



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 11:41 pm BST

PDB ID : 1MYI
Title : HIGH RESOLUTION X-RAY STRUCTURES OF PIG METMYOGLOBIN AND TWO CD3 MUTANTS MB(LYS45-> ARG) AND MB(LYS45-> SER)
Authors : Smerdon, S.J.; Oldfield, T.J.; Wilkinson, A.J.; Dauter, Z.; Petratos, K.; Wilson, K.S.
Deposited on : 1992-02-27
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

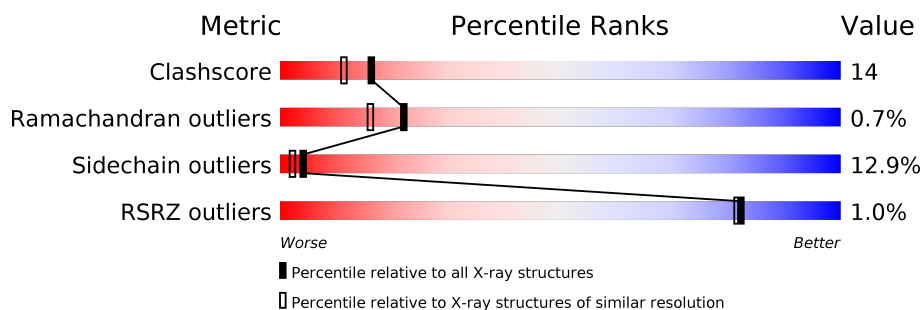
1 Overall quality at a glance

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on 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	<div> <div></div> <div> <div></div> <div>48%</div> <div>37%</div> <div>9%</div> <div>7%</div> </div> </div>
1	B	153	<div> <div></div> <div> <div></div> <div>44%</div> <div>37%</div> <div>16%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2596 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	0	0
			1194	761	207	223	3			
1	B	153	Total	C	N	O	S	0	0	0
			1194	761	207	223	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	SER	LYS	CONFLICT	UNP P02189
B	45	SER	LYS	CONFLICT	UNP P02189

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: 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		

Continued on next page...

Continued from previous page...

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

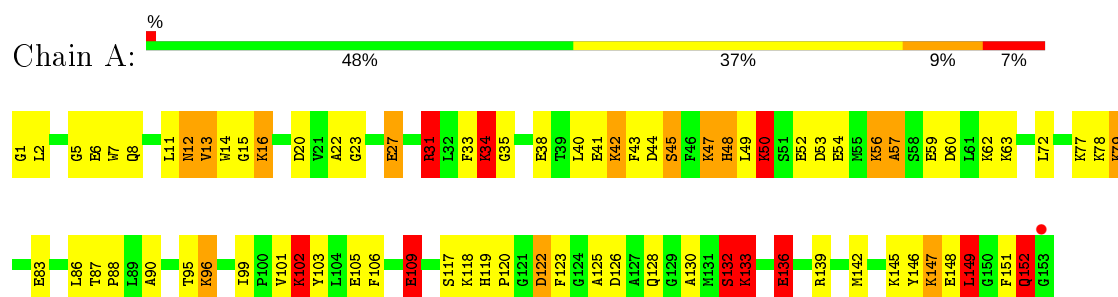
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total	O	0	0
			73	73		
3	B	49	Total	O	0	0
			49	49		

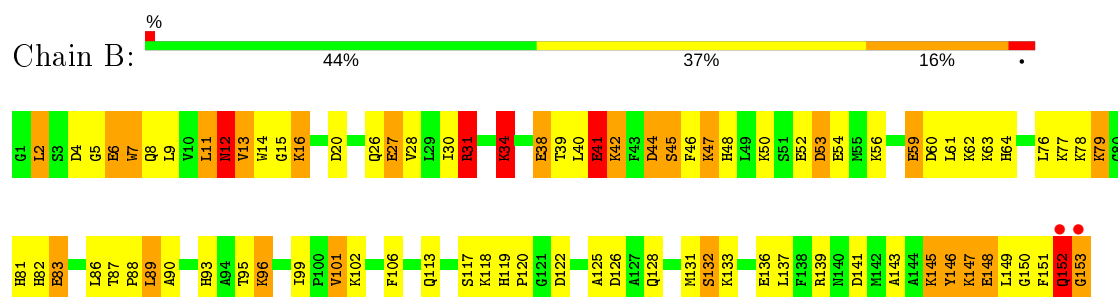
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: MYOGLOBIN



• Molecule 1: MYOGLOBIN



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.92Å 42.92Å 92.95Å 90.00° 92.24° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 25.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 96.6 (25.11-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.01Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.194 , (Not available) 0.181 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 82.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.187 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2596	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 100.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 0.0000e+00. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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	1.57	10/1219 (0.8%)	2.88	115/1634 (7.0%)
1	B	1.53	6/1219 (0.5%)	2.91	127/1634 (7.8%)
All	All	1.55	16/2438 (0.7%)	2.90	242/3268 (7.4%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	SER	CB-OG	9.28	1.54	1.42
1	B	45	SER	CB-OG	8.52	1.53	1.42
1	A	136	GLU	CD-OE2	7.54	1.33	1.25
1	A	136	GLU	CD-OE1	7.49	1.33	1.25
1	B	83	GLU	CD-OE2	7.41	1.33	1.25
1	A	59	GLU	CD-OE1	7.10	1.33	1.25
1	B	31	ARG	NE-CZ	6.94	1.42	1.33
1	A	31	ARG	NE-CZ	6.84	1.42	1.33
1	B	27	GLU	CD-OE2	6.68	1.33	1.25
1	A	27	GLU	CD-OE1	6.56	1.32	1.25
1	A	41	GLU	CD-OE1	6.28	1.32	1.25
1	A	5	GLY	CA-C	5.78	1.61	1.51
1	B	5	GLY	CA-C	5.61	1.60	1.51
1	A	83	GLU	CD-OE1	5.56	1.31	1.25
1	A	109	GLU	CD-OE2	5.54	1.31	1.25
1	B	95	THR	CA-CB	5.07	1.66	1.53

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ASP	CB-CG-OD2	-21.08	99.33	118.30
1	B	122	ASP	CB-CG-OD2	-18.86	101.33	118.30
1	A	60	ASP	CB-CG-OD1	18.09	134.58	118.30
1	B	60	ASP	CB-CG-OD2	-18.04	102.07	118.30
1	B	83	GLU	CB-CG-CD	17.57	161.63	114.20
1	A	136	GLU	OE1-CD-OE2	16.94	143.63	123.30
1	B	12	ASN	OD1-CG-ND2	16.50	159.85	121.90
1	A	53	ASP	CB-CG-OD2	-16.07	103.84	118.30
1	B	60	ASP	CB-CG-OD1	15.06	131.85	118.30
1	A	12	ASN	OD1-CG-ND2	15.02	156.44	121.90
1	A	139	ARG	NE-CZ-NH1	14.32	127.46	120.30
1	A	126	ASP	CB-CG-OD1	13.65	130.58	118.30
1	B	83	GLU	OE1-CD-OE2	-13.44	107.17	123.30
1	B	12	ASN	CB-CG-OD1	-13.34	94.91	121.60
1	A	139	ARG	NE-CZ-NH2	-13.11	113.75	120.30
1	B	132	SER	N-CA-CB	-12.86	91.21	110.50
1	B	41	GLU	CB-CG-CD	12.69	148.46	114.20
1	A	122	ASP	CB-CG-OD1	-12.47	107.08	118.30
1	B	12	ASN	N-CA-CB	-12.36	88.36	110.60
1	A	48	HIS	CA-CB-CG	-12.27	92.73	113.60
1	B	31	ARG	NE-CZ-NH1	-12.18	114.21	120.30
1	B	44	ASP	CB-CG-OD2	-12.15	107.36	118.30
1	A	59	GLU	OE1-CD-OE2	11.65	137.29	123.30
1	B	83	GLU	CG-CD-OE1	11.62	141.54	118.30
1	B	53	ASP	CB-CG-OD1	11.29	128.46	118.30
1	A	12	ASN	CB-CG-OD1	-11.29	99.03	121.60
1	A	12	ASN	N-CA-CB	-11.29	90.28	110.60
1	A	126	ASP	CB-CG-OD2	-11.22	108.20	118.30
1	B	44	ASP	CB-CG-OD1	9.92	127.23	118.30
1	A	34	LYS	CA-CB-CG	9.76	134.88	113.40
1	A	2	LEU	O-C-N	9.71	138.24	122.70
1	B	31	ARG	CB-CG-CD	9.45	136.17	111.60
1	B	152	GLN	CB-CG-CD	9.27	135.70	111.60
1	A	152	GLN	C-N-CA	9.25	141.73	122.30
1	B	12	ASN	CA-CB-CG	-9.18	93.20	113.40
1	B	136	GLU	OE1-CD-OE2	9.11	134.23	123.30
1	B	136	GLU	CG-CD-OE2	-8.99	100.33	118.30
1	A	31	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	B	101	VAL	CA-C-N	8.75	136.46	117.20
1	B	125	ALA	CB-CA-C	8.73	123.20	110.10
1	A	13	VAL	CG1-CB-CG2	-8.56	97.21	110.90
1	B	122	ASP	OD1-CG-OD2	8.39	139.24	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	MET	CA-CB-CG	8.17	127.19	113.30
1	B	27	GLU	CG-CD-OE2	-8.13	102.05	118.30
1	B	146	TYR	CB-CG-CD1	-8.07	116.16	121.00
1	A	105	GLU	OE1-CD-OE2	8.02	132.93	123.30
1	A	53	ASP	N-CA-CB	8.02	125.03	110.60
1	A	146	TYR	CB-CG-CD1	7.95	125.77	121.00
1	A	38	GLU	CA-CB-CG	7.94	130.86	113.40
1	A	43	PHE	CB-CG-CD2	-7.90	115.27	120.80
1	B	53	ASP	CA-CB-CG	-7.79	96.26	113.40
1	B	125	ALA	O-C-N	-7.75	110.30	122.70
1	B	53	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	A	123	PHE	CD1-CE1-CZ	-7.72	110.83	120.10
1	B	34	LYS	CA-C-N	7.69	131.58	116.20
1	B	20	ASP	CB-CG-OD1	7.67	125.20	118.30
1	B	126	ASP	N-CA-CB	-7.64	96.85	110.60
1	B	41	GLU	OE1-CD-OE2	-7.62	114.16	123.30
1	A	101	VAL	CA-C-N	7.59	133.89	117.20
1	A	40	LEU	CB-CG-CD2	-7.52	98.22	111.00
1	B	31	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	A	56	LYS	CB-CG-CD	-7.47	92.18	111.60
1	A	1	GLY	CA-C-N	-7.45	100.82	117.20
1	B	9	LEU	CB-CG-CD1	7.40	123.58	111.00
1	A	54	GLU	CG-CD-OE1	7.38	133.06	118.30
1	B	2	LEU	CB-CG-CD2	-7.35	98.51	111.00
1	B	40	LEU	CB-CG-CD2	-7.33	98.53	111.00
1	A	63	LYS	CA-CB-CG	-7.31	97.33	113.40
1	B	86	LEU	N-CA-CB	-7.27	95.85	110.40
1	B	148	GLU	O-C-N	-7.26	111.09	122.70
1	A	109	GLU	CA-CB-CG	7.24	129.33	113.40
1	B	95	THR	CA-CB-CG2	7.16	122.43	112.40
1	B	89	LEU	CB-CG-CD1	-7.14	98.86	111.00
1	B	47	LYS	C-N-CA	7.11	139.48	121.70
1	B	6	GLU	OE1-CD-OE2	-7.10	114.78	123.30
1	B	62	LYS	CG-CD-CE	-7.04	90.76	111.90
1	A	49	LEU	O-C-N	7.03	133.95	122.70
1	B	86	LEU	CB-CA-C	6.98	123.46	110.20
1	A	79	LYS	CD-CE-NZ	-6.98	95.66	111.70
1	A	102	LYS	CA-CB-CG	-6.94	98.14	113.40
1	B	38	GLU	CA-CB-CG	6.92	128.62	113.40
1	B	139	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	B	79	LYS	CA-C-N	6.86	129.91	116.20
1	A	123	PHE	CG-CD1-CE1	6.81	128.29	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	PHE	CG-CD2-CE2	-6.79	113.33	120.80
1	A	13	VAL	CA-CB-CG1	6.77	121.05	110.90
1	A	136	GLU	CG-CD-OE1	-6.62	105.06	118.30
1	A	40	LEU	CB-CG-CD1	6.61	122.24	111.00
1	B	6	GLU	CG-CD-OE1	6.60	131.50	118.30
1	A	50	LYS	CA-C-N	6.56	131.64	117.20
1	A	35	GLY	CA-C-O	-6.53	108.85	120.60
1	B	132	SER	CA-CB-OG	-6.44	93.81	111.20
1	B	76	LEU	CB-CG-CD1	-6.42	100.09	111.00
1	A	132	SER	N-CA-CB	-6.41	100.89	110.50
1	B	77	LYS	CD-CE-NZ	-6.41	96.97	111.70
1	B	2	LEU	O-C-N	6.40	132.95	122.70
1	B	40	LEU	CB-CG-CD1	6.39	121.87	111.00
1	B	141	ASP	CB-CG-OD2	-6.38	112.55	118.30
1	B	96	LYS	CA-C-O	6.38	133.50	120.10
1	B	146	TYR	CB-CA-C	-6.37	97.66	110.40
1	B	50	LYS	CA-CB-CG	6.35	127.36	113.40
1	B	149	LEU	C-N-CA	6.33	135.60	122.30
1	B	63	LYS	CA-CB-CG	-6.32	99.49	113.40
1	A	53	ASP	O-C-N	6.32	132.81	122.70
1	B	136	GLU	CA-CB-CG	-6.32	99.49	113.40
1	B	90	ALA	CB-CA-C	6.30	119.55	110.10
1	B	54	GLU	OE1-CD-OE2	-6.30	115.74	123.30
1	A	47	LYS	CA-C-O	6.29	133.30	120.10
1	A	31	ARG	CA-CB-CG	-6.28	99.58	113.40
1	A	33	PHE	CB-CG-CD1	-6.28	116.40	120.80
1	B	81	HIS	CA-CB-CG	-6.27	102.94	113.60
1	A	152	GLN	CA-C-N	-6.26	103.67	116.20
1	A	11	LEU	CA-CB-CG	-6.24	100.95	115.30
1	A	41	GLU	CG-CD-OE2	6.21	130.72	118.30
1	A	133	LYS	CA-CB-CG	-6.19	99.78	113.40
1	A	148	GLU	OE1-CD-OE2	6.17	130.71	123.30
1	B	46	PHE	O-C-N	6.17	132.58	122.70
1	A	106	PHE	CB-CG-CD2	-6.17	116.48	120.80
1	B	101	VAL	CB-CA-C	6.16	123.10	111.40
1	B	106	PHE	CD1-CE1-CZ	-6.16	112.71	120.10
1	A	54	GLU	OE1-CD-OE2	-6.15	115.92	123.30
1	B	50	LYS	CA-C-N	6.13	130.69	117.20
1	A	136	GLU	CB-CA-C	-6.12	98.16	110.40
1	B	82	HIS	CG-ND1-CE1	6.11	116.75	108.20
1	A	27	GLU	CB-CG-CD	-6.09	97.76	114.20
1	A	47	LYS	O-C-N	-6.08	112.97	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	SER	CB-CA-C	6.07	121.64	110.10
1	A	128	GLN	CG-CD-OE1	-6.06	109.47	121.60
1	A	14	TRP	CB-CG-CD1	6.06	134.88	127.00
1	B	28	VAL	CG1-CB-CG2	6.05	120.59	110.90
1	A	35	GLY	C-N-CA	6.05	136.83	121.70
1	B	13	VAL	CA-CB-CG1	6.05	119.97	110.90
1	B	133	LYS	CD-CE-NZ	6.05	125.61	111.70
1	A	6	GLU	OE1-CD-OE2	-6.03	116.07	123.30
1	B	145	LYS	CD-CE-NZ	-6.02	97.85	111.70
1	A	56	LYS	CB-CA-C	-5.96	98.49	110.40
1	A	133	LYS	N-CA-CB	-5.96	99.88	110.60
1	B	59	GLU	OE1-CD-OE2	5.95	130.44	123.30
1	A	130	ALA	O-C-N	5.95	132.22	122.70
1	B	26	GLN	CG-CD-OE1	-5.93	109.73	121.60
1	B	44	ASP	CA-C-N	-5.89	104.23	117.20
1	B	61	LEU	CD1-CG-CD2	-5.89	92.83	110.50
1	A	15	GLY	O-C-N	-5.88	113.30	122.70
1	A	63	LYS	CB-CG-CD	-5.87	96.34	111.60
1	B	50	LYS	CB-CG-CD	-5.86	96.36	111.60
1	A	48	HIS	N-CA-CB	-5.86	100.06	110.60
1	A	79	LYS	C-N-CA	-5.85	110.01	122.30
1	A	13	VAL	CA-CB-CG2	5.85	119.68	110.90
1	A	14	TRP	CB-CG-CD2	-5.84	119.01	126.60
1	B	45	SER	N-CA-CB	-5.84	101.74	110.50
1	B	14	TRP	CB-CG-CD2	-5.83	119.02	126.60
1	A	101	VAL	CA-C-O	-5.81	107.90	120.10
1	B	137	LEU	CB-CG-CD2	5.81	120.88	111.00
1	A	31	ARG	CG-CD-NE	5.78	123.95	111.80
1	A	49	LEU	C-N-CA	-5.78	107.24	121.70
1	A	149	LEU	C-N-CA	5.78	134.44	122.30
1	A	57	ALA	C-N-CA	5.76	136.10	121.70
1	B	117	SER	N-CA-CB	5.72	119.08	110.50
1	B	9	LEU	CB-CG-CD2	-5.71	101.29	111.00
1	A	145	LYS	CG-CD-CE	5.70	129.01	111.90
1	B	83	GLU	O-C-N	-5.70	113.58	122.70
1	A	59	GLU	CG-CD-OE1	-5.70	106.91	118.30
1	B	125	ALA	CA-C-O	5.68	132.03	120.10
1	B	27	GLU	OE1-CD-OE2	5.67	130.11	123.30
1	A	96	LYS	N-CA-CB	-5.66	100.41	110.60
1	B	7	TRP	CD1-NE1-CE2	5.66	114.10	109.00
1	A	34	LYS	CB-CA-C	-5.66	99.09	110.40
1	A	62	LYS	CD-CE-NZ	-5.63	98.76	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	GLY	CA-C-O	-5.62	110.48	120.60
1	B	38	GLU	OE1-CD-OE2	-5.62	116.56	123.30
1	A	1	GLY	O-C-N	5.61	131.68	122.70
1	A	96	LYS	O-C-N	5.60	131.67	122.70
1	A	83	GLU	CA-CB-CG	-5.60	101.08	113.40
1	A	42	LYS	CA-C-O	-5.59	108.36	120.10
1	A	79	LYS	CB-CA-C	-5.56	99.28	110.40
1	B	125	ALA	N-CA-CB	-5.54	102.34	110.10
1	A	136	GLU	N-CA-CB	5.53	120.55	110.60
1	B	13	VAL	CA-CB-CG2	-5.51	102.63	110.90
1	A	90	ALA	CB-CA-C	5.50	118.35	110.10
1	A	15	GLY	C-N-CA	5.49	135.43	121.70
1	B	101	VAL	O-C-N	-5.49	113.92	122.70
1	B	11	LEU	CA-C-O	5.48	131.60	120.10
1	A	77	LYS	CA-CB-CG	-5.47	101.37	113.40
1	A	12	ASN	CA-CB-CG	-5.46	101.38	113.40
1	A	79	LYS	CA-CB-CG	-5.46	101.39	113.40
1	A	77	LYS	CD-CE-NZ	-5.46	99.15	111.70
1	B	152	GLN	OE1-CD-NE2	-5.43	109.42	121.90
1	B	79	LYS	O-C-N	-5.41	114.00	123.20
1	A	11	LEU	CB-CA-C	5.36	120.39	110.20
1	B	147	LYS	CB-CA-C	5.36	121.12	110.40
1	A	53	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	146	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	A	2	LEU	CA-C-N	-5.32	105.49	117.20
1	B	126	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	31	ARG	CD-NE-CZ	-5.31	116.17	123.60
1	B	153	GLY	N-CA-C	5.30	126.35	113.10
1	B	126	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	61	LEU	CB-CG-CD2	-5.29	102.00	111.00
1	B	11	LEU	CA-CB-CG	-5.29	103.14	115.30
1	B	41	GLU	CG-CD-OE2	5.28	128.85	118.30
1	A	133	LYS	CD-CE-NZ	5.27	123.83	111.70
1	A	101	VAL	CB-CA-C	5.26	121.39	111.40
1	B	9	LEU	CA-C-O	-5.24	109.09	120.10
1	B	136	GLU	N-CA-CB	-5.24	101.17	110.60
1	B	152	GLN	CA-CB-CG	5.24	124.92	113.40
1	B	93	HIS	CA-CB-CG	-5.23	104.72	113.60
1	B	39	THR	CA-CB-CG2	5.23	119.72	112.40
1	B	63	LYS	CB-CG-CD	5.22	125.18	111.60
1	B	4	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	B	102	LYS	O-C-N	5.22	131.05	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	GLU	CB-CG-CD	-5.22	100.12	114.20
1	B	131	MET	CA-C-O	5.22	131.06	120.10
1	A	22	ALA	N-CA-CB	-5.21	102.81	110.10
1	B	14	TRP	CB-CG-CD1	5.20	133.76	127.00
1	B	16	LYS	CB-CG-CD	-5.20	98.08	111.60
1	B	15	GLY	O-C-N	-5.20	114.39	122.70
1	A	117	SER	CB-CA-C	-5.18	100.26	110.10
1	A	63	LYS	CB-CA-C	-5.18	100.05	110.40
1	B	113	GLN	OE1-CD-NE2	-5.16	110.04	121.90
1	B	117	SER	CB-CA-C	-5.16	100.30	110.10
1	A	20	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	B	152	GLN	CB-CA-C	-5.15	100.10	110.40
1	B	42	LYS	CA-C-N	5.15	128.53	117.20
1	A	105	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	A	125	ALA	CA-C-O	5.14	130.89	120.10
1	A	117	SER	N-CA-CB	5.14	118.21	110.50
1	A	118	LYS	CA-C-O	-5.13	109.32	120.10
1	A	12	ASN	CB-CG-ND2	-5.13	104.39	116.70
1	B	34	LYS	CA-C-O	-5.13	109.33	120.10
1	A	40	LEU	O-C-N	5.11	130.87	122.70
1	B	101	VAL	CA-C-O	-5.10	109.39	120.10
1	A	101	VAL	CA-CB-CG1	5.10	118.55	110.90
1	B	44	ASP	CA-C-O	5.08	130.78	120.10
1	A	72	LEU	CA-C-N	5.08	126.35	116.20
1	B	34	LYS	CD-CE-NZ	5.06	123.35	111.70
1	B	118	LYS	CB-CG-CD	-5.06	98.45	111.60
1	B	54	GLU	CG-CD-OE1	5.05	128.40	118.30
1	B	137	LEU	CB-CG-CD1	-5.04	102.44	111.00
1	B	64	HIS	O-C-N	-5.03	114.66	123.20
1	A	35	GLY	CA-C-N	5.01	128.23	117.20
1	A	53	ASP	OD1-CG-OD2	5.01	132.82	123.30
1	A	109	GLU	N-CA-CB	5.01	119.62	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	ARG	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	1194	0	1197	32	0
1	B	1194	0	1197	39	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
3	A	73	0	0	5	0
3	B	49	0	0	4	0
All	All	2596	0	2454	71	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 14.

All (71) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:TYR:HB2	1:B:153:GLY:OXT	1.42	1.16
1:B:146:TYR:CB	1:B:153:GLY:OXT	2.06	1.02
1:A:34:LYS:HE2	1:A:34:LYS:HA	1.49	0.93
1:B:38:GLU:O	1:B:41:GLU:HG3	1.71	0.91
1:B:8:GLN:O	1:B:12:ASN:HB2	1.77	0.85
1:A:151:PHE:O	1:A:152:GLN:HB2	1.79	0.81
1:B:38:GLU:O	1:B:41:GLU:OE2	2.04	0.76
1:B:52:GLU:HG2	1:B:56:LYS:HE2	1.68	0.75
1:A:109:GLU:HG2	3:A:222:HOH:O	1.86	0.75
1:B:44:ASP:O	1:B:47:LYS:HG2	1.88	0.73
1:B:151:PHE:O	1:B:153:GLY:N	2.19	0.71
1:B:87:THR:N	1:B:88:PRO:HD2	2.05	0.71
1:A:151:PHE:O	1:A:152:GLN:CB	2.40	0.69
1:B:146:TYR:HB3	1:B:153:GLY:OXT	1.94	0.67
1:B:7:TRP:HB3	1:B:79:LYS:HE2	1.78	0.66
1:A:78:LYS:HE2	1:A:78:LYS:HA	1.76	0.66
1:B:27:GLU:OE1	3:B:196:HOH:O	2.14	0.66
1:B:30:ILE:O	1:B:34:LYS:HG3	1.98	0.64
1:A:8:GLN:O	1:A:12:ASN:HB2	1.99	0.62
1:A:102:LYS:HD2	1:A:103:TYR:CD1	2.35	0.62
1:A:34:LYS:CA	1:A:34:LYS:HE2	2.22	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:HG2	3:B:196:HOH:O	2.01	0.61
1:A:44:ASP:O	1:A:47:LYS:HG2	2.01	0.60
1:B:101:VAL:HG13	1:B:152:GLN:HE22	1.69	0.58
1:A:133:LYS:HA	1:A:136:GLU:HG3	1.86	0.58
1:B:52:GLU:O	1:B:56:LYS:HG3	2.03	0.57
1:B:87:THR:N	1:B:88:PRO:CD	2.67	0.57
1:A:48:HIS:O	1:A:50:LYS:HD2	2.05	0.57
1:A:147:LYS:HG2	1:A:152:GLN:NE2	2.19	0.57
1:B:52:GLU:CG	1:B:56:LYS:HE2	2.34	0.57
1:B:146:TYR:CD2	1:B:151:PHE:HD2	2.24	0.56
1:B:146:TYR:CE2	1:B:151:PHE:HE2	2.25	0.55
1:A:87:THR:HB	1:A:88:PRO:HD3	1.89	0.54
1:B:146:TYR:CD2	1:B:151:PHE:CD2	2.96	0.54
1:B:38:GLU:O	1:B:41:GLU:CD	2.45	0.54
1:B:31:ARG:CG	3:B:196:HOH:O	2.56	0.54
1:B:38:GLU:O	1:B:41:GLU:CG	2.49	0.54
1:A:23:GLY:O	1:A:27:GLU:HG3	2.08	0.53
1:A:87:THR:N	1:A:88:PRO:CD	2.72	0.52
1:B:146:TYR:CE2	1:B:151:PHE:CE2	2.97	0.52
1:B:101:VAL:CG1	1:B:152:GLN:HE22	2.23	0.51
1:B:128:GLN:O	1:B:132:SER:HB3	2.10	0.51
1:A:7:TRP:CG	1:A:79:LYS:HG2	2.45	0.51
1:B:2:LEU:HA	1:B:6:GLU:OE1	2.11	0.50
1:B:13:VAL:O	1:B:16:LYS:HB2	2.10	0.50
1:A:34:LYS:HD3	1:A:52:GLU:OE1	2.12	0.49
1:B:143:ALA:O	1:B:153:GLY:OXT	2.30	0.48
1:A:132:SER:O	1:A:136:GLU:HG2	2.14	0.48
1:B:101:VAL:HG12	1:B:146:TYR:CD2	2.49	0.47
1:A:99:ILE:HD12	2:A:154:HEM:HAC	1.96	0.47
1:A:109:GLU:CG	3:A:222:HOH:O	2.56	0.46
1:A:87:THR:N	1:A:88:PRO:HD2	2.30	0.46
1:A:16:LYS:HA	1:A:16:LYS:HD2	1.36	0.46
1:A:87:THR:CB	1:A:88:PRO:HD3	2.45	0.46
1:B:78:LYS:N	1:B:78:LYS:HD2	2.30	0.45
1:B:99:ILE:HD12	2:B:154:HEM:CAC	2.47	0.44
1:A:147:LYS:HE3	1:A:152:GLN:HB3	1.99	0.44
1:A:102:LYS:HD2	1:A:103:TYR:CE1	2.53	0.44
1:A:7:TRP:CD2	1:A:79:LYS:HG2	2.53	0.44
1:A:31:ARG:HD2	3:A:201:HOH:O	2.17	0.43
1:B:146:TYR:CG	1:B:151:PHE:HD2	2.37	0.43
1:B:8:GLN:NE2	3:B:184:HOH:O	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:HIS:N	1:B:120:PRO:CD	2.82	0.42
1:B:101:VAL:HG12	1:B:146:TYR:CE2	2.54	0.42
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.73	0.42
1:A:122:ASP:HB3	3:A:193:HOH:O	2.20	0.41
1:B:11:LEU:HA	1:B:11:LEU:HD23	1.66	0.41
1:A:119:HIS:N	1:A:120:PRO:CD	2.84	0.41
1:B:87:THR:HB	1:B:88:PRO:HD3	2.03	0.41
1:A:57:ALA:O	3:A:211:HOH:O	2.22	0.40
1:A:95:THR:HG22	1:A:151:PHE:CZ	2.57	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	151/153 (99%)	146 (97%)	4 (3%)	1 (1%)	22	16
1	B	151/153 (99%)	144 (95%)	6 (4%)	1 (1%)	22	16
All	All	302/306 (99%)	290 (96%)	10 (3%)	2 (1%)	22	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	B	152	GLN

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	124/124 (100%)	108 (87%)	16 (13%)	4	2
1	B	124/124 (100%)	108 (87%)	16 (13%)	4	2
All	All	248/248 (100%)	216 (87%)	32 (13%)	4	2

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	16	LYS
1	A	34	LYS
1	A	42	LYS
1	A	45	SER
1	A	50	LYS
1	A	56	LYS
1	A	86	LEU
1	A	96	LYS
1	A	102	LYS
1	A	109	GLU
1	A	132	SER
1	A	133	LYS
1	A	136	GLU
1	A	147	LYS
1	A	149	LEU
1	B	12	ASN
1	B	31	ARG
1	B	34	LYS
1	B	41	GLU
1	B	42	LYS
1	B	45	SER
1	B	48	HIS
1	B	53	ASP
1	B	59	GLU
1	B	83	GLU
1	B	89	LEU
1	B	96	LYS
1	B	145	LYS
1	B	147	LYS
1	B	148	GLU
1	B	152	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	113	GLN
1	A	152	GLN
1	B	8	GLN
1	B	91	GLN
1	B	128	GLN
1	B	140	ASN
1	B	152	GLN

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 carbohydrates 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	154	1,3	27,50,50	2.25	8 (29%)	17,82,82	4.02	8 (47%)
2	HEM	A	154	1,3	27,50,50	2.36	10 (37%)	17,82,82	4.16	11 (64%)

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	154	1,3	-	1/6/54/54	-
2	HEM	A	154	1,3	-	0/6/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	154	HEM	C3C-CAC	5.76	1.59	1.47
2	A	154	HEM	C3B-CAB	5.47	1.59	1.47
2	A	154	HEM	CAA-C2A	4.86	1.59	1.52
2	A	154	HEM	C3B-C2B	-4.41	1.34	1.40
2	B	154	HEM	C3B-CAB	4.37	1.56	1.47
2	B	154	HEM	C3B-C2B	-4.36	1.34	1.40
2	A	154	HEM	C3C-CAC	4.14	1.56	1.47
2	A	154	HEM	C4A-NA	3.69	1.43	1.36
2	B	154	HEM	CAA-C2A	3.29	1.56	1.52
2	B	154	HEM	C1A-NA	3.24	1.42	1.36
2	B	154	HEM	CMB-C2B	2.91	1.58	1.51
2	A	154	HEM	C3C-C2C	-2.82	1.36	1.40
2	B	154	HEM	C4A-NA	2.56	1.41	1.36
2	A	154	HEM	CMB-C2B	2.50	1.57	1.51
2	B	154	HEM	C1D-ND	2.31	1.40	1.36
2	A	154	HEM	C1A-NA	2.21	1.40	1.36
2	A	154	HEM	C1B-C2B	2.11	1.47	1.42
2	A	154	HEM	C3D-C2D	-2.02	1.31	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	HEM	CMD-C2D-C1D	-9.47	113.91	128.46
2	A	154	HEM	CBD-CAD-C3D	-8.87	96.14	112.48
2	B	154	HEM	CMD-C2D-C3D	8.46	140.89	124.94
2	B	154	HEM	CBD-CAD-C3D	-7.96	97.81	112.48
2	A	154	HEM	CMD-C2D-C1D	-6.49	118.48	128.46
2	A	154	HEM	CAA-CBA-CGA	6.16	123.00	112.67
2	A	154	HEM	CAD-CBD-CGD	-5.72	103.07	112.67
2	A	154	HEM	CMD-C2D-C3D	5.29	134.91	124.94
2	A	154	HEM	C4C-C3C-C2C	5.14	110.48	106.90
2	A	154	HEM	CMB-C2B-C3B	3.80	131.78	124.68
2	B	154	HEM	CAD-CBD-CGD	-3.48	106.83	112.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	HEM	CMA-C3A-C4A	-3.29	123.41	128.46
2	A	154	HEM	CMC-C2C-C3C	2.95	130.19	124.68
2	A	154	HEM	CMA-C3A-C4A	-2.73	124.27	128.46
2	B	154	HEM	C1D-C2D-C3D	-2.65	105.15	107.00
2	B	154	HEM	CMB-C2B-C3B	2.54	129.43	124.68
2	B	154	HEM	CMA-C3A-C2A	2.40	129.47	124.94
2	A	154	HEM	CBA-CAA-C2A	-2.36	108.14	112.49
2	A	154	HEM	CMA-C3A-C2A	2.29	129.25	124.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

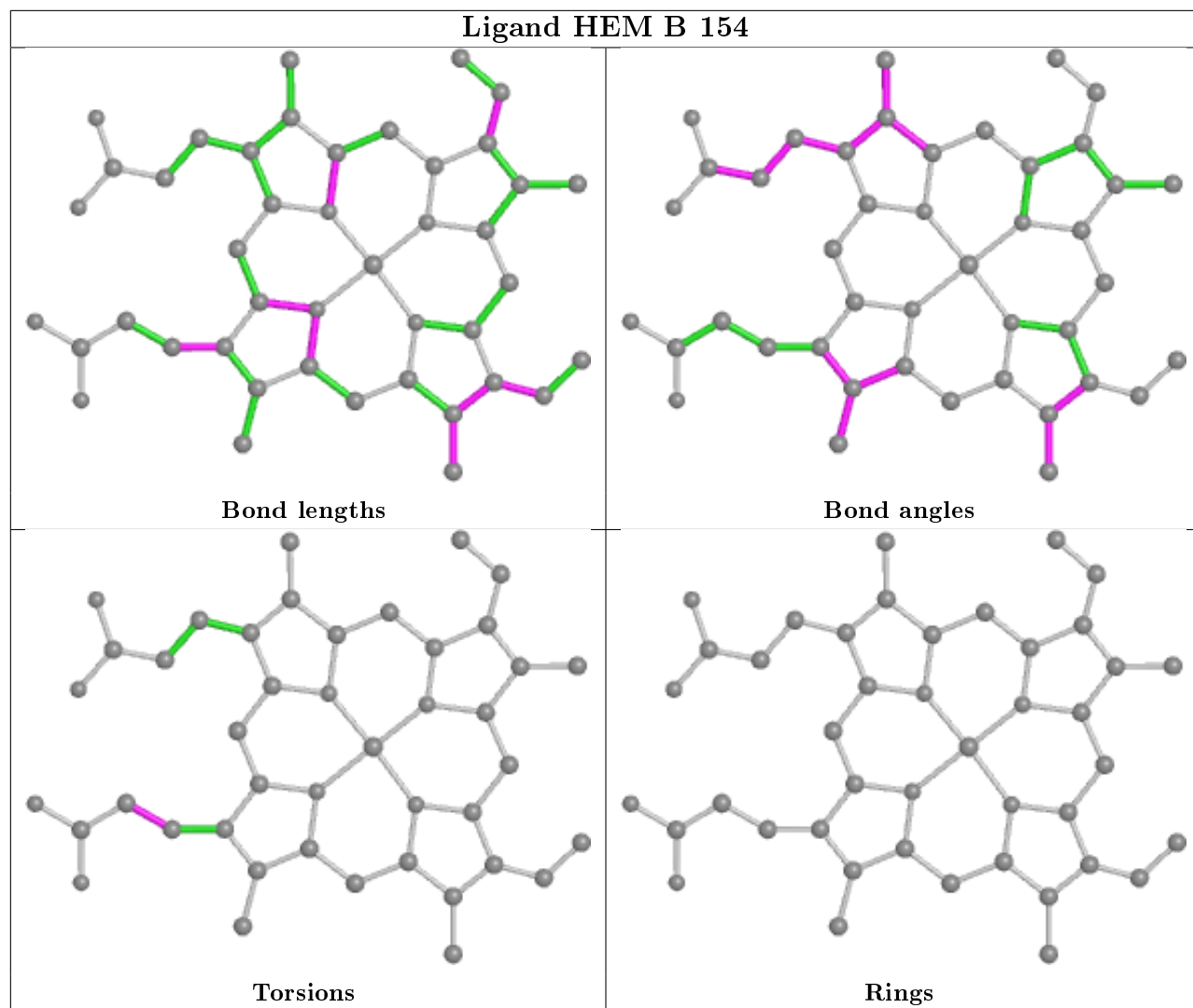
Mol	Chain	Res	Type	Atoms
2	B	154	HEM	C2A-CAA-CBA-CGA

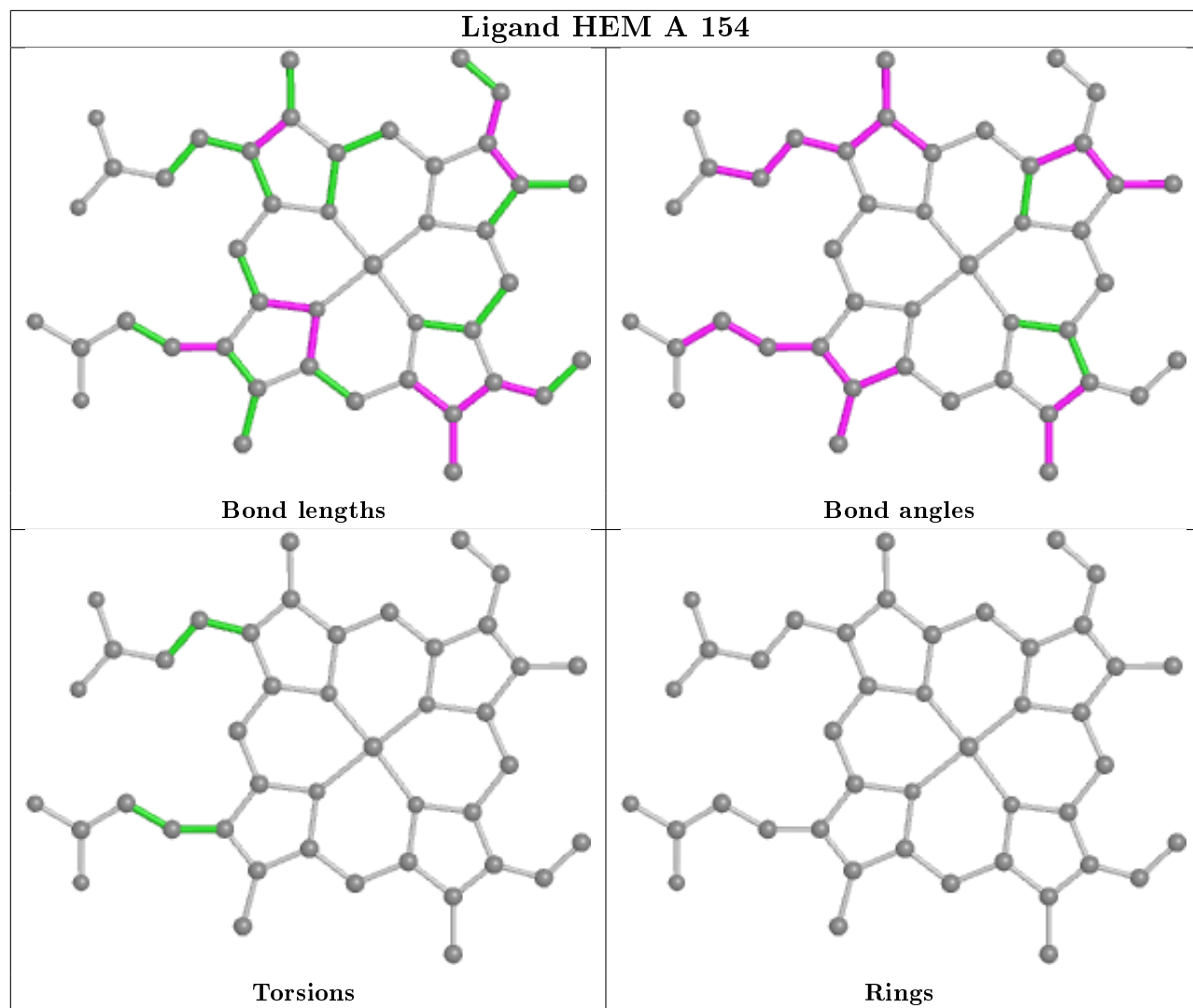
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	154	HEM	1	0
2	A	154	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 [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%)	-0.44	1 (0%) 87 87	16, 30, 53, 81	0
1	B	153/153 (100%)	-0.42	2 (1%) 77 76	16, 30, 51, 73	0
All	All	306/306 (100%)	-0.43	3 (0%) 82 81	16, 30, 51, 81	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	GLY	6.8
1	A	153	GLY	4.6
1	B	152	GLN	2.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

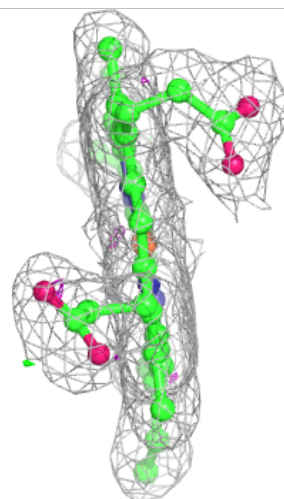
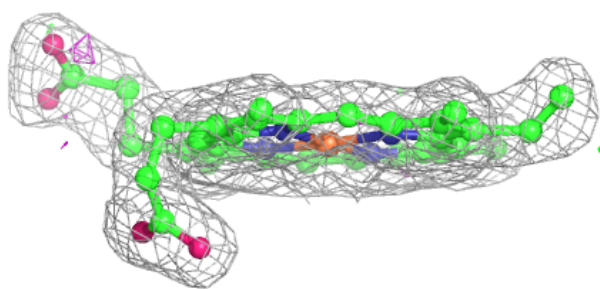
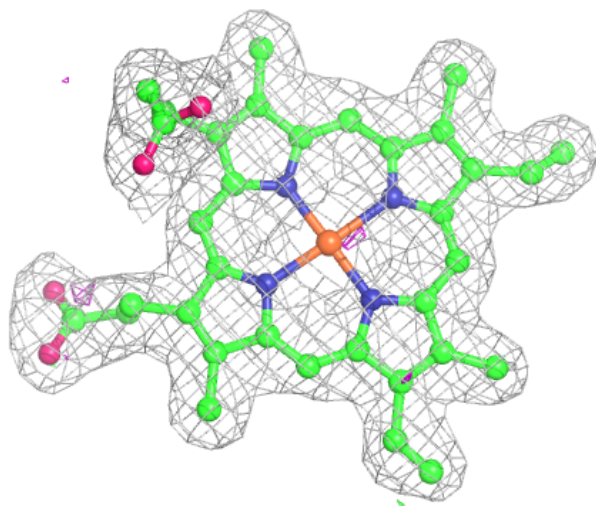
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	HEM	B	154	43/43	0.97	0.10	18,20,35,43	0
2	HEM	A	154	43/43	0.97	0.11	19,22,35,43	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.

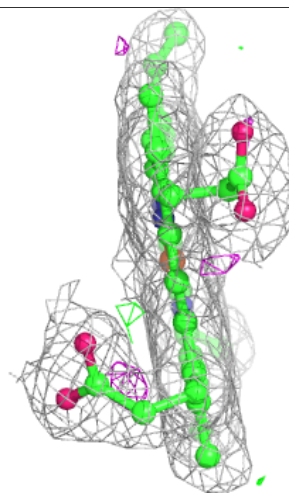
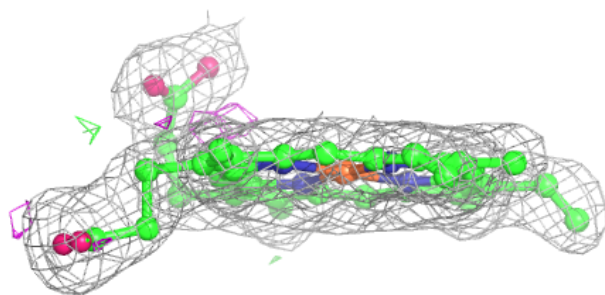
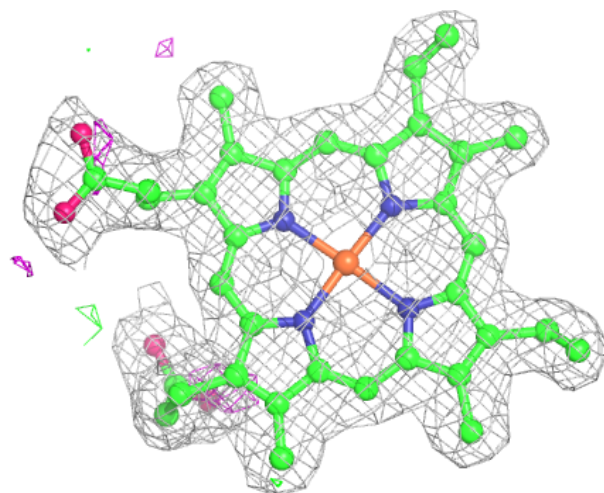
Electron density around HEM B 154:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 154:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.