Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:48 PM GMT

PDB ID	:	1HCO
Title	:	THE STRUCTURE OF HUMAN CARBONMONOXY HAEMOGLOBIN AT 2.7 ANGSTROMS RESOLUTION
Authors	:	Baldwin, J.M.
Deposited on	:	1979-08-07
Resolution	:	2.70 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

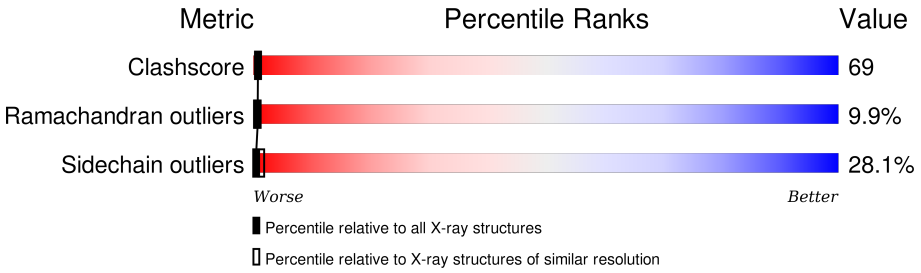
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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 >=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 <=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	32% 36% 26% 6%
2	B	146	19% 32% 34% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2282 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.

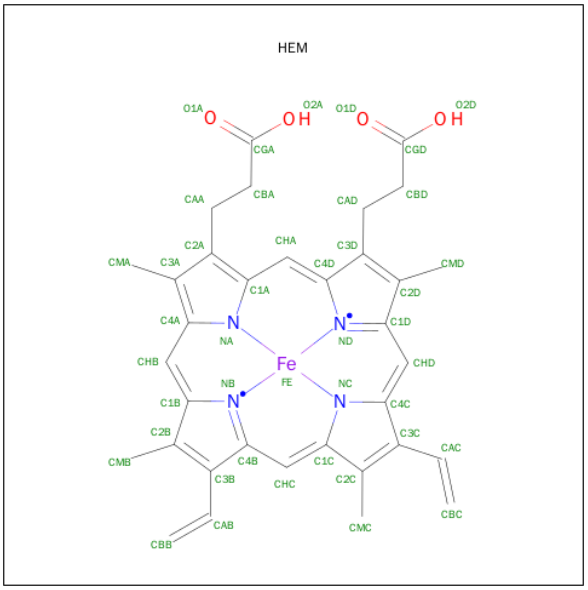
- Molecule 1 is a protein called HEMOGLOBIN (CARBONMONOXY) (ALPHA CHAIN).

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

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

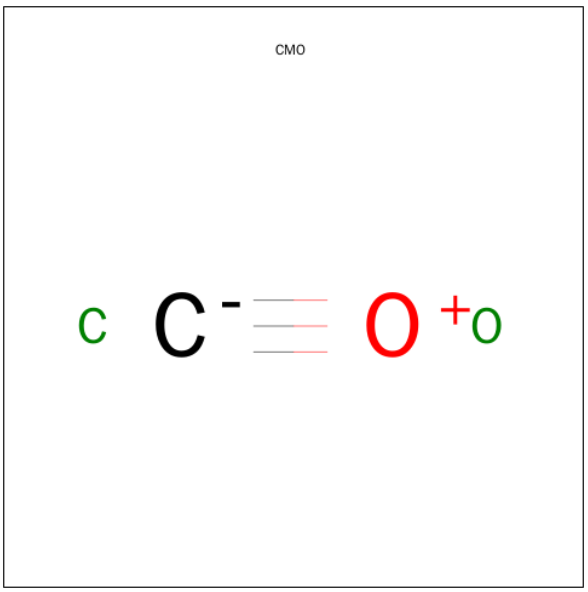
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

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



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

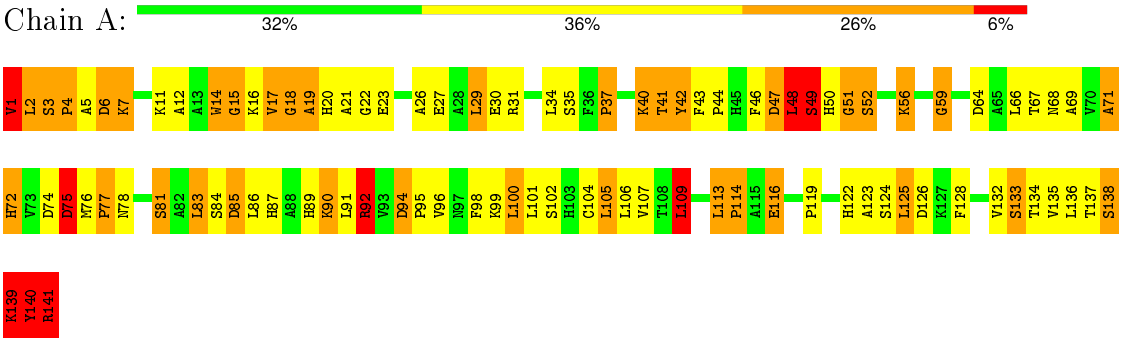
3 Residue-property plots (i)

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 (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.

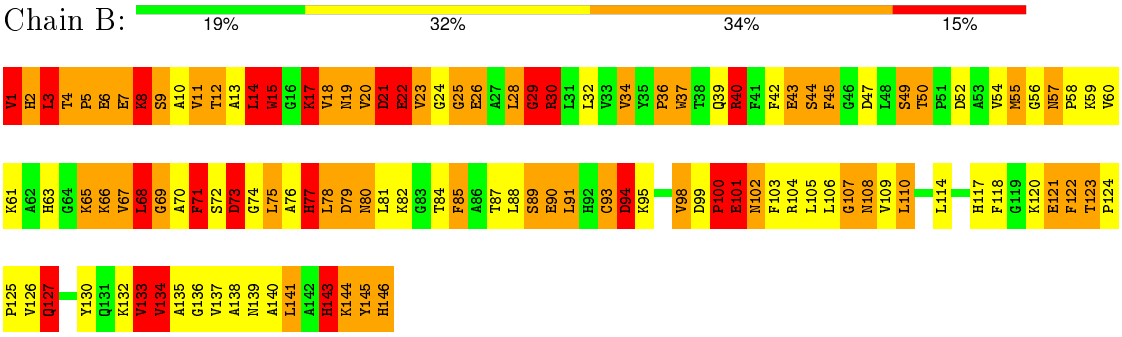
- Molecule 1: HEMOGLOBIN (CARBONMONOXY) (ALPHA CHAIN)

Chain A:



- Molecule 2: HEMOGLOBIN (CARBONMONOXY) (BETA CHAIN)

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	53.70Å 53.70Å 193.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2282	wwPDB-VP
Average B, all atoms (Å^2)	0.0	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: 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	1.43	13/1097 (1.2%)	1.94	55/1491 (3.7%)
2	B	1.16	6/1153 (0.5%)	2.19	87/1566 (5.6%)
All	All	1.30	19/2250 (0.8%)	2.07	142/3057 (4.6%)

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	1	2
2	B	0	2
All	All	1	4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	VAL	CA-CB	-17.51	1.18	1.54
1	A	47	ASP	N-CA	15.23	1.76	1.46
1	A	15	GLY	N-CA	11.07	1.62	1.46
1	A	19	ALA	CA-CB	8.94	1.71	1.52
1	A	49	SER	CA-CB	-7.43	1.41	1.52
1	A	14	TRP	NE1-CE2	-7.29	1.28	1.37
2	B	15	TRP	NE1-CE2	-7.27	1.28	1.37
2	B	37	TRP	NE1-CE2	-7.16	1.28	1.37
1	A	85	ASP	CG-OD2	6.03	1.39	1.25
2	B	26	GLU	CD-OE1	-5.76	1.19	1.25
1	A	27	GLU	CD-OE1	-5.65	1.19	1.25
1	A	23	GLU	CD-OE1	-5.59	1.19	1.25
1	A	138	SER	CA-CB	-5.44	1.44	1.52
2	B	7	GLU	CD-OE1	-5.43	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	ALA	N-CA	5.36	1.57	1.46
2	B	22	GLU	CD-OE1	-5.22	1.20	1.25
2	B	43	GLU	CD-OE1	-5.20	1.20	1.25
1	A	141	ARG	C-OXT	5.17	1.33	1.23
1	A	47	ASP	CA-CB	-5.10	1.42	1.53

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	80	ASN	N-CA-C	-18.45	61.17	111.00
2	B	45	PHE	N-CA-C	17.26	157.60	111.00
1	A	47	ASP	N-CA-C	-16.01	67.78	111.00
2	B	81	LEU	N-CA-C	-15.39	69.43	111.00
2	B	45	PHE	CB-CA-C	-13.82	82.76	110.40
1	A	1	VAL	N-CA-CB	13.78	141.82	111.50
2	B	1	VAL	N-CA-C	11.95	143.26	111.00
2	B	68	LEU	N-CA-C	-11.45	80.08	111.00
1	A	19	ALA	N-CA-CB	-11.27	94.33	110.10
1	A	114	PRO	N-CA-C	10.08	138.30	112.10
2	B	57	ASN	N-CA-C	-10.08	83.79	111.00
1	A	3	SER	N-CA-C	9.91	137.75	111.00
2	B	77	HIS	N-CA-C	-9.88	84.31	111.00
1	A	50	HIS	N-CA-C	9.38	136.34	111.00
2	B	1	VAL	CB-CA-C	-9.38	93.58	111.40
1	A	138	SER	N-CA-C	8.87	134.96	111.00
2	B	36	PRO	N-CA-C	8.85	135.10	112.10
2	B	7	GLU	N-CA-C	-8.70	87.51	111.00
1	A	138	SER	CB-CA-C	-8.60	93.77	110.10
2	B	15	TRP	N-CA-C	8.47	133.88	111.00
1	A	139	LYS	N-CA-C	-8.38	88.37	111.00
2	B	71	PHE	N-CA-C	-8.36	88.44	111.00
1	A	3	SER	CB-CA-C	-8.35	94.23	110.10
1	A	48	LEU	N-CA-C	-8.17	88.94	111.00
2	B	67	VAL	CB-CA-C	-8.05	96.10	111.40
2	B	49	SER	N-CA-C	7.94	132.44	111.00
2	B	80	ASN	CB-CA-C	7.92	126.25	110.40
1	A	6	ASP	CB-CG-OD1	7.91	125.42	118.30
2	B	25	GLY	N-CA-C	7.91	132.86	113.10
2	B	81	LEU	CB-CA-C	7.83	125.08	110.20
1	A	109	LEU	N-CA-C	-7.73	90.13	111.00
2	B	85	PHE	N-CA-C	7.70	131.79	111.00
1	A	1	VAL	CA-CB-CG1	-7.67	99.39	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	75	ASP	CB-CG-OD1	7.60	125.14	118.30
1	A	49	SER	N-CA-CB	7.60	121.89	110.50
2	B	17	LYS	N-CA-C	-7.57	90.57	111.00
2	B	133	VAL	N-CA-C	-7.51	90.73	111.00
2	B	26	GLU	N-CA-C	-7.50	90.75	111.00
2	B	50	THR	N-CA-C	-7.50	90.76	111.00
2	B	73	ASP	CB-CG-OD1	7.47	125.03	118.30
2	B	4	THR	C-N-CD	-7.45	104.22	120.60
1	A	85	ASP	CB-CG-OD1	7.42	124.98	118.30
2	B	122	PHE	N-CA-C	-7.37	91.12	111.00
2	B	68	LEU	CB-CA-C	7.36	124.19	110.20
1	A	94	ASP	CB-CG-OD1	7.33	124.89	118.30
2	B	14	LEU	N-CA-C	-7.29	91.32	111.00
1	A	74	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	113	LEU	N-CA-C	7.09	130.14	111.00
2	B	94	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	126	ASP	CB-CG-OD1	7.06	124.65	118.30
2	B	44	SER	N-CA-C	-7.03	92.01	111.00
2	B	67	VAL	N-CA-C	7.03	129.98	111.00
1	A	47	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	29	LEU	N-CA-C	-6.98	92.16	111.00
2	B	21	ASP	CB-CG-OD1	6.91	124.52	118.30
2	B	52	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	51	GLY	N-CA-C	-6.73	96.28	113.10
2	B	49	SER	CB-CA-C	-6.72	97.33	110.10
1	A	78	ASN	N-CA-C	6.72	129.13	111.00
2	B	100	PRO	CB-CA-C	-6.68	95.31	112.00
1	A	64	ASP	CB-CG-OD1	6.63	124.27	118.30
2	B	79	ASP	CB-CG-OD1	6.62	124.26	118.30
2	B	99	ASP	CB-CG-OD1	6.62	124.26	118.30
2	B	6	GLU	N-CA-C	6.59	128.81	111.00
2	B	47	ASP	CB-CG-OD1	6.54	124.19	118.30
2	B	58	PRO	N-CA-C	-6.50	95.19	112.10
1	A	19	ALA	CB-CA-C	-6.50	100.35	110.10
1	A	23	GLU	OE1-CD-OE2	6.48	131.08	123.30
2	B	6	GLU	CB-CA-C	-6.44	97.53	110.40
1	A	101	LEU	N-CA-C	-6.29	94.01	111.00
2	B	77	HIS	CB-CA-C	6.25	122.90	110.40
2	B	23	VAL	N-CA-C	-6.22	94.20	111.00
2	B	100	PRO	N-CA-C	6.20	128.23	112.10
1	A	37	PRO	CB-CA-C	6.18	127.44	112.00
1	A	6	ASP	N-CA-C	-6.12	94.48	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	102	ASN	N-CA-C	-6.08	94.58	111.00
2	B	15	TRP	CB-CA-C	-6.08	98.25	110.40
1	A	12	ALA	N-CA-CB	-6.02	101.67	110.10
2	B	7	GLU	OE1-CD-OE2	5.99	130.49	123.30
2	B	22	GLU	OE1-CD-OE2	5.98	130.48	123.30
2	B	90	GLU	N-CA-C	-5.98	94.85	111.00
1	A	71	ALA	N-CA-C	-5.96	94.92	111.00
2	B	9	SER	N-CA-C	5.92	126.98	111.00
2	B	101	GLU	OE1-CD-OE2	5.89	130.37	123.30
2	B	6	GLU	OE1-CD-OE2	5.88	130.36	123.30
1	A	113	LEU	CB-CA-C	-5.87	99.05	110.20
2	B	57	ASN	CB-CA-C	5.87	122.13	110.40
2	B	18	VAL	N-CA-C	5.85	126.81	111.00
2	B	13	ALA	N-CA-CB	-5.84	101.92	110.10
2	B	26	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	A	59	GLY	N-CA-C	-5.79	98.63	113.10
1	A	16	LYS	N-CA-C	5.76	126.55	111.00
2	B	93	CYS	N-CA-C	5.76	126.54	111.00
2	B	43	GLU	OE1-CD-OE2	5.75	130.21	123.30
2	B	123	THR	N-CA-C	-5.73	95.54	111.00
1	A	116	GLU	OE1-CD-OE2	5.70	130.14	123.30
1	A	50	HIS	CB-CA-C	-5.70	99.01	110.40
1	A	16	LYS	CB-CA-C	-5.68	99.03	110.40
1	A	47	ASP	CA-CB-CG	-5.67	100.92	113.40
2	B	9	SER	CB-CA-C	-5.62	99.42	110.10
1	A	27	GLU	OE1-CD-OE2	5.61	130.03	123.30
1	A	30	GLU	OE1-CD-OE2	5.61	130.03	123.30
2	B	143	HIS	N-CA-C	5.60	126.11	111.00
2	B	13	ALA	N-CA-C	5.59	126.09	111.00
2	B	85	PHE	CB-CA-C	-5.55	99.29	110.40
2	B	70	ALA	N-CA-C	5.53	125.92	111.00
1	A	47	ASP	N-CA-CB	-5.52	100.66	110.60
1	A	85	ASP	N-CA-C	-5.52	96.10	111.00
2	B	107	GLY	N-CA-C	-5.51	99.32	113.10
1	A	48	LEU	CB-CA-C	5.49	120.64	110.20
2	B	98	VAL	N-CA-C	-5.46	96.27	111.00
2	B	121	GLU	OE1-CD-OE2	5.45	129.84	123.30
2	B	29	GLY	N-CA-C	-5.45	99.48	113.10
2	B	18	VAL	CB-CA-C	-5.44	101.06	111.40
1	A	100	LEU	N-CA-C	5.43	125.66	111.00
2	B	71	PHE	CB-CA-C	5.33	121.06	110.40
1	A	23	GLU	CG-CD-OE2	-5.32	107.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	26	GLU	CG-CD-OE2	-5.31	107.68	118.30
2	B	122	PHE	CB-CA-C	5.29	120.98	110.40
1	A	47	ASP	CB-CA-C	5.28	120.96	110.40
2	B	90	GLU	OE1-CD-OE2	5.28	129.63	123.30
1	A	15	GLY	N-CA-C	-5.27	99.91	113.10
1	A	78	ASN	CB-CA-C	-5.27	99.86	110.40
2	B	30	ARG	N-CA-C	5.26	125.21	111.00
1	A	81	SER	N-CA-C	5.25	125.17	111.00
1	A	30	GLU	CG-CD-OE2	-5.23	107.83	118.30
2	B	127	GLN	N-CA-C	-5.21	96.92	111.00
2	B	22	GLU	CG-CD-OE2	-5.18	107.93	118.30
2	B	84	THR	N-CA-C	-5.16	97.06	111.00
1	A	42	TYR	CB-CG-CD1	-5.16	117.90	121.00
2	B	145	TYR	N-CA-C	-5.15	97.09	111.00
2	B	7	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	A	140	TYR	CB-CG-CD1	-5.13	117.92	121.00
2	B	134	VAL	N-CA-C	5.13	124.85	111.00
2	B	47	ASP	N-CA-C	-5.10	97.24	111.00
2	B	6	GLU	CG-CD-OE2	-5.08	108.14	118.30
1	A	27	GLU	CG-CD-OE2	-5.08	108.15	118.30
2	B	117	HIS	N-CA-C	5.06	124.67	111.00
2	B	145	TYR	CB-CG-CD1	-5.04	117.98	121.00
2	B	10	ALA	N-CA-C	-5.02	97.45	111.00
2	B	43	GLU	CG-CD-OE2	-5.02	108.26	118.30
2	B	90	GLU	CG-CD-OE2	-5.01	108.28	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	VAL	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Sidechain
1	A	92	ARG	Sidechain
2	B	30	ARG	Sidechain
2	B	40	ARG	Sidechain

5.2 Too-close contacts (i)

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	1069	0	1070	123	5
2	B	1123	0	1118	186	2
3	A	43	0	30	9	0
3	B	43	0	30	13	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	2282	0	2248	311	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 69.

All (311) 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:14:LEU:HD21	2:B:118:PHE:CD1	1.43	1.50
1:A:47:ASP:N	1:A:47:ASP:CA	1.76	1.49
2:B:14:LEU:CD2	2:B:118:PHE:CE1	1.99	1.43
1:A:1:VAL:CG2	1:A:2:LEU:H	1.26	1.42
2:B:21:ASP:OD1	2:B:65:LYS:CD	1.72	1.37
1:A:137:THR:O	1:A:140:TYR:HB2	1.21	1.30
2:B:30:ARG:O	2:B:34:VAL:HG23	1.16	1.30
1:A:47:ASP:C	1:A:47:ASP:N	1.84	1.30
2:B:1:VAL:CG1	2:B:78:LEU:O	1.82	1.26
2:B:21:ASP:OD1	2:B:65:LYS:CG	1.83	1.26
1:A:18:GLY:O	1:A:20:HIS:N	1.71	1.22
2:B:1:VAL:HG23	2:B:2:HIS:N	1.27	1.21
2:B:1:VAL:HG11	2:B:78:LEU:O	1.04	1.20
2:B:14:LEU:HD21	2:B:118:PHE:CE1	1.69	1.19
2:B:14:LEU:HD22	2:B:118:PHE:CE1	1.78	1.18
2:B:21:ASP:OD1	2:B:65:LYS:HD2	1.39	1.17
1:A:140:TYR:O	1:A:141:ARG:O	1.59	1.17
1:A:1:VAL:CG2	1:A:2:LEU:N	1.88	1.14
2:B:30:ARG:O	2:B:34:VAL:CG2	1.94	1.14
2:B:20:VAL:HG22	2:B:21:ASP:H	1.07	1.14
2:B:130:TYR:O	2:B:134:VAL:HG23	1.44	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:VAL:CG2	2:B:2:HIS:N	2.02	1.12
1:A:17:VAL:CG2	1:A:113:LEU:HD11	1.80	1.12
1:A:92:ARG:HH11	1:A:92:ARG:HG3	1.12	1.10
1:A:1:VAL:HG23	1:A:2:LEU:N	1.63	1.09
1:A:83:LEU:HD11	3:A:200:HEM:HBA2	1.31	1.08
1:A:3:SER:CB	1:A:4:PRO:HD2	1.79	1.08
1:A:141:ARG:HG2	1:A:141:ARG:HH11	0.91	1.07
2:B:14:LEU:CD2	2:B:118:PHE:CD1	2.30	1.07
2:B:21:ASP:OD1	2:B:65:LYS:HG3	1.53	1.06
2:B:20:VAL:CG2	2:B:21:ASP:N	2.18	1.05
2:B:2:HIS:O	2:B:3:LEU:O	1.73	1.04
2:B:106:LEU:O	2:B:106:LEU:HD12	1.57	1.03
1:A:1:VAL:HG22	1:A:2:LEU:N	1.58	1.02
2:B:20:VAL:HG22	2:B:21:ASP:N	1.66	1.02
1:A:42:TYR:C	1:A:44:PRO:HD3	1.81	1.01
1:A:7:LYS:O	1:A:11:LYS:HG3	1.60	1.00
1:A:3:SER:HB2	1:A:4:PRO:HD2	1.01	1.00
1:A:17:VAL:HG23	1:A:113:LEU:HD11	1.41	1.00
2:B:101:GLU:HG3	2:B:101:GLU:O	1.60	0.99
1:A:141:ARG:HG2	1:A:141:ARG:NH1	1.69	0.99
1:A:14:TRP:HE1	1:A:67:THR:HG1	1.04	0.99
1:A:71:ALA:O	1:A:72:HIS:HB2	1.60	0.98
3:A:200:HEM:HHD	3:A:200:HEM:HBC2	1.45	0.98
2:B:24:GLY:HA2	2:B:68:LEU:HG	1.43	0.97
1:A:141:ARG:CG	1:A:141:ARG:HH11	1.77	0.96
2:B:37:TRP:HE1	2:B:102:ASN:HD21	0.98	0.96
1:A:1:VAL:HG22	1:A:2:LEU:H	0.80	0.95
1:A:3:SER:HB2	1:A:4:PRO:CD	1.95	0.94
2:B:19:ASN:O	2:B:19:ASN:OD1	1.85	0.93
2:B:1:VAL:HG23	2:B:2:HIS:H	1.24	0.93
2:B:42:PHE:O	2:B:45:PHE:HB2	1.69	0.92
1:A:47:ASP:O	1:A:47:ASP:N	2.04	0.90
2:B:130:TYR:O	2:B:134:VAL:CG2	2.20	0.90
2:B:74:GLY:O	2:B:76:ALA:N	2.06	0.89
2:B:14:LEU:CD2	2:B:118:PHE:CZ	2.56	0.88
2:B:15:TRP:CD2	2:B:75:LEU:HD22	2.09	0.87
2:B:67:VAL:CG1	2:B:67:VAL:O	2.24	0.86
2:B:15:TRP:CG	2:B:75:LEU:CD2	2.58	0.86
2:B:105:LEU:O	2:B:109:VAL:CG1	2.24	0.85
2:B:37:TRP:HE1	2:B:102:ASN:ND2	1.75	0.85
2:B:57:ASN:OD1	2:B:59:LYS:HB2	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLY:C	1:A:20:HIS:H	1.80	0.84
2:B:133:VAL:O	2:B:136:GLY:N	2.09	0.84
2:B:15:TRP:CE2	2:B:75:LEU:HD22	2.14	0.83
1:A:139:LYS:O	1:A:139:LYS:HD2	1.79	0.83
2:B:143:HIS:CD2	2:B:143:HIS:O	2.32	0.82
1:A:85:ASP:O	1:A:89:HIS:HB2	1.79	0.82
2:B:66:LYS:O	2:B:69:GLY:HA3	1.78	0.82
2:B:18:VAL:O	2:B:18:VAL:HG12	1.79	0.82
2:B:93:CYS:SG	2:B:145:TYR:CE2	2.72	0.82
2:B:105:LEU:O	2:B:109:VAL:HG13	1.80	0.82
2:B:15:TRP:O	2:B:18:VAL:HB	1.79	0.82
3:B:200:HEM:HMA2	3:B:200:HEM:HBA1	1.59	0.82
2:B:24:GLY:CA	2:B:68:LEU:HG	2.08	0.82
2:B:4:THR:O	2:B:5:PRO:C	2.16	0.82
1:A:137:THR:O	1:A:140:TYR:CB	2.17	0.81
2:B:1:VAL:HG23	2:B:2:HIS:CA	2.11	0.80
1:A:92:ARG:HG3	1:A:92:ARG:NH1	1.88	0.79
2:B:67:VAL:HG12	2:B:67:VAL:O	1.81	0.79
1:A:140:TYR:C	1:A:141:ARG:O	2.20	0.79
1:A:139:LYS:CD	1:A:139:LYS:O	2.31	0.78
1:A:47:ASP:N	1:A:47:ASP:CB	2.46	0.78
2:B:98:VAL:O	2:B:145:TYR:OH	2.01	0.78
2:B:110:LEU:O	2:B:110:LEU:HD22	1.84	0.78
2:B:30:ARG:HD2	2:B:55:MET:HE1	1.65	0.78
1:A:85:ASP:OD2	1:A:89:HIS:HD2	1.66	0.77
2:B:14:LEU:HD21	2:B:118:PHE:CG	2.18	0.77
2:B:137:VAL:O	2:B:141:LEU:HD12	1.85	0.77
2:B:26:GLU:O	2:B:30:ARG:HD3	1.85	0.77
1:A:76:MET:N	1:A:77:PRO:CD	2.47	0.77
2:B:74:GLY:C	2:B:76:ALA:H	1.88	0.77
1:A:47:ASP:OD1	1:A:49:SER:HB3	1.86	0.76
2:B:143:HIS:CG	2:B:143:HIS:O	2.39	0.75
2:B:123:THR:OG1	2:B:126:VAL:HG23	1.87	0.75
1:A:100:LEU:O	1:A:104:CYS:SG	2.45	0.73
2:B:15:TRP:CD2	2:B:75:LEU:CD2	2.72	0.73
2:B:91:LEU:O	2:B:91:LEU:HD22	1.89	0.73
1:A:75:ASP:O	1:A:75:ASP:OD1	2.08	0.72
1:A:85:ASP:OD2	1:A:89:HIS:CD2	2.43	0.71
2:B:77:HIS:O	2:B:80:ASN:O	2.08	0.71
2:B:69:GLY:O	2:B:72:SER:HB2	1.90	0.71
1:A:43:PHE:N	1:A:44:PRO:HD3	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ARG:NH2	2:B:139:ASN:OD1	2.24	0.70
2:B:21:ASP:OD1	2:B:65:LYS:CE	2.39	0.70
1:A:90:LYS:HG2	1:A:91:LEU:HG	1.71	0.70
2:B:91:LEU:O	2:B:95:LYS:HB2	1.92	0.70
1:A:47:ASP:C	1:A:49:SER:H	1.93	0.70
2:B:89:SER:HB2	2:B:141:LEU:O	1.92	0.70
2:B:54:VAL:O	2:B:56:GLY:N	2.24	0.69
1:A:89:HIS:CE1	1:A:139:LYS:HE3	2.26	0.69
2:B:14:LEU:HD23	2:B:118:PHE:CZ	2.28	0.69
2:B:20:VAL:CG2	2:B:65:LYS:HE2	2.23	0.69
1:A:3:SER:CB	1:A:4:PRO:CD	2.60	0.69
2:B:90:GLU:O	2:B:94:ASP:OD1	2.10	0.69
2:B:124:PRO:N	2:B:125:PRO:HD2	2.08	0.68
1:A:46:PHE:HB3	1:A:48:LEU:HD13	1.75	0.68
2:B:45:PHE:CE1	2:B:59:LYS:O	2.47	0.68
2:B:74:GLY:C	2:B:76:ALA:N	2.43	0.68
1:A:132:VAL:O	1:A:136:LEU:HG	1.94	0.68
2:B:105:LEU:O	2:B:109:VAL:HG12	1.94	0.68
2:B:137:VAL:O	2:B:141:LEU:CD1	2.41	0.67
2:B:107:GLY:HA3	2:B:134:VAL:HG13	1.76	0.67
2:B:122:PHE:CE2	2:B:127:GLN:HB2	2.29	0.67
1:A:42:TYR:O	1:A:44:PRO:HD3	1.93	0.67
2:B:11:VAL:HG12	2:B:12:THR:N	2.08	0.67
1:A:76:MET:O	1:A:77:PRO:C	2.32	0.66
2:B:110:LEU:CD2	2:B:110:LEU:O	2.43	0.66
2:B:26:GLU:OE1	2:B:30:ARG:NE	2.28	0.66
2:B:18:VAL:O	2:B:18:VAL:CG1	2.44	0.65
2:B:19:ASN:CG	2:B:19:ASN:O	2.34	0.65
3:B:200:HEM:HBB2	3:B:200:HEM:CMB	2.27	0.65
2:B:20:VAL:HA	2:B:68:LEU:HD12	1.78	0.65
2:B:104:ARG:O	2:B:108:ASN:HB2	1.97	0.65
2:B:4:THR:O	2:B:6:GLU:N	2.29	0.65
1:A:122:HIS:ND1	2:B:30:ARG:NH1	2.44	0.64
2:B:14:LEU:HD22	2:B:118:PHE:HE1	1.56	0.64
2:B:2:HIS:C	2:B:3:LEU:O	2.36	0.64
1:A:92:ARG:HH11	1:A:92:ARG:CG	2.01	0.64
2:B:19:ASN:HD21	2:B:22:GLU:HG3	1.64	0.63
1:A:17:VAL:O	1:A:18:GLY:O	2.15	0.63
2:B:23:VAL:O	2:B:24:GLY:C	2.37	0.63
1:A:76:MET:N	1:A:77:PRO:HD2	2.14	0.63
2:B:14:LEU:O	2:B:17:LYS:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASP:O	1:A:75:ASP:CG	2.37	0.63
1:A:106:LEU:HD21	1:A:125:LEU:HB3	1.81	0.63
3:A:200:HEM:HMA1	3:A:200:HEM:HBA1	1.81	0.62
1:A:122:HIS:O	1:A:122:HIS:HD2	1.82	0.62
2:B:15:TRP:CD1	2:B:75:LEU:CD2	2.82	0.62
1:A:71:ALA:O	1:A:72:HIS:CB	2.38	0.62
2:B:100:PRO:O	2:B:103:PHE:HB2	1.99	0.62
2:B:91:LEU:HD22	2:B:91:LEU:C	2.20	0.61
1:A:37:PRO:O	1:A:40:LYS:HG3	2.01	0.61
2:B:54:VAL:C	2:B:56:GLY:H	2.05	0.61
2:B:43:GLU:C	2:B:45:PHE:N	2.50	0.60
1:A:51:GLY:O	1:A:52:SER:C	2.39	0.60
1:A:17:VAL:HG23	1:A:113:LEU:CD1	2.23	0.60
2:B:124:PRO:N	2:B:125:PRO:CD	2.64	0.60
1:A:139:LYS:C	1:A:139:LYS:HD2	2.22	0.60
1:A:76:MET:O	1:A:77:PRO:O	2.20	0.59
1:A:68:ASN:O	1:A:72:HIS:HB2	2.03	0.59
1:A:122:HIS:O	1:A:122:HIS:CD2	2.56	0.59
2:B:57:ASN:HB3	2:B:60:VAL:HB	1.85	0.59
2:B:63:HIS:CE1	3:B:200:HEM:CHA	2.86	0.59
2:B:4:THR:HB	2:B:5:PRO:HD2	1.85	0.58
3:B:200:HEM:HBB2	3:B:200:HEM:HMB1	1.87	0.57
1:A:139:LYS:CD	1:A:139:LYS:C	2.73	0.57
1:A:85:ASP:O	1:A:89:HIS:N	2.34	0.57
2:B:146:HIS:N	2:B:146:HIS:ND1	2.50	0.57
1:A:139:LYS:O	1:A:139:LYS:HD3	2.02	0.57
2:B:11:VAL:CG1	2:B:12:THR:N	2.66	0.57
1:A:133:SER:O	1:A:137:THR:HG23	2.05	0.57
1:A:7:LYS:CG	1:A:7:LYS:O	2.53	0.57
1:A:51:GLY:O	1:A:52:SER:O	2.23	0.56
2:B:4:THR:CB	2:B:5:PRO:HD2	2.34	0.56
2:B:19:ASN:ND2	2:B:22:GLU:HG3	2.19	0.56
2:B:30:ARG:HD2	2:B:55:MET:CE	2.34	0.56
2:B:89:SER:O	2:B:93:CYS:HB2	2.04	0.56
2:B:20:VAL:HG23	2:B:21:ASP:N	2.14	0.56
2:B:7:GLU:O	2:B:9:SER:N	2.39	0.55
2:B:42:PHE:HE1	3:B:200:HEM:HBC2	1.71	0.55
1:A:98:PHE:HB3	1:A:133:SER:HB3	1.88	0.55
2:B:123:THR:OG1	2:B:126:VAL:CG2	2.55	0.55
1:A:86:LEU:HD12	1:A:90:LYS:HG2	1.89	0.55
2:B:4:THR:O	2:B:7:GLU:N	2.29	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:TRP:CG	2:B:75:LEU:HD22	2.34	0.55
2:B:110:LEU:C	2:B:110:LEU:HD22	2.28	0.55
2:B:106:LEU:C	2:B:106:LEU:HD12	2.24	0.54
1:A:76:MET:HE1	1:A:128:PHE:CE1	2.42	0.54
2:B:88:LEU:O	2:B:91:LEU:HB3	2.06	0.54
2:B:19:ASN:C	2:B:19:ASN:OD1	2.46	0.54
2:B:45:PHE:CZ	2:B:59:LYS:O	2.61	0.54
1:A:76:MET:CE	1:A:128:PHE:CE1	2.91	0.54
2:B:77:HIS:C	2:B:79:ASP:H	2.12	0.53
2:B:7:GLU:O	2:B:8:LYS:C	2.47	0.53
1:A:123:ALA:HA	2:B:34:VAL:HG13	1.90	0.53
2:B:15:TRP:CD1	2:B:75:LEU:HD23	2.43	0.53
1:A:49:SER:O	1:A:52:SER:HB2	2.08	0.53
2:B:85:PHE:HD1	2:B:140:ALA:HB1	1.75	0.52
1:A:42:TYR:CD2	3:A:200:HEM:HBC1	2.45	0.52
1:A:46:PHE:C	1:A:47:ASP:CA	2.68	0.52
1:A:87:HIS:HE1	3:A:200:HEM:NA	2.08	0.52
2:B:138:ALA:HA	2:B:141:LEU:HD12	1.91	0.52
1:A:119:PRO:CG	2:B:55:MET:CE	2.88	0.52
3:A:200:HEM:CBA	3:A:200:HEM:CMA	2.87	0.52
2:B:110:LEU:C	2:B:110:LEU:CD2	2.79	0.52
1:A:76:MET:HB3	1:A:135:VAL:HG21	1.90	0.51
2:B:106:LEU:HD23	3:B:200:HEM:CHC	2.41	0.51
1:A:31:ARG:HG2	2:B:124:PRO:HB3	1.92	0.51
1:A:17:VAL:HG22	1:A:113:LEU:HD11	1.86	0.51
1:A:90:LYS:HG3	1:A:90:LYS:O	2.04	0.51
1:A:3:SER:O	1:A:5:ALA:N	2.44	0.50
1:A:119:PRO:CB	2:B:55:MET:HE2	2.41	0.50
3:B:200:HEM:HMB1	3:B:200:HEM:CBB	2.41	0.50
2:B:20:VAL:HG21	2:B:65:LYS:HE2	1.92	0.50
1:A:119:PRO:CG	2:B:55:MET:HE2	2.42	0.50
2:B:135:ALA:O	2:B:139:ASN:ND2	2.44	0.50
3:A:200:HEM:CMA	3:A:200:HEM:HBA1	2.41	0.50
2:B:122:PHE:C	2:B:123:THR:O	2.39	0.50
2:B:43:GLU:C	2:B:45:PHE:H	2.11	0.50
2:B:91:LEU:CD2	2:B:91:LEU:C	2.80	0.50
3:A:200:HEM:CBC	3:A:200:HEM:HHD	2.29	0.49
2:B:73:ASP:O	2:B:77:HIS:HB2	2.12	0.49
2:B:40:ARG:HH11	2:B:40:ARG:HG2	1.76	0.49
2:B:106:LEU:CD1	2:B:106:LEU:O	2.47	0.49
1:A:141:ARG:CG	1:A:141:ARG:NH1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:PRO:O	2:B:39:GLN:HB2	2.11	0.49
2:B:42:PHE:CE1	3:B:200:HEM:HBC2	2.47	0.49
2:B:66:LYS:O	2:B:69:GLY:CA	2.57	0.48
1:A:85:ASP:O	1:A:89:HIS:CB	2.58	0.48
1:A:98:PHE:CE1	1:A:136:LEU:CD1	2.97	0.48
1:A:98:PHE:HE1	1:A:136:LEU:HD13	1.78	0.48
2:B:101:GLU:O	2:B:105:LEU:HG	2.14	0.48
2:B:63:HIS:HE1	3:B:200:HEM:CHA	2.27	0.48
2:B:132:LYS:O	2:B:133:VAL:O	2.30	0.48
2:B:89:SER:HB2	2:B:141:LEU:HA	1.95	0.47
1:A:43:PHE:N	1:A:44:PRO:CD	2.77	0.47
2:B:5:PRO:HG2	2:B:6:GLU:H	1.79	0.47
1:A:119:PRO:HB3	2:B:55:MET:HE2	1.97	0.47
2:B:29:GLY:HA3	2:B:55:MET:SD	2.55	0.47
2:B:23:VAL:HG12	2:B:68:LEU:HD11	1.97	0.47
1:A:89:HIS:CE1	1:A:139:LYS:CE	2.96	0.47
2:B:15:TRP:CD1	2:B:75:LEU:HD22	2.49	0.46
1:A:84:SER:OG	1:A:135:VAL:O	2.27	0.46
1:A:56:LYS:HB2	1:A:56:LYS:HE3	1.29	0.46
2:B:40:ARG:CG	2:B:40:ARG:NH1	2.78	0.46
2:B:28:LEU:O	2:B:29:GLY:O	2.33	0.46
2:B:107:GLY:HA3	2:B:134:VAL:CG1	2.45	0.46
1:A:66:LEU:HD11	1:A:105:LEU:HD21	1.98	0.46
2:B:102:ASN:O	3:B:200:HEM:CMC	2.64	0.46
2:B:67:VAL:HG13	2:B:67:VAL:O	2.15	0.46
1:A:105:LEU:HA	1:A:105:LEU:HD12	1.75	0.46
1:A:87:HIS:HE1	3:A:200:HEM:C4A	2.33	0.46
2:B:26:GLU:OE1	2:B:30:ARG:NH2	2.47	0.46
1:A:14:TRP:O	1:A:15:GLY:C	2.54	0.45
2:B:4:THR:OG1	2:B:7:GLU:HG3	2.16	0.45
1:A:83:LEU:HA	1:A:83:LEU:HD13	1.79	0.45
1:A:140:TYR:O	1:A:141:ARG:C	2.41	0.45
1:A:47:ASP:CG	1:A:49:SER:HB3	2.36	0.45
2:B:74:GLY:O	2:B:75:LEU:C	2.55	0.45
2:B:30:ARG:CD	2:B:55:MET:HE1	2.43	0.45
2:B:15:TRP:CG	2:B:75:LEU:HD21	2.47	0.45
2:B:144:LYS:HD3	2:B:144:LYS:HA	1.33	0.45
2:B:21:ASP:HA	2:B:65:LYS:HG2	1.98	0.45
2:B:19:ASN:O	2:B:20:VAL:C	2.54	0.45
3:B:200:HEM:HHA	3:B:200:HEM:CBD	2.47	0.45
2:B:15:TRP:CG	2:B:75:LEU:HD23	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:200:HEM:CMB	3:B:200:HEM:CBB	2.92	0.44
1:A:99:LYS:O	1:A:102:SER:HB2	2.17	0.44
1:A:98:PHE:CE1	1:A:136:LEU:HD12	2.52	0.44
1:A:48:LEU:HA	1:A:48:LEU:HD12	1.71	0.44
2:B:71:PHE:CE1	3:B:200:HEM:CBB	3.01	0.44
1:A:26:ALA:HB2	1:A:59:GLY:HA3	1.99	0.44
2:B:77:HIS:O	2:B:79:ASP:N	2.50	0.44
2:B:95:LYS:HA	2:B:95:LYS:HD3	1.76	0.43
1:A:20:HIS:O	1:A:22:GLY:N	2.52	0.43
2:B:1:VAL:O	2:B:2:HIS:HB2	2.18	0.43
2:B:126:VAL:O	2:B:126:VAL:HG12	2.19	0.43
2:B:76:ALA:O	2:B:77:HIS:HB2	2.18	0.43
1:A:46:PHE:CB	1:A:48:LEU:HD13	2.44	0.43
2:B:91:LEU:O	2:B:91:LEU:CD2	2.64	0.43
1:A:6:ASP:OD1	1:A:124:SER:OG	2.21	0.43
2:B:93:CYS:SG	2:B:145:TYR:CD2	3.10	0.43
2:B:54:VAL:O	2:B:57:ASN:N	2.52	0.42
1:A:76:MET:CE	1:A:128:PHE:HE1	2.30	0.42
2:B:79:ASP:O	2:B:79:ASP:OD2	2.37	0.42
1:A:69:ALA:HB1	1:A:76:MET:CE	2.50	0.42
2:B:28:LEU:O	2:B:29:GLY:C	2.58	0.42
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.94	0.42
2:B:28:LEU:O	2:B:32:LEU:HG	2.19	0.42
1:A:119:PRO:HG2	2:B:55:MET:CE	2.49	0.42
1:A:87:HIS:HA	1:A:91:LEU:HD12	2.01	0.42
2:B:77:HIS:C	2:B:79:ASP:N	2.72	0.42
2:B:23:VAL:O	2:B:25:GLY:N	2.53	0.41
2:B:24:GLY:N	2:B:68:LEU:HG	2.34	0.41
2:B:110:LEU:HD22	2:B:114:LEU:HG	2.02	0.41
1:A:109:LEU:HA	1:A:109:LEU:HD12	1.86	0.41
1:A:51:GLY:O	1:A:56:LYS:CE	2.69	0.41
1:A:66:LEU:O	1:A:69:ALA:HB3	2.20	0.41
2:B:54:VAL:C	2:B:56:GLY:N	2.68	0.41
1:A:92:ARG:HA	1:A:140:TYR:OH	2.20	0.41
2:B:11:VAL:HG12	2:B:12:THR:H	1.82	0.41
1:A:29:LEU:HD23	1:A:29:LEU:HA	1.95	0.41
2:B:4:THR:C	2:B:6:GLU:N	2.73	0.40
2:B:68:LEU:HD22	2:B:68:LEU:HA	1.84	0.40
1:A:119:PRO:HG2	2:B:55:MET:HE3	2.02	0.40
2:B:127:GLN:O	2:B:130:TYR:N	2.46	0.40
1:A:69:ALA:HB1	1:A:76:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASP:HA	1:A:95:PRO:HD2	1.87	0.40
2:B:21:ASP:HA	2:B:65:LYS:CG	2.51	0.40
1:A:43:PHE:HB3	1:A:46:PHE:HB2	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:47:ASP:OD2	1:A:68:ASN:ND2[5_645]	1.23	0.97
1:A:47:ASP:CG	1:A:68:ASN:ND2[5_645]	1.71	0.49
1:A:92:ARG:NH2	2:B:39:GLN:OE1[7_555]	1.75	0.45
1:A:94:ASP:OD2	2:B:102:ASN:OD1[7_555]	2.04	0.16
1:A:47:ASP:OD1	1:A:68:ASN:ND2[5_645]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	120 (86%)	9 (6%)	10 (7%)	1	1
2	B	144/146 (99%)	108 (75%)	18 (12%)	18 (12%)	0	0
All	All	283/287 (99%)	228 (81%)	27 (10%)	28 (10%)	1	0

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY
1	A	19	ALA
1	A	52	SER
1	A	77	PRO
2	B	3	LEU
2	B	20	VAL

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Mol	Chain	Res	Type
2	B	55	MET
2	B	75	LEU
2	B	77	HIS
2	B	134	VAL
2	B	143	HIS
1	A	4	PRO
1	A	21	ALA
1	A	140	TYR
2	B	2	HIS
2	B	8	LYS
2	B	15	TRP
2	B	21	ASP
2	B	30	ARG
2	B	133	VAL
1	A	72	HIS
2	B	5	PRO
2	B	78	LEU
1	A	41	THR
1	A	75	ASP
2	B	19	ASN
2	B	29	GLY
2	B	69	GLY

5.3.2 Protein sidechains (i)

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%)	85 (75%)	28 (25%)	1 2
2	B	118/118 (100%)	81 (69%)	37 (31%)	0 0
All	All	231/231 (100%)	166 (72%)	65 (28%)	0 1

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL

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Mol	Chain	Res	Type
1	A	2	LEU
1	A	7	LYS
1	A	17	VAL
1	A	34	LEU
1	A	35	SER
1	A	40	LYS
1	A	41	THR
1	A	48	LEU
1	A	49	SER
1	A	56	LYS
1	A	75	ASP
1	A	81	SER
1	A	83	LEU
1	A	90	LYS
1	A	92	ARG
1	A	96	VAL
1	A	105	LEU
1	A	107	VAL
1	A	109	LEU
1	A	114	PRO
1	A	116	GLU
1	A	125	LEU
1	A	133	SER
1	A	134	THR
1	A	138	SER
1	A	139	LYS
1	A	141	ARG
2	B	1	VAL
2	B	3	LEU
2	B	8	LYS
2	B	11	VAL
2	B	12	THR
2	B	14	LEU
2	B	17	LYS
2	B	21	ASP
2	B	22	GLU
2	B	28	LEU
2	B	30	ARG
2	B	34	VAL
2	B	40	ARG
2	B	44	SER
2	B	49	SER

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Mol	Chain	Res	Type
2	B	50	THR
2	B	61	LYS
2	B	65	LYS
2	B	66	LYS
2	B	68	LEU
2	B	71	PHE
2	B	73	ASP
2	B	82	LYS
2	B	87	THR
2	B	89	SER
2	B	91	LEU
2	B	94	ASP
2	B	100	PRO
2	B	101	GLU
2	B	108	ASN
2	B	110	LEU
2	B	120	LYS
2	B	121	GLU
2	B	127	GLN
2	B	141	LEU
2	B	144	LYS
2	B	146	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	89	HIS
1	A	97	ASN
2	B	102	ASN
2	B	108	ASN
2	B	143	HIS

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	$\#\|Z\| > 2$
3	HEM	A	200	1	30,50,50	2.32	6 (20%)	24,82,82	2.18	8 (33%)
4	CMO	A	201	-	0,1,1	0.00	-	0,0,0	0.00	-
3	HEM	B	200	2	30,50,50	2.32	6 (20%)	24,82,82	2.22	10 (41%)
4	CMO	B	201	-	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	200	1	-	0/10/54/54	0/0/8/8
4	CMO	A	201	-	-	0/0/0/0	0/0/0/0
3	HEM	B	200	2	-	0/10/54/54	0/0/8/8
4	CMO	B	201	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	200	HEM	C3B-C4B	-7.36	1.45	1.51
3	A	200	HEM	C3B-C4B	-7.33	1.45	1.51
3	B	200	HEM	C2D-C3D	-7.05	1.33	1.54
3	A	200	HEM	C2D-C3D	-6.77	1.34	1.54
3	A	200	HEM	C3D-C4D	-4.32	1.46	1.51
3	B	200	HEM	C3D-C4D	-3.92	1.46	1.51
3	A	200	HEM	C2C-C1C	-3.61	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	200	HEM	C2C-C1C	-3.56	1.45	1.52
3	B	200	HEM	C2B-C1B	-2.00	1.45	1.51
3	A	200	HEM	C4C-NC	2.40	1.39	1.36
3	B	200	HEM	C1C-NC	2.67	1.39	1.36
3	A	200	HEM	C1C-NC	2.68	1.39	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	200	HEM	CAA-CBA-CGA	-2.82	107.58	112.75
3	B	200	HEM	C3C-CAC-CBC	-2.80	120.16	124.46
3	A	200	HEM	C3C-CAC-CBC	-2.73	120.27	124.46
3	A	200	HEM	C3B-CAB-CBB	-2.62	120.43	124.46
3	B	200	HEM	CBA-CAA-C2A	-2.56	107.94	112.53
3	B	200	HEM	C3B-CAB-CBB	-2.49	120.64	124.46
3	B	200	HEM	CMD-C2D-C3D	2.55	125.63	114.35
3	A	200	HEM	CMD-C2D-C3D	2.56	125.69	114.35
3	B	200	HEM	C2D-C3D-C4D	3.42	107.30	101.50
3	A	200	HEM	C2D-C3D-C4D	3.48	107.40	101.50
3	B	200	HEM	CMB-C2B-C3B	3.57	125.44	116.53
3	A	200	HEM	CMC-C2C-C3C	3.64	125.63	116.53
3	A	200	HEM	CMB-C2B-C3B	3.67	125.69	116.53
3	B	200	HEM	CMC-C2C-C3C	3.68	125.72	116.53
3	B	200	HEM	CAD-C3D-C4D	4.07	126.81	112.47
3	A	200	HEM	CAD-C3D-C4D	4.15	127.09	112.47
3	A	200	HEM	CAD-C3D-C2D	4.27	125.50	113.22
3	B	200	HEM	CAD-C3D-C2D	4.41	125.89	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	200	HEM	9	0
3	B	200	HEM	13	0

5.7 Other polymers (i)

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.