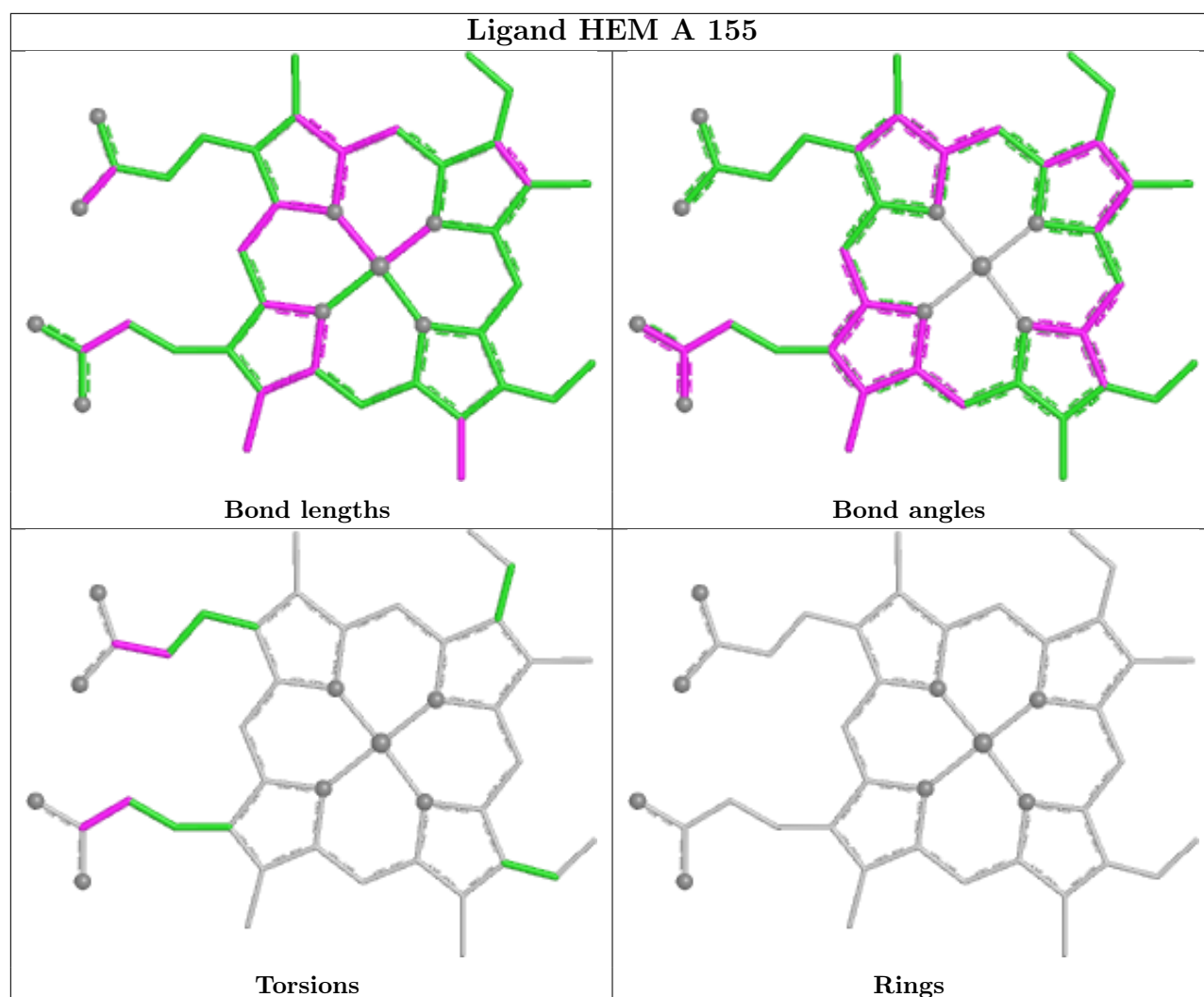
Mol	Chain	Res	Type	Atoms
3	A	155	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	155	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.