



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:36 AM GMT

PDB ID : 3PI9
Title : Site-specific Glycosylation of Hemoglobin Utilizing Oxime Ligation Chemistry as a Viable Alternative to PEGylation
Authors : Bhatt, V.S.; Styslinger, T.J.; Zhang, N.; Wang, P.G.; Palmer, A.F.
Deposited on : 2010-11-05
Resolution : 2.90 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

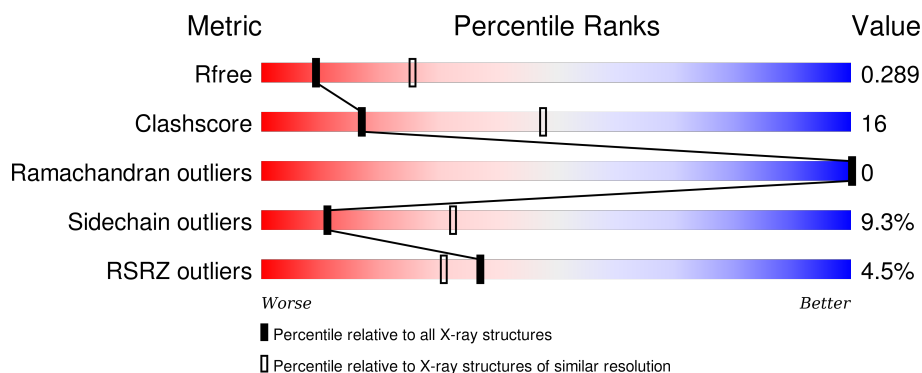
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 ≥ 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	141	<div> <div>2%</div> <div>71% 25% . .</div> </div>
1	C	141	<div> <div>2%</div> <div>70% 25% . .</div> </div>
2	B	145	<div> <div>2%</div> <div>62% 30% 8%</div> </div>
2	D	145	<div> <div>12%</div> <div>59% 30% 10% .</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
4	CMO	A	143	-	-	-	X
4	CMO	B	148	-	-	X	X
4	CMO	C	143	-	-	-	X
4	CMO	D	148	-	-	-	X

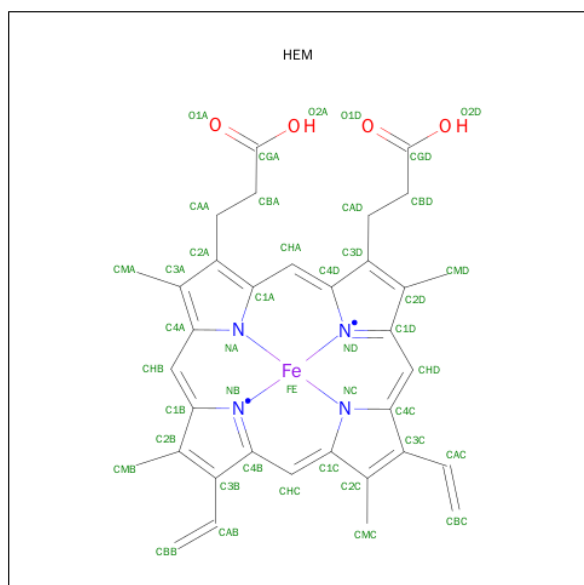
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 2 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total 1066	C 683	N 186	O 196	S 1	10	0	0
1	C	141	Total 1066	C 683	N 186	O 196	S 1	1	0	0

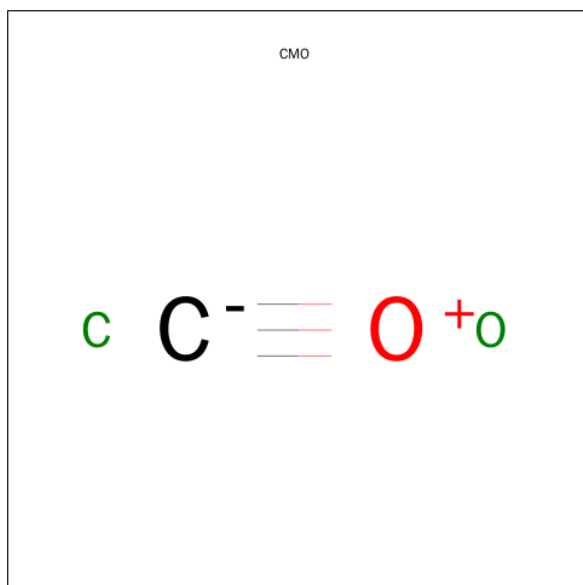
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total 1127	C 726	N 194	O 203	S 4	3	0	0
2	D	145	Total 1127	C 726	N 194	O 203	S 4	6	0	0

- 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		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



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

- Molecule 5 is water.

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

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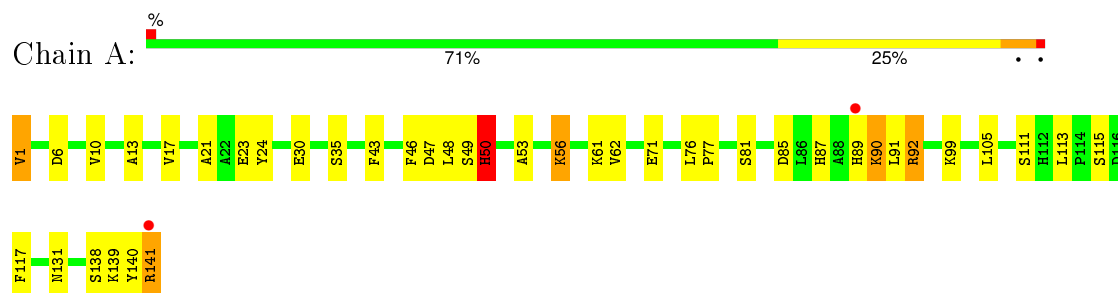
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	O	0	0
			2	2		
5	D	4	Total	O	0	0
			4	4		

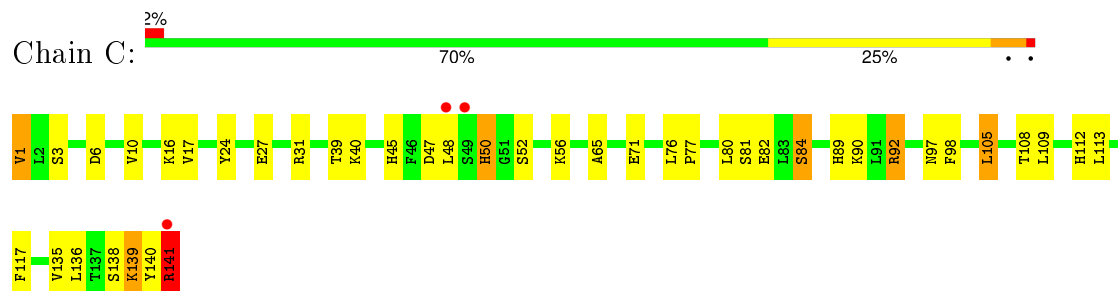
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

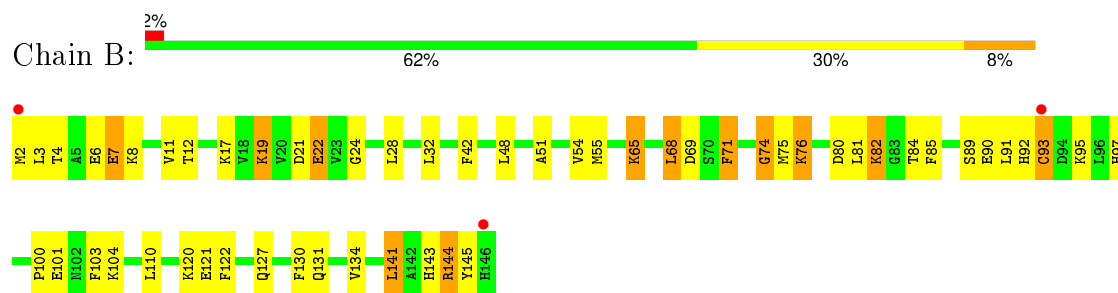
- Molecule 1: Hemoglobin subunit alpha



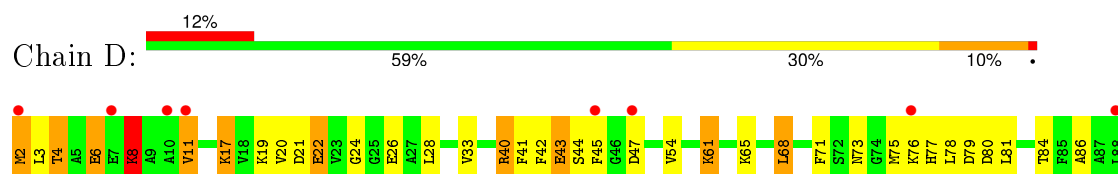
- Molecule 1: Hemoglobin subunit alpha

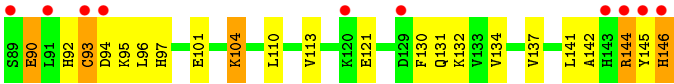


- Molecule 2: Hemoglobin subunit beta



- Molecule 2: Hemoglobin subunit beta





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.18Å 74.01Å 131.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.57 – 2.90 37.57 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.2 (37.57-2.90) 95.3 (37.57-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.09 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.261 , 0.293 0.255 , 0.289	Depositor DCC
R_{free} test set	614 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 12596 reflections (0.016%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4578	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	1.46	15/1093 (1.4%)	1.01	5/1483 (0.3%)
1	C	1.49	14/1093 (1.3%)	1.01	7/1483 (0.5%)
2	B	1.47	11/1152 (1.0%)	1.10	4/1556 (0.3%)
2	D	1.86	20/1152 (1.7%)	1.25	12/1556 (0.8%)
All	All	1.58	60/4490 (1.3%)	1.10	28/6078 (0.5%)

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
1	C	0	1
All	All	0	2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	GLU	CG-CD	28.30	1.94	1.51
1	C	50	HIS	CD2-NE2	23.37	1.91	1.42
2	B	22	GLU	CG-CD	22.20	1.85	1.51
1	A	92	ARG	CZ-NH1	17.81	1.56	1.33
2	D	146	HIS	C-OXT	15.56	1.52	1.23
2	D	44	SER	CB-OG	15.18	1.61	1.42
2	D	101	GLU	CD-OE1	13.56	1.40	1.25
1	C	89	HIS	CG-ND1	12.87	1.67	1.38
1	A	90	LYS	CE-NZ	12.78	1.80	1.49
2	D	61	LYS	CE-NZ	11.80	1.78	1.49
1	A	23	GLU	CD-OE2	11.49	1.38	1.25
2	D	43	GLU	CD-OE2	11.15	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	144	ARG	CZ-NH1	10.60	1.46	1.33
2	B	76	LYS	CD-CE	9.55	1.75	1.51
1	A	30	GLU	CD-OE1	9.46	1.36	1.25
1	C	89	HIS	CE1-NE2	9.40	1.54	1.32
2	D	101	GLU	CD-OE2	9.09	1.35	1.25
2	D	4	THR	CB-OG1	8.91	1.61	1.43
2	B	93	CYS	CB-SG	8.79	1.97	1.82
2	B	7	GLU	CB-CG	8.67	1.68	1.52
2	D	6	GLU	CB-CG	8.59	1.68	1.52
2	B	80	ASP	CG-OD2	7.62	1.42	1.25
1	C	82	GLU	CG-CD	7.44	1.63	1.51
1	C	50	HIS	CE1-NE2	-7.32	1.15	1.32
2	B	97	HIS	CE1-NE2	7.30	1.49	1.32
1	A	50	HIS	C-O	7.03	1.36	1.23
1	A	23	GLU	CD-OE1	6.80	1.33	1.25
1	C	139	LYS	CE-NZ	6.73	1.65	1.49
2	D	146	HIS	C-O	6.68	1.36	1.23
1	A	92	ARG	CG-CD	6.65	1.68	1.51
1	C	82	GLU	CD-OE2	6.64	1.32	1.25
2	D	93	CYS	CB-SG	6.61	1.93	1.82
2	B	82	LYS	CD-CE	6.54	1.67	1.51
2	D	43	GLU	CD-OE1	6.54	1.32	1.25
2	D	132	LYS	CE-NZ	6.44	1.65	1.49
2	B	8	LYS	CE-NZ	6.41	1.65	1.49
2	D	4	THR	CB-CG2	6.25	1.73	1.52
1	A	56	LYS	CE-NZ	6.24	1.64	1.49
1	C	141	ARG	CZ-NH1	6.18	1.41	1.33
2	B	101	GLU	CD-OE1	6.12	1.32	1.25
1	A	71	GLU	CG-CD	6.07	1.61	1.51
1	C	141	ARG	CD-NE	5.96	1.56	1.46
1	A	99	LYS	CE-NZ	5.96	1.64	1.49
1	C	50	HIS	CB-CG	5.84	1.60	1.50
1	A	50	HIS	CB-CG	-5.72	1.39	1.50
2	D	17	LYS	CD-CE	5.68	1.65	1.51
1	C	141	ARG	NE-CZ	5.66	1.40	1.33
2	D	97	HIS	CE1-NE2	5.65	1.45	1.32
2	D	97	HIS	CG-ND1	5.54	1.50	1.38
2	D	104	LYS	CD-CE	5.53	1.65	1.51
2	D	22	GLU	CB-CG	5.51	1.62	1.52
2	B	74	GLY	C-O	-5.47	1.14	1.23
2	B	97	HIS	CG-ND1	5.45	1.50	1.38
1	A	92	ARG	CZ-NH2	5.38	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	ASP	CG-OD1	-5.20	1.13	1.25
1	A	53	ALA	CA-CB	-5.10	1.41	1.52
1	C	71	GLU	CD-OE1	-5.09	1.20	1.25
1	C	82	GLU	CD-OE1	5.07	1.31	1.25
1	A	85	ASP	CB-CG	5.05	1.62	1.51
1	C	16	LYS	CE-NZ	5.01	1.61	1.49

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	144	ARG	NE-CZ-NH1	24.42	132.51	120.30
2	B	80	ASP	CB-CG-OD2	-13.93	105.77	118.30
2	D	144	ARG	NH1-CZ-NH2	-13.09	105.00	119.40
1	A	50	HIS	CA-CB-CG	11.11	132.49	113.60
2	D	40	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	C	141	ARG	NE-CZ-NH1	9.86	125.23	120.30
2	B	22	GLU	CG-CD-OE2	-9.25	99.81	118.30
1	C	50	HIS	CG-CD2-NE2	-8.45	93.14	109.20
2	B	22	GLU	CG-CD-OE1	8.42	135.15	118.30
1	C	82	GLU	OE1-CD-OE2	8.03	132.93	123.30
2	D	43	GLU	CG-CD-OE1	-7.48	103.34	118.30
2	D	43	GLU	CB-CG-CD	6.86	132.72	114.20
1	C	89	HIS	CG-CD2-NE2	-6.84	96.20	109.20
1	A	71	GLU	OE1-CD-OE2	-6.56	115.43	123.30
2	D	6	GLU	CG-CD-OE2	-6.38	105.53	118.30
1	A	53	ALA	CB-CA-C	6.28	119.51	110.10
2	D	6	GLU	CB-CA-C	-6.15	98.11	110.40
1	C	141	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	D	8	LYS	CB-CG-CD	-6.02	95.95	111.60
2	D	6	GLU	CG-CD-OE1	5.91	130.11	118.30
1	C	50	HIS	CE1-NE2-CD2	-5.59	92.61	106.60
2	B	12	THR	OG1-CB-CG2	5.52	122.70	110.00
2	D	43	GLU	CG-CD-OE2	5.52	129.33	118.30
2	D	47	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	30	GLU	OE1-CD-OE2	5.40	129.78	123.30
2	D	79	ASP	O-C-N	5.30	131.18	122.70
1	C	89	HIS	CE1-NE2-CD2	5.20	119.61	106.60
1	A	21	ALA	N-CA-CB	-5.12	102.94	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	HIS	Sidechain
1	C	50	HIS	Sidechain

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	1066	0	1069	32	0
1	C	1066	0	1069	30	0
2	B	1127	0	1129	34	0
2	D	1127	0	1129	41	0
3	A	43	0	30	9	0
3	B	43	0	30	7	0
3	C	43	0	30	7	0
3	D	43	0	30	7	0
4	A	2	0	0	0	0
4	B	2	0	0	5	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	4	0	0	3	0
All	All	4578	0	4516	147	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:LYS:CD	2:B:76:LYS:CE	1.75	1.55
2:D:61:LYS:NZ	2:D:61:LYS:CE	1.78	1.45
1:A:90:LYS:NZ	1:A:90:LYS:CE	1.81	1.43
1:A:140:TYR:O	1:A:141:ARG:OXT	1.69	1.11
2:D:11:VAL:HG13	2:D:75:MET:HE1	1.49	0.95
1:A:92:ARG:HH22	1:A:139:LYS:NZ	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:HIS:NE2	3:C:142:HEM:O1D	2.06	0.88
3:B:147:HEM:FE	4:B:148:CMO:C	1.61	0.81
3:B:147:HEM:NB	4:B:148:CMO:C	2.45	0.80
2:D:19:LYS:HE2	5:D:149:HOH:O	1.80	0.79
2:D:11:VAL:HG13	2:D:75:MET:CE	2.13	0.78
2:B:76:LYS:CE	2:B:76:LYS:CG	2.62	0.78
1:C:40:LYS:HG2	1:C:48:LEU:HD13	1.68	0.76
2:D:11:VAL:HG22	2:D:130:PHE:CE2	2.23	0.74
3:B:147:HEM:NC	4:B:148:CMO:C	2.51	0.73
1:C:139:LYS:HA	1:C:141:ARG:HH22	1.56	0.71
2:D:19:LYS:CE	5:D:149:HOH:O	2.35	0.71
2:B:11:VAL:HG22	2:B:130:PHE:CE2	2.25	0.71
3:A:142:HEM:HMB2	3:A:142:HEM:HBB2	1.72	0.71
2:B:11:VAL:HG22	2:B:130:PHE:CD2	2.26	0.70
1:A:76:LEU:N	1:A:77:PRO:HD2	2.08	0.69
2:B:89:SER:OG	2:B:144:ARG:HG2	1.93	0.69
2:B:2:MET:HG3	2:B:3:LEU:H	1.57	0.69
1:A:61:LYS:HE2	3:A:142:HEM:O1A	1.94	0.68
2:B:32:LEU:HD21	2:B:42:PHE:CD2	2.29	0.67
2:D:3:LEU:O	2:D:8:LYS:NZ	2.29	0.65
3:B:147:HEM:ND	4:B:148:CMO:C	2.60	0.64
2:D:81:LEU:HD22	2:D:137:VAL:HG22	1.79	0.64
2:D:2:MET:HG2	2:D:3:LEU:HD22	1.79	0.63
2:B:19:LYS:H	2:B:19:LYS:HE2	1.63	0.63
1:C:3:SER:HB2	1:C:6:ASP:H	1.64	0.63
1:C:92:ARG:HH22	1:C:139:LYS:HZ2	1.45	0.62
1:C:98:PHE:HE2	1:C:136:LEU:HD12	1.65	0.62
2:B:4:THR:OG1	2:B:7:GLU:HG3	1.98	0.62
1:A:47:ASP:OD2	1:A:49:SER:OG	2.17	0.61
3:B:147:HEM:NA	4:B:148:CMO:C	2.64	0.61
1:A:6:ASP:O	1:A:10:VAL:HG23	2.01	0.60
2:B:81:LEU:HD22	2:B:85:PHE:HE2	1.67	0.60
1:A:140:TYR:O	1:A:141:ARG:C	2.39	0.59
1:C:105:LEU:O	1:C:109:LEU:HG	2.02	0.58
3:C:142:HEM:CMC	3:C:142:HEM:HBC2	2.34	0.58
2:D:11:VAL:HG22	2:D:130:PHE:CZ	2.39	0.57
1:A:92:ARG:HH22	1:A:139:LYS:HZ3	1.48	0.57
2:B:93:CYS:HA	2:B:145:TYR:OH	2.05	0.56
2:D:42:PHE:HA	5:D:150:HOH:O	2.04	0.56
1:C:76:LEU:N	1:C:77:PRO:HD2	2.19	0.56
1:A:140:TYR:HB3	1:C:1:VAL:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:HIS:HE1	3:D:147:HEM:C4A	2.24	0.56
2:D:92:HIS:HA	2:D:96:LEU:HD12	1.88	0.55
2:D:20:VAL:HG13	2:D:68:LEU:HB3	1.88	0.55
1:A:17:VAL:HG13	1:A:24:TYR:CD2	2.40	0.55
2:B:93:CYS:SG	2:B:141:LEU:O	2.64	0.55
2:B:92:HIS:CE1	3:B:147:HEM:NA	2.75	0.54
3:D:147:HEM:CBA	3:D:147:HEM:CMA	2.84	0.54
2:B:71:PHE:CZ	2:B:134:VAL:HG12	2.42	0.54
1:A:61:LYS:HE2	3:A:142:HEM:CGA	2.37	0.54
2:D:19:LYS:HZ2	2:D:22:GLU:HG3	1.73	0.53
1:A:76:LEU:N	1:A:77:PRO:CD	2.71	0.53
2:D:73:ASN:HA	2:D:76:LYS:HE3	1.90	0.52
3:D:147:HEM:HBA1	3:D:147:HEM:HMA1	1.92	0.52
3:D:147:HEM:HBA1	3:D:147:HEM:CMA	2.40	0.52
1:A:91:LEU:O	2:D:40:ARG:HD2	2.10	0.51
2:B:6:GLU:O	2:B:7:GLU:C	2.48	0.51
1:A:92:ARG:HH22	1:A:139:LYS:HZ2	1.51	0.51
3:C:142:HEM:HBA2	3:C:142:HEM:HHA	1.93	0.51
2:D:86:ALA:HB1	2:D:144:ARG:HH22	1.76	0.51
1:A:90:LYS:NZ	1:A:90:LYS:CD	2.67	0.50
2:B:90:GLU:HG3	2:B:144:ARG:NH2	2.27	0.50
2:B:100:PRO:HD3	2:B:145:TYR:CE2	2.47	0.49
3:C:142:HEM:CBA	3:C:142:HEM:HHA	2.42	0.49
2:B:71:PHE:HZ	2:B:134:VAL:HG12	1.78	0.49
2:D:4:THR:O	2:D:8:LYS:HB2	2.12	0.49
2:B:48:LEU:HD22	2:B:54:VAL:HG22	1.95	0.49
1:A:76:LEU:H	1:A:77:PRO:HD2	1.74	0.49
1:C:139:LYS:HA	1:C:141:ARG:NH2	2.27	0.48
2:D:24:GLY:CA	2:D:68:LEU:HG	2.43	0.48
2:D:86:ALA:O	2:D:144:ARG:NH2	2.47	0.48
2:D:61:LYS:CD	2:D:61:LYS:NZ	2.69	0.48
2:B:3:LEU:HB3	2:B:7:GLU:HB2	1.95	0.48
2:D:77:HIS:HB2	2:D:84:THR:OG1	2.14	0.48
1:C:6:ASP:O	1:C:10:VAL:HG23	2.14	0.47
2:B:91:LEU:HD12	2:B:95:LYS:HD2	1.96	0.47
1:C:76:LEU:N	1:C:77:PRO:CD	2.76	0.47
2:B:81:LEU:HD22	2:B:85:PHE:CE2	2.49	0.47
2:B:100:PRO:HA	2:B:103:PHE:CD2	2.50	0.47
1:A:43:PHE:O	1:A:48:LEU:HD11	2.15	0.47
2:D:142:ALA:HB3	2:D:146:HIS:HE1	1.80	0.47
1:C:17:VAL:HG13	1:C:24:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:O	1:A:117:PHE:HB2	2.15	0.47
3:C:142:HEM:CBC	3:C:142:HEM:HMC1	2.46	0.46
2:B:65:LYS:NZ	2:B:69:ASP:OD1	2.45	0.46
1:A:87:HIS:HE1	3:A:142:HEM:C4A	2.33	0.46
2:D:4:THR:OG1	2:D:6:GLU:HB3	2.15	0.46
1:A:140:TYR:CB	1:C:1:VAL:HG22	2.46	0.46
1:C:39:THR:HG22	1:C:97:ASN:HD22	1.80	0.46
1:A:1:VAL:HG22	1:C:140:TYR:CB	2.46	0.46
2:D:11:VAL:CG2	2:D:130:PHE:CE2	2.97	0.46
2:D:26:GLU:CD	2:D:113:VAL:HG13	2.37	0.45
1:C:80:LEU:HB2	1:C:135:VAL:HG11	1.98	0.45
1:C:108:THR:O	1:C:112:HIS:HD2	1.99	0.45
2:D:90:GLU:HG2	2:D:94:ASP:OD2	2.17	0.45
2:B:2:MET:CE	2:B:3:LEU:HG	2.47	0.45
2:D:42:PHE:O	2:D:45:PHE:HB2	2.16	0.45
2:D:19:LYS:HZ2	2:D:21:ASP:HB2	1.81	0.44
1:A:138:SER:CB	1:C:1:VAL:HG13	2.46	0.44
2:D:80:ASP:O	2:D:84:THR:OG1	2.30	0.44
2:D:75:MET:HA	2:D:78:LEU:HG	1.99	0.44
2:B:76:LYS:CD	2:B:76:LYS:NZ	2.72	0.43
1:A:62:VAL:HG22	3:A:142:HEM:CHB	2.48	0.43
2:B:122:PHE:CZ	2:B:127:GLN:HA	2.52	0.43
1:C:138:SER:O	1:C:141:ARG:NH2	2.51	0.43
3:D:147:HEM:CMB	3:D:147:HEM:HBB2	2.49	0.43
2:D:90:GLU:HG3	2:D:144:ARG:HE	1.84	0.43
1:C:39:THR:HG22	1:C:97:ASN:ND2	2.34	0.43
2:B:11:VAL:HG13	2:B:75:MET:HE1	2.00	0.43
1:A:46:PHE:CE1	3:A:142:HEM:O1D	2.72	0.43
1:A:13:ALA:O	1:A:17:VAL:HG23	2.18	0.43
1:C:113:LEU:O	1:C:117:PHE:HB2	2.19	0.42
3:C:142:HEM:HMC1	3:C:142:HEM:HBC2	2.01	0.42
1:A:35:SER:HB3	2:B:131:GLN:HG3	2.00	0.42
2:D:19:LYS:NZ	2:D:21:ASP:HB2	2.35	0.42
2:B:11:VAL:HG13	2:B:75:MET:CE	2.50	0.42
1:A:87:HIS:CE1	3:A:142:HEM:C4A	3.07	0.42
2:D:92:HIS:CE1	3:D:147:HEM:C4A	3.00	0.42
2:D:33:VAL:HG23	2:D:54:VAL:HG11	2.02	0.42
1:A:17:VAL:HG13	1:A:24:TYR:HD2	1.84	0.41
1:C:112:HIS:O	1:C:113:LEU:HD23	2.20	0.41
1:C:27:GLU:O	1:C:31:ARG:HG3	2.20	0.41
2:D:41:PHE:HB3	3:D:147:HEM:HMD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:GLY:HA2	2:B:84:THR:HG21	2.02	0.41
2:D:17:LYS:HE3	2:D:121:GLU:OE2	2.20	0.41
2:B:51:ALA:O	2:B:55:MET:HG2	2.20	0.41
2:B:24:GLY:HA2	2:B:68:LEU:HD23	2.02	0.41
1:C:84:SER:HB2	1:C:141:ARG:HE	1.85	0.41
3:A:142:HEM:HHA	3:A:142:HEM:HAA1	1.80	0.41
2:D:131:GLN:HA	2:D:134:VAL:HG22	2.03	0.41
1:C:84:SER:HB2	1:C:141:ARG:HH21	1.86	0.41
1:C:52:SER:O	1:C:56:LYS:HD3	2.20	0.41
2:B:17:LYS:NZ	2:B:121:GLU:OE2	2.27	0.41
1:C:65:ALA:HB2	3:C:142:HEM:HMA2	2.03	0.41
2:D:68:LEU:HA	2:D:68:LEU:HD22	1.83	0.41
1:A:1:VAL:HG22	1:C:140:TYR:CG	2.56	0.41
2:D:93:CYS:HA	2:D:145:TYR:OH	2.20	0.40
1:A:131:ASN:N	1:A:131:ASN:HD22	2.19	0.40
1:A:62:VAL:HG13	3:A:142:HEM:CMB	2.51	0.40
3:B:147:HEM:HBB2	3:B:147:HEM:HMB2	2.02	0.40
1:C:47:ASP:CG	1:C:52:SER:HB2	2.42	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	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
1	C	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
2	B	143/145 (99%)	137 (96%)	6 (4%)	0	100	100
2	D	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
All	All	564/572 (99%)	540 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	112/112 (100%)	103 (92%)	9 (8%)	15	40
1	C	112/112 (100%)	105 (94%)	7 (6%)	22	54
2	B	118/118 (100%)	104 (88%)	14 (12%)	6	19
2	D	118/118 (100%)	105 (89%)	13 (11%)	8	23
All	All	460/460 (100%)	417 (91%)	43 (9%)	11	32

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	50	HIS
1	A	56	LYS
1	A	81	SER
1	A	89	HIS
1	A	105	LEU
1	A	111	SER
1	A	115	SER
1	A	141	ARG
2	B	19	LYS
2	B	21	ASP
2	B	22	GLU
2	B	28	LEU
2	B	65	LYS
2	B	68	LEU
2	B	71	PHE
2	B	82	LYS
2	B	104	LYS
2	B	110	LEU
2	B	120	LYS
2	B	141	LEU
2	B	143	HIS
2	B	144	ARG
1	C	1	VAL

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Mol	Chain	Res	Type
1	C	81	SER
1	C	84	SER
1	C	90	LYS
1	C	92	ARG
1	C	105	LEU
1	C	141	ARG
2	D	2	MET
2	D	8	LYS
2	D	11	VAL
2	D	28	LEU
2	D	43	GLU
2	D	65	LYS
2	D	68	LEU
2	D	71	PHE
2	D	90	GLU
2	D	95	LYS
2	D	104	LYS
2	D	110	LEU
2	D	141	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
2	B	108	ASN
1	C	89	HIS
1	C	97	ASN
2	D	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

8 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	142	1	30,50,50	3.32	8 (26%)	24,82,82	3.53	13 (54%)
4	CMO	A	143	-	0,1,1	0.00	-	0,0,0	0.00	-
3	HEM	B	147	2,4	30,50,50	3.59	10 (33%)	24,82,82	2.87	11 (45%)
4	CMO	B	148	3	0,1,1	0.00	-	0,0,0	0.00	-
3	HEM	C	142	1	30,50,50	2.95	10 (33%)	24,82,82	2.73	10 (41%)
4	CMO	C	143	-	0,1,1	0.00	-	0,0,0	0.00	-
3	HEM	D	147	2	30,50,50	3.11	7 (23%)	24,82,82	3.24	14 (58%)
4	CMO	D	148	-	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
3	HEM	A	142	1	-	0/10/54/54	0/0/8/8
4	CMO	A	143	-	-	0/0/0/0	0/0/0/0
3	HEM	B	147	2,4	-	0/10/54/54	0/0/8/8
4	CMO	B	148	3	-	0/0/0/0	0/0/0/0
3	HEM	C	142	1	-	0/10/54/54	0/0/8/8
4	CMO	C	143	-	-	0/0/0/0	0/0/0/0
3	HEM	D	147	2	-	0/10/54/54	0/0/8/8
4	CMO	D	148	-	-	0/0/0/0	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	C3B-C4B	-13.47	1.39	1.51
3	A	142	HEM	C3B-C4B	-13.02	1.40	1.51
3	D	147	HEM	C3B-C4B	-12.52	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	142	HEM	C3B-C4B	-9.22	1.43	1.51
3	B	147	HEM	C3D-C4D	-9.16	1.39	1.51
3	C	142	HEM	C3D-C4D	-8.19	1.41	1.51
3	A	142	HEM	C3D-C4D	-8.17	1.41	1.51
3	B	147	HEM	C2C-C1C	-7.16	1.39	1.52
3	D	147	HEM	C3D-C4D	-6.19	1.43	1.51
3	D	147	HEM	C2C-C1C	-5.55	1.42	1.52
3	A	142	HEM	C2C-C1C	-5.16	1.42	1.52
3	C	142	HEM	C2C-C1C	-5.12	1.42	1.52
3	A	142	HEM	FE-NB	-3.90	1.76	1.97
3	D	147	HEM	C2D-C1D	-3.86	1.39	1.51
3	C	142	HEM	FE-ND	-3.84	1.77	1.97
3	C	142	HEM	C2B-C1B	-3.75	1.39	1.51
3	C	142	HEM	C2D-C1D	-3.29	1.41	1.51
3	A	142	HEM	C2D-C1D	-3.16	1.41	1.51
3	B	147	HEM	FE-NB	-3.11	1.81	1.97
3	D	147	HEM	C2B-C1B	-2.98	1.42	1.51
3	B	147	HEM	C2D-C1D	-2.96	1.42	1.51
3	D	147	HEM	C2A-C3A	-2.85	1.29	1.37
3	C	142	HEM	C2A-C3A	-2.78	1.29	1.37
3	B	147	HEM	C2B-C1B	-2.57	1.43	1.51
3	D	147	HEM	CHD-C1D	-2.49	1.32	1.38
3	A	142	HEM	C2B-C1B	-2.44	1.43	1.51
3	C	142	HEM	C4A-CHB	-2.23	1.33	1.39
3	A	142	HEM	CHC-C4B	-2.15	1.32	1.38
3	B	147	HEM	CHC-C1C	-2.14	1.31	1.36
3	B	147	HEM	CHC-C4B	-2.14	1.33	1.38
3	C	142	HEM	C1A-CHA	-2.13	1.34	1.39
3	B	147	HEM	C1A-CHA	-2.08	1.34	1.39
3	A	142	HEM	C1A-CHA	-2.08	1.34	1.39
3	B	147	HEM	FE-ND	-2.00	1.86	1.97
3	C	142	HEM	C3B-CAB	2.30	1.55	1.51

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	142	HEM	CAA-C2A-C1A	-8.16	118.15	127.01
3	D	147	HEM	CAA-CBA-CGA	-7.11	99.71	112.75
3	A	142	HEM	CAA-CBA-CGA	-6.26	101.28	112.75
3	D	147	HEM	C1D-CHD-C4C	-5.07	117.34	125.82
3	B	147	HEM	CBD-CAD-C3D	-4.65	100.03	113.55
3	C	142	HEM	CAA-CBA-CGA	-3.96	105.48	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	147	HEM	C1D-CHD-C4C	-3.85	119.38	125.82
3	A	142	HEM	CMA-C3A-C4A	-3.49	122.58	128.36
3	D	147	HEM	C3C-CAC-CBC	-3.48	119.12	124.46
3	D	147	HEM	C3B-C4B-CHC	-3.45	118.30	123.16
3	B	147	HEM	C4B-CHC-C1C	-3.42	120.10	125.82
3	D	147	HEM	C3B-CAB-CBB	-3.37	119.29	124.46
3	C	142	HEM	C4B-CHC-C1C	-3.37	120.19	125.82
3	B	147	HEM	C3B-C4B-CHC	-3.37	118.43	123.16
3	B	147	HEM	CMA-C3A-C4A	-3.16	123.14	128.36
3	D	147	HEM	CBA-CAA-C2A	-3.03	107.10	112.53
3	B	147	HEM	CAA-C2A-C1A	-2.92	123.84	127.01
3	C	142	HEM	C3C-CAC-CBC	-2.79	120.17	124.46
3	C	142	HEM	CBD-CAD-C3D	-2.29	106.89	113.55
3	A	142	HEM	C1D-CHD-C4C	-2.16	122.21	125.82
3	D	147	HEM	C4B-CHC-C1C	-2.11	122.29	125.82
3	C	142	HEM	CAA-C2A-C1A	2.00	129.18	127.01
3	A	142	HEM	CMA-C3A-C2A	2.04	129.51	125.24
3	A	142	HEM	C2D-C3D-C4D	2.12	105.10	101.50
3	D	147	HEM	CHC-C4B-NB	2.27	129.99	124.52
3	A	142	HEM	CAA-C2A-C3A	2.48	136.09	129.00
3	B	147	HEM	CMD-C2D-C3D	2.67	126.18	114.35
3	D	147	HEM	C2D-C3D-C4D	2.94	106.48	101.50
3	A	142	HEM	CMD-C2D-C3D	3.08	127.96	114.35
3	C	142	HEM	CMD-C2D-C3D	3.56	130.10	114.35
3	C	142	HEM	CMC-C2C-C3C	3.80	126.01	116.53
3	C	142	HEM	CAD-C3D-C4D	3.82	125.95	112.47
3	A	142	HEM	CAD-C3D-C4D	3.96	126.44	112.47
3	D	147	HEM	CAD-C3D-C4D	4.02	126.66	112.47
3	D	147	HEM	CMD-C2D-C3D	4.14	132.65	114.35
3	B	147	HEM	CAD-C3D-C4D	4.21	127.33	112.47
3	A	142	HEM	CMB-C2B-C3B	4.39	127.48	116.53
3	B	147	HEM	CMC-C2C-C3C	4.54	127.87	116.53
3	D	147	HEM	CMC-C2C-C3C	4.56	127.92	116.53
3	D	147	HEM	CAD-C3D-C2D	4.74	126.86	113.22
3	A	142	HEM	CMC-C2C-C3C	4.87	128.68	116.53
3	B	147	HEM	CMB-C2B-C3B	5.00	129.01	116.53
3	D	147	HEM	CMB-C2B-C3B	5.01	129.03	116.53
3	B	147	HEM	CAD-C3D-C2D	5.06	127.76	113.22
3	A	142	HEM	CAD-C3D-C2D	5.30	128.45	113.22
3	C	142	HEM	CAD-C3D-C2D	6.25	131.20	113.22
3	C	142	HEM	CMB-C2B-C3B	6.47	132.68	116.53
3	A	142	HEM	CBA-CAA-C2A	6.71	124.56	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	142	HEM	9	0
3	B	147	HEM	7	0
4	B	148	CMO	5	0
3	C	142	HEM	7	0
3	D	147	HEM	7	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 ⓘ

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	141/141 (100%)	-0.10	2 (1%) 78 76	16, 28, 45, 57	2 (1%)
1	C	141/141 (100%)	-0.07	3 (2%) 67 62	20, 34, 46, 59	0
2	B	145/145 (100%)	0.13	3 (2%) 67 62	15, 31, 62, 79	1 (0%)
2	D	145/145 (100%)	0.60	18 (12%) 5 3	19, 43, 74, 94	2 (1%)
All	All	572/572 (100%)	0.14	26 (4%) 37 31	15, 33, 60, 94	5 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	93	CYS	7.3
2	B	93	CYS	4.9
2	D	89	SER	4.4
2	B	2	MET	4.4
2	B	146	HIS	4.1
1	A	141	ARG	4.1
2	D	2	MET	4.0
2	D	146	HIS	3.8
2	D	143	HIS	3.6
1	C	141	ARG	3.5
2	D	145	TYR	3.3
2	D	91	LEU	3.2
2	D	10	ALA	3.2
2	D	129	ASP	3.1
2	D	94	ASP	2.9
1	C	48	LEU	2.8
2	D	144	ARG	2.7
2	D	76	LYS	2.7
2	D	47	ASP	2.6
2	D	11	VAL	2.6
2	D	120	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	7	GLU	2.2
1	C	49	SER	2.1
2	D	88	LEU	2.1
2	D	45	PHE	2.0
1	A	89	HIS	2.0

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
4	CMO	D	148	2/2	0.89	0.46	7.60	17,17,17,18	0
4	CMO	B	148	2/2	0.98	0.31	6.30	13,13,13,15	0
4	CMO	A	143	2/2	0.90	0.30	3.36	7,7,7,10	0
4	CMO	C	143	2/2	0.91	0.27	2.60	11,11,11,15	0
3	HEM	C	142	43/43	0.95	0.20	0.55	3,13,29,40	0
3	HEM	D	147	43/43	0.94	0.26	0.20	16,27,54,59	0
3	HEM	B	147	43/43	0.94	0.20	-0.01	7,15,44,48	0
3	HEM	A	142	43/43	0.96	0.16	-0.57	3,13,29,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.