



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:11 PM UTC

PDB ID : 1YMB / pdb_00001ymb
Title : HIGH RESOLUTION STUDY OF THE THREE-DIMENSIONAL STRUCTURE OF HORSE HEART METMYOGLOBIN
Authors : Evans, S.V.; Brayer, G.D.
Deposited on : 1993-09-27
Resolution : 1.90 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

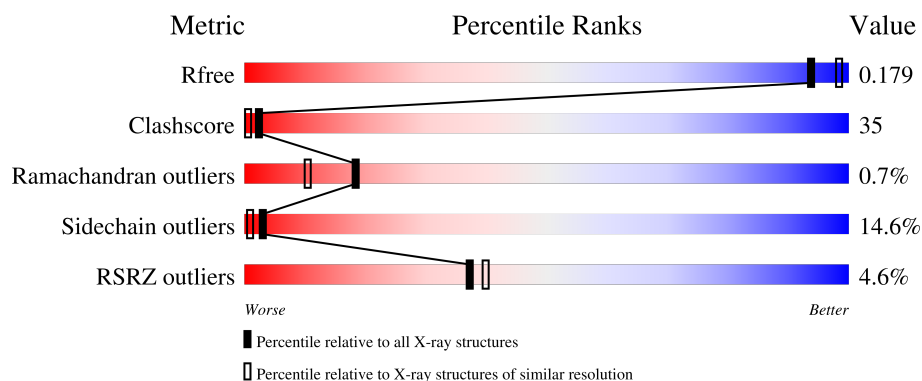
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	153	5% 25% 45% 25% 5%

2 Entry composition [i](#)

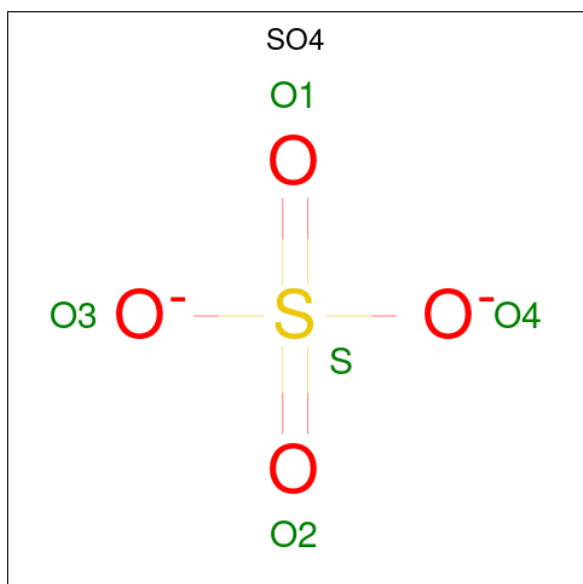
There are 4 unique types of molecules in this entry. The entry contains 1401 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 METMYOGLOBIN.

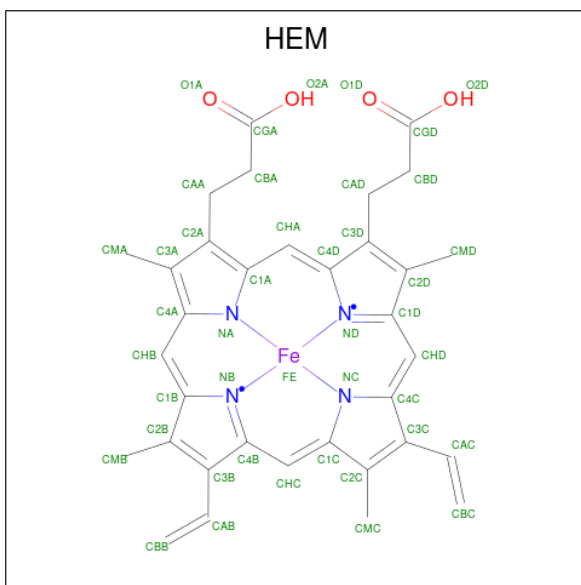
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1199	769	210	218	2	0	0	0

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



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

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	154	Total O 154 154	0	0

- Molecule 1: METMYOGLOBIN

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.27Å 28.92Å 35.93Å 90.00° 107.10° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90 61.43 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90) 85.5 (61.43-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.90Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.155 , (Not available) 0.220 , 0.179	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.045 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	1401	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.85	15/1226 (1.2%)	2.80	128/1645 (7.8%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	LYS	C-O	6.99	1.32	1.24
1	A	143	ALA	C-N	-6.56	1.25	1.33
1	A	64	HIS	N-CA	6.52	1.54	1.46
1	A	74	GLY	C-O	6.51	1.31	1.23
1	A	134	ALA	N-CA	6.00	1.54	1.46
1	A	93	HIS	ND1-CE1	5.99	1.38	1.32
1	A	100	PRO	C-O	5.92	1.30	1.23
1	A	129	GLY	C-O	5.81	1.30	1.23
1	A	132	THR	CB-OG1	5.71	1.52	1.43
1	A	116	HIS	ND1-CE1	5.51	1.38	1.32
1	A	81	HIS	ND1-CE1	5.43	1.38	1.32
1	A	37	PRO	C-O	5.34	1.31	1.24
1	A	44	ASP	C-N	-5.32	1.25	1.33
1	A	86	LEU	N-CA	5.15	1.52	1.46
1	A	88	PRO	C-N	-5.05	1.27	1.33

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ASN	CA-CB-CG	17.54	130.14	112.60
1	A	123	PHE	CA-CB-CG	10.82	124.62	113.80
1	A	140	ASN	OD1-CG-ND2	-10.68	111.92	122.60
1	A	102	LYS	CB-CG-CD	10.47	135.39	111.30
1	A	147	LYS	O-C-N	10.44	132.89	122.03
1	A	151	PHE	CA-CB-CG	10.07	123.87	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	HIS	CA-CB-CG	-9.72	104.08	113.80
1	A	105	GLU	CA-C-O	9.68	130.67	120.70
1	A	44	ASP	CA-CB-CG	9.66	122.27	112.60
1	A	114	VAL	CA-C-O	-9.45	111.44	121.27
1	A	142	ILE	N-CA-C	-9.37	101.43	110.42
1	A	113	HIS	CA-C-O	9.34	130.80	121.00
1	A	106	PHE	CA-CB-CG	9.16	122.96	113.80
1	A	58	SER	N-CA-C	9.13	122.82	108.67
1	A	44	ASP	CA-C-N	8.83	137.20	121.66
1	A	44	ASP	C-N-CA	8.83	137.20	121.66
1	A	41	GLU	CB-CG-CD	8.82	127.60	112.60
1	A	26	GLN	OE1-CD-NE2	8.63	131.23	122.60
1	A	51	THR	CA-C-O	8.55	131.27	121.87
1	A	99	ILE	CB-CG1-CD1	8.11	130.82	113.80
1	A	86	LEU	CB-CA-C	8.00	125.76	109.67
1	A	125	ALA	CA-C-O	-7.97	112.45	120.82
1	A	138	PHE	CA-C-N	7.85	130.65	120.44
1	A	138	PHE	C-N-CA	7.85	130.65	120.44
1	A	122	ASP	CA-CB-CG	7.75	120.35	112.60
1	A	83	GLU	CA-C-O	7.58	129.02	120.90
1	A	4	ASP	O-C-N	7.42	129.71	122.07
1	A	148	GLU	CA-CB-CG	7.42	128.94	114.10
1	A	29	LEU	CB-CA-C	7.34	122.41	110.88
1	A	115	LEU	CA-C-N	-7.27	110.75	120.63
1	A	115	LEU	C-N-CA	-7.27	110.75	120.63
1	A	112	ILE	CA-C-O	-7.21	113.20	120.85
1	A	61	LEU	CA-C-N	7.15	129.73	120.44
1	A	61	LEU	C-N-CA	7.15	129.73	120.44
1	A	66	THR	CA-C-O	-7.14	113.33	120.82
1	A	41	GLU	CA-CB-CG	7.13	128.37	114.10
1	A	83	GLU	CB-CG-CD	7.09	124.66	112.60
1	A	111	ILE	CB-CA-C	7.07	121.02	111.97
1	A	46	PHE	CA-CB-CG	7.06	120.86	113.80
1	A	33	PHE	CA-C-O	-7.03	111.88	119.97
1	A	88	PRO	CA-C-N	6.95	130.16	120.29
1	A	88	PRO	C-N-CA	6.95	130.16	120.29
1	A	132	THR	CA-C-N	6.91	129.54	120.28
1	A	132	THR	C-N-CA	6.91	129.54	120.28
1	A	32	LEU	O-C-N	6.87	129.14	122.07
1	A	27	GLU	CA-C-O	-6.80	113.34	120.55
1	A	21	ILE	O-C-N	6.75	128.42	121.87
1	A	98	LYS	CA-C-O	6.71	130.46	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	LEU	CA-C-N	6.67	129.93	120.53
1	A	29	LEU	C-N-CA	6.67	129.93	120.53
1	A	94	ALA	CA-C-N	6.62	131.89	120.58
1	A	94	ALA	C-N-CA	6.62	131.89	120.58
1	A	52	GLU	CB-CG-CD	6.56	123.75	112.60
1	A	4	ASP	N-CA-C	-6.53	104.09	111.07
1	A	75	ILE	CB-CA-C	6.50	120.30	111.97
1	A	4	ASP	N-CA-CB	6.49	119.42	110.01
1	A	147	LYS	N-CA-C	-6.48	103.91	110.97
1	A	116	HIS	N-CA-CB	6.41	119.27	109.98
1	A	90	ALA	CA-C-N	6.32	128.99	120.65
1	A	90	ALA	C-N-CA	6.32	128.99	120.65
1	A	111	ILE	N-CA-C	-6.30	104.38	110.42
1	A	98	LYS	O-C-N	-6.29	115.13	122.86
1	A	132	THR	CA-CB-CG2	6.28	121.18	110.50
1	A	109	ASP	N-CA-C	-6.28	104.53	111.82
1	A	22	ALA	N-CA-C	-6.27	104.55	111.82
1	A	22	ALA	CA-C-N	6.25	126.87	120.00
1	A	22	ALA	C-N-CA	6.25	126.87	120.00
1	A	31	ARG	CA-C-O	6.21	127.00	120.42
1	A	148	GLU	CB-CG-CD	6.20	123.14	112.60
1	A	132	THR	CA-CB-OG1	-6.19	100.31	109.60
1	A	31	ARG	NE-CZ-NH1	6.19	127.69	121.50
1	A	82	HIS	CA-C-N	6.16	128.85	120.54
1	A	82	HIS	C-N-CA	6.16	128.85	120.54
1	A	145	LYS	CB-CG-CD	6.09	125.30	111.30
1	A	33	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	36	HIS	CA-C-N	5.98	126.41	119.47
1	A	36	HIS	C-N-CA	5.98	126.41	119.47
1	A	75	ILE	CA-CB-CG2	5.98	120.67	110.50
1	A	37	PRO	N-CD-CG	-5.98	94.23	103.20
1	A	82	HIS	N-CA-C	5.95	120.14	112.41
1	A	73	GLY	CA-C-N	5.92	126.67	119.99
1	A	73	GLY	C-N-CA	5.92	126.67	119.99
1	A	29	LEU	O-C-N	-5.88	116.02	122.07
1	A	27	GLU	CG-CD-OE2	5.86	131.88	118.40
1	A	94	ALA	O-C-N	-5.86	115.70	122.03
1	A	133	LYS	N-CA-C	5.86	117.67	111.28
1	A	145	LYS	CA-CB-CG	5.83	125.76	114.10
1	A	140	ASN	CA-C-O	-5.79	114.42	120.55
1	A	146	TYR	CA-C-N	5.78	128.28	120.65
1	A	146	TYR	C-N-CA	5.78	128.28	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	GLN	CB-CG-CD	5.77	122.41	112.60
1	A	128	GLN	CB-CA-C	-5.77	101.22	110.79
1	A	10	VAL	CA-CB-CG2	5.74	120.16	110.40
1	A	6	GLU	CB-CG-CD	5.73	122.35	112.60
1	A	134	ALA	CA-C-O	-5.72	113.04	119.79
1	A	81	HIS	N-CA-C	-5.66	101.74	109.71
1	A	29	LEU	N-CA-CB	-5.65	101.81	110.01
1	A	31	ARG	NE-CZ-NH2	-5.65	114.12	119.20
1	A	108	SER	CA-C-O	-5.64	114.45	120.42
1	A	128	GLN	O-C-N	5.62	128.07	122.12
1	A	9	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	A	26	GLN	CG-CD-NE2	-5.51	108.14	116.40
1	A	134	ALA	N-CA-C	-5.44	105.38	112.23
1	A	58	SER	N-CA-CB	-5.38	101.33	109.94
1	A	109	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	70	THR	CB-CA-C	5.38	120.00	110.85
1	A	114	VAL	O-C-N	5.37	127.31	121.94
1	A	21	ILE	N-CA-C	5.34	116.06	110.62
1	A	18	GLU	CB-CG-CD	5.27	121.56	112.60
1	A	45	LYS	CA-C-N	-5.26	113.93	121.98
1	A	45	LYS	C-N-CA	-5.26	113.93	121.98
1	A	25	GLY	O-C-N	5.26	127.23	122.18
1	A	109	ASP	N-CA-CB	5.26	118.43	110.28
1	A	128	GLN	CB-CG-CD	5.18	121.41	112.60
1	A	70	THR	N-CA-C	-5.17	105.73	111.36
1	A	94	ALA	N-CA-C	5.14	116.74	111.03
1	A	111	ILE	CB-CG1-CD1	5.11	124.52	113.80
1	A	21	ILE	CA-C-N	-5.09	112.58	120.31
1	A	21	ILE	C-N-CA	-5.09	112.58	120.31
1	A	83	GLU	CA-CB-CG	5.09	124.27	114.10
1	A	87	LYS	CA-C-O	-5.08	113.20	120.16
1	A	46	PHE	CA-C-N	5.05	127.75	120.38
1	A	46	PHE	C-N-CA	5.05	127.75	120.38
1	A	85	GLU	CB-CG-CD	5.02	121.14	112.60
1	A	8	GLN	N-CA-C	-5.02	105.70	111.07
1	A	52	GLU	O-C-N	5.02	127.51	122.09
1	A	15	GLY	CA-C-N	5.00	127.24	120.44
1	A	15	GLY	C-N-CA	5.00	127.24	120.44

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	1199	0	1212	87	0
2	A	5	0	0	1	0
3	A	43	0	30	3	0
4	A	154	0	0	36	1
All	All	1401	0	1242	88	1

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 35.

All (88) 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:1:GLY:HA2	4:A:276:HOH:O	1.61	1.00
1:A:52:GLU:HA	1:A:55:MET:HE3	1.52	0.90
1:A:98:LYS:HG3	4:A:225:HOH:O	1.76	0.85
1:A:145:LYS:HE3	4:A:218:HOH:O	1.76	0.85
1:A:21:ILE:HD12	1:A:66:THR:HG23	1.59	0.84
1:A:13:VAL:HG13	1:A:16:LYS:HZ2	1.51	0.74
1:A:45:LYS:HE3	4:A:173:HOH:O	1.87	0.74
1:A:78:LYS:CG	4:A:261:HOH:O	2.36	0.73
1:A:78:LYS:HG2	4:A:261:HOH:O	1.86	0.73
1:A:9:GLN:HG3	4:A:165:HOH:O	1.89	0.73
1:A:44:ASP:HA	1:A:47:LYS:HD2	1.71	0.70
1:A:98:LYS:HB2	4:A:237:HOH:O	1.93	0.69
1:A:98:LYS:HD3	1:A:151:PHE:HE1	1.58	0.69
1:A:21:ILE:CD1	1:A:66:THR:HG23	2.23	0.68
1:A:98:LYS:HD3	1:A:151:PHE:CE1	2.29	0.68
1:A:3:SER:HB2	4:A:284:HOH:O	1.95	0.66
1:A:98:LYS:CB	4:A:237:HOH:O	2.44	0.65
1:A:98:LYS:HE3	4:A:292:HOH:O	1.95	0.65
1:A:96:LYS:HE3	4:A:248:HOH:O	1.97	0.65
1:A:118:LYS:C	1:A:120:PRO:HD3	2.21	0.65
1:A:98:LYS:CE	4:A:292:HOH:O	2.46	0.63
1:A:75:ILE:O	1:A:78:LYS:HB2	1.99	0.63
1:A:119:HIS:N	1:A:120:PRO:HD3	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PHE:HA	4:A:234:HOH:O	1.98	0.62
1:A:101:ILE:HG12	1:A:146:TYR:CD2	2.35	0.62
1:A:96:LYS:CE	4:A:248:HOH:O	2.48	0.62
1:A:83:GLU:H	1:A:83:GLU:CD	2.09	0.61
1:A:2:LEU:HD12	1:A:133:LYS:HZ2	1.67	0.60
1:A:3:SER:OG	1:A:6:GLU:HG3	2.02	0.59
1:A:126:ASP:HB2	4:A:227:HOH:O	2.02	0.59
1:A:30:ILE:HD13	1:A:56:LYS:HG3	1.83	0.59
1:A:131:MET:HA	4:A:264:HOH:O	2.03	0.58
1:A:78:LYS:HE2	4:A:158:HOH:O	2.02	0.58
1:A:99:ILE:HD12	3:A:154:HEM:HAC	1.86	0.57
1:A:101:ILE:H	1:A:152:GLN:HE22	1.52	0.57
1:A:98:LYS:NZ	4:A:292:HOH:O	2.36	0.57
1:A:88:PRO:HD3	4:A:199:HOH:O	2.05	0.55
1:A:78:LYS:CE	4:A:261:HOH:O	2.53	0.55
1:A:82:HIS:HE1	1:A:137:LEU:HD23	1.70	0.55
1:A:51:THR:OG1	1:A:54:GLU:HB2	2.07	0.55
1:A:86:LEU:HD21	1:A:141:ASP:HB3	1.88	0.54
1:A:13:VAL:HG21	1:A:127:ALA:HB1	1.89	0.53
3:A:154:HEM:CGA	4:A:283:HOH:O	2.55	0.53
1:A:95:THR:HA	1:A:98:LYS:HE2	1.90	0.53
1:A:9:GLN:HG2	1:A:127:ALA:HA	1.91	0.52
1:A:118:LYS:HG3	4:A:279:HOH:O	2.09	0.51
1:A:10:VAL:HG22	4:A:264:HOH:O	2.09	0.51
1:A:44:ASP:CA	1:A:47:LYS:HD2	2.42	0.49
1:A:3:SER:HB3	4:A:270:HOH:O	2.12	0.49
1:A:73:GLY:O	1:A:77:LYS:HG3	2.12	0.49
1:A:82:HIS:HE1	1:A:137:LEU:CD2	2.25	0.49
1:A:14:TRP:O	1:A:18:GLU:HG3	2.12	0.49
1:A:16:LYS:HE3	4:A:229:HOH:O	2.13	0.49
1:A:60:ASP:HB2	2:A:155:SO4:O4	2.13	0.49
1:A:101:ILE:H	1:A:152:GLN:NE2	2.10	0.49
1:A:131:MET:HE2	4:A:264:HOH:O	2.13	0.49
1:A:146:TYR:HD2	1:A:152:GLN:HE21	1.59	0.49
1:A:33:PHE:HE2	1:A:61:LEU:HD11	1.78	0.48
1:A:146:TYR:HD2	1:A:152:GLN:NE2	2.12	0.47
1:A:151:PHE:C	1:A:152:GLN:HG3	2.39	0.47
1:A:99:ILE:CD1	3:A:154:HEM:HAC	2.44	0.46
1:A:2:LEU:HA	1:A:6:GLU:OE1	2.14	0.46
1:A:27:GLU:CD	1:A:118:LYS:HE3	2.40	0.46
1:A:116:HIS:NE2	1:A:128:GLN:NE2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ILE:HD13	1:A:104:LEU:HD12	1.98	0.46
1:A:95:THR:HG21	4:A:190:HOH:O	2.16	0.45
1:A:52:GLU:O	1:A:55:MET:HB2	2.17	0.45
1:A:107:ILE:O	1:A:110:ALA:HB3	2.17	0.45
1:A:112:ILE:HG12	4:A:198:HOH:O	2.17	0.45
1:A:148:GLU:C	1:A:150:GLY:H	2.24	0.45
1:A:14:TRP:CH2	1:A:17:VAL:HG11	2.52	0.44
1:A:123:PHE:HD1	4:A:234:HOH:O	1.99	0.44
1:A:133:LYS:HD2	4:A:161:HOH:O	2.17	0.44
1:A:117:SER:O	1:A:120:PRO:HG3	2.17	0.44
1:A:4:ASP:O	1:A:5:GLY:C	2.60	0.44
1:A:10:VAL:HA	4:A:264:HOH:O	2.19	0.43
1:A:10:VAL:HG13	4:A:264:HOH:O	2.19	0.42
1:A:115:LEU:HD12	1:A:123:PHE:CZ	2.54	0.42
1:A:112:ILE:HD11	1:A:135:LEU:HD12	2.00	0.42
1:A:57:ALA:HB1	4:A:170:HOH:O	2.19	0.42
1:A:133:LYS:HD2	4:A:222:HOH:O	2.20	0.41
1:A:24:HIS:O	1:A:28:VAL:HG23	2.20	0.41
1:A:33:PHE:CE2	1:A:61:LEU:HD11	2.54	0.41
1:A:146:TYR:CD2	1:A:152:GLN:NE2	2.88	0.41
1:A:2:LEU:HD11	1:A:133:LYS:HG2	2.02	0.41
1:A:87:LYS:NZ	4:A:282:HOH:O	2.53	0.40
1:A:6:GLU:OE1	1:A:133:LYS:HE3	2.20	0.40
1:A:102:LYS:HE3	1:A:106:PHE:CE1	2.57	0.40

All (1) 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:168:HOH:O	4:A:309:HOH:O[2_656]	1.98	0.22

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	151/153 (99%)	137 (91%)	13 (9%)	1 (1%)	18 10

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	123/123 (100%)	105 (85%)	18 (15%)	3 1

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	16	LYS
1	A	27	GLU
1	A	41	GLU
1	A	50	LYS
1	A	54	GLU
1	A	78	LYS
1	A	83	GLU
1	A	87	LYS
1	A	91	GLN
1	A	95	THR
1	A	101	ILE
1	A	118	LYS
1	A	133	LYS
1	A	139	ARG
1	A	140	ASN
1	A	145	LYS
1	A	152	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	82	HIS
1	A	97	HIS
1	A	128	GLN
1	A	140	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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	SO4	A	155	-	4,4,4	0.93	0	6,6,6	0.68	0
3	HEM	A	154	4,1	50,50,50	1.48	10 (20%)	67,82,82	1.51	11 (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
3	HEM	A	154	4,1	-	5/14/54/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	154	HEM	FE-NB	3.47	2.05	1.94
3	A	154	HEM	CAB-C3B	2.84	1.55	1.47
3	A	154	HEM	CBA-CAA	2.81	1.61	1.51
3	A	154	HEM	C3B-C2B	-2.39	1.32	1.37
3	A	154	HEM	C4A-C3A	2.37	1.48	1.43
3	A	154	HEM	CMD-C2D	2.30	1.55	1.50
3	A	154	HEM	CMB-C2B	2.24	1.55	1.50
3	A	154	HEM	CAC-C3C	2.10	1.53	1.47
3	A	154	HEM	C2A-C3A	-2.09	1.33	1.38
3	A	154	HEM	CHD-C4C	2.01	1.42	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	154	HEM	O1A-CGA-CBA	-4.36	109.25	123.09
3	A	154	HEM	CHC-C4B-NB	4.32	129.07	124.42
3	A	154	HEM	CHC-C1C-NC	3.77	128.56	124.45
3	A	154	HEM	C1C-CHC-C4B	-2.84	119.98	126.02
3	A	154	HEM	CMA-C3A-C2A	2.46	130.84	125.62
3	A	154	HEM	O2A-CGA-CBA	2.44	121.72	114.00
3	A	154	HEM	C3B-C2B-C1B	2.36	108.19	106.41
3	A	154	HEM	CMA-C3A-C4A	-2.20	122.07	125.42
3	A	154	HEM	CHB-C4A-NA	2.16	127.78	123.86
3	A	154	HEM	O2A-CGA-O1A	2.11	128.76	123.33
3	A	154	HEM	CMC-C2C-C1C	-2.05	121.11	124.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

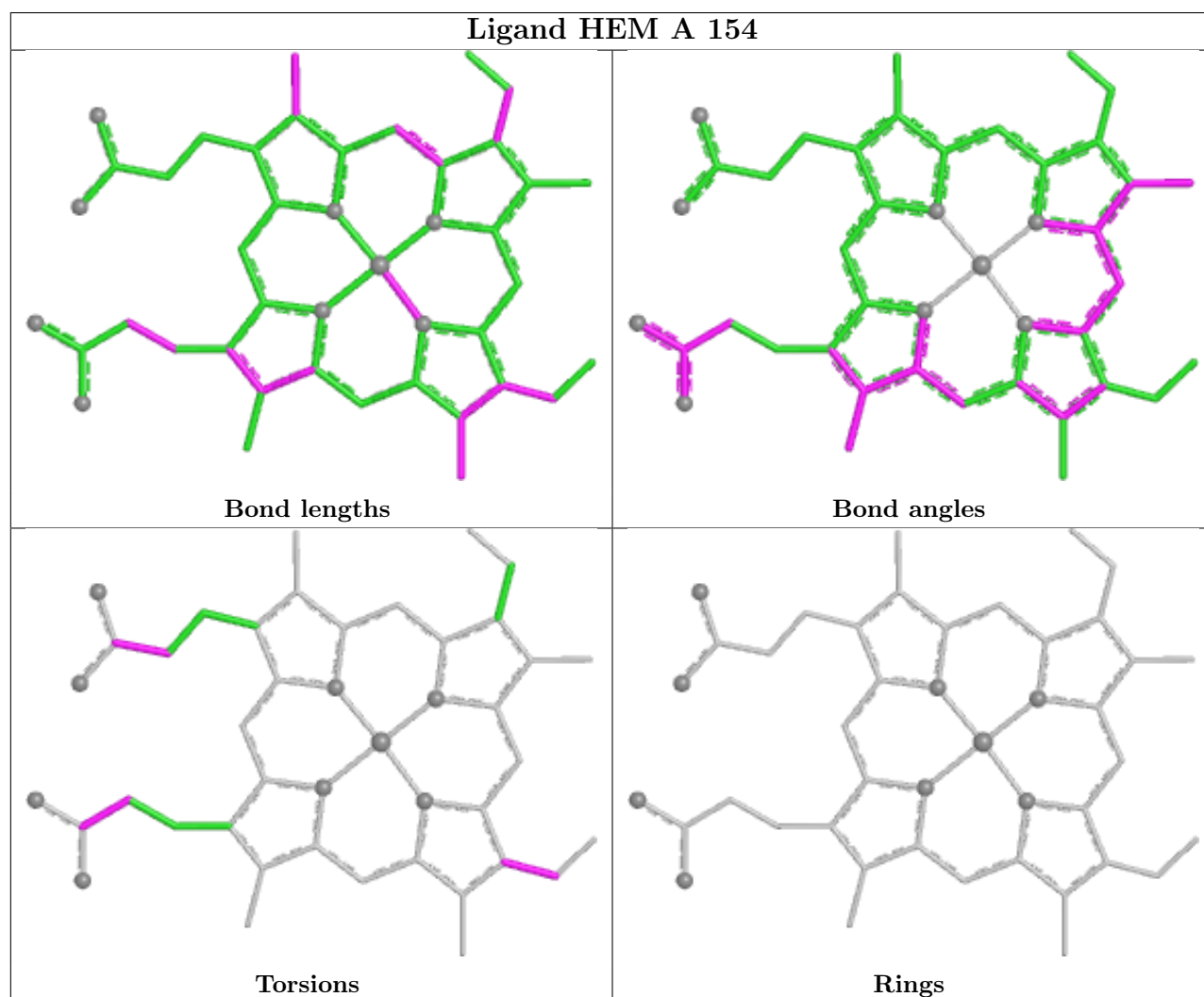
Mol	Chain	Res	Type	Atoms
3	A	154	HEM	C2B-C3B-CAB-CBB
3	A	154	HEM	C4B-C3B-CAB-CBB
3	A	154	HEM	CAA-CBA-CGA-O2A
3	A	154	HEM	CAD-CBD-CGD-O2D
3	A	154	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	155	SO4	1	0
3	A	154	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	153/153 (100%)	0.36	7 (4%) 37 40	5, 12, 26, 34	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	GLY	7.0
1	A	1	GLY	3.0
1	A	151	PHE	2.4
1	A	152	GLN	2.3
1	A	49	LEU	2.1
1	A	4	ASP	2.1
1	A	53	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

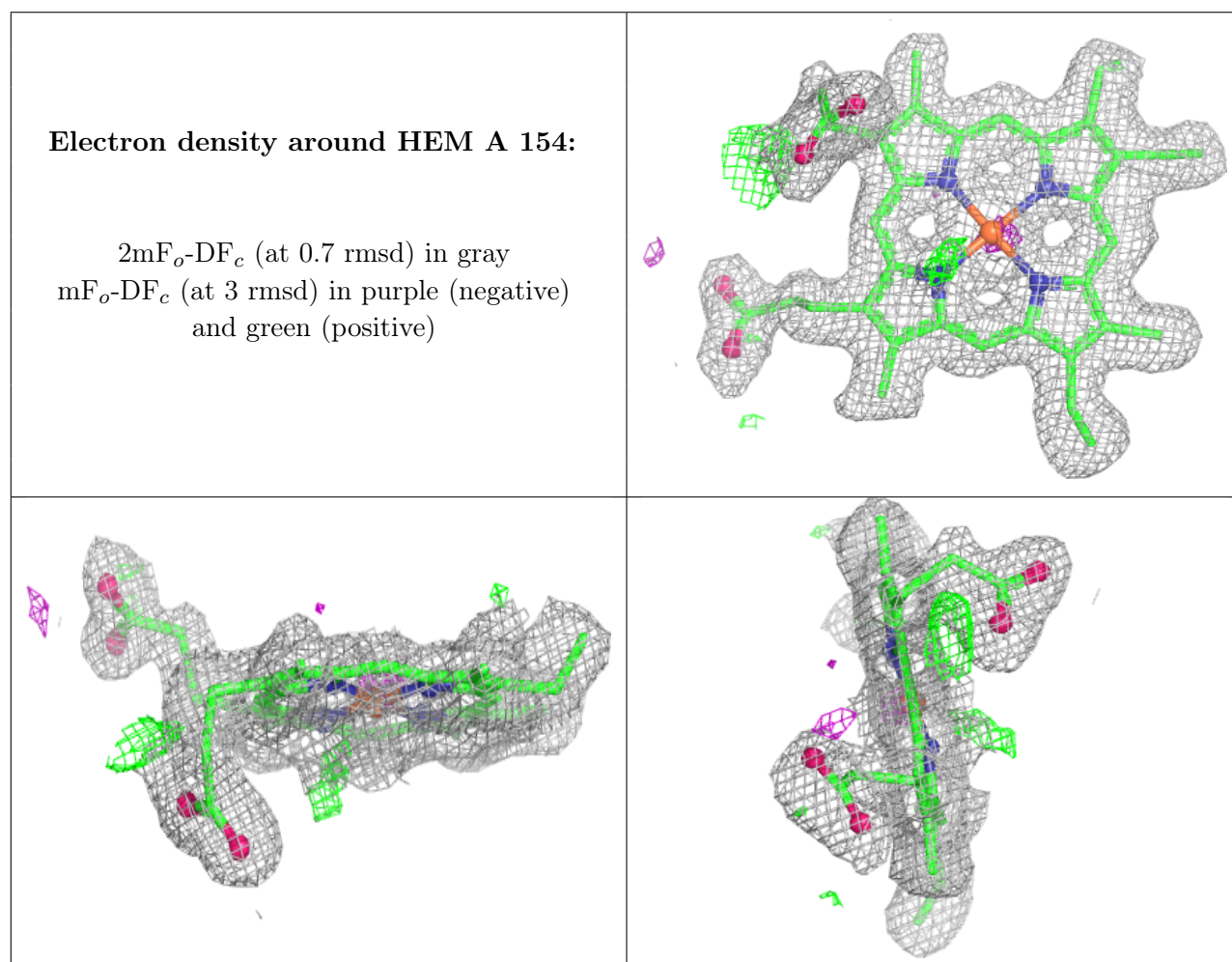
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	155	5/5	0.82	0.14	45,45,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEM	A	154	43/43	0.95	0.08	3,6,9,11	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.