



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:58 PM GMT

PDB ID : 1MYG
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.; Wil-
son, K.S.
Deposited on : 1992-02-27
Resolution : 1.75 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

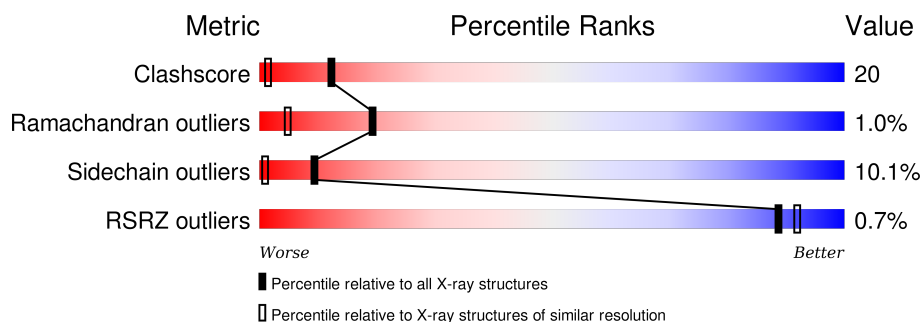
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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. 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>48%</div> <div>38%</div> <div>12%</div> <div></div> </div>
1	B	153	<div> <div>44%</div> <div>39%</div> <div>16%</div> <div></div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	300	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2746 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	3	0
			1210	772	212	223	3			
1	B	153	Total	C	N	O	S	0	3	0
			1207	771	210	223	3			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

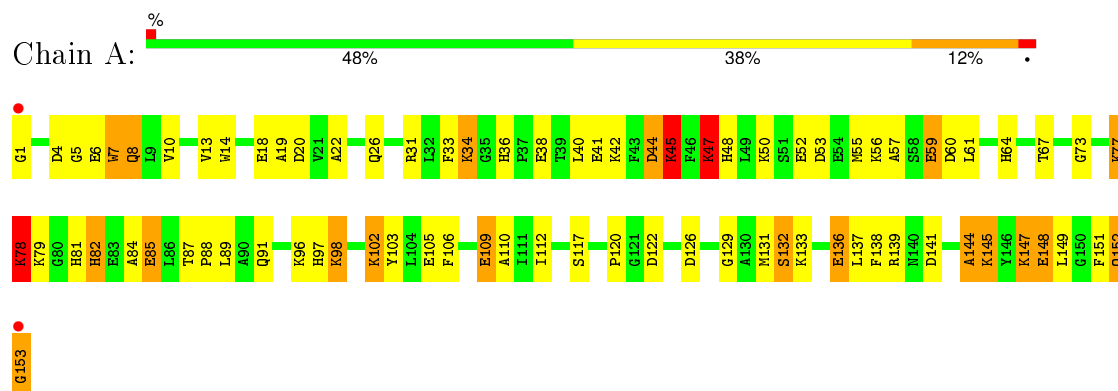
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	111	Total O 111 111	0	0
4	B	122	Total O 122 122	0	2

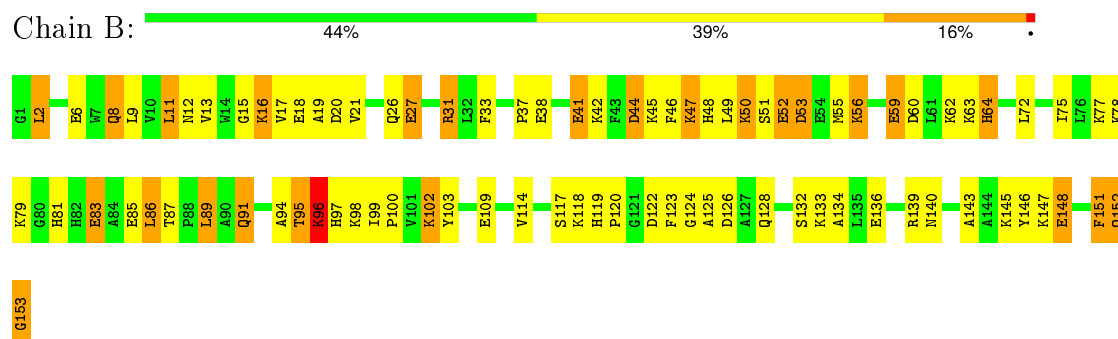
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 21	Depositor
Cell constants a, b, c, α , β , γ	125.26 Å 42.49 Å 92.37 Å 90.00° 92.29° 90.00°	Depositor
Resolution (Å)	10.00 – 1.75 7.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.75) 94.3 (7.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.198 , (Not available) 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 74.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Outliers	(Not available)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2746	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, SO4

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	1.28	2/1251 (0.2%)	2.61	91/1675 (5.4%)
1	B	1.27	1/1248 (0.1%)	2.55	82/1671 (4.9%)
All	All	1.27	3/2499 (0.1%)	2.58	173/3346 (5.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	GLU	CD-OE2	-6.27	1.18	1.25
1	A	18	GLU	CD-OE2	-5.29	1.19	1.25
1	A	5	GLY	N-CA	5.19	1.53	1.46

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	GLU	OE1-CD-OE2	19.82	147.09	123.30
1	B	44	ASP	CB-CG-OD2	-17.10	102.91	118.30
1	A	44	ASP	CB-CG-OD1	14.58	131.42	118.30
1	A	31	ARG	NE-CZ-NH2	-14.54	113.03	120.30
1	B	27	GLU	OE1-CD-OE2	13.35	139.32	123.30
1	B	139	ARG	NE-CZ-NH2	-12.73	113.94	120.30
1	B	53	ASP	CB-CG-OD1	-11.64	107.83	118.30
1	A	44	ASP	CB-CG-OD2	-11.61	107.85	118.30
1	B	59	GLU	CA-CB-CG	11.53	138.76	113.40
1	B	122	ASP	CB-CG-OD1	-11.51	107.94	118.30
1	A	31	ARG	NE-CZ-NH1	11.32	125.96	120.30
1	A	60	ASP	CB-CG-OD2	-11.02	108.38	118.30
1	A	8[A]	GLN	CA-CB-CG	10.52	136.54	113.40
1	A	8[B]	GLN	CA-CB-CG	10.52	136.54	113.40
1	B	20	ASP	CB-CG-OD1	10.44	127.69	118.30
1	A	152	GLN	C-N-CA	10.32	143.98	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	ASP	CB-CG-OD2	-10.16	109.16	118.30
1	A	139	ARG	NE-CZ-NH2	-9.85	115.37	120.30
1	B	60	ASP	CB-CG-OD2	-9.59	109.67	118.30
1	B	148	GLU	OE1-CD-OE2	9.57	134.79	123.30
1	B	85	GLU	OE1-CD-OE2	9.48	134.68	123.30
1	A	38	GLU	CA-CB-CG	9.35	133.98	113.40
1	B	44	ASP	CB-CG-OD1	9.07	126.46	118.30
1	B	122	ASP	OD1-CG-OD2	9.06	140.51	123.30
1	A	6	GLU	OE1-CD-OE2	8.60	133.62	123.30
1	A	136	GLU	OE1-CD-OE2	8.47	133.47	123.30
1	B	103	TYR	CB-CG-CD2	-8.13	116.12	121.00
1	B	12	ASN	CB-CG-OD1	-8.04	105.51	121.60
1	A	31	ARG	CD-NE-CZ	8.02	134.82	123.60
1	A	18	GLU	OE1-CD-OE2	7.84	132.71	123.30
1	A	8[A]	GLN	CG-CD-OE1	7.83	137.27	121.60
1	A	8[B]	GLN	CG-CD-OE1	7.83	137.27	121.60
1	A	40	LEU	CB-CG-CD2	-7.81	97.72	111.00
1	A	139	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	53	ASP	CB-CG-OD2	-7.76	111.31	118.30
1	A	138	PHE	CB-CG-CD1	-7.69	115.41	120.80
1	A	117	SER	N-CA-CB	7.58	121.86	110.50
1	B	122	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	78	LYS	CA-CB-CG	7.50	129.90	113.40
1	B	96	LYS	CD-CE-NZ	7.48	128.91	111.70
1	A	132	SER	CB-CA-C	-7.47	95.90	110.10
1	A	141	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	A	50	LYS	CD-CE-NZ	-7.32	94.87	111.70
1	A	122	ASP	CB-CG-OD1	-7.31	111.72	118.30
1	A	78	LYS	CB-CA-C	-7.25	95.89	110.40
1	B	132	SER	CB-CA-C	-7.23	96.37	110.10
1	B	16	LYS	CB-CA-C	-7.17	96.05	110.40
1	A	98	LYS	CA-CB-CG	-7.17	97.64	113.40
1	A	40	LEU	O-C-N	7.15	134.14	122.70
1	A	117	SER	O-C-N	7.13	134.10	122.70
1	A	136	GLU	CG-CD-OE1	-7.11	104.08	118.30
1	A	136	GLU	CA-CB-CG	-7.08	97.82	113.40
1	B	109	GLU	OE1-CD-OE2	6.93	131.62	123.30
1	A	77	LYS	O-C-N	6.87	133.69	122.70
1	A	110	ALA	N-CA-CB	-6.86	100.50	110.10
1	A	117	SER	CB-CA-C	-6.85	97.08	110.10
1	B	148	GLU	N-CA-CB	-6.81	98.35	110.60
1	B	103	TYR	CD1-CE1-CZ	-6.79	113.69	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	56	LYS	CD-CE-NZ	6.73	127.19	111.70
1	B	47	LYS	CB-CG-CD	-6.68	94.22	111.60
1	B	41	GLU	CG-CD-OE1	6.67	131.64	118.30
1	A	8[A]	GLN	CB-CG-CD	6.65	128.90	111.60
1	A	8[B]	GLN	CB-CG-CD	6.65	128.90	111.60
1	A	59	GLU	CG-CD-OE1	-6.65	105.01	118.30
1	A	20	ASP	CB-CG-OD1	6.64	124.28	118.30
1	B	89[A]	LEU	O-C-N	-6.61	112.12	122.70
1	B	89[B]	LEU	O-C-N	-6.61	112.12	122.70
1	A	112	ILE	CB-CG1-CD1	-6.58	95.47	113.90
1	B	26	GLN	O-C-N	-6.57	112.20	122.70
1	A	148	GLU	CA-CB-CG	6.54	127.78	113.40
1	B	123	PHE	O-C-N	6.46	134.18	123.20
1	B	2	LEU	CB-CG-CD2	-6.42	100.09	111.00
1	B	9	LEU	CB-CG-CD2	-6.30	100.30	111.00
1	B	15	GLY	C-N-CA	6.29	137.42	121.70
1	B	21	VAL	CA-CB-CG1	6.27	120.30	110.90
1	A	1	GLY	O-C-N	-6.26	112.68	122.70
1	A	132	SER	N-CA-CB	6.24	119.86	110.50
1	B	11	LEU	CB-CA-C	6.23	122.04	110.20
1	A	84	ALA	O-C-N	6.22	132.65	122.70
1	B	27	GLU	CG-CD-OE1	-6.22	105.86	118.30
1	B	89[A]	LEU	CA-C-O	6.21	133.13	120.10
1	B	89[B]	LEU	CA-C-O	6.21	133.13	120.10
1	A	109	GLU	OE1-CD-OE2	6.20	130.74	123.30
1	B	38	GLU	CA-CB-CG	6.16	126.96	113.40
1	B	18	GLU	CA-C-O	-6.14	107.21	120.10
1	B	148	GLU	CA-CB-CG	6.11	126.84	113.40
1	A	22	ALA	C-N-CA	6.09	135.09	122.30
1	A	89	LEU	CA-C-O	5.96	132.61	120.10
1	A	67	THR	CA-CB-OG1	-5.95	96.50	109.00
1	B	49	LEU	CB-CG-CD2	-5.95	100.89	111.00
1	B	132	SER	N-CA-CB	5.93	119.39	110.50
1	B	89[A]	LEU	CA-CB-CG	5.92	128.92	115.30
1	B	89[B]	LEU	CA-CB-CG	5.92	128.92	115.30
1	B	62	LYS	CA-CB-CG	-5.88	100.47	113.40
1	A	152	GLN	CA-C-N	-5.88	104.45	116.20
1	B	136	GLU	CA-CB-CG	-5.88	100.47	113.40
1	A	33	PHE	CB-CG-CD2	-5.79	116.74	120.80
1	A	78	LYS	CD-CE-NZ	-5.77	98.43	111.70
1	B	153	GLY	CA-C-O	-5.77	110.22	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	GLY	N-CA-C	-5.77	98.69	113.10
1	B	8[A]	GLN	CB-CA-C	-5.76	98.87	110.40
1	B	8[B]	GLN	CB-CA-C	-5.76	98.87	110.40
1	A	132	SER	O-C-N	5.76	131.91	122.70
1	B	85	GLU	CG-CD-OE2	-5.75	106.80	118.30
1	A	55	MET	O-C-N	-5.75	113.51	122.70
1	B	33	PHE	CG-CD2-CE2	-5.73	114.49	120.80
1	A	1	GLY	C-N-CA	5.73	136.03	121.70
1	A	82	HIS	CG-ND1-CE1	5.69	116.17	108.20
1	A	97	HIS	O-C-N	5.67	131.78	122.70
1	B	41	GLU	CG-CD-OE2	-5.67	106.97	118.30
1	B	18	GLU	O-C-N	5.65	131.74	122.70
1	B	86	LEU	N-CA-CB	-5.65	99.10	110.40
1	A	77	LYS	CA-C-O	-5.65	108.24	120.10
1	B	132	SER	CA-CB-OG	-5.64	95.96	111.20
1	B	53	ASP	OD1-CG-OD2	5.64	134.02	123.30
1	A	33	PHE	CD1-CG-CD2	5.61	125.59	118.30
1	A	33	PHE	O-C-N	5.58	131.62	122.70
1	B	134	ALA	CB-CA-C	5.57	118.45	110.10
1	A	38	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	A	122	ASP	OD1-CG-OD2	5.54	133.82	123.30
1	B	72	LEU	CA-C-N	5.54	127.27	116.20
1	B	18	GLU	OE1-CD-OE2	5.53	129.93	123.30
1	A	132	SER	CA-CB-OG	-5.51	96.32	111.20
1	B	55	MET	O-C-N	-5.50	113.91	122.70
1	B	87	THR	CA-CB-CG2	-5.49	104.71	112.40
1	A	151	PHE	O-C-N	5.45	131.42	122.70
1	A	105	GLU	CG-CD-OE2	-5.45	107.41	118.30
1	A	126	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	26	GLN	CA-CB-CG	-5.38	101.57	113.40
1	A	53	ASP	CA-CB-CG	-5.38	101.57	113.40
1	B	117	SER	CB-CA-C	-5.37	99.89	110.10
1	A	61	LEU	CD1-CG-CD2	-5.37	94.40	110.50
1	B	31	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	B	151	PHE	C-N-CA	5.33	135.03	121.70
1	A	50	LYS	CA-C-N	5.32	128.91	117.20
1	A	138	PHE	CG-CD1-CE1	-5.32	114.95	120.80
1	A	26	GLN	CB-CG-CD	-5.31	97.78	111.60
1	B	52	GLU	CA-C-O	5.31	131.25	120.10
1	B	125	ALA	CB-CA-C	5.31	118.06	110.10
1	B	31	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	B	27	GLU	CB-CG-CD	-5.27	99.96	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ALA	N-CA-CB	-5.27	102.72	110.10
1	B	64	HIS	O-C-N	-5.27	114.25	123.20
1	A	81	HIS	CA-CB-CG	-5.23	104.71	113.60
1	A	153	GLY	CA-C-O	-5.23	111.19	120.60
1	A	59	GLU	CG-CD-OE2	-5.21	107.87	118.30
1	A	19	ALA	N-CA-CB	5.21	117.39	110.10
1	A	105	GLU	OE1-CD-OE2	5.21	129.55	123.30
1	A	137	LEU	CB-CG-CD1	-5.21	102.15	111.00
1	A	122	ASP	CA-CB-CG	-5.18	102.01	113.40
1	B	86	LEU	CA-C-O	5.16	130.94	120.10
1	B	148	GLU	CG-CD-OE1	-5.16	107.98	118.30
1	B	20	ASP	OD1-CG-OD2	-5.15	113.51	123.30
1	A	85	GLU	CG-CD-OE1	5.15	128.60	118.30
1	A	47	LYS	CA-CB-CG	-5.15	102.07	113.40
1	B	55	MET	CA-C-O	5.15	130.91	120.10
1	A	120	PRO	C-N-CA	5.14	133.09	122.30
1	A	40	LEU	CB-CG-CD1	5.13	119.72	111.00
1	B	126	ASP	N-CA-CB	-5.13	101.37	110.60
1	B	31	ARG	CD-NE-CZ	-5.11	116.44	123.60
1	B	77	LYS	CA-C-N	5.10	128.42	117.20
1	A	34	LYS	N-CA-CB	5.08	119.74	110.60
1	B	46	PHE	C-N-CA	-5.08	109.00	121.70
1	A	36	HIS	CA-CB-CG	-5.08	104.97	113.60
1	A	7	TRP	O-C-N	-5.07	114.58	122.70
1	A	96	LYS	O-C-N	5.07	130.81	122.70
1	B	27	GLU	CA-CB-CG	-5.06	102.26	113.40
1	B	17	VAL	CA-CB-CG1	5.06	118.49	110.90
1	B	46	PHE	O-C-N	5.05	130.77	122.70
1	B	152	GLN	CB-CA-C	-5.02	100.36	110.40
1	A	148	GLU	CG-CD-OE2	5.00	128.31	118.30
1	B	140	ASN	CB-CG-OD1	-5.00	111.60	121.60

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	1210	0	1220	48	1
1	B	1207	0	1220	49	1
2	A	5	0	0	1	0
2	B	5	0	0	1	0
3	A	43	0	30	0	0
3	B	43	0	30	2	0
4	A	111	0	0	3	0
4	B	122	0	0	8	0
All	All	2746	0	2500	99	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (99) 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:47:LYS:NZ	1:A:47:LYS:HB2	1.65	1.09
1:A:47:LYS:HZ2	1:A:47:LYS:HB2	1.17	1.07
1:B:16:LYS:HE2	1:B:16:LYS:HA	1.41	1.00
1:A:47:LYS:NZ	1:A:47:LYS:CB	2.25	0.99
1:A:78:LYS:HE2	1:A:78:LYS:HA	1.41	0.97
1:A:52:GLU:HG2	1:A:56:LYS:HE3	1.55	0.87
1:B:16:LYS:CE	1:B:16:LYS:HA	2.07	0.84
1:A:45:LYS:O	1:A:48[A]:HIS:HE1	1.64	0.80
1:B:59:GLU:O	1:B:63[A]:LYS:HD3	1.83	0.79
1:A:102[B]:LYS:HD2	1:A:103:TYR:CE1	2.20	0.76
1:B:8[B]:GLN:NE2	4:B:329:HOH:O	2.22	0.73
1:B:96:LYS:HD2	1:B:97:HIS:CE1	2.24	0.72
1:B:146:TYR:CD2	1:B:151:PHE:HD2	2.07	0.71
1:A:47:LYS:HZ3	1:A:47:LYS:CB	2.02	0.71
1:B:63[A]:LYS:NZ	4:B:320:HOH:O	2.24	0.71
1:A:102[A]:LYS:NZ	1:A:153:GLY:C	2.44	0.70
1:A:78:LYS:CA	1:A:78:LYS:HE2	2.06	0.70
1:A:87:THR:HB	1:A:88:PRO:HD3	1.72	0.70
1:A:45:LYS:O	1:A:48[A]:HIS:CE1	2.44	0.69
1:B:45:LYS:O	1:B:48:HIS:HE1	1.74	0.69
1:B:146:TYR:HB2	1:B:153:GLY:OXT	1.91	0.69
1:B:83:GLU:HB3	4:B:377:HOH:O	1.91	0.68
1:B:114:VAL:HG13	1:B:118:LYS:HD2	1.78	0.66
1:B:16:LYS:HE2	1:B:16:LYS:CA	2.16	0.65
1:A:73:GLY:O	1:A:77:LYS:HG3	1.96	0.65
1:B:16:LYS:CE	1:B:16:LYS:CA	2.72	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102[A]:LYS:HZ1	1:A:153:GLY:C	2.01	0.64
1:A:52:GLU:O	1:A:56:LYS:HG3	1.99	0.63
1:B:31:ARG:HD2	4:B:303:HOH:O	1.99	0.63
1:B:2:LEU:HG	1:B:133:LYS:HE2	1.82	0.62
1:B:143:ALA:O	1:B:153:GLY:OXT	2.18	0.62
1:B:95:THR:O	1:B:98:LYS:HE2	2.00	0.61
1:A:47:LYS:HB2	1:A:47:LYS:HZ3	1.61	0.61
1:B:83:GLU:CD	1:B:83:GLU:H	2.03	0.61
3:B:154:HEM:HMC1	3:B:154:HEM:HBC2	1.84	0.60
1:B:45:LYS:O	1:B:48:HIS:CE1	2.55	0.60
1:B:146:TYR:CD2	1:B:151:PHE:CD2	2.89	0.60
1:B:44:ASP:HA	1:B:47:LYS:HE2	1.86	0.58
1:B:146:TYR:CB	1:B:153:GLY:OXT	2.53	0.56
1:A:10:VAL:O	1:A:13:VAL:HG22	2.06	0.56
1:B:146:TYR:O	1:B:151:PHE:N	2.33	0.56
1:A:102[B]:LYS:HD2	1:A:103:TYR:CD1	2.40	0.56
1:B:83:GLU:OE1	1:B:83:GLU:N	2.39	0.56
1:A:47:LYS:HZ3	1:A:47:LYS:HB3	1.71	0.55
1:B:91:GLN:O	1:B:95:THR:HG23	2.07	0.55
1:B:146:TYR:CG	1:B:151:PHE:HD2	2.25	0.55
1:A:87:THR:CB	1:A:88:PRO:HD3	2.37	0.55
1:A:78:LYS:HG3	1:A:82:HIS:HA	1.88	0.55
1:B:19:ALA:HB1	4:B:391:HOH:O	2.07	0.55
1:A:78:LYS:HG3	1:A:82:HIS:CA	2.37	0.55
1:A:64:HIS:ND1	2:A:301:SO4:O2	2.40	0.54
1:A:7:TRP:CG	1:A:79:LYS:HG2	2.44	0.53
1:B:50:LYS:O	1:B:51:SER:HB3	2.09	0.53
1:A:102[A]:LYS:NZ	1:A:153:GLY:O	2.41	0.53
1:B:81:HIS:HD2	4:B:374:HOH:O	1.92	0.53
1:A:57:ALA:HB3	4:A:318:HOH:O	2.08	0.52
1:B:114:VAL:CG1	1:B:118:LYS:HD2	2.39	0.52
1:A:102[A]:LYS:HZ3	1:A:153:GLY:C	2.13	0.52
1:A:132:SER:HB2	4:A:394:HOH:O	2.09	0.51
1:B:11:LEU:CD1	1:B:79:LYS:HE3	2.41	0.51
1:A:78:LYS:HG3	1:A:82:HIS:HB3	1.94	0.50
1:B:11:LEU:HD11	1:B:79:LYS:HE3	1.93	0.50
1:A:87:THR:N	1:A:88:PRO:CD	2.75	0.49
1:A:13:VAL:HG23	1:A:14:TRP:N	2.28	0.49
1:A:129:GLY:O	1:A:133:LYS:HG3	2.13	0.49
1:A:88:PRO:HA	1:A:91:GLN:HE21	1.79	0.48
1:B:64:HIS:ND1	2:B:300:SO4:O3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLU:O	1:A:136:GLU:HG2	2.14	0.48
1:B:151:PHE:O	1:B:153:GLY:N	2.47	0.47
1:A:13:VAL:HG21	1:A:131:MET:CE	2.44	0.47
1:A:147:LYS:CB	1:A:147:LYS:NZ	2.78	0.47
1:B:75:ILE:HD11	1:B:89[A]:LEU:HD23	1.97	0.46
1:A:44:ASP:O	1:A:47:LYS:HG2	2.15	0.46
1:B:42:LYS:HG2	1:B:99:ILE:CD1	2.45	0.46
1:B:81:HIS:CD2	4:B:374:HOH:O	2.69	0.45
1:B:100:PRO:HB2	1:B:102:LYS:HG2	1.98	0.45
1:B:133:LYS:HB3	1:B:133:LYS:HE3	1.39	0.45
1:A:144:ALA:HA	1:A:147:LYS:HE3	1.99	0.45
3:B:154:HEM:CMC	3:B:154:HEM:HBC2	2.47	0.44
1:A:106:PHE:O	1:A:109:GLU:HG2	2.17	0.44
1:B:42:LYS:HG2	1:B:99:ILE:HD12	1.99	0.44
1:B:13:VAL:O	1:B:16:LYS:HG2	2.18	0.43
1:A:78:LYS:HG3	1:A:82:HIS:CB	2.49	0.43
1:B:78:LYS:HD2	1:B:78:LYS:HA	1.65	0.43
1:B:52:GLU:O	1:B:56:LYS:HG3	2.19	0.42
1:A:78:LYS:CE	1:A:78:LYS:CA	2.89	0.42
1:A:13:VAL:CG2	1:A:14:TRP:N	2.82	0.42
1:A:7:TRP:CD2	1:A:79:LYS:HG2	2.54	0.42
1:B:119:HIS:N	1:B:120:PRO:CD	2.82	0.42
1:A:78:LYS:HD2	1:A:85:GLU:CD	2.40	0.42
1:A:42:LYS:HG2	1:A:42:LYS:H	1.52	0.42
1:B:124:GLY:O	1:B:128:GLN:HG3	2.19	0.41
1:B:94:ALA:O	1:B:98:LYS:HD2	2.20	0.41
1:B:119:HIS:N	1:B:120:PRO:HD3	2.36	0.41
1:A:145:LYS:HD3	1:A:148:GLU:CG	2.50	0.41
1:B:27:GLU:HG2	4:B:340:HOH:O	2.21	0.40
1:A:78:LYS:HE3	4:A:362:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48[A]:HIS:CD2	1:B:48:HIS:CD2[1_546]	2.19	0.01

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	154/153 (101%)	148 (96%)	4 (3%)	2 (1%)	15	3
1	B	154/153 (101%)	147 (96%)	6 (4%)	1 (1%)	30	12
All	All	308/306 (101%)	295 (96%)	10 (3%)	3 (1%)	19	5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	B	152	GLN
1	A	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	127/124 (102%)	113 (89%)	14 (11%)	8	1
1	B	127/124 (102%)	114 (90%)	13 (10%)	9	1
All	All	254/248 (102%)	227 (89%)	27 (11%)	9	1

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8[A]	GLN
1	A	8[B]	GLN
1	A	34	LYS

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Mol	Chain	Res	Type
1	A	41	GLU
1	A	45	LYS
1	A	47	LYS
1	A	59	GLU
1	A	78	LYS
1	A	98	LYS
1	A	102[A]	LYS
1	A	102[B]	LYS
1	A	145	LYS
1	A	147	LYS
1	A	149	LEU
1	B	37	PRO
1	B	41	GLU
1	B	50	LYS
1	B	53	ASP
1	B	83	GLU
1	B	86	LEU
1	B	91	GLN
1	B	95	THR
1	B	96	LYS
1	B	102	LYS
1	B	145	LYS
1	B	147	LYS
1	B	148	GLU

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	36	HIS
1	A	91	GLN
1	A	140	ASN
1	A	152	GLN
1	B	12	ASN
1	B	48	HIS
1	B	116	GLN
1	B	128	GLN
1	B	140	ASN

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 ⓘ

4 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	$\# Z > 2$
3	HEM	A	154	1,4	30,50,50	2.45	10 (33%)	24,82,82	3.12	11 (45%)
2	SO4	A	301	-	4,4,4	1.56	1 (25%)	6,6,6	0.97	0
3	HEM	B	154	1,4	30,50,50	2.99	12 (40%)	24,82,82	3.39	12 (50%)
2	SO4	B	300	-	4,4,4	1.49	0	6,6,6	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	154	1,4	-	0/10/54/54	0/0/8/8
2	SO4	A	301	-	-	0/0/0/0	0/0/0/0
3	HEM	B	154	1,4	-	0/10/54/54	0/0/8/8
2	SO4	B	300	-	-	0/0/0/0	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	154	HEM	C3B-C4B	-7.92	1.44	1.51
3	B	154	HEM	C2D-C3D	-7.66	1.31	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	154	HEM	C2D-C3D	-6.60	1.34	1.54
3	B	154	HEM	C3D-C4D	-5.08	1.45	1.51
3	A	154	HEM	C3B-C4B	-4.89	1.47	1.51
3	A	154	HEM	C2C-C1C	-4.35	1.44	1.52
3	B	154	HEM	C2C-C1C	-3.03	1.46	1.52
3	B	154	HEM	C2B-C1B	-2.24	1.44	1.51
3	A	154	HEM	C3D-C4D	-2.14	1.48	1.51
3	A	154	HEM	C2B-C1B	-2.01	1.45	1.51
2	A	301	SO4	O1-S	2.15	1.54	1.47
3	B	154	HEM	C3C-CAC	2.33	1.55	1.51
3	B	154	HEM	C4C-NC	2.41	1.39	1.36
3	B	154	HEM	FE-NB	2.46	2.10	1.97
3	A	154	HEM	C3B-CAB	2.50	1.56	1.51
3	A	154	HEM	FE-NB	2.67	2.11	1.97
3	B	154	HEM	C3B-CAB	2.74	1.56	1.51
3	A	154	HEM	CAA-C2A	3.08	1.57	1.52
3	B	154	HEM	CHC-C1C	3.42	1.44	1.36
3	A	154	HEM	C4C-NC	3.69	1.40	1.36
3	B	154	HEM	CAA-C2A	3.84	1.58	1.52
3	A	154	HEM	C1C-NC	5.33	1.42	1.36
3	B	154	HEM	C1C-NC	5.77	1.43	1.36

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	154	HEM	CBD-CAD-C3D	-6.05	95.95	113.55
3	A	154	HEM	CBD-CAD-C3D	-4.99	99.04	113.55
3	A	154	HEM	CAA-C2A-C1A	-3.90	122.78	127.01
3	A	154	HEM	CAA-CBA-CGA	-3.45	106.43	112.75
3	B	154	HEM	CAD-CBD-CGD	-2.84	101.41	113.02
3	B	154	HEM	C3C-CAC-CBC	-2.38	120.81	124.46
3	B	154	HEM	CMA-C3A-C4A	-2.30	124.55	128.36
3	B	154	HEM	CAA-C2A-C1A	-2.05	124.78	127.01
3	B	154	HEM	CMA-C3A-C2A	2.13	129.69	125.24
3	A	154	HEM	CAD-C3D-C4D	2.51	121.32	112.47
3	B	154	HEM	C3B-CAB-CBB	2.78	128.72	124.46
3	A	154	HEM	C3B-C4B-CHC	3.10	127.52	123.16
3	A	154	HEM	CMD-C2D-C3D	3.44	129.58	114.35
3	A	154	HEM	C3C-CAC-CBC	3.78	130.26	124.46
3	A	154	HEM	C2D-C3D-C4D	4.60	109.29	101.50
3	A	154	HEM	CMC-C2C-C3C	5.34	129.85	116.53
3	B	154	HEM	CMC-C2C-C3C	5.44	130.12	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	154	HEM	CMD-C2D-C3D	5.47	138.56	114.35
3	A	154	HEM	CAD-C3D-C2D	5.54	129.14	113.22
3	B	154	HEM	CMB-C2B-C3B	6.15	131.88	116.53
3	A	154	HEM	CMB-C2B-C3B	6.22	132.06	116.53
3	B	154	HEM	CAD-C3D-C2D	6.39	131.58	113.22
3	B	154	HEM	C2D-C3D-C4D	6.78	112.99	101.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	SO4	1	0
3	B	154	HEM	2	0
2	B	300	SO4	1	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 [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%)	-0.58	2 (1%) 79 85	13, 28, 56, 97	0
1	B	153/153 (100%)	-0.63	0 100 100	14, 28, 55, 88	0
All	All	306/306 (100%)	-0.60	2 (0%) 89 92	13, 28, 56, 97	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	GLY	5.6
1	A	1	GLY	3.6

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	B	300	5/5	0.98	0.13	2.28	74,74,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	HEM	B	154	43/43	0.98	0.06	-0.28	16,21,33,46	0
3	HEM	A	154	43/43	0.99	0.06	-0.30	17,21,34,42	0
2	SO4	A	301	5/5	0.97	0.10	-	76,77,77,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.