



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:06 am GMT

PDB ID : 1PMB  
Title : THE DETERMINATION OF THE CRYSTAL STRUCTURE OF RECOMBINANT PIG MYOGLOBIN BY MOLECULAR REPLACEMENT AND ITS REFINEMENT  
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Deposited on : 1989-11-27  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

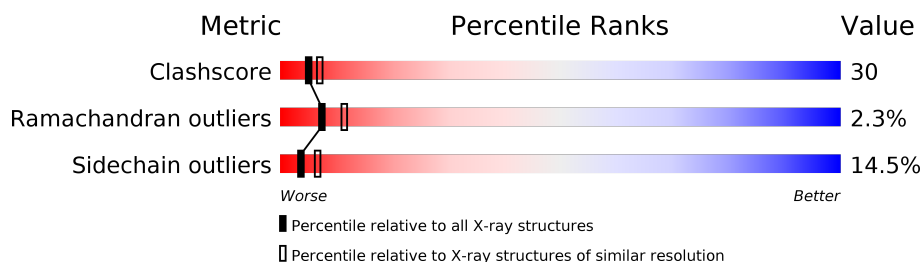
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

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 2537 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
			1197	764	208	222	3			
1	B	153	Total	C	N	O	S	0	0	0
			1197	764	208	222	3			

- 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		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

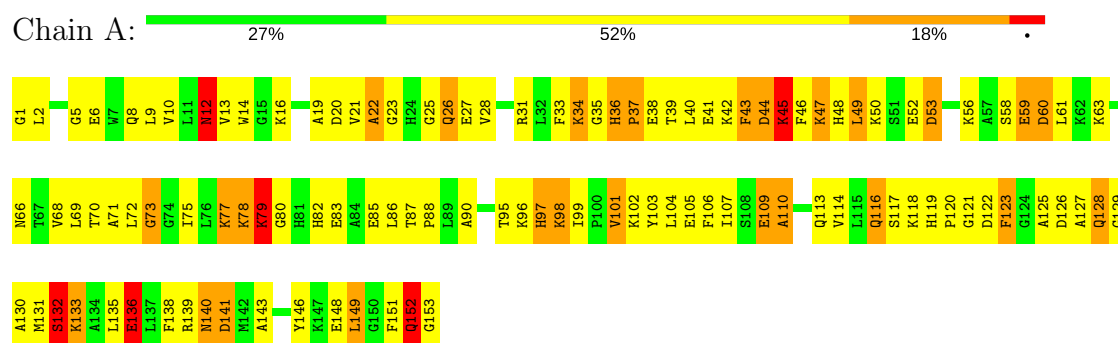
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total 29	O 29	0	0
3	B	28	Total 28	O 28	0	0

### 3 Residue-property plots

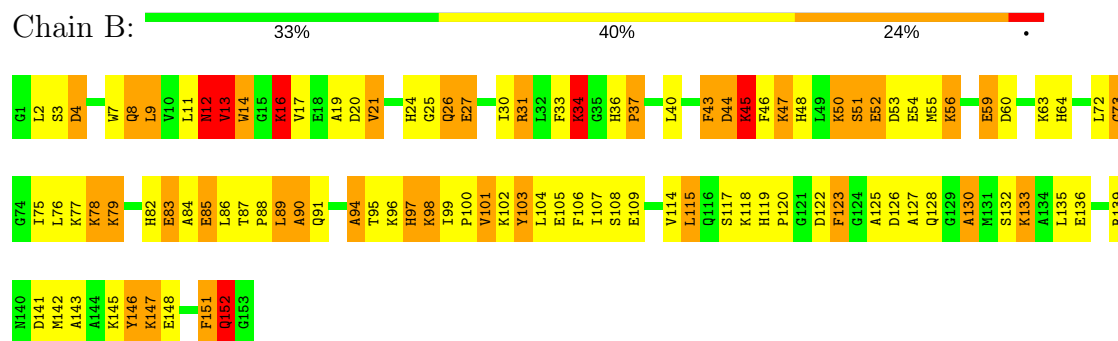
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

#### • Molecule 1: MYOGLOBIN



#### • Molecule 1: MYOGLOBIN



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.91Å 42.63Å 92.20Å 90.00° 92.16° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2537	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

## 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	1.02	0/1222	2.69	99/1637 (6.0%)
1	B	1.07	1/1222 (0.1%)	2.74	110/1637 (6.7%)
All	All	1.04	1/2444 (0.0%)	2.71	209/3274 (6.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	GLU	CD-OE2	6.76	1.33	1.25

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	NE-CZ-NH2	-16.28	112.16	120.30
1	B	83	GLU	OE1-CD-OE2	13.82	139.88	123.30
1	A	109	GLU	CA-CB-CG	13.67	143.47	113.40
1	B	31	ARG	NE-CZ-NH2	13.66	127.13	120.30
1	A	31	ARG	NE-CZ-NH1	13.06	126.83	120.30
1	A	141	ASP	CB-CG-OD2	12.78	129.80	118.30
1	B	109	GLU	OE1-CD-OE2	12.52	138.32	123.30
1	A	20	ASP	CB-CG-OD2	-12.40	107.14	118.30
1	B	132	SER	N-CA-CB	-12.05	92.42	110.50
1	B	53	ASP	CB-CG-OD1	12.02	129.11	118.30
1	A	132	SER	N-CA-CB	-11.51	93.23	110.50
1	B	4	ASP	CB-CG-OD1	-11.41	108.03	118.30
1	A	103	TYR	O-C-N	10.72	139.85	122.70
1	A	60	ASP	CB-CG-OD1	-10.61	108.75	118.30
1	B	123	PHE	CB-CG-CD1	-10.33	113.57	120.80
1	A	12	ASN	OD1-CG-ND2	10.17	145.29	121.90
1	B	12	ASN	OD1-CG-ND2	10.12	145.17	121.90
1	B	31	ARG	NE-CZ-NH1	-10.08	115.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	GLN	OE1-CD-NE2	9.99	144.87	121.90
1	B	103	TYR	O-C-N	9.68	138.19	122.70
1	B	126	ASP	CB-CG-OD2	9.60	126.94	118.30
1	B	136	GLU	OE1-CD-OE2	9.46	134.65	123.30
1	A	141	ASP	CB-CG-OD1	-9.23	109.99	118.30
1	B	139	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	B	59	GLU	CA-CB-CG	8.90	132.97	113.40
1	B	72	LEU	C-N-CA	8.73	140.64	122.30
1	B	60	ASP	CB-CG-OD1	8.72	126.15	118.30
1	A	5	GLY	O-C-N	8.56	136.40	122.70
1	B	83	GLU	CB-CA-C	-8.49	93.41	110.40
1	A	59	GLU	CA-CB-CG	8.32	131.71	113.40
1	A	126	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	A	72	LEU	C-N-CA	8.27	139.66	122.30
1	B	51	SER	N-CA-CB	-8.25	98.13	110.50
1	B	44	ASP	CA-C-N	-8.19	99.18	117.20
1	B	97	HIS	CA-CB-CG	-8.17	99.71	113.60
1	A	69	LEU	O-C-N	8.15	135.74	122.70
1	B	37	PRO	O-C-N	8.08	135.63	122.70
1	B	53	ASP	CB-CA-C	8.06	126.53	110.40
1	B	9	LEU	O-C-N	8.04	135.56	122.70
1	A	14	TRP	CB-CG-CD1	8.00	137.40	127.00
1	A	53	ASP	CB-CG-OD1	-7.99	111.11	118.30
1	A	19	ALA	C-N-CA	7.92	141.50	121.70
1	B	103	TYR	CB-CG-CD2	-7.87	116.28	121.00
1	A	77	LYS	CG-CD-CE	7.77	135.21	111.90
1	B	13	VAL	CB-CA-C	7.76	126.14	111.40
1	A	128	GLN	CG-CD-OE1	-7.70	106.19	121.60
1	A	83	GLU	CG-CD-OE1	7.64	133.58	118.30
1	A	33	PHE	CB-CG-CD1	-7.62	115.47	120.80
1	B	146	TYR	O-C-N	7.60	134.86	122.70
1	B	136	GLU	CG-CD-OE2	-7.53	103.23	118.30
1	A	83	GLU	CB-CG-CD	7.52	134.51	114.20
1	A	12	ASN	N-CA-CB	-7.47	97.16	110.60
1	A	45	LYS	N-CA-CB	-7.41	97.27	110.60
1	B	34	LYS	CB-CA-C	-7.36	95.68	110.40
1	B	14	TRP	CB-CG-CD1	7.36	136.56	127.00
1	A	71	ALA	CA-C-N	7.34	133.36	117.20
1	B	44	ASP	CA-C-O	7.32	135.47	120.10
1	B	19	ALA	C-N-CA	7.29	139.93	121.70
1	B	123	PHE	O-C-N	7.29	135.59	123.20
1	B	12	ASN	CB-CG-OD1	-7.26	107.08	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ASP	CB-CG-OD1	7.24	124.82	118.30
1	A	38	GLU	CA-CB-CG	7.18	129.21	113.40
1	B	53	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	B	20	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	44	ASP	CA-C-O	6.99	134.78	120.10
1	A	149	LEU	C-N-CA	6.97	136.94	122.30
1	A	12	ASN	CB-CG-ND2	-6.97	99.97	116.70
1	B	86	LEU	CB-CA-C	6.91	123.34	110.20
1	A	135	LEU	O-C-N	6.91	133.76	122.70
1	A	136	GLU	OE1-CD-OE2	6.88	131.56	123.30
1	A	117	SER	N-CA-CB	6.85	120.78	110.50
1	B	105	GLU	OE1-CD-OE2	6.73	131.38	123.30
1	A	60	ASP	CB-CG-OD2	6.73	124.36	118.30
1	A	83	GLU	OE1-CD-OE2	-6.72	115.24	123.30
1	A	126	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	73	GLY	C-N-CA	6.70	136.37	122.30
1	A	58	SER	C-N-CA	6.67	138.37	121.70
1	A	97	HIS	O-C-N	6.65	133.34	122.70
1	A	78	LYS	CB-CA-C	-6.64	97.11	110.40
1	B	64	HIS	C-N-CA	6.64	136.24	122.30
1	B	103	TYR	N-CA-CB	6.62	122.52	110.60
1	B	75	ILE	N-CA-CB	-6.62	95.58	110.80
1	A	14	TRP	CB-CG-CD2	-6.61	118.01	126.60
1	A	59	GLU	OE1-CD-OE2	6.58	131.19	123.30
1	A	25	GLY	C-N-CA	6.54	138.05	121.70
1	A	123	PHE	CB-CG-CD1	-6.53	116.23	120.80
1	B	82	HIS	N-CA-CB	-6.48	98.94	110.60
1	A	103	TYR	CB-CG-CD1	6.46	124.88	121.00
1	B	14	TRP	CB-CG-CD2	-6.43	118.24	126.60
1	B	152	GLN	CA-CB-CG	6.42	127.53	113.40
1	A	14	TRP	CG-CD2-CE3	-6.38	128.16	133.90
1	B	135	LEU	O-C-N	6.37	132.89	122.70
1	A	2	LEU	O-C-N	6.36	132.88	122.70
1	B	130	ALA	CB-CA-C	6.36	119.64	110.10
1	B	103	TYR	CB-CG-CD1	6.36	124.82	121.00
1	B	19	ALA	CB-CA-C	6.32	119.58	110.10
1	B	34	LYS	N-CA-CB	6.31	121.95	110.60
1	A	135	LEU	CA-C-O	-6.31	106.86	120.10
1	A	127	ALA	CB-CA-C	6.30	119.56	110.10
1	B	117	SER	CB-CA-C	-6.28	98.17	110.10
1	B	125	ALA	C-N-CA	6.26	137.35	121.70
1	B	59	GLU	CG-CD-OE2	-6.25	105.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ASP	CA-C-N	-6.22	103.51	117.20
1	B	146	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	A	49	LEU	CB-CA-C	6.18	121.94	110.20
1	A	149	LEU	CB-CA-C	6.17	121.92	110.20
1	A	79	LYS	CA-CB-CG	6.14	126.92	113.40
1	B	14	TRP	CG-CD2-CE3	-6.12	128.39	133.90
1	B	141	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	34	LYS	N-CA-CB	6.10	121.58	110.60
1	A	53	ASP	OD1-CG-OD2	6.09	134.86	123.30
1	A	53	ASP	CA-CB-CG	-6.07	100.04	113.40
1	A	125	ALA	CB-CA-C	6.05	119.18	110.10
1	B	106	PHE	O-C-N	6.02	132.34	122.70
1	B	14	TRP	CA-C-N	6.02	128.24	116.20
1	A	139	ARG	CB-CA-C	-5.96	98.47	110.40
1	A	71	ALA	CA-C-O	-5.94	107.62	120.10
1	B	44	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	B	8	GLN	CB-CG-CD	5.92	126.99	111.60
1	B	122	ASP	CA-C-N	-5.91	104.19	117.20
1	B	108	SER	CA-C-N	-5.91	104.20	117.20
1	B	25	GLY	C-N-CA	5.91	136.47	121.70
1	B	122	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	153	GLY	N-CA-C	5.89	127.82	113.10
1	A	97	HIS	CA-CB-CG	-5.87	103.61	113.60
1	B	4	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	20	ASP	N-CA-CB	-5.85	100.07	110.60
1	B	59	GLU	CB-CA-C	-5.85	98.70	110.40
1	A	36	HIS	O-C-N	5.84	132.20	121.10
1	B	89	LEU	CA-CB-CG	5.78	128.60	115.30
1	B	151	PHE	C-N-CA	5.77	136.12	121.70
1	A	75	ILE	C-N-CA	5.77	136.12	121.70
1	B	115	LEU	O-C-N	-5.74	113.51	122.70
1	A	70	THR	O-C-N	-5.74	113.52	122.70
1	B	27	GLU	CG-CD-OE1	5.74	129.78	118.30
1	B	152	GLN	CB-CG-CD	5.74	126.52	111.60
1	B	43	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	A	103	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	B	103	TYR	CZ-CE2-CD2	-5.71	114.66	119.80
1	A	6	GLU	CA-CB-CG	-5.70	100.86	113.40
1	B	12	ASN	CA-CB-CG	-5.70	100.86	113.40
1	B	127	ALA	CB-CA-C	5.69	118.64	110.10
1	A	121	GLY	CA-C-O	-5.68	110.37	120.60
1	A	148	GLU	N-CA-CB	-5.63	100.46	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	GLU	O-C-N	5.62	131.70	122.70
1	B	117	SER	N-CA-CB	5.62	118.92	110.50
1	B	53	ASP	N-CA-CB	-5.57	100.58	110.60
1	B	52	GLU	CA-C-O	5.57	131.79	120.10
1	B	101	VAL	CB-CA-C	5.55	121.95	111.40
1	B	103	TYR	CA-CB-CG	-5.54	102.88	113.40
1	B	132	SER	CA-CB-OG	-5.53	96.27	111.20
1	B	14	TRP	O-C-N	-5.51	113.83	123.20
1	B	24	HIS	C-N-CA	5.50	133.85	122.30
1	B	148	GLU	N-CA-CB	-5.49	100.72	110.60
1	B	146	TYR	CA-C-O	-5.48	108.59	120.10
1	B	12	ASN	N-CA-CB	-5.47	100.75	110.60
1	B	102	LYS	CD-CE-NZ	5.45	124.25	111.70
1	B	73	GLY	C-N-CA	5.44	133.72	122.30
1	B	16	LYS	CA-C-O	5.42	131.49	120.10
1	B	128	GLN	OE1-CD-NE2	5.41	134.34	121.90
1	B	123	PHE	CA-C-N	-5.41	105.39	116.20
1	A	22	ALA	CB-CA-C	5.39	118.19	110.10
1	A	28	VAL	CA-CB-CG1	5.37	118.95	110.90
1	B	85	GLU	N-CA-CB	5.36	120.24	110.60
1	A	103	TYR	CA-C-O	-5.35	108.86	120.10
1	A	42	LYS	O-C-N	5.34	131.25	122.70
1	A	42	LYS	CA-CB-CG	-5.34	101.64	113.40
1	A	33	PHE	CG-CD1-CE1	-5.34	114.93	120.80
1	A	121	GLY	C-N-CA	5.34	135.04	121.70
1	B	9	LEU	CA-C-O	-5.33	108.90	120.10
1	B	36	HIS	O-C-N	5.33	131.23	121.10
1	A	132	SER	O-C-N	-5.33	114.18	122.70
1	B	9	LEU	CA-CB-CG	-5.31	103.08	115.30
1	A	59	GLU	CG-CD-OE2	-5.30	107.69	118.30
1	A	90	ALA	N-CA-CB	-5.30	102.68	110.10
1	B	109	GLU	CG-CD-OE2	-5.29	107.72	118.30
1	B	34	LYS	O-C-N	5.29	132.19	123.20
1	B	21	VAL	CA-CB-CG1	5.27	118.81	110.90
1	A	135	LEU	C-N-CA	-5.26	108.54	121.70
1	B	146	TYR	CZ-CE2-CD2	-5.25	115.07	119.80
1	A	14	TRP	CE2-CD2-CE3	5.24	124.99	118.70
1	A	123	PHE	O-C-N	5.24	132.11	123.20
1	B	27	GLU	O-C-N	-5.22	114.35	122.70
1	A	37	PRO	O-C-N	5.21	131.03	122.70
1	B	3	SER	CA-C-O	5.20	131.02	120.10
1	B	52	GLU	CA-C-N	-5.20	105.76	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ASP	O-C-N	5.19	131.01	122.70
1	A	90	ALA	CB-CA-C	5.19	117.88	110.10
1	A	132	SER	C-N-CA	5.17	134.62	121.70
1	B	152	GLN	C-N-CA	5.17	133.15	122.30
1	B	126	ASP	N-CA-CB	-5.13	101.37	110.60
1	A	43	PHE	CB-CG-CD2	-5.12	117.21	120.80
1	A	69	LEU	CA-C-O	-5.12	109.35	120.10
1	B	90	ALA	CB-CA-C	5.12	117.78	110.10
1	A	33	PHE	O-C-N	5.12	130.88	122.70
1	A	152	GLN	CA-CB-CG	5.08	124.58	113.40
1	A	110	ALA	N-CA-CB	-5.08	102.99	110.10
1	B	36	HIS	CA-CB-CG	-5.08	104.97	113.60
1	B	103	TYR	CA-C-O	-5.07	109.45	120.10
1	A	85	GLU	CG-CD-OE2	-5.07	108.16	118.30
1	A	122	ASP	CA-C-O	5.04	130.69	120.10
1	A	140	ASN	CB-CG-ND2	5.04	128.80	116.70
1	A	35	GLY	CA-C-O	-5.04	111.53	120.60
1	A	33	PHE	CD1-CG-CD2	5.04	124.85	118.30
1	B	105	GLU	N-CA-CB	-5.03	101.54	110.60
1	B	94	ALA	C-N-CA	5.03	134.26	121.70
1	B	103	TYR	CB-CA-C	-5.03	100.35	110.40
1	A	71	ALA	C-N-CA	5.02	134.26	121.70
1	B	75	ILE	CB-CA-C	5.01	121.63	111.60

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	1197	0	1202	74	0
1	B	1197	0	1203	73	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
3	A	29	0	0	2	0
3	B	28	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2537	0	2465	147	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 30.

All (147) 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:99:ILE:HD12	2:A:154:HEM:HAC	1.26	1.13
1:B:2:LEU:HD11	1:B:133:LYS:HB3	1.38	1.05
1:B:52:GLU:HG2	1:B:56:LYS:HE2	1.09	1.04
1:B:52:GLU:CG	1:B:56:LYS:HE2	1.90	1.00
1:B:52:GLU:HG2	1:B:56:LYS:CE	1.97	0.94
1:A:37:PRO:O	1:A:40:LEU:HB3	1.72	0.88
1:B:143:ALA:O	1:B:147:LYS:HE2	1.79	0.82
1:A:99:ILE:CD1	2:A:154:HEM:HAC	2.10	0.81
1:B:44:ASP:HA	1:B:47:LYS:HE3	1.63	0.81
1:A:23:GLY:O	1:A:27:GLU:HG3	1.79	0.80
1:B:59:GLU:O	1:B:63:LYS:HG3	1.83	0.79
1:B:44:ASP:O	1:B:47:LYS:HG2	1.83	0.78
1:A:8:GLN:O	1:A:12:ASN:HB2	1.84	0.77
1:B:8:GLN:O	1:B:12:ASN:HB2	1.83	0.77
1:B:96:LYS:HE2	1:B:97:HIS:CE1	2.21	0.76
1:B:2:LEU:CD1	1:B:133:LYS:HB3	2.19	0.72
1:A:116:GLN:HG2	1:A:123:PHE:HD2	1.54	0.71
1:B:147:LYS:N	1:B:147:LYS:HD3	2.03	0.71
1:A:78:LYS:HE2	1:A:78:LYS:HA	1.73	0.70
1:B:98:LYS:O	1:B:100:PRO:HD3	1.92	0.70
1:B:52:GLU:O	1:B:56:LYS:HG2	1.92	0.69
1:A:102:LYS:O	1:A:105:GLU:HB3	1.93	0.68
1:A:101:VAL:H	1:A:152:GLN:HE22	1.42	0.67
1:A:102:LYS:HG3	1:A:106:PHE:CZ	2.30	0.66
1:A:119:HIS:N	1:A:120:PRO:HD3	2.10	0.66
1:B:48:HIS:O	1:B:50:LYS:HD3	1.95	0.65
1:A:95:THR:HG22	1:A:151:PHE:CZ	2.31	0.65
1:A:110:ALA:HA	1:A:113:GLN:HE21	1.61	0.65
1:B:96:LYS:HE2	1:B:97:HIS:HE1	1.60	0.63
1:A:96:LYS:O	1:A:98:LYS:HD3	1.99	0.63
1:A:101:VAL:HG13	1:A:152:GLN:HE22	1.63	0.62
1:B:99:ILE:HD12	2:B:154:HEM:HAC	1.81	0.61
1:A:46:PHE:HB3	1:A:49:LEU:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ASP:HA	1:A:47:LYS:HE2	1.83	0.61
1:B:94:ALA:HA	1:B:151:PHE:CD2	2.37	0.60
1:B:104:LEU:O	1:B:107:ILE:HG22	2.01	0.60
1:A:132:SER:O	1:A:136:GLU:CG	2.51	0.59
1:A:132:SER:O	1:A:136:GLU:HG2	2.03	0.58
1:A:59:GLU:O	1:A:63:LYS:HG3	2.02	0.58
1:A:78:LYS:O	1:A:79:LYS:C	2.40	0.57
1:B:119:HIS:N	1:B:120:PRO:HD3	2.19	0.57
1:B:99:ILE:HD12	2:B:154:HEM:CAC	2.35	0.57
1:B:34:LYS:HD2	1:B:52:GLU:OE2	2.03	0.56
1:B:4:ASP:O	1:B:8:GLN:HG2	2.03	0.56
1:B:73:GLY:O	1:B:77:LYS:HG3	2.05	0.56
1:B:84:ALA:O	1:B:88:PRO:HD3	2.06	0.56
1:A:36:HIS:HB2	1:A:39:THR:CG2	2.36	0.56
1:A:116:GLN:HG2	1:A:123:PHE:CD2	2.40	0.55
1:B:87:THR:N	1:B:88:PRO:HD2	2.21	0.55
1:A:95:THR:HG22	1:A:151:PHE:CE2	2.42	0.55
1:B:31:ARG:HD2	3:B:156:HOH:O	2.06	0.55
1:B:118:LYS:C	1:B:120:PRO:HD3	2.27	0.54
1:A:99:ILE:HD12	2:A:154:HEM:CAC	2.19	0.54
1:A:13:VAL:HG21	1:A:123:PHE:CD1	2.43	0.53
1:A:36:HIS:CB	1:A:39:THR:HG23	2.38	0.53
1:A:82:HIS:O	1:A:86:LEU:HB2	2.09	0.53
1:B:87:THR:N	1:B:88:PRO:CD	2.71	0.52
1:A:95:THR:O	1:A:98:LYS:HE2	2.09	0.52
1:A:21:VAL:HG12	1:A:66:ASN:ND2	2.25	0.52
1:A:86:LEU:HD11	1:A:138:PHE:CE2	2.45	0.52
1:B:151:PHE:CE1	1:B:152:GLN:HG3	2.44	0.51
1:B:103:TYR:HB3	2:B:154:HEM:HMC1	1.93	0.51
1:A:10:VAL:HG23	1:A:130:ALA:HB1	1.92	0.51
1:B:44:ASP:HA	1:B:47:LYS:CE	2.39	0.51
1:A:34:LYS:HE2	1:A:52:GLU:HB2	1.92	0.51
1:B:101:VAL:HG13	1:B:152:GLN:HE22	1.75	0.51
1:B:90:ALA:O	1:B:94:ALA:CB	2.59	0.51
1:A:36:HIS:HB2	1:A:39:THR:HG23	1.93	0.50
1:A:40:LEU:HD12	1:A:40:LEU:O	2.11	0.50
1:A:102:LYS:HG3	1:A:106:PHE:CE1	2.46	0.50
1:A:37:PRO:O	1:A:40:LEU:CB	2.54	0.49
1:A:119:HIS:N	1:A:120:PRO:CD	2.75	0.49
1:A:143:ALA:O	1:A:146:TYR:HB2	2.12	0.49
1:B:30:ILE:HG12	1:B:55:MET:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HG21	1:A:123:PHE:HD1	1.76	0.49
1:A:1:GLY:O	1:A:133:LYS:NZ	2.46	0.48
1:B:101:VAL:CG1	1:B:152:GLN:HE22	2.26	0.48
1:B:84:ALA:O	1:B:88:PRO:CD	2.61	0.48
1:A:78:LYS:O	1:A:80:GLY:N	2.46	0.48
1:B:143:ALA:O	1:B:147:LYS:CE	2.59	0.48
1:A:13:VAL:CG1	1:A:131:MET:CE	2.91	0.48
1:B:104:LEU:CD1	1:B:142:MET:HG2	2.44	0.48
1:B:97:HIS:HB2	1:B:99:ILE:HG12	1.95	0.48
1:A:118:LYS:C	1:A:120:PRO:HD3	2.34	0.47
1:A:110:ALA:O	1:A:114:VAL:HG23	2.14	0.47
1:A:132:SER:O	1:A:136:GLU:HG3	2.14	0.47
1:B:146:TYR:HD1	1:B:152:GLN:NE2	2.13	0.47
1:A:82:HIS:C	1:A:82:HIS:CD2	2.88	0.47
1:B:101:VAL:HG12	1:B:146:TYR:CD1	2.50	0.47
1:A:101:VAL:HG13	1:A:152:GLN:NE2	2.30	0.47
1:B:83:GLU:HG2	1:B:83:GLU:H	1.28	0.46
1:A:22:ALA:O	1:A:26:GLN:HB2	2.16	0.46
1:A:60:ASP:HB2	3:A:168:HOH:O	2.15	0.46
1:A:119:HIS:O	1:A:123:PHE:HB2	2.16	0.46
1:B:13:VAL:O	1:B:16:LYS:HB2	2.16	0.46
1:B:21:VAL:HG23	3:B:171:HOH:O	2.16	0.46
1:A:16:LYS:HA	1:A:16:LYS:HD2	1.63	0.46
1:B:130:ALA:O	1:B:133:LYS:HB2	2.15	0.46
1:B:143:ALA:O	1:B:146:TYR:HB2	2.16	0.46
1:B:7:TRP:HB3	1:B:79:LYS:HE3	1.97	0.46
1:A:45:LYS:O	1:A:48:HIS:HE1	1.99	0.45
1:A:97:HIS:HB2	1:A:99:ILE:HG12	1.97	0.45
1:B:7:TRP:CD2	1:B:79:LYS:HG2	2.52	0.45
1:A:73:GLY:O	1:A:77:LYS:HG3	2.16	0.45
1:A:129:GLY:O	1:A:133:LYS:HB2	2.16	0.44
1:A:9:LEU:HA	1:A:9:LEU:HD23	1.82	0.44
1:B:98:LYS:HB3	1:B:98:LYS:HE2	1.80	0.44
1:B:56:LYS:HG2	1:B:56:LYS:H	1.35	0.44
1:B:85:GLU:O	1:B:88:PRO:HD2	2.18	0.44
1:B:114:VAL:O	1:B:118:LYS:HG3	2.17	0.44
1:A:140:ASN:O	1:A:143:ALA:HB3	2.17	0.44
1:A:104:LEU:O	1:A:107:ILE:HG22	2.18	0.43
1:B:119:HIS:O	1:B:123:PHE:HB2	2.17	0.43
1:B:90:ALA:O	1:B:94:ALA:HB3	2.17	0.43
1:A:107:ILE:O	1:A:110:ALA:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:HIS:NE2	1:A:141:ASP:OD2	2.38	0.43
1:A:36:HIS:O	1:A:39:THR:HG23	2.19	0.43
1:B:45:LYS:O	1:B:48:HIS:HE1	2.02	0.43
1:B:95:THR:O	1:B:98:LYS:HD2	2.18	0.43
1:A:152:GLN:HB3	1:A:152:GLN:HE21	1.55	0.43
1:A:118:LYS:HE3	1:A:118:LYS:HB3	1.91	0.43
1:B:17:VAL:CG2	1:B:115:LEU:HD21	2.49	0.43
1:B:13:VAL:HG21	1:B:123:PHE:HD1	1.82	0.43
1:A:110:ALA:HA	1:A:113:GLN:NE2	2.30	0.42
1:A:21:VAL:HG12	1:A:66:ASN:HD22	1.83	0.42
1:A:43:PHE:O	1:A:44:ASP:C	2.58	0.42
1:B:50:LYS:HB2	1:B:54:GLU:OE1	2.20	0.42
1:B:43:PHE:CB	1:B:46:PHE:CD2	3.02	0.42
1:B:43:PHE:CD2	1:B:43:PHE:N	2.86	0.42
1:B:90:ALA:HB2	1:B:142:MET:CE	2.50	0.42
1:B:91:GLN:HB2	1:B:91:GLN:HE21	1.52	0.42
1:B:11:LEU:HD21	1:B:76:LEU:O	2.18	0.42
1:B:33:PHE:O	1:B:37:PRO:HA	2.19	0.42
1:A:87:THR:HB	1:A:88:PRO:HD3	2.02	0.41
1:A:68:VAL:HG21	3:A:156:HOH:O	2.21	0.41
1:B:78:LYS:O	1:B:79:LYS:C	2.59	0.41
1:A:149:LEU:HA	1:A:149:LEU:HD23	1.84	0.41
1:B:16:LYS:HA	1:B:16:LYS:HD3	1.32	0.41
1:A:101:VAL:H	1:A:152:GLN:NE2	2.12	0.41
1:B:26:GLN:HG3	3:B:155:HOH:O	2.21	0.41
1:B:47:LYS:HB3	1:B:47:LYS:HE2	1.66	0.41
1:A:78:LYS:CE	1:A:78:LYS:HA	2.41	0.41
1:B:97:HIS:CB	1:B:99:ILE:HG12	2.51	0.41
1:B:14:TRP:NE1	1:B:73:GLY:HA2	2.36	0.40
1:A:78:LYS:HE2	1:A:78:LYS:CA	2.48	0.40
1:B:9:LEU:HD23	1:B:9:LEU:HA	1.28	0.40
1:A:43:PHE:CD2	1:A:43:PHE:N	2.90	0.40

There are no symmetry-related clashes.

## 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%)	138 (91%)	9 (6%)	4 (3%)	6	9
1	B	151/153 (99%)	140 (93%)	8 (5%)	3 (2%)	9	14
All	All	302/306 (99%)	278 (92%)	17 (6%)	7 (2%)	7	11

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	B	79	LYS
1	A	45	LYS
1	B	152	GLN
1	A	79	LYS
1	A	128	GLN
1	B	45	LYS

### 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	124/124 (100%)	107 (86%)	17 (14%)	4	8
1	B	124/124 (100%)	105 (85%)	19 (15%)	3	6
All	All	248/248 (100%)	212 (86%)	36 (14%)	4	7

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	26	GLN
1	A	41	GLU
1	A	45	LYS
1	A	47	LYS

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Mol	Chain	Res	Type
1	A	50	LYS
1	A	53	ASP
1	A	56	LYS
1	A	61	LEU
1	A	98	LYS
1	A	101	VAL
1	A	109	GLU
1	A	116	GLN
1	A	132	SER
1	A	133	LYS
1	A	136	GLU
1	A	152	GLN
1	B	12	ASN
1	B	13	VAL
1	B	16	LYS
1	B	26	GLN
1	B	27	GLU
1	B	34	LYS
1	B	40	LEU
1	B	45	LYS
1	B	47	LYS
1	B	50	LYS
1	B	51	SER
1	B	56	LYS
1	B	78	LYS
1	B	89	LEU
1	B	98	LYS
1	B	133	LYS
1	B	145	LYS
1	B	147	LYS
1	B	152	GLN

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

Mol	Chain	Res	Type
1	A	48	HIS
1	A	66	ASN
1	A	113	GLN
1	A	116	GLN
1	A	152	GLN
1	B	91	GLN
1	B	116	GLN

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Mol	Chain	Res	Type
1	B	140	ASN
1	B	152	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	HEM	A	154	1,3	28,50,50	2.13	10 (35%)	17,82,82	2.53	4 (23%)
2	HEM	B	154	1,3	28,50,50	2.25	12 (42%)	17,82,82	2.59	5 (29%)

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	A	154	1,3	-	0/6/54/54	0/0/8/8
2	HEM	B	154	1,3	-	0/6/54/54	0/0/8/8

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	C3B-C2B	-5.33	1.33	1.40
2	B	154	HEM	C3B-C2B	-5.15	1.33	1.40
2	B	154	HEM	C3C-C2C	-3.91	1.35	1.40
2	A	154	HEM	C3C-C2C	-2.87	1.36	1.40
2	B	154	HEM	CAA-C2A	2.01	1.55	1.52
2	B	154	HEM	CMD-C2D	2.08	1.55	1.51
2	A	154	HEM	C4C-NC	2.14	1.39	1.36
2	B	154	HEM	CMB-C2B	2.26	1.56	1.51
2	B	154	HEM	C4C-NC	2.28	1.39	1.36
2	A	154	HEM	C4D-ND	2.35	1.39	1.36
2	B	154	HEM	C4B-NB	2.51	1.41	1.36
2	A	154	HEM	CMB-C2B	2.55	1.57	1.51
2	A	154	HEM	C1C-NC	2.62	1.39	1.36
2	B	154	HEM	C1A-NA	2.66	1.41	1.36
2	A	154	HEM	CAA-C2A	2.72	1.56	1.52
2	A	154	HEM	C4A-NA	2.78	1.42	1.36
2	B	154	HEM	C4D-ND	3.05	1.40	1.36
2	B	154	HEM	C1C-NC	3.37	1.40	1.36
2	A	154	HEM	C3C-CAC	3.53	1.54	1.47
2	B	154	HEM	C3B-CAB	3.94	1.55	1.47
2	A	154	HEM	C3B-CAB	4.27	1.56	1.47
2	B	154	HEM	C3C-CAC	4.29	1.56	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	HEM	CMD-C2D-C1D	-6.04	119.18	128.46
2	A	154	HEM	CMD-C2D-C1D	-4.01	122.30	128.46
2	B	154	HEM	CMA-C3A-C4A	-3.74	122.72	128.46
2	B	154	HEM	CMA-C3A-C2A	2.80	130.21	124.94
2	A	154	HEM	CMD-C2D-C3D	3.12	130.83	124.94
2	B	154	HEM	CMB-C2B-C3B	4.21	132.70	124.89
2	A	154	HEM	CMB-C2B-C3B	4.60	133.43	124.89
2	B	154	HEM	CMD-C2D-C3D	5.06	134.49	124.94
2	A	154	HEM	CAA-CBA-CGA	7.28	125.11	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	154	HEM	3	0
2	B	154	HEM	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.