



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2018 – 02:12 am GMT

PDB ID : 1A4F  
Title : BAR-HEADED GOOSE HEMOGLOBIN (OXY FORM)  
Authors : Zhang, J.; Gu, X.  
Deposited on : 1998-01-29  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

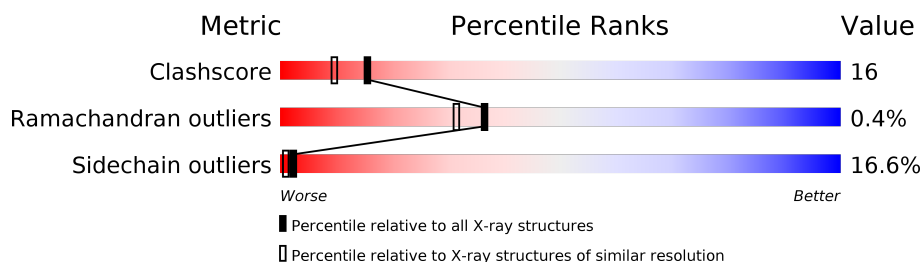
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122078	8264 (2.00-2.00)
Ramachandran outliers	120005	8163 (2.00-2.00)
Sidechain outliers	119972	8162 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	141	
2	B	146	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2448 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 (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	1	0
			1086	698	189	195	4			

- Molecule 2 is a protein called HEMOGLOBIN (BETA CHAIN).

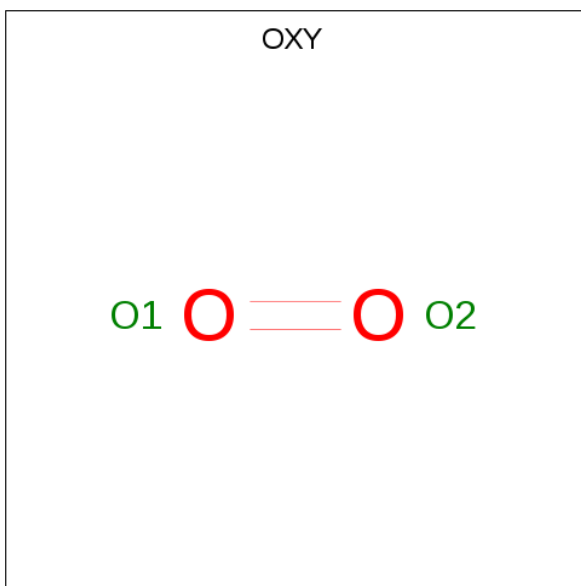
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	2	0
			1164	751	207	202	4			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



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

- Molecule 5 is water.

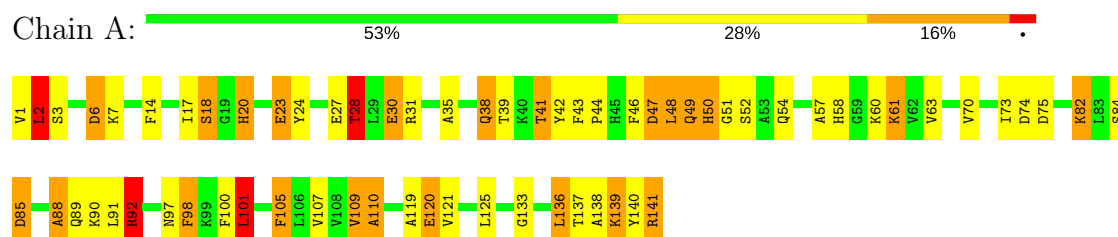
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total	O	0	0
			51	51		
5	B	57	Total	O	0	0
			57	57		

### 3 Residue-property plots

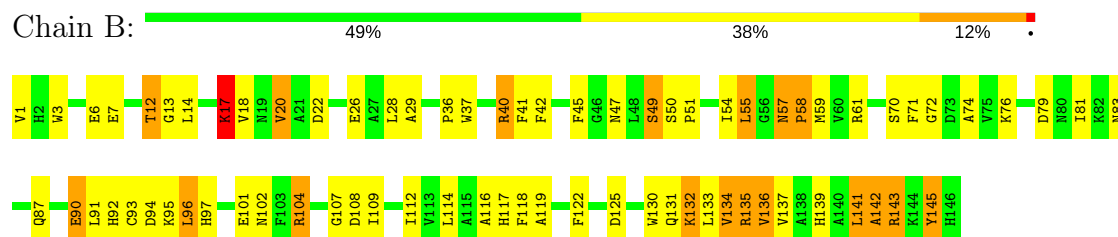
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



#### • Molecule 2: HEMOGLOBIN (BETA CHAIN)



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.59Å 81.59Å 107.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	87.1 (10.00-2.00)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2448	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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, OXY

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	1.00	0/1115	2.46	54/1509 (3.6%)
2	B	1.05	0/1201	2.29	51/1628 (3.1%)
All	All	1.03	0/2316	2.37	105/3137 (3.3%)

There are no bond length outliers.

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	NE-CZ-NH1	31.00	135.80	120.30
2	B	61	ARG	NE-CZ-NH1	16.05	128.32	120.30
2	B	40[A]	ARG	NE-CZ-NH1	14.46	127.53	120.30
2	B	40[B]	ARG	NE-CZ-NH1	14.46	127.53	120.30
2	B	61	ARG	NE-CZ-NH2	-14.25	113.18	120.30
2	B	22	ASP	CB-CG-OD1	13.87	130.78	118.30
1	A	82	LYS	CA-CB-CG	12.42	140.72	113.40
1	A	28	THR	CA-CB-CG2	12.40	129.76	112.40
1	A	92	ARG	NE-CZ-NH1	-12.20	114.20	120.30
1	A	31	ARG	NH1-CZ-NH2	-11.84	106.37	119.40
2	B	79	ASP	CB-CG-OD1	10.21	127.49	118.30
2	B	87	GLN	CA-CB-CG	10.14	135.72	113.40
2	B	104	ARG	NE-CZ-NH1	-9.52	115.54	120.30
1	A	141	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	A	107	VAL	CA-CB-CG2	8.77	124.06	110.90
2	B	40[A]	ARG	CD-NE-CZ	8.66	135.73	123.60
2	B	40[B]	ARG	CD-NE-CZ	8.66	135.73	123.60
1	A	49	GLN	CA-CB-CG	8.34	131.74	113.40
1	A	92	ARG	NH1-CZ-NH2	8.15	128.36	119.40
1	A	75	ASP	CA-CB-CG	8.14	131.32	113.40
2	B	20	VAL	CA-CB-CG2	8.08	123.02	110.90
1	A	91	LEU	O-C-N	7.55	134.78	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	LEU	CB-CG-CD2	-7.46	98.32	111.00
1	A	141	ARG	CD-NE-CZ	7.41	133.97	123.60
1	A	138	ALA	N-CA-CB	7.19	120.16	110.10
2	B	28	LEU	CB-CA-C	7.17	123.81	110.20
1	A	121	VAL	CG1-CB-CG2	-7.06	99.60	110.90
2	B	134	VAL	CA-CB-CG1	7.02	121.43	110.90
2	B	135	ARG	NE-CZ-NH2	-6.84	116.88	120.30
2	B	90	GLU	OE1-CD-OE2	6.78	131.43	123.30
2	B	134	VAL	N-CA-CB	-6.74	96.67	111.50
2	B	122	PHE	O-C-N	6.62	133.28	122.70
1	A	47	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	A	31	ARG	CG-CD-NE	-6.58	97.99	111.80
2	B	134	VAL	CB-CA-C	6.57	123.89	111.40
1	A	92	ARG	CD-NE-CZ	-6.56	114.42	123.60
2	B	141	LEU	CA-CB-CG	6.49	130.23	115.30
1	A	41	THR	CA-CB-CG2	6.38	121.33	112.40
1	A	85	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	30	GLU	CG-CD-OE2	6.33	130.97	118.30
2	B	79	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	58	HIS	CA-CB-CG	-6.17	103.12	113.60
2	B	18	VAL	CA-C-O	-6.08	107.34	120.10
1	A	27	GLU	O-C-N	6.06	132.39	122.70
1	A	119	ALA	CB-CA-C	6.03	119.15	110.10
1	A	82	LYS	CG-CD-CE	6.02	129.95	111.90
1	A	46	PHE	CB-CG-CD1	6.02	125.01	120.80
1	A	30	GLU	CB-CG-CD	6.00	130.39	114.20
2	B	87	GLN	CB-CA-C	5.97	122.34	110.40
1	A	110	ALA	CB-CA-C	-5.87	101.30	110.10
1	A	82	LYS	CB-CG-CD	5.84	126.79	111.60
2	B	142	ALA	O-C-N	-5.78	113.46	122.70
1	A	92	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	2	LEU	CA-C-O	5.74	132.14	120.10
1	A	98	PHE	CB-CG-CD1	-5.70	116.81	120.80
2	B	101	GLU	O-C-N	-5.69	113.60	122.70
2	B	41	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	A	31	ARG	CD-NE-CZ	5.62	131.47	123.60
2	B	41	PHE	CD1-CG-CD2	5.61	125.59	118.30
2	B	109	ILE	CA-C-O	-5.58	108.39	120.10
1	A	82	LYS	CB-CA-C	5.55	121.50	110.40
2	B	108	ASP	CB-CG-OD2	-5.52	113.33	118.30
2	B	125	ASP	CB-CG-OD2	-5.51	113.34	118.30
2	B	145	TYR	N-CA-CB	5.49	120.49	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	A	31	ARG	NE-CZ-NH2	-5.43	117.58	120.30
2	B	119	ALA	CB-CA-C	5.43	118.24	110.10
2	B	137	VAL	CA-C-O	-5.42	108.71	120.10
1	A	42	TYR	CD1-CE1-CZ	-5.42	114.92	119.80
1	A	75	ASP	CB-CG-OD2	5.41	123.17	118.30
2	B	137	VAL	O-C-N	5.41	131.35	122.70
1	A	109	VAL	O-C-N	-5.40	114.06	122.70
2	B	122	PHE	CD1-CE1-CZ	-5.39	113.63	120.10
2	B	104	ARG	NH1-CZ-NH2	5.39	125.33	119.40
1	A	30	GLU	CG-CD-OE1	-5.38	107.54	118.30
1	A	139	LYS	CB-CG-CD	5.38	125.59	111.60
1	A	84	SER	N-CA-CB	5.34	118.51	110.50
1	A	141	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
1	A	88	ALA	CA-C-N	-5.29	105.55	117.20
1	A	101	LEU	CB-CA-C	5.29	120.25	110.20
1	A	48	LEU	N-CA-CB	-5.28	99.85	110.40
1	A	109	VAL	CA-CB-CG1	5.28	118.81	110.90
1	A	109	VAL	CA-C-N	5.26	128.77	117.20
1	A	120	GLU	O-C-N	-5.23	114.33	122.70
2	B	22	ASP	OD1-CG-OD2	-5.21	113.39	123.30
1	A	91	LEU	CB-CG-CD1	-5.18	102.20	111.00
2	B	90	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	A	74	ASP	CB-CG-OD2	5.16	122.94	118.30
2	B	42	PHE	CD1-CE1-CZ	-5.16	113.91	120.10
2	B	83	ASN	C-N-CA	5.15	134.58	121.70
2	B	17	LYS	CA-CB-CG	-5.14	102.09	113.40
2	B	112	ILE	CA-CB-CG2	5.13	121.16	110.90
1	A	100	PHE	O-C-N	5.12	130.90	122.70
2	B	45	PHE	CB-CG-CD1	-5.12	117.22	120.80
2	B	139	HIS	CA-CB-CG	5.12	122.30	113.60
2	B	36	PRO	N-CA-CB	5.11	109.44	103.30
2	B	13	GLY	O-C-N	5.11	130.88	122.70
1	A	105	PHE	O-C-N	-5.11	114.53	122.70
2	B	132	LYS	CD-CE-NZ	-5.10	99.97	111.70
2	B	7	GLU	CG-CD-OE1	-5.08	108.14	118.30
2	B	20	VAL	CB-CA-C	5.05	120.99	111.40
2	B	58	PRO	C-N-CA	-5.05	109.08	121.70
1	A	31	ARG	O-C-N	5.04	130.77	122.70
2	B	58	PRO	N-CD-CG	-5.04	95.63	103.20
2	B	1	VAL	CA-CB-CG1	5.01	118.41	110.90

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	1086	0	1096	31	0
2	B	1164	0	1174	42	0
3	A	43	0	30	1	0
3	B	43	0	30	6	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	51	0	0	0	0
5	B	57	0	0	4	0
All	All	2448	0	2330	74	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 16.

All (74) 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:92:ARG:HA	1:A:140:TYR:HH	1.18	1.03
2:B:141:LEU:CD1	3:B:150:HEM:HBB2	1.93	0.99
1:A:92:ARG:HA	1:A:140:TYR:OH	1.62	0.98
2:B:141:LEU:HD12	3:B:150:HEM:HBB2	1.49	0.92
2:B:3:TRP:CZ3	2:B:132:LYS:HD2	2.04	0.92
2:B:91:LEU:O	2:B:96:LEU:HD22	1.74	0.88
2:B:143:ARG:HD3	5:B:180:HOH:O	1.84	0.76
2:B:91:LEU:HG	2:B:96:LEU:CD2	2.20	0.70
2:B:92:HIS:HA	2:B:96:LEU:HD23	1.74	0.70
2:B:57:ASN:HD22	2:B:59:MET:H	1.39	0.69
2:B:40[A]:ARG:NH2	5:B:167:HOH:O	2.20	0.69
1:A:92:ARG:CA	1:A:140:TYR:OH	2.39	0.68
3:B:150:HEM:HMC2	3:B:150:HEM:HBC2	1.75	0.67
2:B:96:LEU:O	2:B:97:HIS:HB2	1.95	0.66
1:A:14:PHE:O	1:A:18:SER:HB2	1.96	0.65
1:A:70:VAL:O	1:A:73:ILE:HB	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:TRP:HE1	2:B:102:ASN:HD21	1.43	0.65
2:B:132:LYS:O	2:B:136:VAL:HG13	1.97	0.65
2:B:91:LEU:HG	2:B:96:LEU:HD21	1.78	0.63
2:B:141:LEU:HD11	3:B:150:HEM:HBB2	1.79	0.62
2:B:93:CYS:SG	2:B:145:TYR:CE2	2.93	0.62
2:B:26[A]:GLU:OE1	2:B:117:HIS:NE2	2.31	0.59
2:B:51:PRO:O	2:B:55:LEU:HB2	2.03	0.58
3:B:150:HEM:CMC	3:B:150:HEM:HBC2	2.34	0.58
1:A:57:ALA:O	1:A:61:LYS:HG2	2.03	0.57
2:B:107:GLY:HA3	2:B:134:VAL:HG13	1.86	0.56
2:B:57:ASN:ND2	2:B:59:MET:H	2.03	0.56
2:B:71:PHE:O	2:B:74:ALA:HB3	2.05	0.56
2:B:72:GLY:O	2:B:76:LYS:HG2	2.06	0.56
2:B:142:ALA:O	2:B:145:TYR:HB2	2.05	0.56
2:B:47:ASN:OD1	2:B:49:SER:HB3	2.06	0.55
2:B:130:TRP:CE3	2:B:133:LEU:HD23	2.42	0.55
1:A:101:LEU:O	1:A:101:LEU:HD12	2.07	0.54
2:B:12:THR:HG22	5:B:202:HOH:O	2.07	0.54
2:B:130:TRP:CZ3	2:B:133:LEU:HD23	2.43	0.54
1:A:28:THR:HG21	1:A:105:PHE:HD1	1.74	0.53
1:A:47:ASP:N	1:A:54:GLN:OE1	2.35	0.52
2:B:3:TRP:CH2	2:B:132:LYS:HD2	2.45	0.51
1:A:49:GLN:O	1:A:50:HIS:C	2.49	0.51
2:B:93:CYS:SG	2:B:145:TYR:CD2	3.03	0.51
1:A:110:ALA:HB1	2:B:116:ALA:HB2	1.95	0.49
1:A:17:ILE:CD1	1:A:105:PHE:HZ	2.26	0.49
1:A:3:SER:O	1:A:6:ASP:HB2	2.13	0.49
2:B:90:GLU:O	2:B:94:ASP:HB2	2.13	0.48
1:A:61:LYS:HE3	3:A:150:HEM:O2A	2.12	0.48
1:A:88:ALA:O	1:A:140:TYR:CE1	2.67	0.48
2:B:17:LYS:HB3	2:B:118:PHE:CE1	2.49	0.48
2:B:29:ALA:HB1	2:B:55:LEU:HD13	1.95	0.48
2:B:76:LYS:HD2	2:B:76:LYS:N	2.20	0.47
1:A:101:LEU:HD12	1:A:101:LEU:C	2.35	0.47
1:A:51:GLY:O	1:A:52:SER:C	2.50	0.47
2:B:17:LYS:HB3	2:B:118:PHE:HE1	1.80	0.46
2:B:50:SER:O	2:B:54:ILE:N	2.44	0.46
1:A:14:PHE:CE2	1:A:17:ILE:HD11	2.50	0.46
2:B:57:ASN:HA	2:B:58:PRO:HD3	1.75	0.46
1:A:20:HIS:HB3	1:A:23:GLU:HG2	1.99	0.45
2:B:81:ILE:HD12	2:B:136:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:THR:CG2	5:B:202:HOH:O	2.63	0.44
2:B:51:PRO:O	2:B:55:LEU:HD22	2.18	0.43
1:A:2:LEU:HD12	1:A:2:LEU:N	2.33	0.43
1:A:43:PHE:N	1:A:44:PRO:CD	2.81	0.43
3:B:150:HEM:CBC	3:B:150:HEM:HMC2	2.47	0.43
1:A:133:GLY:O	1:A:137:THR:HG23	2.19	0.42
1:A:92:ARG:C	1:A:140:TYR:OH	2.57	0.42
1:A:98:PHE:CE1	1:A:137:THR:HG22	2.54	0.42
2:B:92:HIS:HA	2:B:96:LEU:CD2	2.46	0.42
2:B:114:LEU:HD22	2:B:118:PHE:HE2	1.83	0.42
1:A:125:LEU:HA	1:A:125:LEU:HD23	1.87	0.42
1:A:17:ILE:HB	1:A:24:TYR:HD2	1.85	0.41
1:A:38:GLN:HE21	1:A:38:GLN:H	1.68	0.41
1:A:136:LEU:HA	1:A:136:LEU:HD23	1.67	0.41
1:A:39:THR:HG22	1:A:97:ASN:HD22	1.86	0.41
1:A:24:TYR:O	1:A:28:THR:HG23	2.20	0.40
1:A:35:ALA:HB1	2:B:131:GLN:HG3	2.03	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	140/141 (99%)	134 (96%)	5 (4%)	1 (1%)	24	17
2	B	146/146 (100%)	141 (97%)	5 (3%)	0	100	100
All	All	286/287 (100%)	275 (96%)	10 (4%)	1 (0%)	36	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU

### 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	115/114 (101%)	91 (79%)	24 (21%)	1	0
2	B	123/121 (102%)	108 (88%)	15 (12%)	5	3
All	All	238/235 (101%)	199 (84%)	39 (16%)	2	1

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	7	LYS
1	A	18	SER
1	A	20	HIS
1	A	23	GLU
1	A	28	THR
1	A	30	GLU
1	A	38	GLN
1	A	41	THR
1	A	48	LEU
1	A	50	HIS
1	A	60	LYS
1	A	61	LYS
1	A	63	VAL
1	A	82	LYS
1	A	85	ASP
1	A	89	GLN
1	A	90	LYS
1	A	92	ARG
1	A	101	LEU
1	A	109	VAL
1	A	120	GLU
1	A	139	LYS
1	A	141	ARG
2	B	6	GLU
2	B	12	THR
2	B	14	LEU

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Mol	Chain	Res	Type
2	B	17	LYS
2	B	20	VAL
2	B	49	SER
2	B	55	LEU
2	B	57	ASN
2	B	70	SER
2	B	95	LYS
2	B	96	LEU
2	B	104	ARG
2	B	135	ARG
2	B	136	VAL
2	B	143	ARG

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	9	ASN
1	A	20	HIS
1	A	38	GLN
1	A	97	ASN
2	B	57	ASN
2	B	83	ASN
2	B	102	ASN
2	B	146	HIS

### 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	150	1,4	27,50,50	1.87	6 (22%)	17,82,82	2.30	7 (41%)
4	OXY	A	151	3	1,1,1	0.11	0	0,0,0	0.00	-
3	HEM	B	150	2,4	27,50,50	2.08	7 (25%)	17,82,82	1.77	4 (23%)
4	OXY	B	151	3	1,1,1	0.03	0	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
3	HEM	A	150	1,4	-	0/6/54/54	0/0/8/8
4	OXY	A	151	3	-	0/0/0/0	0/0/0/0
3	HEM	B	150	2,4	-	0/6/54/54	0/0/8/8
4	OXY	B	151	3	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	150	HEM	C3B-C2B	-5.24	1.33	1.40
3	B	150	HEM	C3C-C2C	-4.66	1.33	1.40
3	A	150	HEM	C3B-C2B	-4.36	1.34	1.40
3	A	150	HEM	C3C-C2C	-3.72	1.35	1.40
3	B	150	HEM	C3D-C2D	-2.25	1.31	1.37
3	B	150	HEM	CMA-C3A	2.09	1.55	1.51
3	B	150	HEM	C1A-NA	2.25	1.40	1.36
3	A	150	HEM	CAD-C3D	2.49	1.56	1.52
3	A	150	HEM	C1A-NA	2.62	1.41	1.36
3	B	150	HEM	C3C-CAC	2.90	1.53	1.47
3	A	150	HEM	C3B-CAB	3.63	1.55	1.47
3	A	150	HEM	C3C-CAC	3.78	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	150	HEM	C3B-CAB	4.13	1.56	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	150	HEM	CMA-C3A-C4A	-4.46	121.61	128.46
3	B	150	HEM	CAD-CBD-CGD	-2.67	108.10	112.66
3	A	150	HEM	CMD-C2D-C1D	-2.54	124.56	128.46
3	A	150	HEM	CMD-C2D-C3D	2.41	129.48	124.94
3	A	150	HEM	C4C-C3C-C2C	2.59	108.71	106.90
3	B	150	HEM	CMB-C2B-C3B	2.81	129.99	124.88
3	A	150	HEM	CMA-C3A-C2A	2.87	130.35	124.94
3	B	150	HEM	CAA-CBA-CGA	2.93	117.67	112.66
3	A	150	HEM	CAA-CBA-CGA	3.07	117.91	112.66
3	B	150	HEM	CBA-CAA-C2A	4.24	120.59	112.48
3	A	150	HEM	CMB-C2B-C3B	4.80	133.62	124.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	150	HEM	1	0
3	B	150	HEM	6	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.