



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:09 PM GMT

PDB ID : 1CLS  
Title : CROSS-LINKED HUMAN HEMOGLOBIN DEOXY  
Authors : Ji, X.; Fronticelli, C.; Bucci, E.; Gilliland, G.L.  
Deposited on : 1995-08-29  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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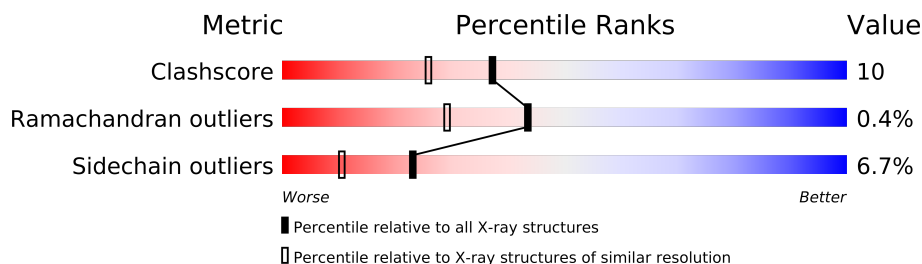
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	141	
1	C	141	
2	B	146	
2	D	146	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5058 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

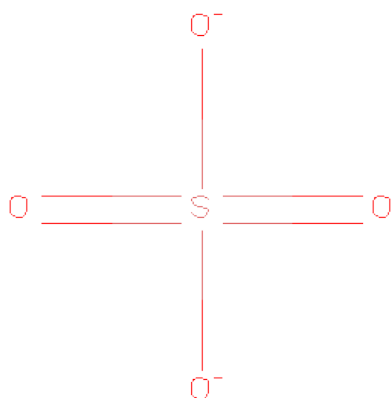
- Molecule 1 is a protein called HEMOGLOBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	C	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

- Molecule 2 is a protein called HEMOGLOBIN.

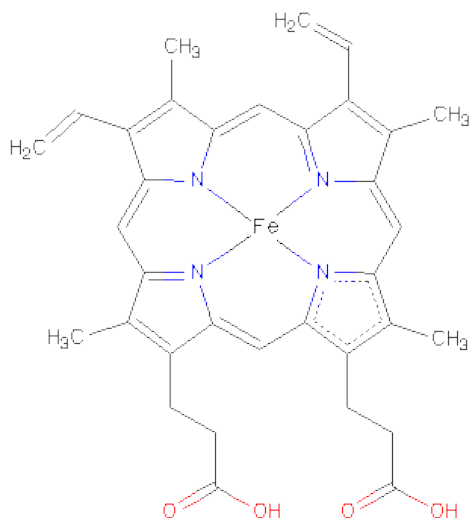
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	D	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).

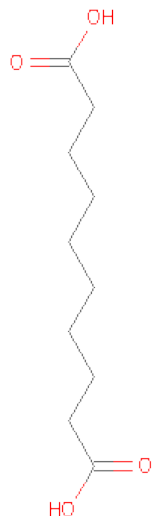


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	C	1	Total	O	0	0
			1	1		

- Molecule 6 is SEBACIC ACID (three-letter code: DEC) (formula:  $C_{10}H_{18}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			12	10	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	115	Total	O	0	0
			115	115		
7	B	127	Total	O	0	0
			127	127		
7	C	130	Total	O	0	0
			130	130		
7	D	106	Total	O	0	0
			106	106		

### 3 Residue-property plots

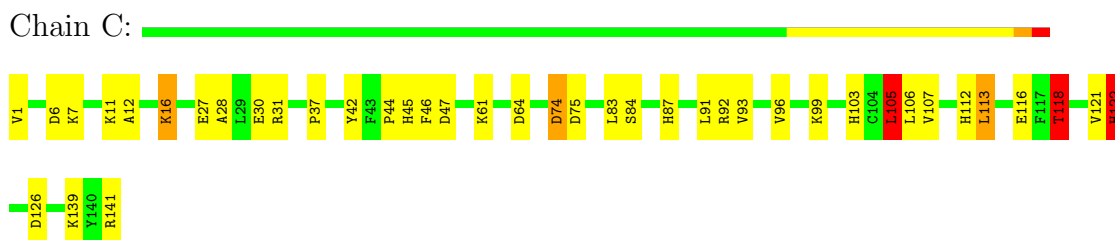
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

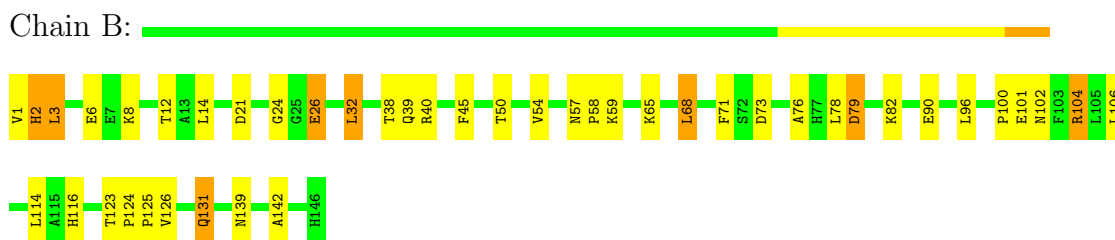
#### • Molecule 1: HEMOGLOBIN



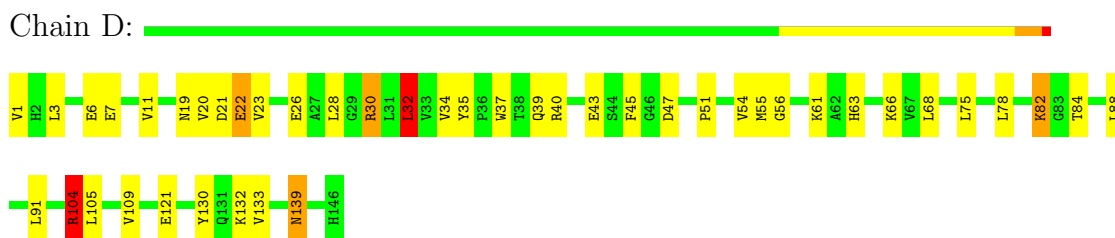
#### • Molecule 1: HEMOGLOBIN



#### • Molecule 2: HEMOGLOBIN



#### • Molecule 2: HEMOGLOBIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.80Å 82.47Å 53.30Å 90.00° 99.24° 90.00°	Depositor
Resolution (Å)	6.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.90)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, $R_{free}$	0.168 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5058	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, DEC, SO4, O

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	0.92	0/1097	1.63	15/1491 (1.0%)
1	C	0.89	0/1097	1.62	19/1491 (1.3%)
2	B	0.91	0/1153	1.62	14/1566 (0.9%)
2	D	0.88	0/1153	1.66	21/1566 (1.3%)
All	All	0.90	0/4500	1.63	69/6114 (1.1%)

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	C	0	1

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	40	ARG	NE-CZ-NH2	-12.87	113.86	120.30
2	D	30	ARG	NE-CZ-NH2	-12.65	113.97	120.30
1	A	126	ASP	CB-CG-OD1	12.08	129.18	118.30
2	B	40	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	C	141	ARG	NE-CZ-NH1	11.08	125.84	120.30
1	A	64	ASP	CB-CG-OD1	10.13	127.42	118.30
1	C	31	ARG	NE-CZ-NH1	9.36	124.98	120.30
2	D	30	ARG	NH1-CZ-NH2	9.03	129.33	119.40
2	B	73	ASP	CB-CG-OD1	8.62	126.06	118.30
2	D	40	ARG	NE-CZ-NH1	8.46	124.53	120.30
2	D	21	ASP	CB-CG-OD1	8.00	125.50	118.30
1	C	118	THR	N-CA-CB	-7.80	95.47	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	30	ARG	NE-CZ-NH1	-7.75	116.43	120.30
1	A	92	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	C	92	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	64	ASP	CB-CG-OD2	-7.38	111.66	118.30
2	B	26	GLU	OE1-CD-OE2	7.27	132.03	123.30
1	C	96	VAL	CA-CB-CG2	7.02	121.43	110.90
2	D	35	TYR	CB-CG-CD1	-6.91	116.85	121.00
1	C	74	ASP	CB-CG-OD1	6.90	124.51	118.30
2	D	22	GLU	OE1-CD-OE2	-6.86	115.07	123.30
2	B	40	ARG	NE-CZ-NH1	6.75	123.67	120.30
2	D	32	LEU	CB-CG-CD1	6.73	122.45	111.00
1	C	30	GLU	OE1-CD-OE2	-6.66	115.31	123.30
1	A	42	TYR	CG-CD2-CE2	-6.65	115.98	121.30
1	A	116	GLU	OE1-CD-OE2	-6.48	115.53	123.30
1	A	31	ARG	CD-NE-CZ	6.42	132.59	123.60
2	D	45	PHE	CB-CG-CD1	6.37	125.26	120.80
1	A	106	LEU	CB-CG-CD2	-6.33	100.24	111.00
1	C	105	LEU	CA-CB-CG	6.33	129.86	115.30
2	D	30	ARG	CD-NE-CZ	6.19	132.26	123.60
1	C	47	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	76	MET	CG-SD-CE	6.09	109.94	100.20
2	B	104	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	B	114	LEU	CB-CG-CD2	-5.80	101.14	111.00
2	D	21	ASP	OD1-CG-OD2	-5.72	112.42	123.30
1	A	43	PHE	CB-CG-CD2	-5.71	116.80	120.80
2	B	126	VAL	CA-CB-CG2	-5.68	102.38	110.90
2	D	54	VAL	CG1-CB-CG2	-5.65	101.86	110.90
1	A	116	GLU	CG-CD-OE1	5.55	129.41	118.30
2	D	47	ASP	CB-CG-OD1	5.55	123.30	118.30
1	C	6	ASP	CB-CG-OD2	-5.51	113.34	118.30
2	B	101	GLU	OE1-CD-OE2	5.50	129.91	123.30
1	C	118	THR	CA-CB-CG2	5.50	120.10	112.40
1	C	46	PHE	CB-CG-CD1	5.46	124.62	120.80
1	C	126	ASP	CB-CG-OD2	5.36	123.12	118.30
2	B	79	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	113	LEU	CA-CB-CG	5.36	127.62	115.30
2	D	28	LEU	CA-C-N	5.34	126.89	116.20
1	A	141	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	126	ASP	OD1-CG-OD2	-5.32	113.19	123.30
2	D	84	THR	CA-CB-CG2	5.32	119.85	112.40
1	C	122	HIS	CA-CB-CG	5.29	122.60	113.60
2	D	104	ARG	CB-CG-CD	5.26	125.29	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	C	30	GLU	CG-CD-OE1	5.16	128.62	118.30
1	C	64	ASP	CB-CG-OD1	5.15	122.94	118.30
1	C	106	LEU	CB-CG-CD1	5.15	119.75	111.00
2	D	133	VAL	CB-CA-C	-5.13	101.66	111.40
2	B	71	PHE	CB-CG-CD1	-5.12	117.21	120.80
1	A	140	TYR	CB-CG-CD1	5.11	124.07	121.00
2	B	106	LEU	O-C-N	-5.11	114.52	123.20
2	B	76	ALA	CB-CA-C	-5.09	102.46	110.10
2	B	26	GLU	CG-CD-OE1	-5.09	108.12	118.30
2	D	21	ASP	CA-CB-CG	5.03	124.47	113.40
2	B	131	GLN	O-C-N	5.03	130.75	122.70
2	D	22	GLU	CB-CG-CD	5.01	127.74	114.20
2	D	34	VAL	CG1-CB-CG2	-5.01	102.89	110.90
1	C	46	PHE	CB-CG-CD2	-5.01	117.30	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	37	PRO	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1069	0	1073	22	0
1	C	1069	0	1073	24	0
2	B	1123	0	1116	22	0
2	D	1123	0	1115	24	0
3	B	5	0	0	0	0
3	D	5	0	0	1	0
4	A	43	0	30	4	0
4	B	43	0	30	3	0
4	C	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	43	0	30	3	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	D	12	0	16	3	0
7	A	115	0	0	4	0
7	B	127	0	0	2	0
7	C	130	0	0	4	0
7	D	106	0	0	4	0
All	All	5058	0	4513	92	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (92) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:82:LYS:HE3	6:D:149:DEC:H32	1.51	0.90
1:C:12:ALA:O	1:C:16:LYS:HE2	1.80	0.81
2:D:20:VAL:HG13	2:D:68:LEU:HB3	1.61	0.80
1:A:76:MET:N	1:A:77:PRO:HD2	1.99	0.77
1:A:56:LYS:O	1:A:60:LYS:HD3	1.87	0.75
1:A:74:ASP:HA	7:A:254:HOH:O	1.87	0.74
2:B:1:VAL:HB	2:B:2:HIS:CD2	2.24	0.73
1:C:118:THR:HG22	1:C:121:VAL:H	1.56	0.68
1:C:45:HIS:HE1	4:C:142:HEM:O2D	1.77	0.67
2:D:43:GLU:HA	7:D:219:HOH:O	1.94	0.66
2:B:2:HIS:N	2:B:2:HIS:CD2	2.62	0.65
2:B:45:PHE:HA	2:B:59:LYS:HD3	1.78	0.65
1:C:45:HIS:CD2	1:C:45:HIS:H	2.12	0.64
2:D:139:ASN:HB3	6:D:149:DEC:O3	1.99	0.63
2:B:2:HIS:CD2	2:B:2:HIS:H	2.17	0.63
2:D:105:LEU:O	2:D:109:VAL:HG23	2.01	0.60
1:C:42:TYR:CE1	1:C:93:VAL:HA	2.37	0.59
1:C:83:LEU:HD11	4:C:142:HEM:HMA3	1.85	0.59
1:A:61:LYS:NZ	4:A:142:HEM:O1A	2.36	0.58
1:A:137:THR:HG22	7:A:231:HOH:O	2.03	0.58
1:C:122:HIS:HD2	2:D:30:ARG:HH11	1.52	0.58
1:C:27:GLU:OE1	1:C:112:HIS:HE1	1.87	0.58
1:C:84:SER:OG	1:C:139:LYS:HD2	2.05	0.57
2:B:32:LEU:HG	2:B:39:GLN:HG2	1.87	0.56
1:A:28:ALA:HB2	1:A:105:LEU:HD13	1.86	0.56
1:A:76:MET:N	1:A:77:PRO:CD	2.68	0.55
1:A:28:ALA:CB	1:A:105:LEU:HD13	2.37	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2:HIS:O	2:B:3:LEU:HD22	2.07	0.55
1:C:45:HIS:CE1	4:C:142:HEM:O2D	2.59	0.54
2:B:38:THR:HG22	2:B:102:ASN:OD1	2.07	0.54
2:D:51:PRO:O	2:D:55:MET:HG2	2.08	0.54
1:A:14:TRP:O	1:A:17:VAL:HB	2.08	0.53
2:D:32:LEU:HG	2:D:39:GLN:HG2	1.90	0.53
2:B:123:THR:HA	7:B:165:HOH:O	2.07	0.53
1:A:76:MET:H	1:A:77:PRO:HD2	1.70	0.53
1:A:21:ALA:HB1	1:A:63:ALA:HB1	1.91	0.52
1:C:113:LEU:HB3	1:C:116:GLU:HG2	1.90	0.51
2:D:3:LEU:HD22	2:D:7:GLU:HB3	1.91	0.51
1:C:45:HIS:CD2	7:C:263:HOH:O	2.63	0.51
1:C:122:HIS:CD2	2:D:30:ARG:HH11	2.29	0.51
2:B:82:LYS:CE	6:D:149:DEC:H32	2.33	0.50
4:D:148:HEM:HMC2	4:D:148:HEM:HBC2	1.94	0.50
2:D:22:GLU:HB2	7:D:177:HOH:O	2.11	0.50
2:D:121:GLU:HB2	7:D:243:HOH:O	2.11	0.50
2:B:90:GLU:HG2	7:B:260:HOH:O	2.11	0.50
1:A:83:LEU:HD11	4:A:142:HEM:C3A	2.46	0.49
4:D:148:HEM:HHC	4:D:148:HEM:HBB2	1.95	0.49
1:A:11:LYS:HE3	7:A:163:HOH:O	2.13	0.49
1:A:13:ALA:O	1:A:16:LYS:HB3	2.12	0.49
1:A:60:LYS:HE3	7:A:199:HOH:O	2.13	0.48
2:D:104:ARG:HG2	7:D:194:HOH:O	2.14	0.48
1:C:83:LEU:HD21	4:C:142:HEM:HMA3	1.96	0.47
1:A:42:TYR:CE2	1:A:93:VAL:HA	2.50	0.47
2:D:75:LEU:HA	2:D:78:LEU:HD13	1.97	0.47
1:C:112:HIS:HD2	7:C:251:HOH:O	1.96	0.47
1:C:103:HIS:O	1:C:107:VAL:HG23	2.15	0.47
1:A:92:ARG:HB3	2:D:37:TRP:HB2	1.97	0.47
1:C:28:ALA:CB	1:C:105:LEU:HD13	2.45	0.47
4:B:148:HEM:HMB1	4:B:148:HEM:HBB2	1.96	0.47
2:D:19:ASN:HB3	2:D:22:GLU:HG2	1.97	0.47
1:C:44:PRO:HD2	1:C:45:HIS:HD2	1.80	0.46
1:C:112:HIS:CD2	7:C:251:HOH:O	2.68	0.46
4:B:148:HEM:CMB	4:B:148:HEM:HBB2	2.46	0.46
1:A:83:LEU:HD11	4:A:142:HEM:CMA	2.46	0.45
2:B:24:GLY:HA2	2:B:68:LEU:HG	1.97	0.45
2:B:57:ASN:HA	2:B:58:PRO:HD2	1.83	0.45
1:A:114:PRO:HA	2:B:116:HIS:CD2	2.52	0.45
1:C:87:HIS:HA	1:C:91:LEU:HB2	1.98	0.44
1:C:27:GLU:OE1	1:C:112:HIS:CE1	2.69	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:3:LEU:HD12	2:D:78:LEU:CD2	2.48	0.44
2:D:56:GLY:HA2	2:D:61:LYS:HZ1	1.81	0.44
1:C:7:LYS:O	1:C:11:LYS:HG3	2.18	0.44
2:B:50:THR:O	2:B:54:VAL:HG23	2.17	0.44
1:C:61:LYS:HD2	7:C:227:HOH:O	2.18	0.43
2:D:11:VAL:HA	2:D:130:TYR:CE2	2.54	0.43
2:B:104:ARG:NH2	2:B:139:ASN:OD1	2.52	0.43
2:B:21:ASP:CG	2:B:65:LYS:HD3	2.39	0.43
2:D:23:VAL:HG12	2:D:68:LEU:HD21	2.01	0.43
2:D:82:LYS:HB2	3:D:147:SO4:O4	2.19	0.42
2:B:100:PRO:HB3	2:B:142:ALA:HB2	2.00	0.42
2:D:3:LEU:HD23	2:D:132:LYS:HD3	2.01	0.42
2:B:8:LYS:O	2:B:12:THR:HG23	2.20	0.42
2:D:63:HIS:O	2:D:66:LYS:HB2	2.19	0.42
1:C:83:LEU:HD22	1:C:87:HIS:HE1	1.85	0.42
1:A:140:TYR:HD2	2:D:37:TRP:CE3	2.36	0.42
1:A:96:VAL:HG22	1:A:96:VAL:O	2.19	0.42
1:A:83:LEU:HD21	4:A:142:HEM:HMA1	2.02	0.41
4:D:148:HEM:HHC	4:D:148:HEM:CBB	2.50	0.41
2:B:124:PRO:N	2:B:125:PRO:CD	2.84	0.41
2:D:88:LEU:HD23	2:D:91:LEU:HD23	2.02	0.41
2:B:1:VAL:N	2:B:78:LEU:O	2.54	0.41
2:B:96:LEU:HD13	4:B:148:HEM:C3D	2.55	0.41

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	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	30	15
1	C	139/141 (99%)	138 (99%)	0	1 (1%)	30	15
2	B	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
2	D	144/146 (99%)	142 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	566/574 (99%)	554 (98%)	10 (2%)	2 (0%)	43	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ASP
1	C	75	ASP

### 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	113/113 (100%)	105 (93%)	8 (7%)	21	9
1	C	113/113 (100%)	106 (94%)	7 (6%)	26	12
2	B	118/118 (100%)	109 (92%)	9 (8%)	19	8
2	D	118/118 (100%)	111 (94%)	7 (6%)	28	14
All	All	462/462 (100%)	431 (93%)	31 (7%)	23	10

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	78	ASN
1	A	84	SER
1	A	90	LYS
1	A	105	LEU
1	A	109	LEU
1	A	119	PRO
1	A	137	THR
2	B	2	HIS
2	B	3	LEU
2	B	6	GLU
2	B	14	LEU
2	B	26	GLU
2	B	32	LEU

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Mol	Chain	Res	Type
2	B	68	LEU
2	B	79	ASP
2	B	131	GLN
1	C	1	VAL
1	C	16	LYS
1	C	74	ASP
1	C	99	LYS
1	C	105	LEU
1	C	118	THR
1	C	122	HIS
2	D	1	VAL
2	D	6	GLU
2	D	26	GLU
2	D	32	LEU
2	D	82	LYS
2	D	104	ARG
2	D	139	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
2	B	2	HIS
1	C	45	HIS
1	C	112	HIS
1	C	122	HIS
2	D	117	HIS
2	D	146	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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
4	HEM	A	142	1,5	49,50,50	2.33	15 (30%)	46,82,82	2.22	10 (21%)
3	SO4	B	147	-	4,4,4	1.78	1 (25%)	6,6,6	0.71	0
4	HEM	B	148	2	49,50,50	3.01	17 (34%)	46,82,82	2.31	11 (23%)
4	HEM	C	142	1,5	49,50,50	2.79	14 (28%)	46,82,82	2.01	11 (23%)
3	SO4	D	147	-	4,4,4	1.43	0	6,6,6	0.42	0
4	HEM	D	148	2	49,50,50	2.61	18 (36%)	46,82,82	1.84	10 (21%)
6	DEC	D	149	2	11,11,13	10.53	2 (18%)	6,10,14	0.52	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
4	HEM	A	142	1,5	-	0/14/114/114	0/0/8/8
3	SO4	B	147	-	-	0/0/0/0	0/0/0/0
4	HEM	B	148	2	-	0/14/114/114	0/0/8/8
4	HEM	C	142	1,5	-	0/14/114/114	0/0/8/8
3	SO4	D	147	-	-	0/0/0/0	0/0/0/0
4	HEM	D	148	2	-	0/14/114/114	0/0/8/8
6	DEC	D	149	2	-	0/7/9/11	0/0/0/0

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	149	DEC	O3-C10	26.36	1.29	1.11
6	D	149	DEC	O1-C1	22.83	1.27	1.11
4	C	142	HEM	C2B-C1B	10.17	1.47	1.44
4	B	148	HEM	C2D-C1D	9.41	1.46	1.44
4	B	148	HEM	C2B-C1B	8.79	1.46	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	142	HEM	C3D-C4D	-7.78	1.42	1.44
4	D	148	HEM	C4A-C3A	7.28	1.49	1.40
4	A	142	HEM	C3D-C2D	-6.30	1.32	1.43
4	C	142	HEM	C3B-C2B	-6.11	1.33	1.43
4	B	148	HEM	C3D-C2D	-5.92	1.33	1.43
4	D	148	HEM	C2D-C1D	5.89	1.46	1.44
4	B	148	HEM	C4A-C3A	5.75	1.47	1.40
4	B	148	HEM	C3B-C2B	-5.66	1.33	1.43
4	D	148	HEM	C3B-C2B	-5.47	1.34	1.43
4	D	148	HEM	C3D-C2D	-5.29	1.34	1.43
4	C	142	HEM	C3B-CAB	5.29	1.57	1.40
4	D	148	HEM	C3C-C2C	-5.16	1.34	1.43
4	A	142	HEM	C3B-C2B	-5.11	1.34	1.43
4	A	142	HEM	C3B-CAB	5.03	1.56	1.40
4	C	142	HEM	C3D-C2D	-5.02	1.35	1.43
4	D	148	HEM	C2B-C1B	4.90	1.45	1.44
4	A	142	HEM	C3C-C2C	-4.86	1.35	1.43
4	B	148	HEM	C3B-CAB	4.84	1.55	1.40
4	A	142	HEM	C2B-C1B	-4.63	1.43	1.44
4	D	148	HEM	C3B-CAB	4.60	1.54	1.40
4	B	148	HEM	C3C-C2C	-4.57	1.35	1.43
4	D	148	HEM	C3C-CAC	4.46	1.54	1.40
4	A	142	HEM	C3C-CAC	4.43	1.54	1.40
4	B	148	HEM	CHB-C1B	4.29	1.42	1.35
4	C	142	HEM	C3C-CAC	4.00	1.53	1.40
4	A	142	HEM	C4A-C3A	3.92	1.45	1.40
4	C	142	HEM	C4A-C3A	3.71	1.44	1.40
4	B	148	HEM	C3D-C4D	3.69	1.45	1.44
4	D	148	HEM	C3D-C4D	3.64	1.45	1.44
4	C	142	HEM	CAA-C2A	3.50	1.58	1.52
4	B	148	HEM	C3C-CAC	3.48	1.51	1.40
4	C	142	HEM	C3C-C2C	-3.42	1.37	1.43
4	D	148	HEM	CHB-C1B	3.32	1.40	1.35
4	A	142	HEM	CAA-C2A	3.18	1.57	1.52
4	B	148	HEM	C3B-C4B	3.06	1.48	1.44
4	B	148	HEM	FE-NA	3.06	2.05	1.92
4	B	148	HEM	CHD-C4C	3.01	1.41	1.36
4	B	148	HEM	CMC-C2C	2.91	1.56	1.47
4	D	148	HEM	FE-NA	2.80	2.04	1.92
4	C	142	HEM	CMC-C2C	2.70	1.55	1.47
4	B	148	HEM	CHA-C4D	2.63	1.39	1.35
4	A	142	HEM	FE-NB	2.57	2.07	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	142	HEM	O2D-CGD	-2.57	1.21	1.30
3	B	147	SO4	O2-S	2.57	1.55	1.47
4	A	142	HEM	CHB-C1B	2.54	1.39	1.35
4	B	148	HEM	FE-NB	2.51	2.07	1.97
4	A	142	HEM	CMC-C2C	2.47	1.55	1.47
4	A	142	HEM	FE-NC	2.40	2.06	1.97
4	A	142	HEM	CMB-C2B	2.33	1.54	1.47
4	B	148	HEM	CMD-C2D	2.31	1.54	1.47
4	D	148	HEM	CMD-C2D	2.29	1.54	1.47
4	D	148	HEM	CMC-C2C	2.26	1.54	1.47
4	D	148	HEM	CMB-C2B	2.21	1.54	1.47
4	A	142	HEM	CBD-CGD	2.19	1.56	1.50
4	C	142	HEM	CHB-C1B	2.20	1.39	1.35
4	D	148	HEM	CHD-C4C	2.19	1.40	1.36
4	A	142	HEM	CMD-C2D	2.18	1.54	1.47
4	D	148	HEM	CAA-C2A	2.13	1.55	1.52
4	D	148	HEM	C1A-C2A	2.12	1.47	1.43
4	C	142	HEM	C4C-NC	2.09	1.41	1.38
4	C	142	HEM	CMB-C2B	2.07	1.53	1.47
4	D	148	HEM	CAD-CBD	2.06	1.58	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	142	HEM	C3B-C4B-NB	-9.39	107.28	114.00
4	C	142	HEM	C3B-C4B-NB	-7.67	108.51	114.00
4	D	148	HEM	C3B-C4B-NB	-6.79	109.14	114.00
4	B	148	HEM	C4A-CHB-C1B	-6.23	119.27	127.47
4	B	148	HEM	CMA-C3A-C4A	-6.12	119.21	128.62
4	B	148	HEM	C3B-C4B-NB	-5.90	109.78	114.00
4	B	148	HEM	CMA-C3A-C2A	5.16	134.67	124.94
4	D	148	HEM	C4A-CHB-C1B	-5.09	120.78	127.47
4	A	142	HEM	O2D-CGD-O1D	5.00	136.01	123.30
4	A	142	HEM	O2A-CGA-O1A	4.62	135.05	123.30
4	C	142	HEM	CMA-C3A-C4A	-3.82	122.75	128.62
4	A	142	HEM	CMA-C3A-C4A	-3.80	122.77	128.62
4	B	148	HEM	O1D-CGD-CBD	-3.79	110.00	123.03
4	A	142	HEM	O1A-CGA-CBA	-3.73	110.20	123.03
4	C	142	HEM	C1A-C2A-C3A	3.67	110.72	106.92
4	C	142	HEM	CMA-C3A-C2A	3.67	131.86	124.94
4	D	148	HEM	CMA-C3A-C4A	-3.55	123.17	128.62
4	C	142	HEM	CHC-C4B-NB	-3.53	121.65	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	148	HEM	O2D-CGD-O1D	3.47	132.12	123.30
4	C	142	HEM	O1A-CGA-CBA	-3.25	111.86	123.03
4	B	148	HEM	CHB-C4A-NA	3.16	129.86	124.58
4	B	148	HEM	C2D-C1D-ND	-3.16	109.20	112.93
4	A	142	HEM	CMA-C3A-C2A	3.03	130.66	124.94
4	B	148	HEM	CHC-C1C-NC	3.01	127.35	124.73
4	A	142	HEM	O1D-CGD-CBD	-2.92	112.97	123.03
4	D	148	HEM	CMA-C3A-C2A	2.91	130.42	124.94
4	C	142	HEM	O2A-CGA-O1A	2.88	130.63	123.30
4	B	148	HEM	C3A-C4A-CHB	-2.85	120.59	126.00
4	D	148	HEM	C2D-C1D-ND	-2.77	109.65	112.93
4	A	142	HEM	CHC-C1C-NC	-2.74	122.36	124.73
4	C	142	HEM	CHC-C1C-NC	-2.56	122.51	124.73
4	C	142	HEM	C2D-C1D-ND	-2.43	110.06	112.93
4	A	142	HEM	C1A-C2A-C3A	2.39	109.40	106.92
4	C	142	HEM	C4A-C3A-C2A	-2.34	105.37	107.00
4	D	148	HEM	CBA-CAA-C2A	2.28	116.70	112.69
4	A	142	HEM	C1B-NB-C4B	2.26	107.48	105.16
4	B	148	HEM	CMB-C2B-C3B	2.21	131.38	126.16
4	D	148	HEM	CBD-CAD-C3D	-2.13	109.72	114.37
4	D	148	HEM	C3A-C4A-CHB	-2.10	122.03	126.00
4	D	148	HEM	CMB-C2B-C3B	2.06	131.01	126.16
4	D	148	HEM	O1D-CGD-CBD	-2.06	115.95	123.03
4	C	142	HEM	CMB-C2B-C3B	2.06	131.00	126.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.