



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 09:24 pm GMT

PDB ID : 1I3D  
Title : HUMAN CARBONMONOXY HEMOGLOBIN BART'S (GAMMA4)  
Authors : Kidd, R.D.; Baker, H.M.; Mathews, A.J.; Brittain, T.; Baker, E.N.  
Deposited on : 2001-02-15  
Resolution : 1.70 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

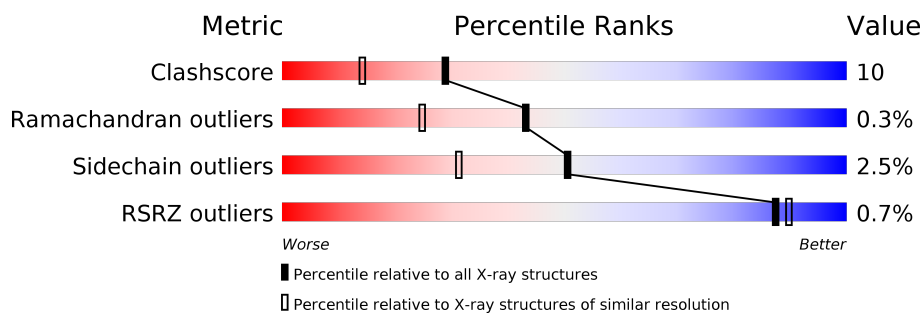
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	122126	4167 (1.70-1.70)
Ramachandran outliers	120053	4100 (1.70-1.70)
Sidechain outliers	120020	4100 (1.70-1.70)
RSRZ outliers	108989	3718 (1.70-1.70)

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.

Mol	Chain	Length	Quality of chain
1	A	146	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div>5%</div> </div> </div>
1	B	146	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>32%</div> <div>8%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2638 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 HEMOGLOBIN GAMMA CHAINS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	7	0	0
			1131	724	193	211	3			
1	B	146	Total	C	N	O	S	5	0	0
			1131	724	193	211	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 CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			2	1	1		
3	B	1	Total	C	O	0	0
			2	1	1		

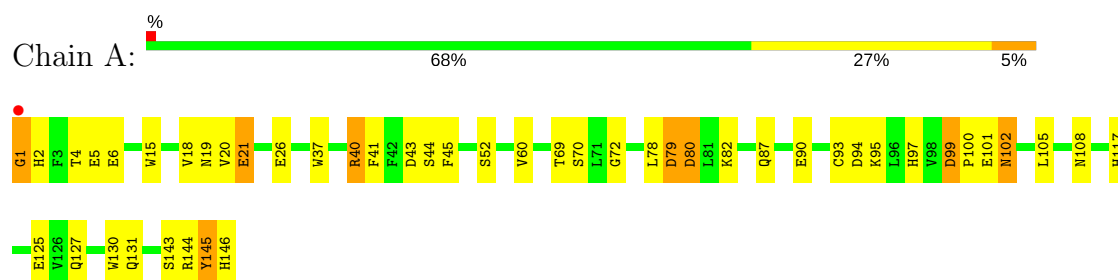
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	143	Total	O	0	0
			143	143		
4	B	143	Total	O	0	0
			143	143		

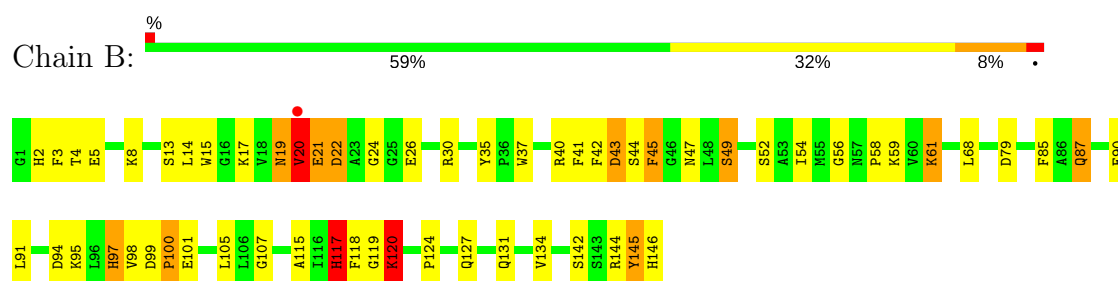
### 3 Residue-property plots [i](#)

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: HEMOGLOBIN GAMMA CHAINS



#### • Molecule 1: HEMOGLOBIN GAMMA CHAINS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.62Å 82.84Å 53.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 21.09 – 1.70	Depositor EDS
% Data completeness (in resolution range)	88.5 (20.00-1.70) 88.6 (21.09-1.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.211 , 0.244 0.200 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.4	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2638	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: CMO, 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	2.95	72/1157 (6.2%)	2.07	25/1565 (1.6%)
1	B	3.04	83/1157 (7.2%)	1.92	26/1565 (1.7%)
All	All	3.00	155/2314 (6.7%)	2.00	51/3130 (1.6%)

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 (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	GLU	CD-OE1	25.14	1.53	1.25
1	B	26	GLU	CD-OE1	22.37	1.50	1.25
1	B	101	GLU	CD-OE1	22.08	1.50	1.25
1	B	26	GLU	CD-OE2	-20.48	1.03	1.25
1	A	40	ARG	CD-NE	20.06	1.80	1.46
1	B	90	GLU	CD-OE1	19.53	1.47	1.25
1	A	144	ARG	CZ-NH2	17.78	1.56	1.33
1	B	20	VAL	CB-CG1	-17.64	1.15	1.52
1	A	6	GLU	CD-OE1	16.33	1.43	1.25
1	A	79	ASP	CA-CB	15.69	1.88	1.53
1	A	21	GLU	CD-OE2	14.96	1.42	1.25
1	A	6	GLU	CD-OE2	-14.56	1.09	1.25
1	B	101	GLU	CG-CD	-14.37	1.30	1.51
1	A	40	ARG	NE-CZ	-14.07	1.14	1.33
1	A	40	ARG	CZ-NH2	13.83	1.51	1.33
1	B	40	ARG	CZ-NH1	-13.46	1.15	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	HIS	CG-CD2	-13.39	1.12	1.35
1	A	5	GLU	CD-OE1	13.29	1.40	1.25
1	A	6	GLU	CG-CD	13.23	1.71	1.51
1	B	45	PHE	CE1-CZ	12.76	1.61	1.37
1	B	21	GLU	N-CA	12.65	1.71	1.46
1	B	40	ARG	NE-CZ	11.97	1.48	1.33
1	A	90	GLU	CD-OE2	11.68	1.38	1.25
1	A	80	ASP	CB-CG	11.41	1.75	1.51
1	A	1	GLY	N-CA	11.18	1.62	1.46
1	B	99	ASP	CB-CG	-11.04	1.28	1.51
1	B	146	HIS	C-O	10.92	1.44	1.23
1	B	19	ASN	CG-ND2	-10.49	1.06	1.32
1	A	2	HIS	CG-CD2	10.38	1.53	1.35
1	A	26	GLU	CD-OE1	10.27	1.36	1.25
1	B	49	SER	CA-CB	10.27	1.68	1.52
1	B	120	LYS	CD-CE	-10.25	1.25	1.51
1	A	1	GLY	C-N	10.23	1.57	1.34
1	B	145	TYR	CE2-CZ	9.78	1.51	1.38
1	B	21	GLU	CB-CG	-9.71	1.33	1.52
1	B	101	GLU	CB-CG	9.34	1.69	1.52
1	B	2	HIS	CG-CD2	9.33	1.51	1.35
1	B	2	HIS	N-CA	-9.22	1.27	1.46
1	B	44	SER	CB-OG	9.21	1.54	1.42
1	B	44	SER	CA-CB	-9.04	1.39	1.52
1	A	20	VAL	CB-CG1	-8.91	1.34	1.52
1	B	117	HIS	CE1-NE2	8.32	1.51	1.32
1	B	99	ASP	CG-OD2	8.29	1.44	1.25
1	B	26	GLU	CG-CD	8.11	1.64	1.51
1	B	56	GLY	CA-C	7.92	1.64	1.51
1	A	43	ASP	CG-OD2	7.91	1.43	1.25
1	B	94	ASP	C-N	7.77	1.51	1.34
1	B	19	ASN	CG-OD1	7.70	1.40	1.24
1	A	101	GLU	CG-CD	-7.64	1.40	1.51
1	A	41	PHE	CE1-CZ	7.55	1.51	1.37
1	B	52	SER	CA-CB	7.53	1.64	1.52
1	B	117	HIS	CD2-NE2	-7.45	1.21	1.38
1	B	21	GLU	C-O	7.42	1.37	1.23
1	A	144	ARG	CZ-NH1	-7.36	1.23	1.33
1	A	146	HIS	CE1-NE2	7.35	1.49	1.32
1	B	98	VAL	CA-CB	7.30	1.70	1.54
1	B	79	ASP	C-N	-7.26	1.17	1.34
1	B	19	ASN	CB-CG	7.18	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	ASP	CG-OD2	7.17	1.41	1.25
1	A	117	HIS	CB-CG	7.12	1.62	1.50
1	B	85	PHE	CG-CD2	7.08	1.49	1.38
1	A	143	SER	CA-CB	7.05	1.63	1.52
1	B	22	ASP	CG-OD1	-7.01	1.09	1.25
1	B	41	PHE	CB-CG	-6.99	1.39	1.51
1	B	41	PHE	CG-CD2	6.98	1.49	1.38
1	B	59	LYS	CE-NZ	6.97	1.66	1.49
1	B	145	TYR	CE1-CZ	6.95	1.47	1.38
1	B	145	TYR	CD2-CE2	-6.94	1.28	1.39
1	B	45	PHE	CG-CD2	6.83	1.49	1.38
1	A	87	GLN	CD-NE2	6.82	1.50	1.32
1	B	2	HIS	CB-CG	-6.80	1.37	1.50
1	A	80	ASP	C-O	6.79	1.36	1.23
1	A	146	HIS	CB-CG	-6.68	1.38	1.50
1	A	78	LEU	CA-C	-6.63	1.35	1.52
1	A	94	ASP	N-CA	6.57	1.59	1.46
1	B	47	ASN	CA-CB	6.56	1.70	1.53
1	B	17	LYS	C-N	6.55	1.49	1.34
1	A	145	TYR	CB-CG	6.51	1.61	1.51
1	B	42	PHE	CB-CG	-6.50	1.40	1.51
1	B	145	TYR	CG-CD2	6.45	1.47	1.39
1	A	130	TRP	CZ3-CH2	6.37	1.50	1.40
1	A	37	TRP	NE1-CE2	-6.36	1.29	1.37
1	B	49	SER	C-N	6.35	1.48	1.34
1	A	43	ASP	CB-CG	-6.31	1.38	1.51
1	B	5	GLU	CD-OE1	6.28	1.32	1.25
1	A	87	GLN	CG-CD	6.20	1.65	1.51
1	B	47	ASN	CG-OD1	6.19	1.37	1.24
1	A	45	PHE	CD1-CE1	6.15	1.51	1.39
1	A	72	GLY	N-CA	6.14	1.55	1.46
1	B	144	ARG	CZ-NH2	6.14	1.41	1.33
1	B	94	ASP	N-CA	6.12	1.58	1.46
1	A	145	TYR	CA-CB	-6.12	1.40	1.53
1	A	144	ARG	CG-CD	6.06	1.67	1.51
1	A	40	ARG	CZ-NH1	-6.04	1.25	1.33
1	A	26	GLU	CD-OE2	6.00	1.32	1.25
1	B	115	ALA	CA-CB	6.00	1.65	1.52
1	A	82	LYS	CA-CB	5.96	1.67	1.53
1	A	37	TRP	CD2-CE2	5.92	1.48	1.41
1	A	94	ASP	CB-CG	-5.92	1.39	1.51
1	B	119	GLY	N-CA	5.92	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	HIS	CE1-NE2	5.85	1.46	1.32
1	B	47	ASN	CB-CG	-5.85	1.37	1.51
1	A	97	HIS	CG-CD2	5.84	1.45	1.35
1	B	117	HIS	CG-CD2	-5.80	1.25	1.35
1	B	146	HIS	C-OXT	-5.79	1.12	1.23
1	A	69	THR	N-CA	5.76	1.57	1.46
1	B	119	GLY	C-O	-5.74	1.14	1.23
1	A	80	ASP	CG-OD2	-5.72	1.12	1.25
1	B	117	HIS	CB-CG	5.71	1.60	1.50
1	A	15	TRP	CE3-CZ3	5.70	1.48	1.38
1	B	100	PRO	N-CA	-5.67	1.37	1.47
1	A	125	GLU	CD-OE1	-5.67	1.19	1.25
1	B	85	PHE	CE2-CZ	5.67	1.48	1.37
1	B	79	ASP	CB-CG	5.66	1.63	1.51
1	A	108	ASN	CG-OD1	5.65	1.36	1.24
1	A	52	SER	CA-CB	5.63	1.61	1.52
1	B	145	TYR	CZ-OH	-5.63	1.28	1.37
1	B	3	PHE	N-CA	5.62	1.57	1.46
1	A	82	LYS	C-N	5.55	1.43	1.33
1	A	99	ASP	CG-OD1	5.52	1.38	1.25
1	B	144	ARG	CG-CD	5.50	1.65	1.51
1	B	4	THR	N-CA	-5.50	1.35	1.46
1	A	102	ASN	CB-CG	5.48	1.63	1.51
1	A	101	GLU	CD-OE2	5.46	1.31	1.25
1	B	54	ILE	N-CA	5.44	1.57	1.46
1	A	131	GLN	CB-CG	-5.41	1.38	1.52
1	B	142	SER	N-CA	5.41	1.57	1.46
1	B	15	TRP	CD2-CE2	5.38	1.47	1.41
1	B	58	PRO	N-CD	5.37	1.55	1.47
1	A	146	HIS	N-CA	5.31	1.56	1.46
1	A	95	LYS	C-O	5.30	1.33	1.23
1	B	59	LYS	CB-CG	5.29	1.66	1.52
1	B	42	PHE	CA-CB	5.28	1.65	1.53
1	A	70	SER	CB-OG	-5.25	1.35	1.42
1	A	40	ARG	CG-CD	5.25	1.65	1.51
1	A	4	THR	N-CA	5.24	1.56	1.46
1	A	18	VAL	CA-CB	5.22	1.65	1.54
1	A	44	SER	CA-C	-5.21	1.39	1.52
1	B	2	HIS	CE1-NE2	5.20	1.44	1.32
1	A	105	LEU	CG-CD1	5.19	1.71	1.51
1	A	2	HIS	C-O	-5.16	1.13	1.23
1	B	37	TRP	CD2-CE2	5.14	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	8	LYS	CD-CE	-5.13	1.38	1.51
1	A	93	CYS	N-CA	5.12	1.56	1.46
1	B	5	GLU	CG-CD	5.09	1.59	1.51
1	B	4	THR	CA-C	-5.09	1.39	1.52
1	A	41	PHE	CE2-CZ	-5.07	1.27	1.37
1	A	117	HIS	CD2-NE2	5.04	1.52	1.42
1	B	144	ARG	CZ-NH1	5.03	1.39	1.33
1	A	20	VAL	N-CA	5.03	1.56	1.46
1	A	60	VAL	C-O	5.03	1.32	1.23
1	A	19	ASN	C-N	-5.03	1.22	1.34
1	B	13	SER	CB-OG	-5.01	1.35	1.42
1	B	3	PHE	CG-CD1	-5.00	1.31	1.38
1	B	97	HIS	CB-CG	5.00	1.59	1.50

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ARG	NE-CZ-NH1	28.39	134.50	120.30
1	A	40	ARG	NE-CZ-NH2	-26.70	106.95	120.30
1	A	144	ARG	NE-CZ-NH1	21.05	130.82	120.30
1	B	43	ASP	CB-CG-OD1	15.74	132.47	118.30
1	B	101	GLU	OE1-CD-OE2	-15.41	104.81	123.30
1	B	20	VAL	CG1-CB-CG2	14.62	134.28	110.90
1	A	43	ASP	CB-CG-OD1	14.12	131.01	118.30
1	B	99	ASP	CB-CG-OD1	13.54	130.48	118.30
1	B	40	ARG	NE-CZ-NH2	-13.16	113.72	120.30
1	A	144	ARG	NE-CZ-NH2	-13.03	113.79	120.30
1	B	146	HIS	CA-C-O	-12.59	93.65	120.10
1	B	45	PHE	CZ-CE2-CD2	11.59	134.01	120.10
1	A	101	GLU	OE1-CD-OE2	-11.02	110.08	123.30
1	A	117	HIS	ND1-CG-CD2	9.45	122.03	108.80
1	A	99	ASP	CB-CG-OD2	9.38	126.74	118.30
1	B	22	ASP	CB-CG-OD2	-8.94	110.25	118.30
1	B	43	ASP	OD1-CG-OD2	-8.73	106.71	123.30
1	A	80	ASP	CB-CG-OD1	-8.62	110.54	118.30
1	A	146	HIS	CA-C-O	8.08	137.06	120.10
1	A	79	ASP	CB-CA-C	-7.95	94.49	110.40
1	B	40	ARG	NH1-CZ-NH2	7.92	128.11	119.40
1	B	22	ASP	CB-CG-OD1	7.92	125.42	118.30
1	B	5	GLU	OE1-CD-OE2	-7.68	114.08	123.30
1	A	5	GLU	OE1-CD-OE2	-7.39	114.43	123.30
1	B	15	TRP	CD1-CG-CD2	7.37	112.20	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	PHE	CB-CG-CD2	-7.23	115.74	120.80
1	B	99	ASP	OD1-CG-OD2	-6.80	110.37	123.30
1	B	85	PHE	CB-CG-CD2	-6.70	116.11	120.80
1	B	42	PHE	CB-CG-CD2	6.67	125.47	120.80
1	A	43	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	26	GLU	OE1-CD-OE2	-6.53	115.46	123.30
1	A	1	GLY	CA-C-O	6.50	132.30	120.60
1	A	1	GLY	O-C-N	-6.46	112.37	122.70
1	B	94	ASP	CB-CG-OD1	6.37	124.04	118.30
1	A	117	HIS	CG-ND1-CE1	-6.35	97.45	105.70
1	B	21	GLU	CA-C-O	-6.33	106.81	120.10
1	B	85	PHE	CB-CG-CD1	6.06	125.04	120.80
1	B	97	HIS	CG-ND1-CE1	5.92	116.49	108.20
1	A	1	GLY	CA-C-N	-5.87	104.28	117.20
1	B	19	ASN	CB-CG-OD1	-5.73	110.13	121.60
1	A	94	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	78	LEU	O-C-N	-5.62	113.70	122.70
1	B	45	PHE	CG-CD2-CE2	-5.58	114.66	120.80
1	A	20	VAL	CG1-CB-CG2	5.49	119.69	110.90
1	A	146	HIS	CG-ND1-CE1	5.39	115.75	108.20
1	B	52	SER	N-CA-CB	-5.38	102.43	110.50
1	A	40	ARG	CD-NE-CZ	-5.35	116.11	123.60
1	B	15	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	B	90	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	A	80	ASP	OD1-CG-OD2	5.08	132.95	123.30
1	A	41	PHE	CD1-CE1-CZ	-5.02	114.08	120.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	GLY	Mainchain

## 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	1131	0	1128	17	3
1	B	1131	0	1126	32	1
2	A	43	0	30	0	0
2	B	43	0	30	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	143	0	0	2	0
4	B	143	0	0	4	5
All	All	2638	0	2314	48	5

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 10.

All (48) 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:21:GLU:N	1:B:21:GLU:CA	1.71	1.53
1:A:79:ASP:CA	1:A:79:ASP:CB	1.88	1.51
1:A:80:ASP:CB	1:A:80:ASP:CG	1.75	1.49
1:A:40:ARG:NE	1:A:40:ARG:CD	1.80	1.44
1:B:61:LYS:NZ	1:B:61:LYS:HB2	1.52	1.17
1:B:87:GLN:NE2	4:B:341:HOH:O	1.82	1.12
1:B:120:LYS:HD2	1:B:120:LYS:H	1.09	1.09
1:A:40:ARG:NH2	4:A:376:HOH:O	1.87	1.05
1:B:61:LYS:HZ3	1:B:61:LYS:HB2	1.12	0.94
1:B:91:LEU:HA	1:B:95:LYS:HD2	1.47	0.93
1:B:120:LYS:CD	1:B:120:LYS:H	1.81	0.93
1:B:61:LYS:NZ	1:B:61:LYS:CB	2.31	0.92
1:A:40:ARG:CD	1:A:40:ARG:CZ	2.52	0.84
1:B:120:LYS:N	1:B:120:LYS:HD2	1.90	0.84
1:B:61:LYS:HZ2	1:B:61:LYS:HB2	1.45	0.79
1:B:21:GLU:N	1:B:21:GLU:C	2.37	0.77
1:A:79:ASP:C	1:A:79:ASP:CB	2.55	0.75
1:B:20:VAL:O	1:B:20:VAL:HG12	1.87	0.75
1:B:21:GLU:N	1:B:21:GLU:CB	2.50	0.75
1:B:87:GLN:HG2	4:B:328:HOH:O	1.88	0.72
1:B:20:VAL:C	1:B:21:GLU:CA	2.58	0.72
1:B:61:LYS:HZ3	1:B:61:LYS:CB	1.96	0.67
1:A:79:ASP:CB	1:A:79:ASP:N	2.58	0.66
1:A:80:ASP:CA	1:A:80:ASP:CG	2.67	0.62
1:A:80:ASP:CB	1:A:80:ASP:OD1	2.40	0.62
1:B:100:PRO:HG3	1:B:145:TYR:CD2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASP:CA	1:A:79:ASP:CG	2.69	0.60
1:B:127:GLN:HE21	1:B:131:GLN:HE21	1.52	0.58
1:A:100:PRO:HG3	1:A:145:TYR:CD2	2.39	0.57
1:A:99:ASP:HB2	4:A:394:HOH:O	2.05	0.57
1:B:19:ASN:HD21	1:B:21:GLU:HB3	1.70	0.56
1:A:40:ARG:CG	1:A:40:ARG:NE	2.67	0.53
1:B:21:GLU:N	1:B:22:ASP:N	2.58	0.52
1:B:35:TYR:CZ	1:B:105:LEU:HD11	2.45	0.52
1:B:120:LYS:CD	1:B:120:LYS:N	2.63	0.51
1:B:107:GLY:HA3	1:B:134:VAL:HG13	1.93	0.51
1:A:99:ASP:HB3	1:A:102:ASN:ND2	2.31	0.45
1:B:19:ASN:ND2	1:B:21:GLU:HB3	2.32	0.44
1:B:24:GLY:HA2	1:B:68:LEU:HD13	1.99	0.44
1:B:45:PHE:HE1	2:B:147:HEM:O1D	2.01	0.43
1:A:127:GLN:OE1	1:B:30:ARG:HD3	2.20	0.42
1:A:21:GLU:CD	1:A:21:GLU:H	2.24	0.41
1:A:80:ASP:CB	1:A:80:ASP:OD2	2.46	0.41
1:B:100:PRO:HG3	1:B:145:TYR:CE2	2.56	0.41
1:B:14:LEU:HD11	1:B:118:PHE:CG	2.56	0.40
1:B:49:SER:HA	4:B:454:HOH:O	2.20	0.40
1:B:24:GLY:N	1:B:68:LEU:HD22	2.36	0.40
1:B:97:HIS:HE1	4:B:426:HOH:O	2.03	0.40

All (5) 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:40:ARG:CD	4:B:298:HOH:O[2_565]	1.43	0.77
4:B:468:HOH:O	4:B:468:HOH:O[2_665]	1.76	0.44
1:A:40:ARG:NH1	4:B:291:HOH:O[2_565]	1.95	0.25
1:A:40:ARG:NE	4:B:298:HOH:O[2_565]	1.98	0.22
1:B:117:HIS:CE1	4:B:368:HOH:O[2_665]	2.01	0.19

## 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	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	B	144/146 (99%)	141 (98%)	2 (1%)	1 (1%)	24	9
All	All	288/292 (99%)	283 (98%)	4 (1%)	1 (0%)	43	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	20	VAL

### 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	122/122 (100%)	122 (100%)	0	100	100
1	B	122/122 (100%)	116 (95%)	6 (5%)	27	10
All	All	244/244 (100%)	238 (98%)	6 (2%)	50	31

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	43	ASP
1	B	61	LYS
1	B	87	GLN
1	B	117	HIS
1	B	120	LYS
1	B	124	PRO

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	102	ASN

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Mol	Chain	Res	Type
1	A	131	GLN
1	B	2	HIS
1	B	19	ASN
1	B	39	GLN
1	B	87	GLN
1	B	97	HIS
1	B	131	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](#)

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	$\# Z  > 2$
2	HEM	A	147	1,3	27,50,50	3.10	11 (40%)	17,82,82	3.19	7 (41%)
3	CMO	A	148	2	0,1,1	0.00	-	0,0,0	0.00	-
2	HEM	B	147	1,3	27,50,50	2.47	11 (40%)	17,82,82	2.35	8 (47%)
3	CMO	B	148	2	0,1,1	0.00	-	0,0,0	0.00	-

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	147	1,3	-	0/6/54/54	0/0/8/8
3	CMO	A	148	2	-	0/0/0/0	0/0/0/0
2	HEM	B	147	1,3	-	0/6/54/54	0/0/8/8
3	CMO	B	148	2	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	147	HEM	C3B-C2B	-7.66	1.29	1.40
2	A	147	HEM	C3C-C2C	-5.25	1.33	1.40
2	B	147	HEM	C3C-C2C	-4.16	1.34	1.40
2	A	147	HEM	CBA-CAA	-2.99	1.32	1.53
2	B	147	HEM	CMD-C2D	2.27	1.56	1.51
2	B	147	HEM	C3B-CAB	2.47	1.52	1.47
2	A	147	HEM	CMC-C2C	2.97	1.58	1.51
2	B	147	HEM	C4A-NA	3.00	1.42	1.36
2	B	147	HEM	CMA-C3A	3.14	1.58	1.51
2	A	147	HEM	CBB-CAB	3.25	1.51	1.29
2	B	147	HEM	C1C-C2C	3.26	1.50	1.42
2	B	147	HEM	CBB-CAB	3.29	1.51	1.29
2	A	147	HEM	CMB-C2B	3.33	1.59	1.51
2	B	147	HEM	CMB-C2B	3.36	1.59	1.51
2	A	147	HEM	CBC-CAC	3.48	1.52	1.29
2	A	147	HEM	CAA-C2A	3.51	1.57	1.52
2	A	147	HEM	C1D-ND	4.28	1.45	1.36
2	B	147	HEM	C3C-CAC	4.31	1.56	1.47
2	B	147	HEM	C1D-ND	4.34	1.45	1.36
2	B	147	HEM	CAD-C3D	5.18	1.61	1.52
2	A	147	HEM	C4A-NA	5.54	1.47	1.36
2	A	147	HEM	C3B-CAB	6.15	1.60	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	147	HEM	C1D-C2D-C3D	-6.44	102.52	107.00
2	B	147	HEM	CAA-CBA-CGA	-3.94	105.93	112.66
2	A	147	HEM	CMA-C3A-C4A	-3.10	123.71	128.46
2	B	147	HEM	CMD-C2D-C1D	-2.99	123.86	128.46
2	B	147	HEM	CBD-CAD-C3D	-2.77	107.17	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	147	HEM	CMD-C2D-C3D	2.05	128.80	124.94
2	B	147	HEM	C3B-C4B-NB	2.31	112.20	109.21
2	B	147	HEM	CMC-C2C-C3C	2.47	129.38	124.88
2	A	147	HEM	CMD-C2D-C3D	2.52	129.69	124.94
2	B	147	HEM	CMB-C2B-C3B	2.94	130.24	124.88
2	A	147	HEM	CAD-CBD-CGD	4.41	120.19	112.66
2	A	147	HEM	CBA-CAA-C2A	4.47	121.03	112.48
2	B	147	HEM	C4C-C3C-C2C	4.93	110.34	106.90
2	A	147	HEM	C4A-C3A-C2A	5.51	110.83	107.00
2	A	147	HEM	CAA-CBA-CGA	5.61	122.25	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	147	HEM	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	79:ASP	C	80:ASP	N	1.17

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	146/146 (100%)	-0.21	1 (0%) 87 90	8, 15, 23, 29	11 (7%)
1	B	146/146 (100%)	-0.13	1 (0%) 87 90	8, 16, 25, 30	15 (10%)
All	All	292/292 (100%)	-0.17	2 (0%) 87 90	8, 15, 25, 30	26 (8%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	VAL	4.0
1	A	1	GLY	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	CMO	A	148	2/2	0.88	0.17	12,12,12,20	0
3	CMO	B	148	2/2	0.91	0.14	14,14,14,19	0
2	HEM	B	147	43/43	0.98	0.10	11,13,23,26	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	147	43/43	0.98	0.09	10,12,16,19	7

## 6.5 Other polymers [i](#)

There are no such residues in this entry.