



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:50 AM UTC

PDB ID : 1QHU / pdb_00001qhu
Title : MAMMALIAN BLOOD SERUM HAEMOPEXIN DEGLYCOSYLATED
AND IN COMPLEX WITH ITS LIGAND HAEM
Authors : Paoli, M.; Baker, H.M.; Morgan, W.T.; Smith, A.; Baker, E.N.
Deposited on : 1999-05-27
Resolution : 2.30 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

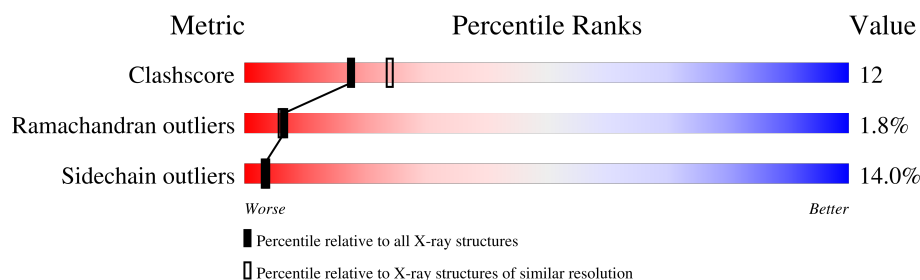
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	460	47% 26% 10% • 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	A	441	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3463 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 PROTEIN (HEMOPEXIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	1	0	0
			3199	2047	561	575	16			

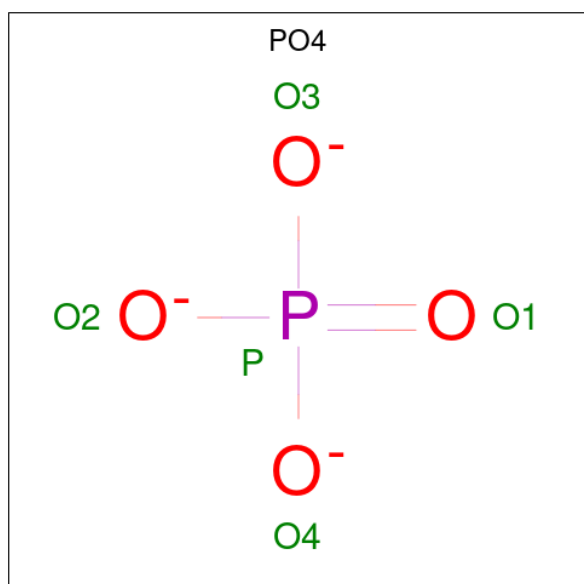
- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

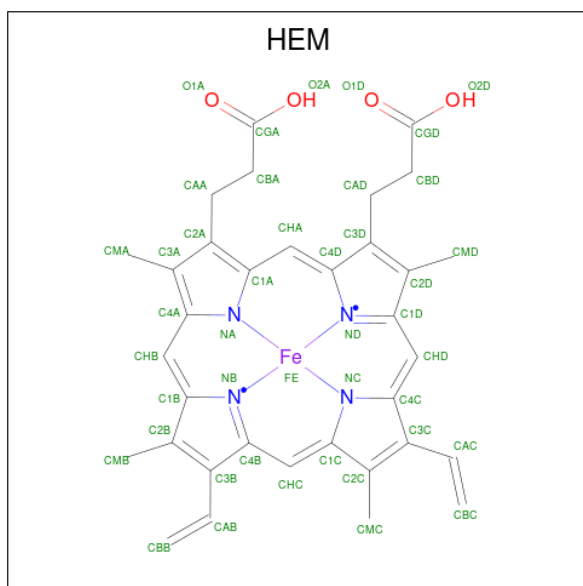
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Na	0	0
			4	4		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

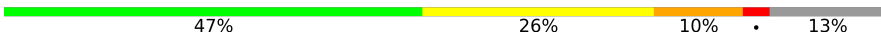


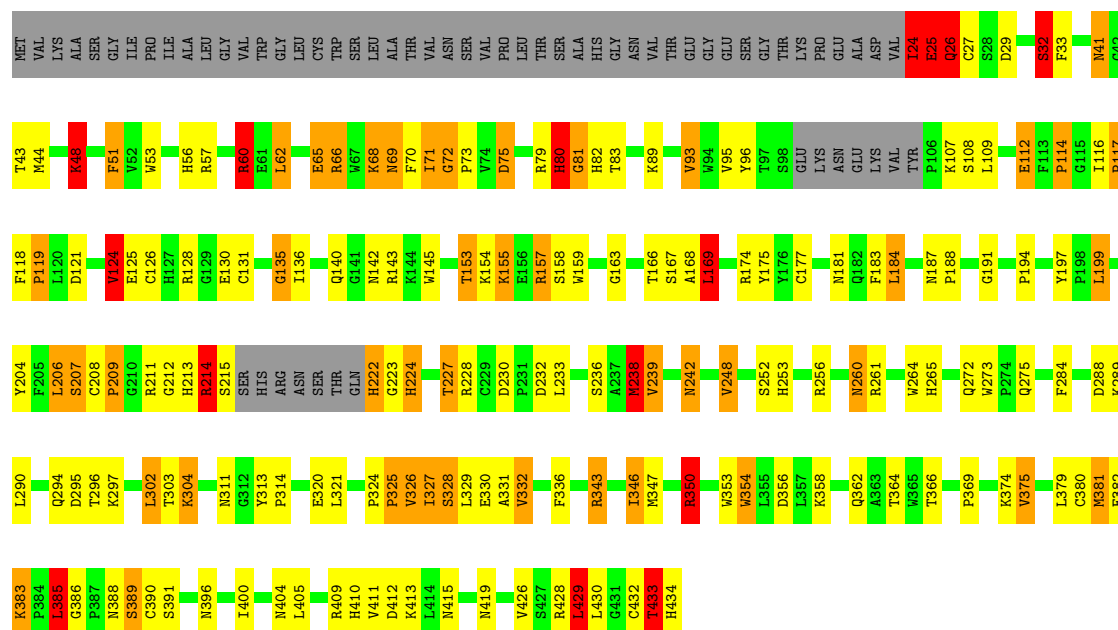
3 Residue-property plots

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: PROTEIN (HEMOPEXIN)

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	44.68 Å 61.95 Å 83.29 Å 90.00° 93.21° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	94.7 (20.00-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3463	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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: NA, HEM, PO4, CL

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	1.12	13/3307 (0.4%)	2.36	187/4498 (4.2%)

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	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	HIS	N-CA	14.27	1.64	1.46
1	A	223	GLY	N-CA	8.91	1.59	1.45
1	A	222	HIS	N-CA	-8.89	1.29	1.46
1	A	223	GLY	C-N	8.59	1.45	1.33
1	A	222	HIS	CA-C	8.10	1.70	1.52
1	A	214	ARG	CD-NE	7.13	1.56	1.46
1	A	223	GLY	CA-C	6.92	1.61	1.51
1	A	222	HIS	C-N	6.46	1.43	1.33
1	A	327	ILE	C-N	6.11	1.44	1.33
1	A	213	HIS	CA-C	6.00	1.60	1.52
1	A	434	HIS	C-O	-5.77	1.12	1.23
1	A	222	HIS	CA-CB	-5.76	1.42	1.53
1	A	434	HIS	C-OXT	-5.54	1.12	1.23

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ARG	O-C-N	-31.51	80.69	122.59
1	A	222	HIS	N-CA-CB	16.15	137.95	110.50
1	A	118	PHE	CA-C-O	-15.54	104.05	119.91
1	A	118	PHE	O-C-N	15.18	132.48	121.85
1	A	197	TYR	CA-C-O	-15.12	101.94	120.54
1	A	214	ARG	CA-C-O	-13.97	100.53	120.51
1	A	313	TYR	CA-C-O	-13.90	106.37	120.97
1	A	343	ARG	NE-CZ-NH2	-13.60	106.96	119.20
1	A	343	ARG	NE-CZ-NH1	13.33	134.83	121.50
1	A	331	ALA	CA-C-O	11.14	133.19	121.38
1	A	197	TYR	O-C-N	10.32	133.57	121.39
1	A	223	GLY	CA-C-N	10.11	134.65	120.29
1	A	223	GLY	C-N-CA	10.11	134.65	120.29
1	A	25	GLU	CB-CG-CD	9.33	128.46	112.60
1	A	350	ARG	CD-NE-CZ	9.20	137.28	124.40
1	A	410	HIS	CA-CB-CG	-9.17	104.63	113.80
1	A	346	ILE	CB-CA-C	9.16	123.71	110.33
1	A	215	SER	CA-C-O	-9.12	105.30	120.80
1	A	181	ASN	CA-CB-CG	8.98	121.58	112.60
1	A	288	ASP	CA-CB-CG	8.78	121.38	112.60
1	A	169	LEU	CA-CB-CG	8.52	146.12	116.30
1	A	325	PRO	O-C-N	8.39	133.71	122.30
1	A	142	ASN	OD1-CG-ND2	-8.38	114.22	122.60
1	A	428	ARG	CD-NE-CZ	8.32	136.05	124.40
1	A	112	GLU	CB-CG-CD	8.27	126.66	112.60
1	A	207	SER	N-CA-CB	8.08	123.05	110.21
1	A	224	HIS	N-CA-C	7.88	119.95	111.36
1	A	311	ASN	CA-CB-CG	7.78	120.38	112.60
1	A	410	HIS	O-C-N	7.67	131.02	123.04
1	A	256	ARG	NH1-CZ-NH2	7.47	129.01	119.30
1	A	131	CYS	N-CA-C	-7.45	99.19	110.14
1	A	412	ASP	CA-CB-CG	7.36	119.96	112.60
1	A	130	GLU	CA-C-O	7.31	128.62	119.78
1	A	369	PRO	CA-C-O	-7.29	112.96	121.86
1	A	119	PRO	N-CA-CB	7.28	110.61	102.60
1	A	336	PHE	CA-CB-CG	7.24	121.04	113.80
1	A	214	ARG	NE-CZ-NH2	7.20	125.68	119.20
1	A	336	PHE	CA-C-N	7.20	133.05	123.11
1	A	336	PHE	C-N-CA	7.20	133.05	123.11
1	A	191	GLY	CA-C-O	7.10	127.01	119.06
1	A	347	MET	CA-C-O	-7.09	113.05	120.70
1	A	214	ARG	N-CA-C	7.08	125.88	110.80
1	A	116	ILE	CA-C-N	7.08	127.04	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ILE	C-N-CA	7.08	127.04	120.03
1	A	389	SER	O-C-N	-7.06	115.03	122.94
1	A	48	LYS	CA-CB-CG	7.03	128.16	114.10
1	A	187	ASN	OD1-CG-ND2	-7.02	115.58	122.60
1	A	381	MET	CA-C-N	7.02	130.25	120.29
1	A	381	MET	C-N-CA	7.02	130.25	120.29
1	A	256	ARG	NE-CZ-NH2	-7.00	112.90	119.20
1	A	33	PHE	CA-C-N	6.98	130.21	120.29
1	A	33	PHE	C-N-CA	6.98	130.21	120.29
1	A	429	LEU	N-CA-CB	6.95	121.93	110.39
1	A	211	ARG	NE-CZ-NH2	-6.93	112.97	119.20
1	A	238	MET	CA-C-N	6.91	131.56	122.51
1	A	238	MET	C-N-CA	6.91	131.56	122.51
1	A	343	ARG	CA-CB-CG	6.88	127.87	114.10
1	A	212	GLY	CA-C-O	-6.88	114.67	121.48
1	A	41	ASN	OD1-CG-ND2	6.87	129.47	122.60
1	A	65	GLU	CB-CG-CD	6.83	124.21	112.60
1	A	32	SER	CA-CB-OG	-6.75	97.59	111.10
1	A	239	VAL	CB-CA-C	-6.73	98.37	110.48
1	A	167	SER	N-CA-CB	6.70	122.82	111.57
1	A	24	ILE	CA-C-O	-6.65	109.50	120.80
1	A	204	TYR	N-CA-C	6.64	121.23	112.72
1	A	433	THR	N-CA-C	6.64	124.94	110.80
1	A	130	GLU	N-CA-C	-6.63	104.84	113.12
1	A	330	GLU	CA-C-O	6.58	126.38	119.14
1	A	214	ARG	CA-C-N	6.58	133.53	121.70
1	A	214	ARG	C-N-CA	6.58	133.53	121.70
1	A	169	LEU	N-CA-C	6.57	118.84	108.79
1	A	95	VAL	N-CA-CB	-6.56	103.12	110.99
1	A	187	ASN	CB-CA-C	6.55	118.82	109.38
1	A	354	TRP	CA-C-N	6.55	133.08	121.75
1	A	354	TRP	C-N-CA	6.55	133.08	121.75
1	A	385	LEU	N-CA-C	-6.54	96.42	107.99
1	A	253	HIS	CA-CB-CG	6.43	120.23	113.80
1	A	230	ASP	CA-C-N	6.42	126.34	119.28
1	A	230	ASP	C-N-CA	6.42	126.34	119.28
1	A	236	SER	O-C-N	-6.39	114.85	122.27
1	A	388	ASN	N-CA-C	6.39	119.31	108.90
1	A	327	ILE	N-CA-CB	-6.36	100.46	110.96
1	A	60	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	A	222	HIS	O-C-N	-6.30	112.92	123.00
1	A	66	ARG	CD-NE-CZ	6.29	133.20	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	PRO	CB-CA-C	-6.27	102.73	110.95
1	A	181	ASN	N-CA-C	-6.27	105.50	113.02
1	A	227	THR	CA-CB-OG1	-6.26	100.20	109.60
1	A	302	LEU	CA-C-O	-6.26	114.74	121.56
1	A	128	ARG	NE-CZ-NH2	-6.19	113.63	119.20
1	A	426	VAL	CA-C-O	-6.14	114.72	121.29
1	A	432	CYS	N-CA-C	6.11	118.41	110.53
1	A	214	ARG	NH1-CZ-NH2	-6.09	111.38	119.30
1	A	213	HIS	CA-C-N	6.09	133.17	121.54
1	A	213	HIS	C-N-CA	6.09	133.17	121.54
1	A	415	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	A	26	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	A	223	GLY	O-C-N	6.05	130.09	122.28
1	A	80	HIS	CA-CB-CG	-6.03	107.77	113.80
1	A	26	GLN	CB-CG-CD	6.03	122.86	112.60
1	A	66	ARG	N-CA-C	-6.02	104.67	112.68
1	A	432	CYS	CA-C-N	6.02	133.04	121.54
1	A	432	CYS	C-N-CA	6.02	133.04	121.54
1	A	81	GLY	N-CA-C	-5.97	107.00	115.30
1	A	329	LEU	N-CA-C	5.97	118.92	109.96
1	A	166	THR	N-CA-C	-5.96	106.01	113.28
1	A	248	VAL	N-CA-C	-5.93	100.53	108.35
1	A	332	VAL	N-CA-CB	-5.91	101.42	112.36
1	A	79	ARG	NE-CZ-NH2	5.91	124.51	119.20
1	A	214	ARG	N-CA-CB	-5.89	100.53	110.49
1	A	354	TRP	O-C-N	-5.89	115.74	123.16
1	A	124	VAL	CB-CA-C	-5.87	100.33	110.65
1	A	313	TYR	O-C-N	5.87	128.31	121.21
1	A	326	VAL	N-CA-C	5.86	120.62	112.35
1	A	374	LYS	CA-C-O	-5.81	114.49	120.99
1	A	289	LYS	N-CA-C	5.79	119.49	110.17
1	A	430	LEU	CA-C-O	5.79	126.71	119.59
1	A	56	HIS	CA-C-O	-5.78	113.32	119.97
1	A	119	PRO	CA-N-CD	-5.78	103.41	111.50
1	A	428	ARG	CA-C-O	-5.76	113.34	119.97
1	A	43	THR	CA-C-N	5.76	129.74	121.50
1	A	43	THR	C-N-CA	5.76	129.74	121.50
1	A	44	MET	CA-C-O	-5.73	114.16	120.69
1	A	136	ILE	O-C-N	5.73	129.53	123.00
1	A	288	ASP	N-CA-C	-5.71	106.21	112.72
1	A	426	VAL	N-CA-C	-5.71	104.76	110.30
1	A	112	GLU	N-CA-CB	-5.68	101.72	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	VAL	N-CA-CB	-5.66	101.90	112.36
1	A	125	GLU	CB-CG-CD	5.65	122.20	112.60
1	A	386	GLY	CA-C-N	5.62	125.31	119.64
1	A	386	GLY	C-N-CA	5.62	125.31	119.64
1	A	79	ARG	CA-C-N	-5.60	112.92	122.33
1	A	79	ARG	C-N-CA	-5.60	112.92	122.33
1	A	124	VAL	N-CA-CB	5.59	121.47	111.63
1	A	126	CYS	CA-CB-SG	-5.58	101.57	114.40
1	A	75	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	320	GLU	CB-CG-CD	5.55	122.04	112.60
1	A	419	ASN	CA-CB-CG	5.55	118.15	112.60
1	A	174	ARG	CD-NE-CZ	5.51	132.11	124.40
1	A	199	LEU	CA-C-O	-5.50	115.19	121.68
1	A	353	TRP	O-C-N	-5.48	116.50	123.24
1	A	121	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	350	ARG	CA-C-O	-5.43	113.31	119.78
1	A	332	VAL	CB-CA-C	5.43	119.47	110.30
1	A	51	PHE	N-CA-C	5.42	118.11	110.14
1	A	314	PRO	N-CA-CB	5.42	108.56	102.60
1	A	96	TYR	N-CA-C	5.41	117.49	108.02
1	A	183	PHE	CA-CB-CG	5.40	119.20	113.80
1	A	72	GLY	O-C-N	5.32	127.09	121.77
1	A	380	CYS	CA-C-N	5.30	131.32	121.62
1	A	380	CYS	C-N-CA	5.30	131.32	121.62
1	A	153	THR	N-CA-C	5.30	117.73	109.52
1	A	275	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	A	325	PRO	CA-C-N	5.29	129.02	120.82
1	A	325	PRO	C-N-CA	5.29	129.02	120.82
1	A	366	THR	CA-C-N	5.28	128.85	121.24
1	A	366	THR	C-N-CA	5.28	128.85	121.24
1	A	131	CYS	N-CA-CB	5.28	118.57	110.70
1	A	211	ARG	NH1-CZ-NH2	5.28	126.16	119.30
1	A	303	THR	CA-C-N	5.27	131.61	121.54
1	A	303	THR	C-N-CA	5.27	131.61	121.54
1	A	214	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	A	207	SER	CA-C-O	5.24	126.19	120.58
1	A	433	THR	CB-CA-C	-5.23	100.01	110.42
1	A	25	GLU	N-CA-C	5.22	121.92	110.80
1	A	121	ASP	CA-C-O	-5.22	113.52	119.41
1	A	29	ASP	CA-C-O	-5.21	116.03	121.55
1	A	232	ASP	CB-CA-C	5.17	119.47	110.94
1	A	284	PHE	CA-CB-CG	5.17	118.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	TRP	CA-C-N	5.16	124.65	119.19
1	A	273	TRP	C-N-CA	5.16	124.65	119.19
1	A	419	ASN	O-C-N	5.12	129.37	123.17
1	A	135	GLY	O-C-N	-5.12	116.04	122.70
1	A	328	SER	CB-CA-C	5.09	119.97	111.22
1	A	140	GLN	CA-C-O	-5.08	113.85	120.25
1	A	404	ASN	N-CA-C	5.08	117.77	109.59
1	A	364	THR	CA-C-O	-5.08	114.93	120.36
1	A	206	LEU	CA-C-O	-5.07	115.22	120.70
1	A	353	TRP	CA-CB-CG	5.07	123.23	113.60
1	A	326	VAL	O-C-N	5.07	129.64	122.04
1	A	136	ILE	CA-C-O	-5.06	115.92	121.28
1	A	214	ARG	CG-CD-NE	-5.05	100.89	112.00
1	A	114	PRO	N-CA-C	5.03	119.46	111.26
1	A	272	GLN	CA-C-N	5.03	130.25	123.46
1	A	272	GLN	C-N-CA	5.03	130.25	123.46
1	A	242	ASN	CA-C-O	5.03	125.59	119.05
1	A	389	SER	CA-CB-OG	5.01	121.11	111.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	ARG	Peptide,Mainchain

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	3199	0	3034	74	0
2	A	2	0	0	0	0
3	A	4	0	0	0	0
4	A	5	0	0	2	0
5	A	43	0	30	6	0
6	A	210	0	0	8	0
All	All	3463	0	3064	78	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 12.

All (78) 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:379:LEU:HA	4:A:441:PO4:O2	1.62	0.99
1:A:227:THR:HG22	1:A:233:LEU:HD13	1.56	0.85
1:A:26:GLN:HE21	1:A:26:GLN:H	1.27	0.81
1:A:326:VAL:HG23	1:A:327:ILE:HD12	1.65	0.78
1:A:302:LEU:HB3	1:A:304:LYS:HE2	1.70	0.72
1:A:68:LYS:O	1:A:69:ASN:HB3	1.90	0.69
1:A:214:ARG:HG2	5:A:500:HEM:CBC	2.23	0.69
1:A:73:PRO:HD2	1:A:89:LYS:HE3	1.75	0.68
1:A:326:VAL:CG2	1:A:327:ILE:HD12	2.23	0.68
1:A:324:PRO:HB2	1:A:326:VAL:HG22	1.76	0.68
1:A:383:LYS:HE2	6:A:709:HOH:O	1.93	0.67
1:A:326:VAL:HG23	1:A:327:ILE:HB	1.77	0.66
1:A:379:LEU:HD12	4:A:441:PO4:O2	1.95	0.66
1:A:214:ARG:HG2	5:A:500:HEM:HBC2	1.78	0.65
1:A:409:ARG:HD2	6:A:555:HOH:O	1.99	0.62
1:A:381:MET:HE2	1:A:385:LEU:HD13	1.81	0.62
1:A:389:SER:HB3	1:A:396:ASN:HD21	1.67	0.60
1:A:26:GLN:H	1:A:26:GLN:NE2	1.96	0.59
5:A:500:HEM:HBB2	5:A:500:HEM:HMB2	1.85	0.59
1:A:328:SER:HB3	6:A:556:HOH:O	2.02	0.58
1:A:117:PRO:HG2	1:A:145:TRP:CH2	2.37	0.58
1:A:325:PRO:HD2	1:A:326:VAL:HG13	1.86	0.56
1:A:326:VAL:HG23	1:A:327:ILE:CD1	2.34	0.56
5:A:500:HEM:HBC2	5:A:500:HEM:HHD	1.88	0.55
1:A:222:HIS:CD2	1:A:224:HIS:H	2.26	0.54
1:A:326:VAL:HG23	1:A:327:ILE:CB	2.38	0.54
5:A:500:HEM:HBB2	5:A:500:HEM:CMB	2.39	0.52
1:A:80:HIS:HE1	1:A:135:GLY:O	1.94	0.51
1:A:390:CYS:O	1:A:409:ARG:HD3	2.13	0.48
1:A:68:LYS:HE3	6:A:627:HOH:O	2.13	0.48
1:A:124:VAL:HG22	1:A:168:ALA:HB1	1.95	0.48
1:A:177:CYS:HB3	1:A:184:LEU:HD12	1.96	0.47
1:A:350:ARG:HG2	1:A:350:ARG:HH11	1.79	0.47
1:A:326:VAL:HG23	1:A:327:ILE:CG1	2.44	0.47
1:A:32:SER:N	6:A:620:HOH:O	2.48	0.47
1:A:68:LYS:O	1:A:69:ASN:CB	2.60	0.47
1:A:391:SER:H	1:A:396:ASN:ND2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:THR:O	1:A:296:THR:HG22	2.15	0.47
1:A:70:PHE:C	1:A:71:ILE:HD13	2.40	0.47
1:A:238:MET:HE2	1:A:400:ILE:HG12	1.96	0.46
1:A:391:SER:H	1:A:396:ASN:HD21	1.64	0.46
1:A:24:ILE:O	1:A:27:CYS:HB2	2.16	0.46
1:A:343:ARG:HG2	1:A:354:TRP:CE3	2.51	0.46
1:A:82:HIS:CE1	1:A:261:ARG:HG2	2.51	0.45
1:A:51:PHE:CZ	1:A:62:LEU:HD13	2.52	0.45
1:A:294:GLN:HE21	1:A:297:LYS:NZ	2.15	0.45
1:A:124:VAL:HG22	1:A:168:ALA:CB	2.47	0.45
1:A:143:ARG:HH21	1:A:145:TRP:HZ2	1.65	0.45
1:A:53:TRP:CE2	1:A:60:ARG:HG3	2.52	0.44
1:A:325:PRO:CD	1:A:326:VAL:HG13	2.46	0.44
1:A:53:TRP:NE1	1:A:60:ARG:HG3	2.32	0.44
1:A:93:VAL:HG22	1:A:109:LEU:HD13	1.98	0.44
1:A:60:ARG:HE	1:A:60:ARG:HB3	1.63	0.44
1:A:124:VAL:HG13	1:A:169:LEU:HA	2.00	0.44
1:A:157:ARG:HG2	1:A:159:TRP:CE2	2.53	0.44
1:A:70:PHE:O	1:A:71:ILE:HD13	2.17	0.43
1:A:390:CYS:H	1:A:396:ASN:ND2	2.16	0.43
1:A:194:PRO:HG3	6:A:662:HOH:O	2.17	0.43
1:A:48:LYS:HZ2	1:A:48:LYS:HG2	1.66	0.43
1:A:242:ASN:HD22	1:A:242:ASN:H	1.66	0.43
1:A:153:THR:HB	1:A:155:LYS:NZ	2.33	0.43
1:A:75:ASP:OD2	1:A:119:PRO:HB3	2.19	0.43
1:A:383:LYS:HG2	6:A:509:HOH:O	2.19	0.43
1:A:260:ASN:HB2	1:A:264:TRP:CZ2	2.53	0.43
1:A:356:ASP:OD1	1:A:358:LYS:HB2	2.19	0.42
1:A:51:PHE:CE2	1:A:62:LEU:HD13	2.54	0.42
1:A:208:CYS:HA	1:A:209:PRO:HD3	1.70	0.42
1:A:242:ASN:H	1:A:242:ASN:ND2	2.17	0.42
1:A:405:LEU:HD22	1:A:429:LEU:HD23	2.01	0.42
1:A:112:GLU:C	1:A:114:PRO:HD3	2.44	0.42
1:A:175:TYR:CE1	1:A:188:PRO:HG3	2.54	0.42
1:A:41:ASN:HD22	1:A:261:ARG:HH21	1.69	0.41
5:A:500:HEM:HAD1	6:A:584:HOH:O	2.20	0.41
1:A:81:GLY:O	1:A:83:THR:HG23	2.19	0.41
1:A:71:ILE:HG22	1:A:72:GLY:N	2.35	0.40
1:A:222:HIS:NE2	1:A:224:HIS:HB3	2.36	0.40
1:A:175:TYR:CD1	1:A:188:PRO:HG3	2.56	0.40
1:A:222:HIS:CD2	1:A:224:HIS:N	2.89	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	392/460 (85%)	369 (94%)	16 (4%)	7 (2%)	6 6

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	THR
1	A	163	GLY
1	A	214	ARG
1	A	25	GLU
1	A	69	ASN
1	A	265	HIS
1	A	295	ASP

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	342/393 (87%)	294 (86%)	48 (14%)	3 3

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE

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Mol	Chain	Res	Type
1	A	25	GLU
1	A	26	GLN
1	A	32	SER
1	A	48	LYS
1	A	57	ARG
1	A	60	ARG
1	A	62	LEU
1	A	65	GLU
1	A	66	ARG
1	A	68	LYS
1	A	71	ILE
1	A	80	HIS
1	A	93	VAL
1	A	107	LYS
1	A	108	SER
1	A	124	VAL
1	A	154	LYS
1	A	155	LYS
1	A	157	ARG
1	A	158	SER
1	A	169	LEU
1	A	184	LEU
1	A	199	LEU
1	A	206	LEU
1	A	207	SER
1	A	209	PRO
1	A	228	ARG
1	A	238	MET
1	A	239	VAL
1	A	248	VAL
1	A	252	SER
1	A	260	ASN
1	A	290	LEU
1	A	304	LYS
1	A	321	LEU
1	A	332	VAL
1	A	346	ILE
1	A	350	ARG
1	A	362	GLN
1	A	375	VAL
1	A	382	GLU
1	A	383	LYS

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Mol	Chain	Res	Type
1	A	385	LEU
1	A	411	VAL
1	A	413	LYS
1	A	429	LEU
1	A	433	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	41	ASN
1	A	80	HIS
1	A	127	HIS
1	A	242	ASN
1	A	253	HIS
1	A	271	HIS
1	A	272	GLN
1	A	294	GLN
1	A	396	ASN
1	A	401	HIS
1	A	415	ASN
1	A	422	GLN
1	A	424	GLN
1	A	434	HIS

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

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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
5	HEM	A	500	1	50,50,50	1.28	6 (12%)	67,82,82	1.35	8 (11%)
4	PO4	A	441	3	4,4,4	1.82	2 (50%)	6,6,6	1.60	1 (16%)

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
5	HEM	A	500	1	-	4/14/54/54	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	HEM	FE-NA	2.49	2.03	1.95
4	A	441	PO4	P-O2	-2.49	1.47	1.54
5	A	500	HEM	CMB-C2B	2.41	1.55	1.50
5	A	500	HEM	CMC-C2C	2.35	1.55	1.50
5	A	500	HEM	CMD-C2D	2.27	1.55	1.50
4	A	441	PO4	P-O4	-2.23	1.48	1.54
5	A	500	HEM	CAC-C3C	2.18	1.53	1.47
5	A	500	HEM	CAB-C3B	2.09	1.53	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	500	HEM	CHB-C1B-NB	3.93	129.23	124.37
5	A	500	HEM	O2A-CGA-O1A	3.42	132.13	123.33
4	A	441	PO4	O4-P-O1	3.18	122.19	110.95
5	A	500	HEM	C4A-CHB-C1B	-2.76	119.75	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	500	HEM	CHB-C4A-NA	2.58	128.54	123.86
5	A	500	HEM	CBA-CAA-C2A	2.35	119.03	112.53
5	A	500	HEM	O2A-CGA-CBA	-2.18	107.13	114.00
5	A	500	HEM	C4C-C3C-C2C	2.16	108.69	106.81
5	A	500	HEM	C2D-C1D-ND	-2.15	107.42	109.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

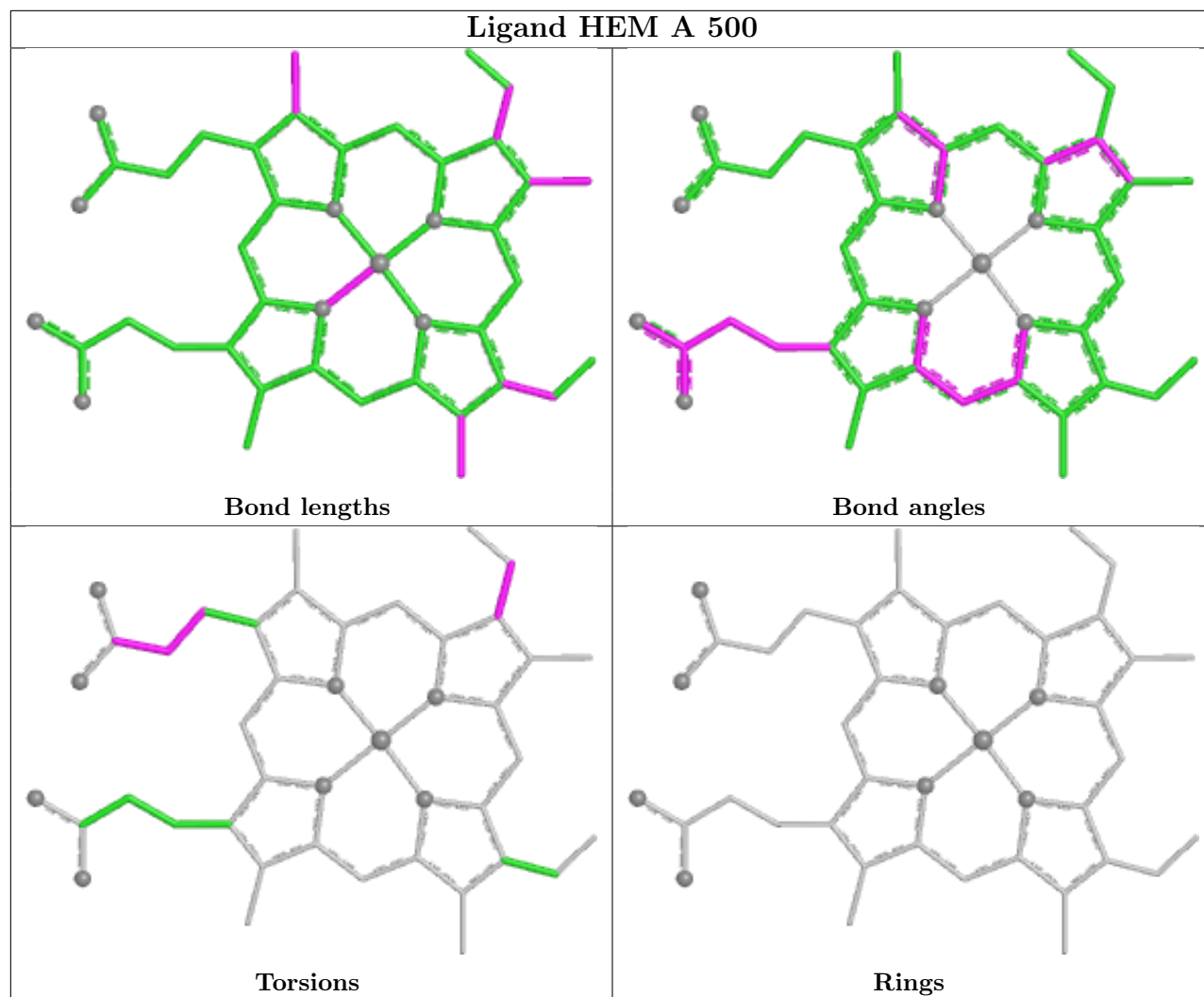
Mol	Chain	Res	Type	Atoms
5	A	500	HEM	C3D-CAD-CBD-CGD
5	A	500	HEM	C4C-C3C-CAC-CBC
5	A	500	HEM	CAD-CBD-CGD-O2D
5	A	500	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	500	HEM	6	0
4	A	441	PO4	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.