



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1MNK / pdb_00001mnk
Title : INTERACTIONS AMONG RESIDUES CD3, E7, E10 AND E11 IN MYOGLOBINS: ATTEMPTS TO SIMULATE THE O₂ AND CO BINDING PROPERTIES OF APLYSIA MYOGLOBIN
Authors : Krzywda, S.; Wilkinson, A.J.
Deposited on : 1995-01-11
Resolution : 2.20 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

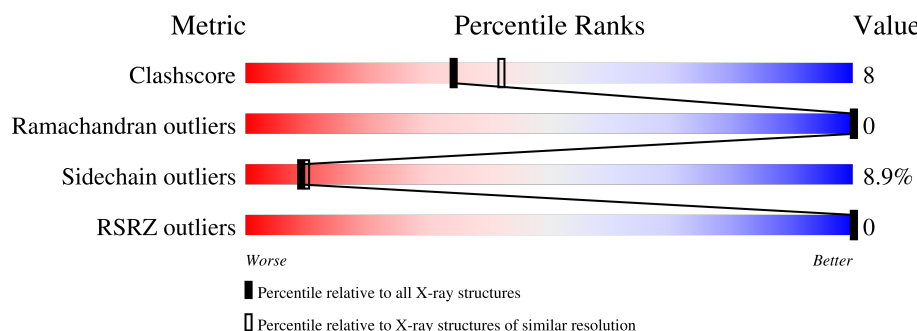
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	
1	B	153	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2651 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	151	Total	C	N	O	S	0	0	0
			1180	755	203	219	3			
1	B	151	Total	C	N	O	S	0	0	0
			1180	755	203	219	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	VAL	HIS	conflict	UNP P02189
A	68	THR	VAL	conflict	UNP P02189
B	64	VAL	HIS	conflict	UNP P02189
B	68	THR	VAL	conflict	UNP P02189

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

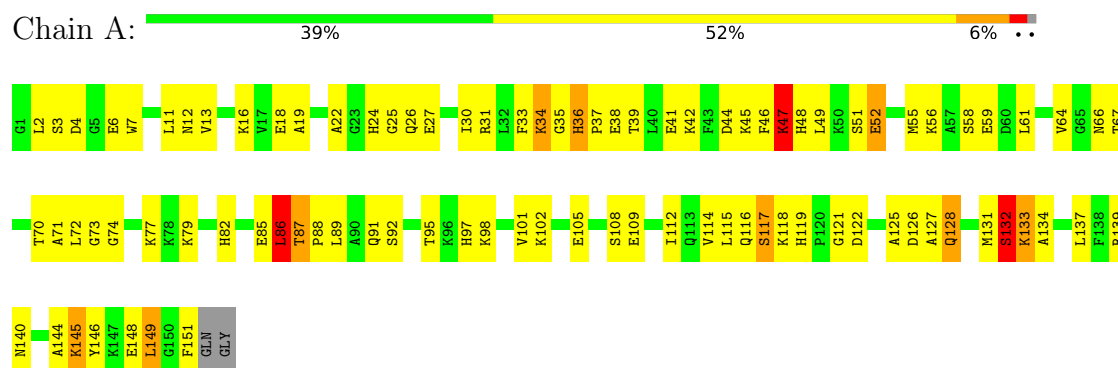
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total 90	O 90	1	0
3	B	115	Total 115	O 115	1	0

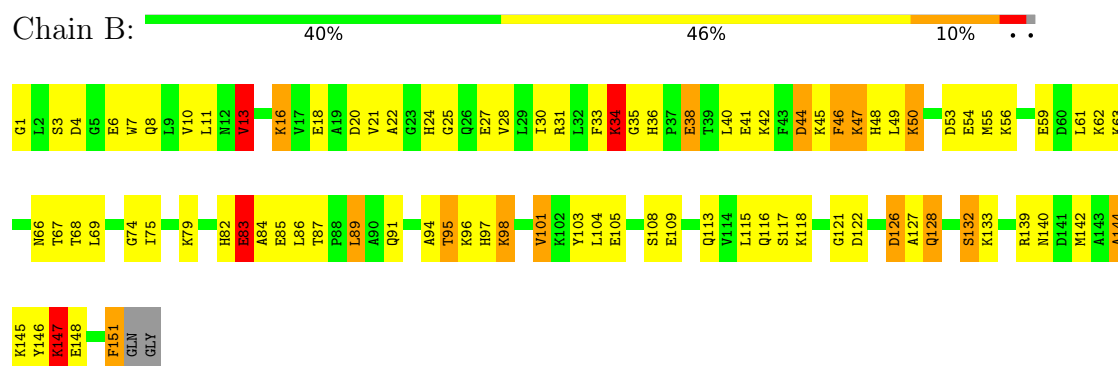
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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	125.26Å 42.49Å 92.37Å 90.00° 92.29° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 10.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.20) 92.5 (10.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.43 (at 2.19Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.164 , (Not available) 0.160 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 94.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.178 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2651	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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.*

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

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	1.33	2/1204 (0.2%)	2.89	145/1615 (9.0%)
1	B	1.36	3/1204 (0.2%)	2.80	126/1615 (7.8%)
All	All	1.34	5/2408 (0.2%)	2.84	271/3230 (8.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	33	PHE	C-N	-5.26	1.26	1.33
1	B	87	THR	CA-CB	5.22	1.60	1.53
1	A	127	ALA	N-CA	5.14	1.52	1.46
1	A	114	VAL	N-CA	5.07	1.52	1.46
1	B	109	GLU	N-CA	5.01	1.52	1.46

All (271) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	HIS	CA-C-N	14.02	135.74	120.03
1	A	24	HIS	C-N-CA	14.02	135.74	120.03
1	A	48	HIS	CA-CB-CG	-13.06	100.74	113.80
1	B	128	GLN	OE1-CD-NE2	12.51	135.11	122.60
1	B	24	HIS	CA-C-N	12.47	133.78	119.94
1	B	24	HIS	C-N-CA	12.47	133.78	119.94
1	A	35	GLY	CA-C-O	-12.46	106.76	120.09
1	A	66	ASN	OD1-CG-ND2	-12.09	110.51	122.60
1	A	35	GLY	CA-C-N	11.94	132.79	122.28
1	A	35	GLY	C-N-CA	11.94	132.79	122.28
1	A	131	MET	CA-C-O	11.77	133.02	120.55
1	A	30	ILE	O-C-N	-11.55	110.66	121.87
1	B	35	GLY	CA-C-N	11.45	132.35	122.28
1	B	35	GLY	C-N-CA	11.45	132.35	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	ARG	NE-CZ-NH2	-10.70	109.57	119.20
1	B	117	SER	CB-CA-C	-10.32	94.59	110.90
1	B	35	GLY	CA-C-O	-9.84	109.56	120.09
1	A	24	HIS	O-C-N	-9.82	111.71	122.12
1	A	47	LYS	CA-C-N	9.78	144.39	121.52
1	A	47	LYS	C-N-CA	9.78	144.39	121.52
1	A	91	GLN	CA-C-O	-9.71	110.80	121.00
1	A	46	PHE	CA-C-O	-9.42	108.85	119.78
1	A	11	LEU	CA-C-O	-9.29	109.28	119.97
1	B	74	GLY	O-C-N	-9.17	113.38	122.18
1	B	118	LYS	CA-C-O	-9.04	109.12	119.79
1	B	53	ASP	CA-CB-CG	-8.91	103.69	112.60
1	B	83	GLU	CB-CG-CD	8.89	127.71	112.60
1	B	116	GLN	CA-C-O	8.88	129.96	120.55
1	A	6	GLU	CG-CD-OE1	8.80	138.65	118.40
1	B	117	SER	N-CA-CB	8.69	122.66	110.07
1	B	139	ARG	NE-CZ-NH2	-8.66	111.41	119.20
1	B	67	THR	CA-CB-OG1	-8.64	96.64	109.60
1	B	25	GLY	CA-C-O	8.53	130.21	121.00
1	A	121	GLY	O-C-N	-8.47	113.26	122.24
1	A	148	GLU	CA-CB-CG	8.47	131.03	114.10
1	A	128	GLN	OE1-CD-NE2	8.45	131.05	122.60
1	A	34	LYS	CA-CB-CG	8.36	130.82	114.10
1	B	69	LEU	O-C-N	8.31	133.46	122.33
1	B	66	ASN	OD1-CG-ND2	-8.30	114.30	122.60
1	B	69	LEU	CA-C-O	-8.13	110.20	119.79
1	A	117	SER	CB-CA-C	-8.10	97.34	110.79
1	B	89	LEU	CB-CA-C	7.67	122.92	110.88
1	B	144	ALA	N-CA-C	-7.67	103.00	111.36
1	A	24	HIS	CA-CB-CG	-7.66	106.14	113.80
1	A	6	GLU	CG-CD-OE2	-7.55	101.02	118.40
1	A	58	SER	CA-C-O	7.55	129.52	120.92
1	A	105	GLU	CA-C-O	-7.43	112.54	120.42
1	B	63	LYS	CA-C-O	-7.40	113.05	120.82
1	B	89	LEU	N-CA-CB	-7.33	99.39	110.01
1	B	132	SER	CA-CB-OG	-7.30	96.50	111.10
1	A	3	SER	O-C-N	-7.25	113.74	122.65
1	A	119	HIS	CA-CB-CG	-7.23	106.57	113.80
1	A	36	HIS	O-C-N	7.22	126.76	121.12
1	B	25	GLY	O-C-N	-7.20	115.27	122.18
1	A	109	GLU	CA-C-O	-7.17	111.72	119.97
1	B	116	GLN	OE1-CD-NE2	-7.17	115.43	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	THR	N-CA-C	7.16	120.12	111.82
1	A	30	ILE	CA-C-N	7.14	129.72	120.44
1	A	30	ILE	C-N-CA	7.14	129.72	120.44
1	A	86	LEU	N-CA-C	7.05	119.04	111.36
1	A	91	GLN	O-C-N	7.04	129.35	122.03
1	B	13	VAL	N-CA-CB	-7.02	100.99	110.54
1	A	34	LYS	N-CA-C	-6.97	103.76	111.36
1	B	101	VAL	O-C-N	-6.96	113.93	121.80
1	A	71	ALA	O-C-N	-6.95	114.76	122.12
1	B	44	ASP	CA-CB-CG	-6.95	105.66	112.60
1	B	6	GLU	CG-CD-OE1	6.94	134.35	118.40
1	B	40	LEU	CA-C-O	6.89	127.85	120.55
1	B	47	LYS	CA-C-N	6.88	134.99	121.58
1	B	47	LYS	C-N-CA	6.88	134.99	121.58
1	A	72	LEU	CA-C-N	6.85	127.59	119.98
1	A	72	LEU	C-N-CA	6.85	127.59	119.98
1	B	21	VAL	O-C-N	-6.83	114.79	121.83
1	A	115	LEU	CA-C-O	6.81	127.77	120.55
1	A	25	GLY	O-C-N	-6.80	115.57	122.17
1	B	50	LYS	CA-C-O	-6.79	111.42	119.15
1	A	140	ASN	CA-C-O	-6.78	113.36	120.55
1	B	144	ALA	CA-C-O	-6.76	113.25	120.42
1	A	39	THR	CA-C-O	6.76	127.70	119.38
1	A	146	TYR	CA-C-N	6.74	129.31	120.28
1	A	146	TYR	C-N-CA	6.74	129.31	120.28
1	B	45	LYS	N-CA-CB	-6.62	99.06	110.32
1	A	108	SER	CA-C-O	6.62	127.57	120.55
1	B	139	ARG	CB-CA-C	-6.62	99.59	110.85
1	B	85	GLU	CG-CD-OE1	6.62	133.62	118.40
1	B	20	ASP	CA-CB-CG	-6.60	106.00	112.60
1	B	33	PHE	CA-C-N	6.60	129.66	120.29
1	B	33	PHE	C-N-CA	6.60	129.66	120.29
1	A	4	ASP	O-C-N	6.59	129.11	122.12
1	A	132	SER	N-CA-CB	-6.58	100.42	110.16
1	B	116	GLN	O-C-N	-6.55	115.17	122.12
1	B	36	HIS	CA-C-N	6.53	126.46	119.28
1	B	36	HIS	C-N-CA	6.53	126.46	119.28
1	B	108	SER	CA-C-O	6.50	127.64	120.82
1	A	52	GLU	CG-CD-OE1	6.43	133.19	118.40
1	A	31	ARG	N-CA-CB	6.43	119.33	110.01
1	A	33	PHE	CA-C-O	-6.42	113.61	120.42
1	B	103	TYR	O-C-N	6.42	130.17	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	THR	CA-CB-OG1	-6.41	99.98	109.60
1	A	98	LYS	CA-C-N	-6.41	117.14	123.04
1	A	98	LYS	C-N-CA	-6.41	117.14	123.04
1	A	149	LEU	CA-C-N	6.37	131.19	121.51
1	A	149	LEU	C-N-CA	6.37	131.19	121.51
1	A	64	VAL	N-CA-C	-6.36	104.30	110.72
1	A	102	LYS	CB-CA-C	-6.34	98.90	110.63
1	B	117	SER	CA-C-N	-6.32	109.93	120.68
1	B	117	SER	C-N-CA	-6.32	109.93	120.68
1	B	94	ALA	CA-C-N	6.31	129.90	120.31
1	B	94	ALA	C-N-CA	6.31	129.90	120.31
1	A	42	LYS	CB-CA-C	-6.29	98.69	110.01
1	A	122	ASP	CA-C-N	-6.28	114.54	123.20
1	A	122	ASP	C-N-CA	-6.28	114.54	123.20
1	A	74	GLY	O-C-N	-6.27	116.17	122.19
1	A	116	GLN	OE1-CD-NE2	-6.25	116.35	122.60
1	B	126	ASP	N-CA-C	6.25	117.89	111.14
1	A	61	LEU	N-CA-C	-6.23	104.42	111.14
1	B	140	ASN	O-C-N	-6.22	115.53	122.12
1	B	67	THR	CA-CB-CG2	6.22	121.07	110.50
1	B	122	ASP	CA-CB-CG	6.20	118.80	112.60
1	B	105	GLU	N-CA-CB	6.20	119.34	110.16
1	B	48	HIS	CA-CB-CG	6.20	120.00	113.80
1	A	33	PHE	CA-C-N	6.18	129.06	120.29
1	A	33	PHE	C-N-CA	6.18	129.06	120.29
1	A	26	GLN	OE1-CD-NE2	6.17	128.77	122.60
1	B	121	GLY	O-C-N	-6.17	115.71	122.68
1	B	104	LEU	N-CA-C	-6.17	104.67	111.82
1	B	3	SER	O-C-N	-6.16	115.47	122.68
1	A	46	PHE	O-C-N	6.15	130.68	122.26
1	B	66	ASN	CA-CB-CG	-6.11	106.49	112.60
1	B	133	LYS	CB-CG-CD	-6.11	97.25	111.30
1	A	132	SER	CA-CB-OG	-6.10	98.89	111.10
1	A	139	ARG	NE-CZ-NH2	-6.10	113.71	119.20
1	A	41	GLU	CB-CG-CD	6.10	122.96	112.60
1	B	53	ASP	CB-CA-C	6.10	121.21	110.85
1	A	7	TRP	CA-C-O	6.07	126.99	120.55
1	B	10	VAL	CA-C-O	-6.06	114.75	121.17
1	A	2	LEU	CA-C-O	-6.05	114.28	121.66
1	B	113	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	B	132	SER	CA-C-N	-6.01	111.75	120.29
1	B	132	SER	C-N-CA	-6.01	111.75	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	GLY	CA-C-N	6.00	126.64	119.98
1	A	73	GLY	C-N-CA	6.00	126.64	119.98
1	A	12	ASN	N-CA-CB	5.99	119.02	110.16
1	A	2	LEU	N-CA-C	-5.98	101.15	110.42
1	A	25	GLY	CA-C-N	5.97	128.56	120.44
1	A	25	GLY	C-N-CA	5.97	128.56	120.44
1	A	49	LEU	N-CA-C	-5.97	100.27	109.76
1	A	79	LYS	CB-CA-C	-5.96	103.43	111.89
1	B	86	LEU	N-CA-CB	-5.96	101.13	110.30
1	A	31	ARG	CB-CA-C	-5.92	101.59	110.88
1	A	59	GLU	CA-C-O	-5.92	114.22	120.55
1	A	95	THR	CA-CB-OG1	-5.90	100.75	109.60
1	A	117	SER	N-CA-CB	5.89	118.78	110.12
1	A	91	GLN	N-CA-CB	5.88	118.50	109.91
1	A	85	GLU	CG-CD-OE1	5.88	131.92	118.40
1	B	79	LYS	CB-CA-C	-5.87	103.55	111.89
1	B	31	ARG	NE-CZ-NH1	5.86	127.36	121.50
1	B	84	ALA	O-C-N	5.85	128.10	122.07
1	B	122	ASP	CA-C-O	5.84	125.47	119.05
1	A	52	GLU	CB-CG-CD	5.82	122.49	112.60
1	A	109	GLU	CG-CD-OE2	-5.82	105.02	118.40
1	B	103	TYR	CA-C-O	-5.81	113.29	119.97
1	A	42	LYS	O-C-N	5.79	130.37	122.37
1	A	109	GLU	OE1-CD-OE2	5.79	136.79	122.90
1	A	59	GLU	OE1-CD-OE2	5.79	136.78	122.90
1	A	133	LYS	CG-CD-CE	5.78	124.59	111.30
1	B	59	GLU	CG-CD-OE1	-5.76	105.14	118.40
1	A	125	ALA	O-C-N	-5.76	116.10	122.09
1	A	101	VAL	CA-C-O	-5.76	115.06	121.05
1	A	91	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	B	147	LYS	CB-CA-C	5.73	119.88	110.88
1	A	22	ALA	CA-C-O	-5.73	114.35	120.42
1	B	28	VAL	CA-C-O	-5.71	115.12	121.17
1	B	46	PHE	CA-C-O	-5.70	113.13	119.34
1	B	151	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	132	SER	CB-CA-C	5.67	120.50	110.85
1	A	18	GLU	CG-CD-OE2	-5.67	105.36	118.40
1	B	62	LYS	CG-CD-CE	-5.66	98.28	111.30
1	B	18	GLU	CG-CD-OE2	-5.62	105.48	118.40
1	B	42	LYS	O-C-N	5.62	130.21	122.46
1	A	18	GLU	CG-CD-OE1	5.60	131.29	118.40
1	B	147	LYS	CA-CB-CG	5.60	125.30	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	GLU	OE1-CD-OE2	5.60	136.34	122.90
1	A	134	ALA	CA-C-O	-5.60	114.49	120.42
1	B	3	SER	N-CA-CB	-5.58	101.94	110.42
1	A	139	ARG	N-CA-CB	5.55	118.28	110.12
1	A	105	GLU	CB-CA-C	-5.55	101.42	110.85
1	A	151	PHE	CA-CB-CG	5.54	119.34	113.80
1	B	127	ALA	CB-CA-C	5.54	119.98	110.79
1	A	47	LYS	CB-CA-C	-5.53	101.66	110.84
1	A	25	GLY	CA-C-O	5.52	126.21	120.80
1	B	54	GLU	CA-C-O	-5.52	114.57	120.42
1	B	74	GLY	N-CA-C	-5.52	106.10	112.50
1	B	101	VAL	CB-CA-C	5.52	121.20	112.26
1	A	95	THR	CA-CB-CG2	5.51	119.86	110.50
1	A	131	MET	CA-C-N	-5.50	112.48	120.29
1	A	131	MET	C-N-CA	-5.50	112.48	120.29
1	A	92	SER	CA-C-O	5.49	126.58	120.82
1	B	115	LEU	CA-C-O	5.49	126.37	120.55
1	B	34	LYS	CB-CA-C	-5.49	101.53	110.85
1	B	109	GLU	N-CA-CB	-5.46	102.09	110.16
1	B	24	HIS	O-C-N	-5.45	116.34	122.12
1	A	87	THR	CA-C-O	5.45	124.07	118.73
1	A	70	THR	N-CA-C	-5.45	105.24	111.07
1	A	36	HIS	CA-CB-CG	-5.44	108.36	113.80
1	B	63	LYS	CA-CB-CG	-5.42	103.26	114.10
1	B	25	GLY	CA-C-N	5.41	127.80	120.44
1	B	25	GLY	C-N-CA	5.41	127.80	120.44
1	A	30	ILE	N-CA-CB	-5.40	103.19	110.54
1	A	137	LEU	N-CA-C	-5.39	105.30	111.07
1	A	3	SER	N-CA-CB	-5.36	102.77	110.44
1	B	7	TRP	N-CA-C	-5.34	105.46	111.28
1	A	7	TRP	O-C-N	-5.34	116.46	122.12
1	A	26	GLN	CG-CD-OE1	-5.33	110.15	120.80
1	A	126	ASP	N-CA-C	5.32	116.76	111.07
1	B	142	MET	CA-C-O	5.31	126.39	120.82
1	A	87	THR	CA-CB-OG1	-5.30	101.65	109.60
1	A	105	GLU	O-C-N	5.30	128.19	122.15
1	B	104	LEU	CA-C-N	-5.29	112.78	120.29
1	B	104	LEU	C-N-CA	-5.29	112.78	120.29
1	A	118	LYS	CA-C-O	-5.29	113.41	119.60
1	B	27	GLU	CB-CG-CD	-5.28	103.63	112.60
1	B	91	GLN	N-CA-CB	5.27	117.61	109.91
1	A	144	ALA	CA-C-O	-5.26	114.84	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	GLU	CG-CD-OE2	-5.26	106.30	118.40
1	A	19	ALA	N-CA-C	-5.26	106.70	113.01
1	B	127	ALA	N-CA-C	-5.25	105.56	111.28
1	B	139	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	B	148	GLU	CB-CA-C	-5.24	100.61	110.67
1	A	128	GLN	CG-CD-OE1	-5.24	110.33	120.80
1	B	139	ARG	CD-NE-CZ	-5.22	117.09	124.40
1	B	13	VAL	CB-CA-C	5.22	119.19	112.14
1	B	10	VAL	O-C-N	5.22	127.02	121.91
1	B	1	GLY	CA-C-N	-5.21	113.78	122.64
1	B	1	GLY	C-N-CA	-5.21	113.78	122.64
1	A	89	LEU	CA-C-N	5.18	127.49	120.44
1	A	89	LEU	C-N-CA	5.18	127.49	120.44
1	B	49	LEU	CA-C-O	5.17	126.49	120.49
1	A	59	GLU	O-C-N	5.17	128.43	122.17
1	B	6	GLU	CG-CD-OE2	-5.17	106.51	118.40
1	B	68	THR	CA-C-O	-5.15	115.41	120.82
1	B	22	ALA	N-CA-C	-5.15	105.75	111.36
1	A	27	GLU	CB-CA-C	-5.14	102.25	110.79
1	B	11	LEU	CA-C-O	-5.14	114.06	119.97
1	A	59	GLU	CG-CD-OE2	-5.13	106.59	118.40
1	B	82	HIS	N-CA-CB	-5.12	102.76	111.20
1	A	95	THR	N-CA-C	5.11	119.60	112.90
1	B	117	SER	O-C-N	5.11	127.61	122.09
1	A	51	SER	O-C-N	5.11	129.39	122.96
1	A	38	GLU	CA-C-O	-5.10	112.41	119.05
1	B	38	GLU	CG-CD-OE2	-5.10	106.67	118.40
1	A	85	GLU	N-CA-C	-5.10	105.81	112.23
1	B	1	GLY	O-C-N	5.10	131.16	123.00
1	A	105	GLU	N-CA-CB	5.10	117.71	110.16
1	A	77	LYS	O-C-N	5.08	129.24	122.43
1	B	16	LYS	CB-CA-C	-5.08	102.21	110.85
1	A	85	GLU	CG-CD-OE2	-5.07	106.73	118.40
1	A	140	ASN	CB-CG-ND2	5.07	124.01	116.40
1	A	91	GLN	CG-CD-NE2	5.07	124.00	116.40
1	A	133	LYS	CD-CE-NZ	5.07	128.12	111.90
1	A	133	LYS	CB-CA-C	-5.06	102.39	110.79
1	A	55	MET	CA-C-O	-5.06	115.49	120.70
1	B	24	HIS	CA-CB-CG	-5.06	108.74	113.80
1	B	75	ILE	CA-C-N	5.05	127.05	120.28
1	B	75	ILE	C-N-CA	5.05	127.05	120.28
1	A	126	ASP	CA-CB-CG	-5.05	107.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	112	ILE	O-C-N	-5.04	116.97	121.91
1	B	44	ASP	O-C-N	5.01	127.43	122.12
1	B	36	HIS	CA-CB-CG	-5.01	108.79	113.80
1	B	47	LYS	CG-CD-CE	5.00	122.81	111.30
1	A	55	MET	N-CA-C	-5.00	105.74	111.14

There are no chirality outliers.

There are no planarity outliers.

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	1180	0	1194	18	0
1	B	1180	0	1194	17	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
3	A	90	0	0	8	0
3	B	115	0	0	9	0
All	All	2651	0	2448	37	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 8.

All (37) 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:13:VAL:HG13	3:A:232:HOH:O	1.51	1.08
1:A:13:VAL:HG22	3:A:232:HOH:O	1.66	0.95
1:B:126:ASP:HB2	3:B:161:HOH:O	1.73	0.88
1:B:128:GLN:HG2	3:B:197:HOH:O	1.78	0.84
1:A:13:VAL:CG2	3:A:232:HOH:O	2.29	0.77
1:A:13:VAL:CB	3:A:232:HOH:O	2.31	0.76
1:B:128:GLN:CG	3:B:197:HOH:O	2.39	0.70
1:B:38:GLU:HG3	3:B:258:HOH:O	1.92	0.69
1:B:144:ALA:HA	1:B:147:LYS:HE3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HA	3:A:232:HOH:O	1.99	0.62
1:A:128:GLN:HB3	3:A:241:HOH:O	1.99	0.61
1:A:47:LYS:HA	1:A:47:LYS:NZ	2.15	0.61
1:B:13:VAL:HG23	3:B:224:HOH:O	2.03	0.58
1:A:52:GLU:HG2	1:A:56:LYS:HE2	1.86	0.57
2:B:154:HEM:HMC1	2:B:154:HEM:HBC2	1.86	0.57
1:A:82:HIS:O	1:A:86:LEU:HB2	2.10	0.51
2:B:154:HEM:HBC2	2:B:154:HEM:CMC	2.39	0.51
1:A:47:LYS:HA	1:A:47:LYS:HZ3	1.75	0.50
1:B:97:HIS:C	1:B:98:LYS:HG2	2.38	0.49
1:B:128:GLN:HB3	3:B:197:HOH:O	2.13	0.47
1:A:97:HIS:NE2	2:A:154:HEM:O1A	2.40	0.47
1:A:128:GLN:O	1:A:132:SER:HB3	2.15	0.46
1:B:128:GLN:CB	3:B:197:HOH:O	2.63	0.46
1:B:46:PHE:CZ	1:B:61:LEU:HA	2.52	0.45
1:A:87:THR:HB	1:A:88:PRO:HD3	1.99	0.45
1:B:4:ASP:O	1:B:8:GLN:HG2	2.17	0.45
1:B:146:TYR:CD2	1:B:151:PHE:HD2	2.34	0.45
1:A:36:HIS:N	1:A:37:PRO:HD3	2.32	0.44
1:A:13:VAL:CG1	3:A:232:HOH:O	2.19	0.44
1:B:41:GLU:HG3	3:B:217:HOH:O	2.16	0.44
1:B:30:ILE:O	1:B:34:LYS:HB2	2.17	0.43
1:B:83:GLU:HG3	3:B:236:HOH:O	2.19	0.43
1:A:45:LYS:HE3	3:A:222:HOH:O	2.19	0.43
1:A:44:ASP:O	1:A:47:LYS:HG2	2.19	0.42
1:B:44:ASP:HA	1:B:47:LYS:HG3	2.01	0.42
1:B:30:ILE:HG12	1:B:55:MET:HB3	2.02	0.41
1:A:145:LYS:O	1:A:149:LEU:HG	2.21	0.41

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	149/153 (97%)	144 (97%)	5 (3%)	0	100	100
1	B	149/153 (97%)	146 (98%)	3 (2%)	0	100	100
All	All	298/306 (97%)	290 (97%)	8 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	123/124 (99%)	115 (94%)	8 (6%)	15	18
1	B	123/124 (99%)	109 (89%)	14 (11%)	5	5
All	All	246/248 (99%)	224 (91%)	22 (9%)	9	10

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	34	LYS
1	A	47	LYS
1	A	86	LEU
1	A	117	SER
1	A	132	SER
1	A	133	LYS
1	A	145	LYS
1	B	13	VAL
1	B	16	LYS
1	B	34	LYS
1	B	50	LYS
1	B	56	LYS
1	B	83	GLU
1	B	89	LEU
1	B	95	THR
1	B	96	LYS
1	B	98	LYS

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Mol	Chain	Res	Type
1	B	101	VAL
1	B	132	SER
1	B	145	LYS
1	B	147	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	66	ASN
1	A	91	GLN
1	A	140	ASN
1	B	12	ASN
1	B	36	HIS
1	B	48	HIS
1	B	66	ASN
1	B	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	HEM	B	154	1,3	50,50,50	1.36	7 (14%)	67,82,82	1.85	20 (29%)
2	HEM	A	154	1,3	50,50,50	1.43	5 (10%)	67,82,82	1.60	15 (22%)

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	-	7/14/54/54	-
2	HEM	A	154	1,3	-	7/14/54/54	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	FE-NB	3.94	2.07	1.94
2	A	154	HEM	CAC-C3C	3.61	1.57	1.47
2	A	154	HEM	CAB-C3B	3.42	1.56	1.47
2	B	154	HEM	CAC-C3C	3.28	1.56	1.47
2	B	154	HEM	FE-NB	3.18	2.04	1.94
2	B	154	HEM	CAB-C3B	2.81	1.54	1.47
2	A	154	HEM	FE-ND	2.54	2.02	1.94
2	B	154	HEM	CMB-C2B	2.35	1.55	1.50
2	B	154	HEM	C2A-C3A	-2.31	1.32	1.38
2	B	154	HEM	CMD-C2D	2.27	1.55	1.50
2	A	154	HEM	CAA-C2A	2.27	1.57	1.51
2	B	154	HEM	FE-ND	2.22	2.01	1.94

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	HEM	CBD-CAD-C3D	-4.77	99.34	112.53
2	A	154	HEM	CBD-CAD-C3D	-4.13	101.11	112.53
2	B	154	HEM	CMB-C2B-C1B	-3.62	119.38	125.03
2	A	154	HEM	CHD-C4C-NC	3.33	128.07	124.45
2	B	154	HEM	CHD-C1D-ND	3.25	127.92	124.42
2	B	154	HEM	C3B-C2B-C1B	3.25	108.85	106.41
2	B	154	HEM	CMA-C3A-C4A	-3.24	120.48	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	154	HEM	CAC-C3C-C4C	-3.11	117.38	124.82
2	B	154	HEM	CBB-CAB-C3B	-3.08	112.16	127.53
2	A	154	HEM	CBB-CAB-C3B	-2.97	112.69	127.53
2	B	154	HEM	C3D-C4D-ND	-2.92	106.97	110.17
2	A	154	HEM	CHB-C1B-NB	2.90	127.95	124.37
2	A	154	HEM	C3B-C4B-NB	-2.90	107.39	109.47
2	B	154	HEM	O2D-CGD-CBD	2.86	123.05	114.00
2	B	154	HEM	C4D-C3D-C2D	2.83	111.01	106.89
2	A	154	HEM	CAD-C3D-C4D	-2.79	119.83	124.70
2	B	154	HEM	CMD-C2D-C1D	-2.78	120.69	125.03
2	B	154	HEM	CMA-C3A-C2A	2.76	131.48	125.62
2	B	154	HEM	CMD-C2D-C3D	2.67	133.37	126.15
2	B	154	HEM	CHC-C1C-NC	2.66	127.35	124.45
2	B	154	HEM	CAA-CBA-CGA	2.55	120.44	113.67
2	A	154	HEM	C4D-C3D-C2D	2.50	110.53	106.89
2	A	154	HEM	CHA-C4D-C3D	2.48	129.80	125.23
2	A	154	HEM	C3D-C4D-ND	-2.44	107.49	110.17
2	A	154	HEM	CHC-C4B-NB	2.41	127.02	124.42
2	B	154	HEM	C1A-CHA-C4D	-2.38	120.64	126.25
2	B	154	HEM	CHA-C1A-NA	2.35	128.12	123.86
2	B	154	HEM	CBC-CAC-C3C	-2.35	115.80	127.53
2	A	154	HEM	CHB-C4A-NA	2.32	128.07	123.86
2	A	154	HEM	C4B-C3B-C2B	2.17	109.27	107.28
2	B	154	HEM	CHA-C4D-ND	2.16	127.04	124.37
2	B	154	HEM	O2A-CGA-CBA	2.15	120.81	114.00
2	B	154	HEM	CMC-C2C-C1C	-2.14	120.96	124.73
2	A	154	HEM	C4A-CHB-C1B	-2.07	121.38	126.25
2	A	154	HEM	O2A-CGA-O1A	-2.01	118.17	123.33

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	154	HEM	C2A-CAA-CBA-CGA
2	A	154	HEM	C2B-C3B-CAB-CBB
2	B	154	HEM	C2B-C3B-CAB-CBB
2	B	154	HEM	C2A-CAA-CBA-CGA
2	A	154	HEM	C4B-C3B-CAB-CBB
2	A	154	HEM	CAA-CBA-CGA-O1A
2	B	154	HEM	CAA-CBA-CGA-O1A
2	A	154	HEM	CAA-CBA-CGA-O2A
2	B	154	HEM	CAA-CBA-CGA-O2A

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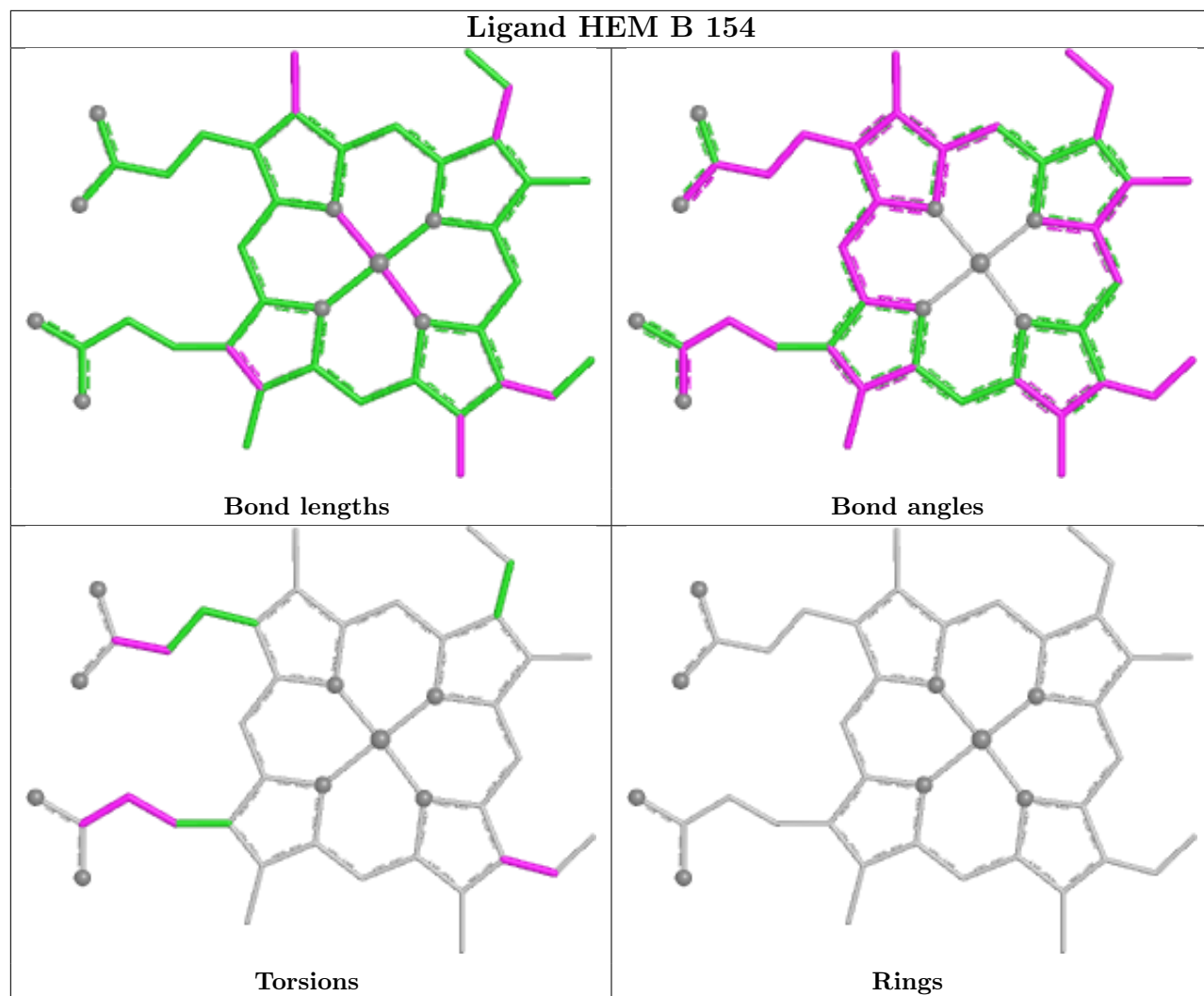
Mol	Chain	Res	Type	Atoms
2	A	154	HEM	CAD-CBD-CGD-O2D
2	B	154	HEM	CAD-CBD-CGD-O2D
2	A	154	HEM	CAD-CBD-CGD-O1D
2	B	154	HEM	C4B-C3B-CAB-CBB
2	B	154	HEM	CAD-CBD-CGD-O1D

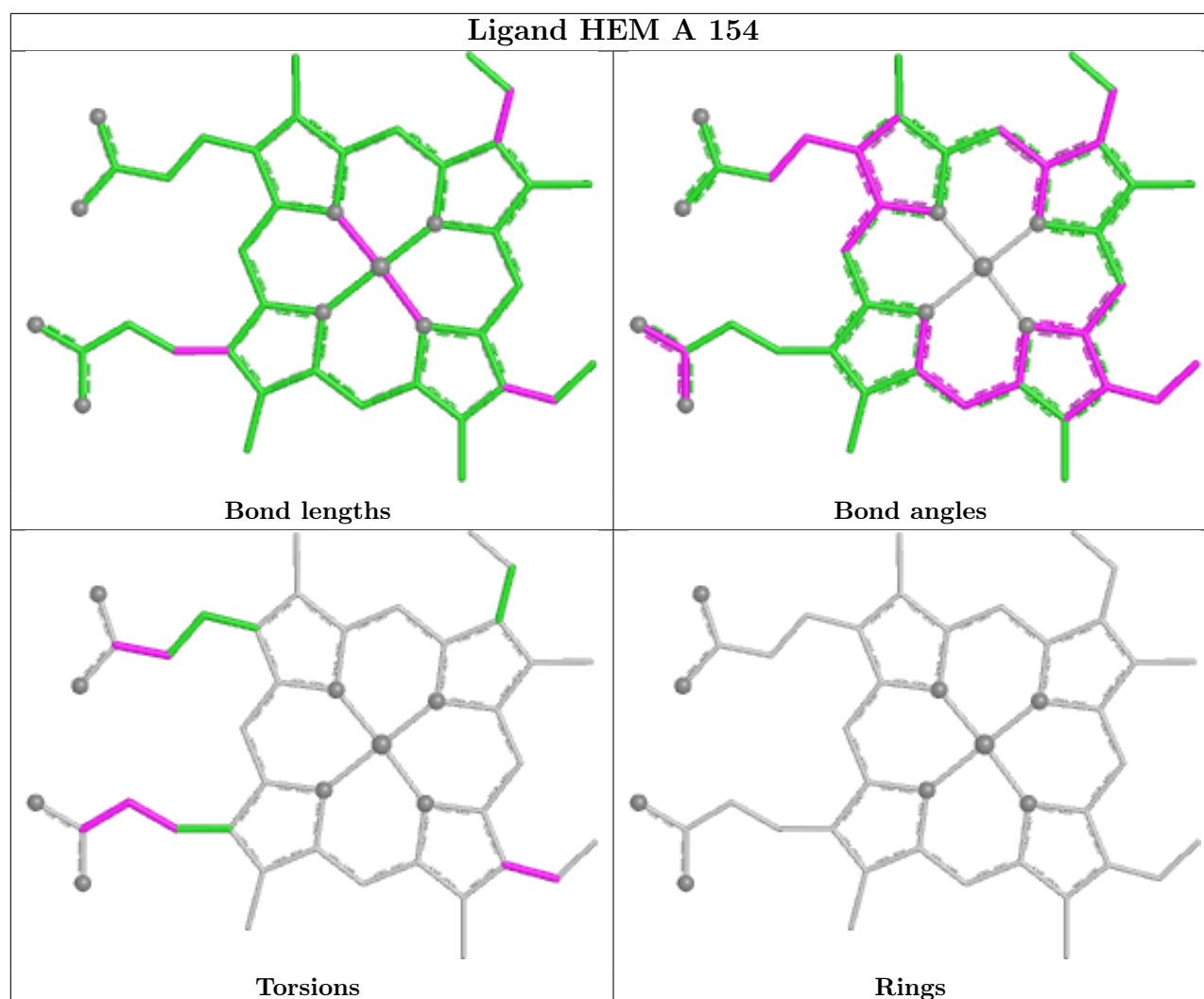
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	154	HEM	2	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	151/153 (98%)	-0.82	0 100 100	9, 23, 50, 63	0
1	B	151/153 (98%)	-0.82	0 100 100	10, 24, 49, 64	0
All	All	302/306 (98%)	-0.82	0 100 100	9, 24, 49, 64	0

There are no RSRZ outliers to report.

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](#)

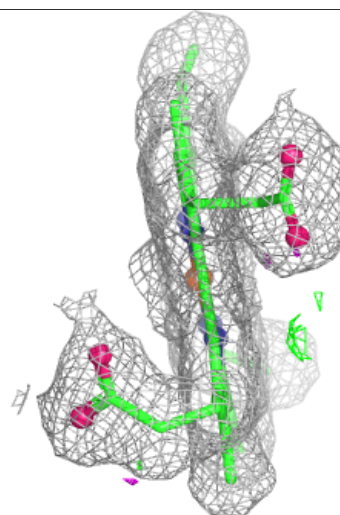
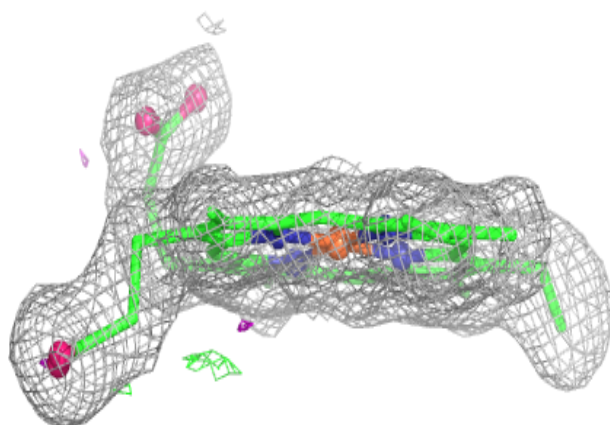
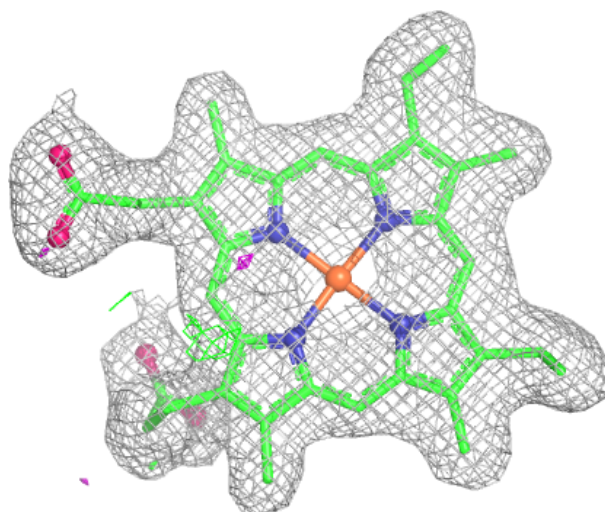
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	HEM	A	154	43/43	0.98	0.05	15,18,25,30	0
2	HEM	B	154	43/43	0.98	0.05	13,18,27,33	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.

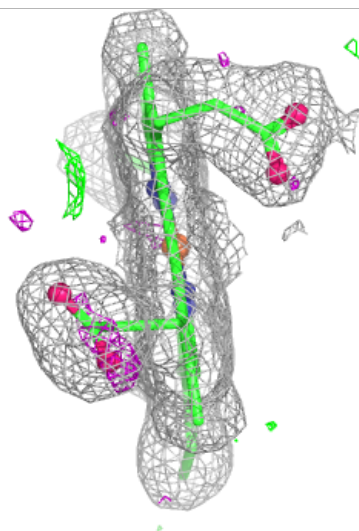
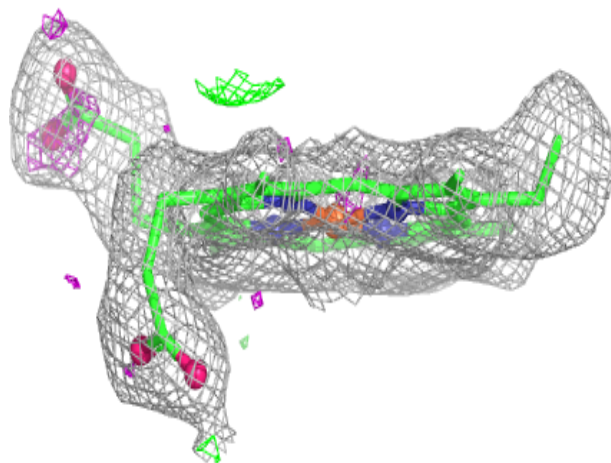
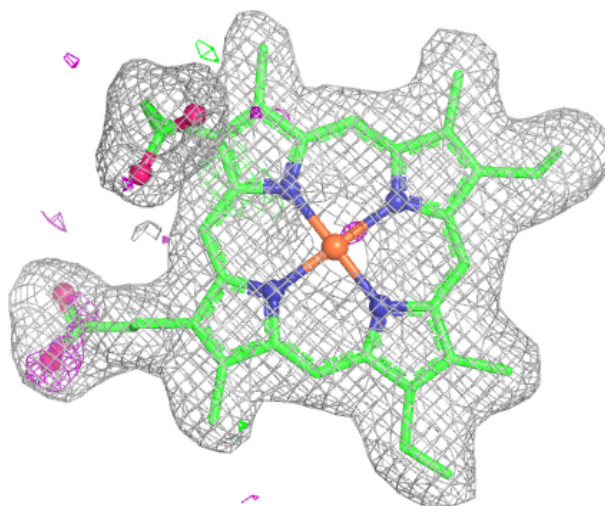
Electron density around HEM A 154:

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



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)



6.5 Other polymers ⓘ

There are no such residues in this entry.