Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:40 PM GMT

PDB ID	:	1LH5
Title	:	X-RAY STRUCTURAL INVESTIGATION OF LEGHEMOGLOBIN. VI. STRUCTURE OF ACETATE-FERRILEGHEMOGLOBIN AT A RESOLUTION OF 2.0 ANGSTROMS (RUSSIAN)
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Deposited on	:	1982-04-23
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
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 (1)) were used in the production of this report:

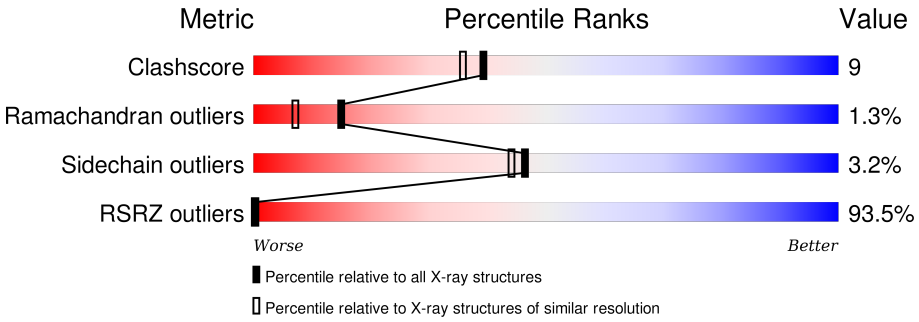
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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.

Mol	Chain	Length	Quality of chain
1	A	153	93% 15% 50% 30% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1291 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 LEGHEMOGLOBIN (FLUORO MET).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	36	1	0
			1180	761	193	225	1			

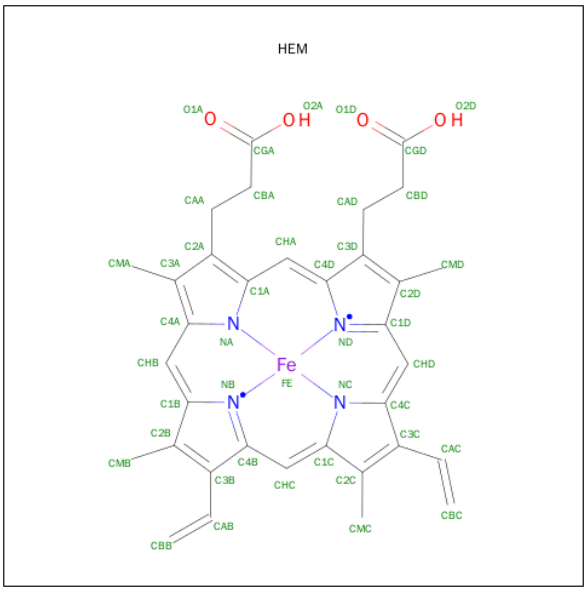
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLU	GLN	CONFLICT	UNP P02240
A	150	ASP	ASN	CONFLICT	UNP P02240

- Molecule 2 is FLUORIDE ION (three-letter code: F) (formula: F).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	F	0	0
			1	1		

- 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	3	0
			43	34	1	4	4		

- Molecule 4 is water.

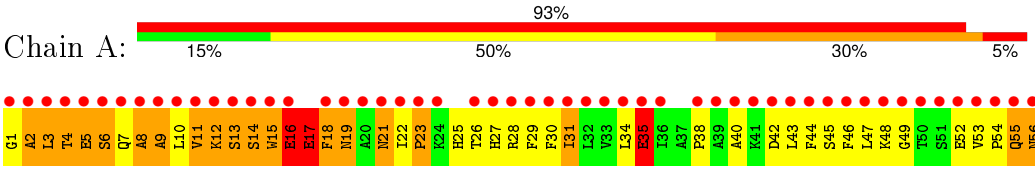
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	67	Total	O	0	0
			67	67		

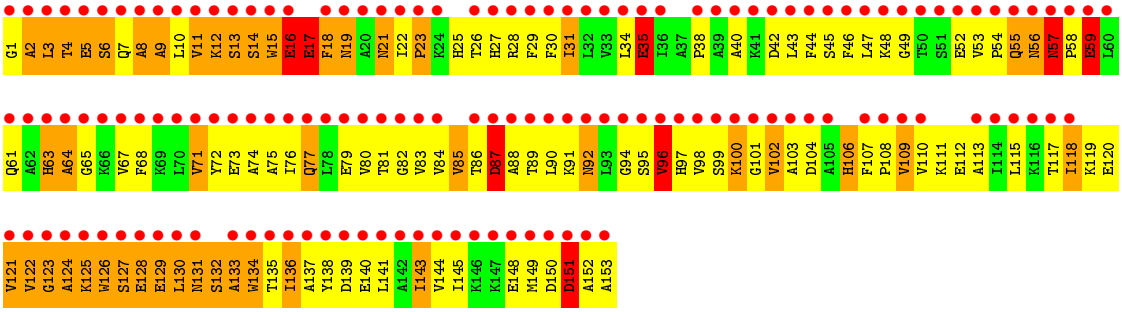
3 Residue-property plots (i)

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.

- Molecule 1: LEGHEMOGLOBIN (FLUORO MET)

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α, β, γ	93.34Å 38.24Å 51.91Å 90.00° 90.00° 98.80°	Depositor
Resolution (Å)	(Not available) – 2.00 9.92 – 1.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 92.5 (9.92-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) 0.503 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	1.36 , 290.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[1]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 11564 reflections	Xtriage
F_o,F_c correlation	0.49	EDS
Total number of atoms	1291	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ 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: HEM, F

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	3.29	148/1214 (12.2%)	2.30	58/1648 (3.5%)

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	13

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	TYR	CB-CG	11.25	1.68	1.51
1	A	15	TRP	CD2-CE2	10.77	1.54	1.41
1	A	95	SER	CB-OG	10.19	1.55	1.42
1	A	138	TYR	CZ-OH	10.04	1.54	1.37
1	A	112	GLU	CG-CD	9.79	1.66	1.51
1	A	13	SER	CA-CB	9.43	1.67	1.52
1	A	120	GLU	CG-CD	9.29	1.65	1.51
1	A	35	GLU	CD-OE2	9.04	1.35	1.25
1	A	13	SER	CB-OG	-8.99	1.30	1.42
1	A	138	TYR	CD2-CE2	8.86	1.52	1.39
1	A	140	GLU	CB-CG	8.75	1.68	1.52
1	A	106	HIS	CB-CG	8.62	1.65	1.50
1	A	11	VAL	CB-CG1	8.55	1.70	1.52
1	A	94	GLY	CA-C	8.55	1.65	1.51
1	A	72	TYR	CE1-CZ	8.42	1.49	1.38
1	A	5	GLU	CD-OE2	8.33	1.34	1.25
1	A	121	VAL	CB-CG2	8.14	1.70	1.52
1	A	72	TYR	CG-CD2	8.09	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	PHE	CB-CG	8.03	1.65	1.51
1	A	79	GLU	CB-CG	7.93	1.67	1.52
1	A	15	TRP	CB-CG	7.92	1.64	1.50
1	A	65	GLY	C-O	7.91	1.36	1.23
1	A	44	PHE	CB-CG	7.88	1.64	1.51
1	A	132[A]	SER	CA-CB	7.81	1.64	1.52
1	A	132[B]	SER	CA-CB	7.81	1.64	1.52
1	A	132[C]	SER	CA-CB	7.81	1.64	1.52
1	A	11	VAL	N-CA	7.53	1.61	1.46
1	A	15	TRP	CG-CD1	7.52	1.47	1.36
1	A	46	PHE	CB-CG	7.49	1.64	1.51
1	A	15	TRP	CZ3-CH2	7.43	1.51	1.40
1	A	102	VAL	CB-CG1	7.35	1.68	1.52
1	A	101	GLY	CA-C	7.31	1.63	1.51
1	A	16	GLU	CD-OE1	7.29	1.33	1.25
1	A	123	GLY	CA-C	7.28	1.63	1.51
1	A	113	ALA	CA-CB	7.25	1.67	1.52
1	A	61	GLN	C-O	7.25	1.37	1.23
1	A	85	VAL	CB-CG2	7.19	1.68	1.52
1	A	134	TRP	N-CA	7.18	1.60	1.46
1	A	124	ALA	N-CA	7.15	1.60	1.46
1	A	99	SER	N-CA	7.11	1.60	1.46
1	A	84	VAL	N-CA	7.07	1.60	1.46
1	A	128	GLU	CD-OE2	-7.07	1.17	1.25
1	A	88	ALA	N-CA	7.05	1.60	1.46
1	A	45	SER	CB-OG	7.04	1.51	1.42
1	A	144	VAL	CB-CG2	7.01	1.67	1.52
1	A	67	VAL	CB-CG2	6.98	1.67	1.52
1	A	73	GLU	CG-CD	6.97	1.62	1.51
1	A	27	HIS	CE1-NE2	6.96	1.48	1.32
1	A	27	HIS	CG-ND1	6.95	1.54	1.38
1	A	86	THR	N-CA	6.88	1.60	1.46
1	A	68	PHE	CG-CD2	6.76	1.48	1.38
1	A	138	TYR	CD1-CE1	6.72	1.49	1.39
1	A	68	PHE	CE1-CZ	6.71	1.50	1.37
1	A	152	ALA	C-O	6.62	1.35	1.23
1	A	72	TYR	C-O	6.62	1.35	1.23
1	A	110	VAL	CB-CG2	6.60	1.66	1.52
1	A	68	PHE	N-CA	6.53	1.59	1.46
1	A	53	VAL	CA-CB	6.53	1.68	1.54
1	A	35	GLU	CD-OE1	-6.50	1.18	1.25
1	A	149	MET	C-O	6.50	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	SER	C-O	6.49	1.35	1.23
1	A	122	VAL	N-CA	6.47	1.59	1.46
1	A	71	VAL	CB-CG1	6.45	1.66	1.52
1	A	40	ALA	CA-CB	6.40	1.65	1.52
1	A	97	HIS	CA-CB	6.37	1.68	1.53
1	A	28	ARG	CZ-NH1	6.35	1.41	1.33
1	A	109	VAL	CA-CB	6.35	1.68	1.54
1	A	30	PHE	N-CA	6.30	1.58	1.46
1	A	59	GLU	CD-OE2	6.28	1.32	1.25
1	A	145	ILE	N-CA	6.23	1.58	1.46
1	A	90	LEU	CA-CB	6.20	1.68	1.53
1	A	130	LEU	N-CA	6.19	1.58	1.46
1	A	124	ALA	C-O	6.13	1.35	1.23
1	A	136	ILE	N-CA	-6.13	1.34	1.46
1	A	15	TRP	C-O	6.09	1.34	1.23
1	A	75	ALA	C-O	6.08	1.34	1.23
1	A	79	GLU	CD-OE1	6.07	1.32	1.25
1	A	68	PHE	C-O	6.06	1.34	1.23
1	A	120	GLU	CA-CB	6.04	1.67	1.53
1	A	133	ALA	CA-C	6.03	1.68	1.52
1	A	102	VAL	N-CA	6.00	1.58	1.46
1	A	95	SER	N-CA	5.99	1.58	1.46
1	A	46	PHE	CD2-CE2	5.98	1.51	1.39
1	A	18	PHE	N-CA	5.97	1.58	1.46
1	A	45	SER	N-CA	5.90	1.58	1.46
1	A	104	ASP	N-CA	5.88	1.58	1.46
1	A	76	ILE	C-O	5.88	1.34	1.23
1	A	16	GLU	CG-CD	5.86	1.60	1.51
1	A	38	PRO	N-CA	5.86	1.57	1.47
1	A	148	GLU	CB-CG	5.84	1.63	1.52
1	A	14	SER	CB-OG	-5.83	1.34	1.42
1	A	2	ALA	CA-CB	5.82	1.64	1.52
1	A	143	ILE	CA-CB	5.82	1.68	1.54
1	A	63	HIS	CA-C	5.79	1.68	1.52
1	A	55	GLN	C-O	5.77	1.34	1.23
1	A	64	ALA	N-CA	5.77	1.57	1.46
1	A	129	GLU	CD-OE1	5.75	1.31	1.25
1	A	111	LYS	N-CA	5.74	1.57	1.46
1	A	79	GLU	CD-OE2	5.70	1.31	1.25
1	A	15	TRP	CD1-NE1	5.69	1.47	1.38
1	A	92	ASN	CB-CG	5.68	1.64	1.51
1	A	92	ASN	C-O	5.64	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	VAL	CB-CG2	5.63	1.64	1.52
1	A	52	GLU	CG-CD	-5.62	1.43	1.51
1	A	43	LEU	CA-CB	5.60	1.66	1.53
1	A	6	SER	CA-CB	5.59	1.61	1.52
1	A	111	LYS	CB-CG	5.59	1.67	1.52
1	A	115	LEU	N-CA	5.58	1.57	1.46
1	A	77	GLN	CG-CD	5.56	1.63	1.51
1	A	87	ASP	CA-C	5.56	1.67	1.52
1	A	58	PRO	N-CD	5.56	1.55	1.47
1	A	4	THR	C-O	5.54	1.33	1.23
1	A	23	PRO	N-CA	5.52	1.56	1.47
1	A	106	HIS	ND1-CE1	5.52	1.48	1.34
1	A	152	ALA	N-CA	5.47	1.57	1.46
1	A	107	PHE	N-CA	5.46	1.57	1.46
1	A	29	PHE	CG-CD2	5.45	1.47	1.38
1	A	97	HIS	CG-CD2	-5.45	1.26	1.35
1	A	110	VAL	CA-C	5.45	1.67	1.52
1	A	77	GLN	CA-CB	5.44	1.66	1.53
1	A	111	LYS	CD-CE	5.44	1.64	1.51
1	A	52	GLU	N-CA	5.41	1.57	1.46
1	A	71	VAL	N-CA	5.40	1.57	1.46
1	A	81	THR	CA-CB	5.39	1.67	1.53
1	A	44	PHE	CD2-CE2	5.35	1.50	1.39
1	A	8	ALA	C-O	5.33	1.33	1.23
1	A	141	LEU	CB-CG	5.33	1.68	1.52
1	A	82	GLY	CA-C	5.32	1.60	1.51
1	A	99	SER	C-O	5.31	1.33	1.23
1	A	29	PHE	CE1-CZ	5.25	1.47	1.37
1	A	2	ALA	C-N	-5.22	1.22	1.34
1	A	140	GLU	CD-OE2	5.21	1.31	1.25
1	A	75	ALA	N-CA	5.20	1.56	1.46
1	A	49	GLY	CA-C	-5.19	1.43	1.51
1	A	136	ILE	CA-CB	5.18	1.66	1.54
1	A	17	GLU	CB-CG	5.16	1.61	1.52
1	A	100	LYS	C-N	-5.15	1.23	1.33
1	A	148	GLU	CG-CD	-5.11	1.44	1.51
1	A	137	ALA	CA-C	5.11	1.66	1.52
1	A	145	ILE	CB-CG2	5.10	1.68	1.52
1	A	96	VAL	C-O	5.09	1.33	1.23
1	A	125	LYS	CD-CE	5.09	1.64	1.51
1	A	144	VAL	CA-C	5.09	1.66	1.52
1	A	55	GLN	CA-CB	-5.05	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	PHE	CA-CB	-5.05	1.42	1.53
1	A	68	PHE	CE2-CZ	5.03	1.47	1.37
1	A	9	ALA	CA-CB	5.01	1.62	1.52
1	A	148	GLU	C-O	5.01	1.32	1.23

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	112	GLU	OE1-CD-OE2	-9.56	111.83	123.30
1	A	28	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	A	72	TYR	CB-CG-CD1	-9.04	115.58	121.00
1	A	17	GLU	OE1-CD-OE2	-8.33	113.31	123.30
1	A	16	GLU	OE1-CD-OE2	-8.30	113.34	123.30
1	A	87	ASP	CB-CG-OD2	-8.22	110.91	118.30
1	A	30	PHE	CB-CG-CD2	-8.22	115.05	120.80
1	A	124	ALA	CB-CA-C	-8.12	97.91	110.10
1	A	15	TRP	CG-CD2-CE3	-8.01	126.69	133.90
1	A	29	PHE	CB-CG-CD1	-7.84	115.31	120.80
1	A	138	TYR	CB-CG-CD2	7.61	125.57	121.00
1	A	73	GLU	OE1-CD-OE2	-7.57	114.22	123.30
1	A	29	PHE	CD1-CG-CD2	7.04	127.45	118.30
1	A	128	GLU	OE1-CD-OE2	-6.97	114.94	123.30
1	A	126	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	A	54	PRO	N-CA-CB	6.78	111.44	103.30
1	A	80	VAL	CA-CB-CG2	-6.62	100.97	110.90
1	A	68	PHE	CB-CG-CD1	-6.61	116.17	120.80
1	A	46	PHE	CB-CG-CD2	6.47	125.33	120.80
1	A	138	TYR	CD1-CE1-CZ	6.46	125.61	119.80
1	A	61	GLN	O-C-N	6.38	132.91	122.70
1	A	15	TRP	CD2-CE3-CZ3	-6.34	110.56	118.80
1	A	15	TRP	CD1-NE1-CE2	-6.33	103.30	109.00
1	A	72	TYR	CG-CD1-CE1	-6.32	116.24	121.30
1	A	126	TRP	NE1-CE2-CD2	6.29	113.59	107.30
1	A	35	GLU	CB-CA-C	-6.11	98.18	110.40
1	A	15	TRP	CH2-CZ2-CE2	-6.07	111.33	117.40
1	A	120	GLU	OE1-CD-OE2	-6.05	116.04	123.30
1	A	124	ALA	N-CA-CB	5.96	118.44	110.10
1	A	110	VAL	O-C-N	-5.96	113.17	122.70
1	A	15	TRP	CB-CG-CD1	5.87	134.63	127.00
1	A	15	TRP	CE2-CD2-CE3	5.82	125.69	118.70
1	A	153	ALA	N-CA-CB	-5.80	101.97	110.10
1	A	48	LYS	CB-CA-C	-5.75	98.91	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3	LEU	N-CA-CB	5.72	121.83	110.40
1	A	134	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	A	117	THR	CA-CB-CG2	5.56	120.19	112.40
1	A	133	ALA	O-C-N	-5.52	113.86	122.70
1	A	15	TRP	NE1-CE2-CZ2	-5.52	124.33	130.40
1	A	89	THR	N-CA-CB	-5.49	99.86	110.30
1	A	104	ASP	CB-CA-C	-5.41	99.58	110.40
1	A	127	SER	O-C-N	5.34	131.25	122.70
1	A	126	TRP	CE2-CD2-CE3	5.29	125.05	118.70
1	A	12	LYS	O-C-N	5.29	131.16	122.70
1	A	57	ASN	CB-CG-OD1	-5.28	111.04	121.60
1	A	76	ILE	O-C-N	5.25	131.11	122.70
1	A	138	TYR	CG-CD2-CE2	5.24	125.50	121.30
1	A	29	PHE	CB-CG-CD2	-5.21	117.15	120.80
1	A	15	TRP	NE1-CE2-CD2	5.18	112.48	107.30
1	A	108	PRO	N-CA-CB	5.17	109.51	103.30
1	A	23	PRO	N-CA-CB	5.16	109.49	103.30
1	A	49	GLY	O-C-N	5.16	130.95	122.70
1	A	126	TRP	CD1-CG-CD2	5.16	110.42	106.30
1	A	131	ASN	O-C-N	5.13	130.91	122.70
1	A	103	ALA	O-C-N	-5.09	114.56	122.70
1	A	31	ILE	CB-CA-C	-5.08	101.43	111.60
1	A	19	ASN	CA-CB-CG	-5.07	102.24	113.40
1	A	151	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ILE	Mainchain
1	A	150	ASP	Sidechain
1	A	151	ASP	Sidechain
1	A	16	GLU	Sidechain
1	A	17	GLU	Sidechain
1	A	19	ASN	Sidechain
1	A	35	GLU	Sidechain
1	A	42	ASP	Sidechain
1	A	56	ASN	Sidechain
1	A	57	ASN	Sidechain
1	A	59	GLU	Sidechain
1	A	83	VAL	Mainchain
1	A	87	ASP	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	1180	0	1200	21	204
2	A	1	0	0	0	0
3	A	43	0	30	3	0
4	A	67	0	0	1	30
All	All	1291	0	1230	21	205

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 9.

All (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASN:O	1:A:96:VAL:HG12	1.91	0.71
1:A:18:PHE:CE1	1:A:25:HIS:HB3	2.31	0.64
1:A:31:ILE:O	1:A:35:GLU:HG3	2.01	0.60
1:A:102:VAL:HG13	3:A:155:HEM:HAC	1.83	0.59
1:A:17:GLU:OE2	1:A:122:VAL:HG12	2.03	0.57
1:A:106:HIS:O	1:A:109:VAL:HB	2.07	0.55
1:A:77:GLN:NE2	1:A:85:VAL:H	2.06	0.54
1:A:87:ASP:O	1:A:91:LYS:HG3	2.08	0.54
1:A:63:HIS:HE1	3:A:155:HEM:C4D	2.26	0.54
1:A:26:THR:HB	1:A:64:ALA:HB3	1.90	0.52
1:A:100:LYS:HG3	3:A:155:HEM:HAD2	1.93	0.50
1:A:21:ASN:HD22	1:A:21:ASN:C	2.15	0.49
1:A:139:ASP:O	1:A:143:ILE:HG13	2.13	0.49
1:A:21:ASN:ND2	1:A:21:ASN:C	2.68	0.46
1:A:71:VAL:O	1:A:74:ALA:HB3	2.16	0.46
1:A:47:LEU:HB3	4:A:220:HOH:O	2.16	0.45
1:A:126:TRP:CZ2	1:A:131:ASN:HB2	2.51	0.45
1:A:57:ASN:OD1	1:A:59:GLU:HB2	2.20	0.42
1:A:25:HIS:CE1	1:A:121:VAL:HG22	2.55	0.41
1:A:22:ILE:HB	1:A:23:PRO:HD3	2.02	0.40

All (205) 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:4:THR:OG1	1:A:17:GLU:CB[2_675]	0.28	1.92
1:A:126:TRP:CD1	1:A:128:GLU:C[2_675]	0.37	1.83
1:A:6:SER:O	1:A:14:SER:N[2_675]	0.40	1.80
1:A:8:ALA:CA	1:A:13:SER:OG[2_675]	0.52	1.68
1:A:6:SER:OG	1:A:14:SER:O[2_675]	0.54	1.66
1:A:127:SER:N	1:A:131:ASN:CA[2_675]	0.56	1.64
1:A:9:ALA:CB	1:A:12:LYS:C[2_675]	0.59	1.61
1:A:10:LEU:CA	1:A:10:LEU:C[2_675]	0.63	1.57
1:A:126:TRP:NE1	1:A:128:GLU:CA[2_675]	0.71	1.49
1:A:119:LYS:CD	1:A:128:GLU:OE2[2_675]	0.77	1.43
1:A:126:TRP:C	1:A:131:ASN:CA[2_675]	0.78	1.42
1:A:8:ALA:C	1:A:13:SER:CB[2_675]	0.81	1.39
1:A:126:TRP:C	1:A:131:ASN:C[2_675]	0.81	1.39
1:A:119:LYS:CE	1:A:128:GLU:CG[2_675]	0.82	1.38
1:A:10:LEU:O	1:A:10:LEU:CB[2_675]	0.84	1.36
1:A:9:ALA:N	1:A:13:SER:CA[2_675]	0.84	1.36
1:A:119:LYS:O	4:A:182:HOH:O[2_675]	0.87	1.33
1:A:126:TRP:CG	1:A:128:GLU:O[2_675]	0.94	1.26
1:A:130:LEU:N	1:A:130:LEU:CD2[2_675]	0.94	1.26
1:A:7:GLN:CA	4:A:203:HOH:O[2_675]	0.96	1.24
1:A:9:ALA:CA	1:A:13:SER:N[2_675]	1.00	1.20
1:A:126:TRP:NE1	1:A:128:GLU:N[2_675]	1.01	1.19
1:A:7:GLN:CB	4:A:203:HOH:O[2_675]	1.01	1.19
1:A:10:LEU:CA	1:A:10:LEU:O[2_675]	1.07	1.13
1:A:127:SER:N	1:A:131:ASN:N[2_675]	1.07	1.13
1:A:9:ALA:O	1:A:9:ALA:O[2_675]	1.12	1.08
1:A:9:ALA:N	1:A:13:SER:CB[2_675]	1.14	1.06
1:A:125:LYS:CB	1:A:133:ALA:CA[2_675]	1.17	1.03
1:A:126:TRP:CD1	1:A:128:GLU:O[2_675]	1.17	1.03
1:A:130:LEU:O	4:A:192:HOH:O[2_675]	1.17	1.03
1:A:126:TRP:O	1:A:131:ASN:C[2_675]	1.18	1.02
1:A:9:ALA:CB	1:A:13:SER:N[2_675]	1.18	1.02
1:A:126:TRP:O	1:A:131:ASN:O[2_675]	1.19	1.01
1:A:119:LYS:CD	1:A:128:GLU:CD[2_675]	1.19	1.01
1:A:7:GLN:CG	1:A:17:GLU:OE2[2_675]	1.20	1.00
1:A:8:ALA:N	1:A:13:SER:OG[2_675]	1.21	0.99
1:A:125:LYS:C	1:A:133:ALA:N[2_675]	1.24	0.96
1:A:4:THR:CB	1:A:17:GLU:CB[2_675]	1.24	0.96
1:A:123:GLY:O	1:A:132[B]:SER:OG[2_675]	1.25	0.95
1:A:6:SER:CB	1:A:14:SER:O[2_675]	1.30	0.90
1:A:134:TRP:N	4:A:219:HOH:O[2_675]	1.31	0.89
1:A:6:SER:O	1:A:14:SER:CA[2_675]	1.32	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLN:OE1	1:A:17:GLU:OE1[2_675]	1.32	0.88
1:A:6:SER:C	1:A:14:SER:CA[2_675]	1.34	0.86
1:A:6:SER:N	1:A:17:GLU:N[2_675]	1.36	0.84
1:A:130:LEU:CA	1:A:130:LEU:CD2[2_675]	1.37	0.83
1:A:9:ALA:CB	1:A:12:LYS:CA[2_675]	1.38	0.82
1:A:7:GLN:NE2	1:A:122:VAL:CA[2_675]	1.38	0.82
1:A:126:TRP:CE2	1:A:128:GLU:CA[2_675]	1.39	0.81
1:A:7:GLN:CD	1:A:17:GLU:OE2[2_675]	1.39	0.81
1:A:6:SER:C	1:A:14:SER:N[2_675]	1.39	0.81
1:A:4:THR:OG1	1:A:17:GLU:CG[2_675]	1.40	0.80
1:A:126:TRP:CD1	1:A:128:GLU:CA[2_675]	1.40	0.80
1:A:8:ALA:C	1:A:13:SER:OG[2_675]	1.42	0.78
1:A:7:GLN:C	4:A:203:HOH:O[2_675]	1.42	0.78
1:A:7:GLN:OE1	1:A:17:GLU:OE2[2_675]	1.44	0.76
1:A:6:SER:C	1:A:13:SER:O[2_675]	1.47	0.73
1:A:126:TRP:CB	1:A:128:GLU:O[2_675]	1.47	0.73
1:A:17:GLU:O	4:A:222:HOH:O[2_675]	1.47	0.73
1:A:9:ALA:N	1:A:13:SER:N[2_675]	1.48	0.72
1:A:6:SER:O	1:A:13:SER:C[2_675]	1.48	0.72
1:A:122:VAL:N	1:A:129:GLU:OE2[2_675]	1.48	0.72
1:A:7:GLN:OE1	1:A:17:GLU:CD[2_675]	1.49	0.71
1:A:123:GLY:C	1:A:132[C]:SER:OG[2_675]	1.49	0.71
1:A:125:LYS:O	1:A:133:ALA:N[2_675]	1.49	0.71
1:A:126:TRP:NE1	1:A:128:GLU:C[2_675]	1.50	0.70
1:A:130:LEU:CB	1:A:130:LEU:CG[2_675]	1.53	0.67
1:A:6:SER:CB	1:A:14:SER:C[2_675]	1.53	0.67
1:A:10:LEU:CA	1:A:10:LEU:CA[2_675]	1.53	0.67
1:A:4:THR:CA	1:A:17:GLU:CG[2_675]	1.54	0.66
1:A:4:THR:O	4:A:206:HOH:O[2_675]	1.54	0.66
1:A:6:SER:C	1:A:13:SER:C[2_675]	1.55	0.65
1:A:9:ALA:C	1:A:9:ALA:O[2_675]	1.56	0.64
1:A:56:ASN:N	4:A:170:HOH:O[1_545]	1.57	0.63
1:A:126:TRP:CA	1:A:131:ASN:C[2_675]	1.57	0.63
1:A:10:LEU:CD2	1:A:11:VAL:CA[2_675]	1.59	0.61
1:A:8:ALA:CA	1:A:13:SER:CB[2_675]	1.61	0.59
1:A:56:ASN:OD1	4:A:171:HOH:O[1_545]	1.61	0.59
1:A:4:THR:CB	1:A:17:GLU:CA[2_675]	1.61	0.59
1:A:129:GLU:C	1:A:130:LEU:CD2[2_675]	1.61	0.59
1:A:10:LEU:CD1	1:A:14:SER:OG[2_675]	1.62	0.58
1:A:118:ILE:O	1:A:129:GLU:OE2[2_675]	1.63	0.57
1:A:17:GLU:C	4:A:222:HOH:O[2_675]	1.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLN:N	1:A:13:SER:O[2_675]	1.64	0.56
1:A:126:TRP:CG	1:A:128:GLU:C[2_675]	1.64	0.56
1:A:127:SER:N	1:A:131:ASN:CB[2_675]	1.64	0.56
1:A:125:LYS:CA	1:A:133:ALA:N[2_675]	1.64	0.56
1:A:126:TRP:O	1:A:131:ASN:CA[2_675]	1.64	0.56
1:A:126:TRP:CD1	1:A:129:GLU:N[2_675]	1.64	0.56
1:A:6:SER:CB	1:A:15:TRP:N[2_675]	1.64	0.56
1:A:10:LEU:CG	1:A:14:SER:OG[2_675]	1.65	0.55
1:A:126:TRP:CH2	1:A:126:TRP:CH2[2_675]	1.65	0.55
1:A:4:THR:N	1:A:17:GLU:CG[2_675]	1.66	0.54
1:A:126:TRP:NE1	1:A:127:SER:C[2_675]	1.66	0.54
1:A:7:GLN:CB	1:A:17:GLU:OE2[2_675]	1.67	0.53
1:A:56:ASN:CB	4:A:189:HOH:O[1_545]	1.67	0.53
1:A:6:SER:OG	1:A:14:SER:C[2_675]	1.68	0.52
1:A:126:TRP:C	1:A:131:ASN:CB[2_675]	1.68	0.52
1:A:10:LEU:C	1:A:10:LEU:CB[2_675]	1.68	0.52
1:A:6:SER:CB	1:A:15:TRP:CA[2_675]	1.68	0.52
1:A:10:LEU:N	1:A:10:LEU:O[2_675]	1.69	0.51
1:A:10:LEU:O	1:A:10:LEU:CG[2_675]	1.70	0.50
1:A:122:VAL:CG2	1:A:132[A]:SER:OG[2_675]	1.70	0.50
1:A:5:GLU:CB	1:A:16:GLU:CB[2_675]	1.70	0.50
1:A:127:SER:CA	1:A:131:ASN:CA[2_675]	1.71	0.49
1:A:118:ILE:CG2	1:A:129:GLU:CB[2_675]	1.72	0.48
1:A:15:TRP:CB	4:A:221:HOH:O[2_675]	1.73	0.47
1:A:5:GLU:C	1:A:16:GLU:CB[2_675]	1.73	0.47
1:A:11:VAL:O	4:A:221:HOH:O[2_675]	1.74	0.46
1:A:9:ALA:CB	1:A:12:LYS:O[2_675]	1.76	0.44
1:A:130:LEU:CA	1:A:130:LEU:CB[2_675]	1.76	0.44
1:A:119:LYS:CG	1:A:128:GLU:CB[2_675]	1.76	0.44
1:A:125:LYS:CB	1:A:133:ALA:N[2_675]	1.77	0.43
1:A:5:GLU:CG	1:A:16:GLU:CB[2_675]	1.77	0.43
1:A:6:SER:CB	1:A:15:TRP:C[2_675]	1.78	0.42
1:A:4:THR:OG1	1:A:17:GLU:CA[2_675]	1.78	0.42
1:A:126:TRP:C	1:A:131:ASN:N[2_675]	1.79	0.41
1:A:123:GLY:O	1:A:132[C]:SER:OG[2_675]	1.80	0.40
1:A:130:LEU:CA	1:A:130:LEU:CG[2_675]	1.80	0.40
1:A:9:ALA:CA	1:A:13:SER:CA[2_675]	1.80	0.40
1:A:128:GLU:N	4:A:212:HOH:O[2_675]	1.82	0.38
1:A:6:SER:CA	1:A:16:GLU:N[2_675]	1.82	0.38
1:A:7:GLN:N	1:A:14:SER:CA[2_675]	1.82	0.38
1:A:10:LEU:N	1:A:10:LEU:C[2_675]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:THR:CB	1:A:17:GLU:CG[2_675]	1.83	0.37
1:A:4:THR:N	1:A:17:GLU:CD[2_675]	1.83	0.37
1:A:119:LYS:CD	1:A:128:GLU:CG[2_675]	1.83	0.37
1:A:15:TRP:N	4:A:221:HOH:O[2_675]	1.83	0.37
1:A:126:TRP:N	1:A:131:ASN:C[2_675]	1.84	0.36
1:A:124:ALA:O	1:A:135:THR:CB[2_675]	1.84	0.36
1:A:7:GLN:CG	1:A:122:VAL:CG1[2_675]	1.86	0.34
1:A:7:GLN:NE2	1:A:122:VAL:C[2_675]	1.86	0.34
1:A:119:LYS:C	4:A:182:HOH:O[2_675]	1.86	0.34
1:A:4:THR:C	1:A:17:GLU:CG[2_675]	1.87	0.33
1:A:9:ALA:C	1:A:13:SER:N[2_675]	1.87	0.33
1:A:122:VAL:O	1:A:132[C]:SER:OG[2_675]	1.88	0.32
1:A:8:ALA:O	1:A:13:SER:CB[2_675]	1.88	0.32
1:A:6:SER:C	1:A:14:SER:C[2_675]	1.89	0.31
1:A:126:TRP:CE2	1:A:128:GLU:N[2_675]	1.90	0.30
1:A:7:GLN:NE2	1:A:122:VAL:CB[2_675]	1.91	0.29
1:A:125:LYS:O	1:A:130:LEU:O[2_675]	1.91	0.29
1:A:127:SER:N	1:A:131:ASN:C[2_675]	1.91	0.29
1:A:134:TRP:CA	4:A:219:HOH:O[2_675]	1.92	0.28
1:A:118:ILE:O	1:A:129:GLU:CD[2_675]	1.92	0.28
1:A:126:TRP:C	1:A:131:ASN:O[2_675]	1.92	0.28
1:A:10:LEU:CD1	1:A:14:SER:CB[2_675]	1.93	0.27
1:A:130:LEU:N	1:A:130:LEU:CG[2_675]	1.94	0.26
1:A:126:TRP:CB	1:A:132[B]:SER:OG[2_675]	1.94	0.26
1:A:6:SER:N	1:A:16:GLU:N[2_675]	1.95	0.25
1:A:6:SER:CA	1:A:14:SER:C[2_675]	1.95	0.25
1:A:5:GLU:CA	1:A:16:GLU:CB[2_675]	1.95	0.25
1:A:10:LEU:C	1:A:10:LEU:C[2_675]	1.95	0.25
1:A:6:SER:CA	1:A:15:TRP:N[2_675]	1.96	0.24
1:A:6:SER:CA	1:A:13:SER:O[2_675]	1.97	0.23
1:A:6:SER:N	1:A:16:GLU:C[2_675]	1.97	0.23
1:A:8:ALA:CB	1:A:13:SER:OG[2_675]	1.98	0.22
4:A:159:HOH:O	4:A:177:HOH:O[2_675]	1.98	0.22
1:A:56:ASN:OD1	4:A:170:HOH:O[1_545]	1.98	0.22
1:A:7:GLN:C	1:A:13:SER:OG[2_675]	1.99	0.21
1:A:126:TRP:O	1:A:131:ASN:CG[2_675]	2.00	0.20
1:A:7:GLN:NE2	1:A:122:VAL:O[2_675]	2.00	0.20
1:A:16:GLU:O	4:A:222:HOH:O[2_675]	2.01	0.19
1:A:122:VAL:CG2	1:A:129:GLU:CA[2_675]	2.01	0.19
1:A:5:GLU:CG	1:A:16:GLU:CG[2_675]	2.03	0.17
1:A:135:THR:OG1	4:A:159:HOH:O[2_675]	2.03	0.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:N	1:A:13:SER:CB[2_675]	2.04	0.16
1:A:122:VAL:CG2	1:A:129:GLU:O[2_675]	2.05	0.15
1:A:9:ALA:CB	1:A:12:LYS:CB[2_675]	2.05	0.15
1:A:5:GLU:O	1:A:13:SER:O[2_675]	2.05	0.15
1:A:9:ALA:CA	1:A:12:LYS:C[2_675]	2.05	0.15
1:A:6:SER:N	1:A:16:GLU:CA[2_675]	2.05	0.15
1:A:119:LYS:CG	1:A:128:GLU:OE2[2_675]	2.06	0.14
1:A:1:GLY:N	4:A:193:HOH:O[2_675]	2.06	0.14
1:A:6:SER:N	1:A:13:SER:O[2_675]	2.06	0.14
1:A:125:LYS:CA	1:A:133:ALA:CA[2_675]	2.07	0.13
1:A:130:LEU:C	4:A:192:HOH:O[2_675]	2.08	0.12
1:A:8:ALA:C	1:A:13:SER:CA[2_675]	2.08	0.12
1:A:5:GLU:C	1:A:13:SER:O[2_675]	2.09	0.11
1:A:119:LYS:NZ	1:A:128:GLU:CG[2_675]	2.09	0.11
1:A:7:GLN:N	1:A:14:SER:N[2_675]	2.10	0.10
1:A:7:GLN:N	1:A:13:SER:C[2_675]	2.10	0.10
1:A:4:THR:N	1:A:17:GLU:OE1[2_675]	2.10	0.10
1:A:126:TRP:CG	1:A:128:GLU:CA[2_675]	2.11	0.09
1:A:9:ALA:N	1:A:13:SER:OG[2_675]	2.12	0.08
1:A:126:TRP:N	1:A:133:ALA:N[2_675]	2.12	0.08
1:A:126:TRP:CZ3	1:A:126:TRP:CH2[2_675]	2.13	0.07
1:A:133:ALA:C	4:A:219:HOH:O[2_675]	2.13	0.07
1:A:119:LYS:CE	1:A:128:GLU:CB[2_675]	2.13	0.07
1:A:5:GLU:O	1:A:16:GLU:CB[2_675]	2.14	0.06
1:A:55:GLN:OE1	4:A:172:HOH:O[1_545]	2.14	0.06
1:A:124:ALA:N	1:A:132[C]:SER:OG[2_675]	2.15	0.05
1:A:122:VAL:CG1	1:A:129:GLU:CG[2_675]	2.15	0.05
1:A:127:SER:CA	1:A:131:ASN:CB[2_675]	2.15	0.05
1:A:125:LYS:O	1:A:133:ALA:CA[2_675]	2.15	0.05
1:A:127:SER:N	1:A:130:LEU:C[2_675]	2.16	0.04
1:A:119:LYS:CB	1:A:128:GLU:CB[2_675]	2.16	0.04
1:A:18:PHE:N	4:A:222:HOH:O[2_675]	2.16	0.04
1:A:8:ALA:N	4:A:203:HOH:O[2_675]	2.16	0.04
1:A:15:TRP:CA	4:A:221:HOH:O[2_675]	2.16	0.04
1:A:5:GLU:N	1:A:17:GLU:N[2_675]	2.16	0.04
1:A:6:SER:CB	1:A:16:GLU:N[2_675]	2.16	0.04
1:A:126:TRP:O	1:A:131:ASN:CB[2_675]	2.16	0.04
1:A:4:THR:O	1:A:17:GLU:CG[2_675]	2.17	0.03
1:A:56:ASN:CB	4:A:170:HOH:O[1_545]	2.18	0.02
1:A:126:TRP:CD2	1:A:128:GLU:CA[2_675]	2.19	0.01

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	153/153 (100%)	147 (96%)	4 (3%)	2 (1%)	15 7

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	2	ALA

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	127/125 (102%)	123 (97%)	4 (3%)	47 46

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	34	LEU
1	A	96	VAL
1	A	151	ASP

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	21	ASN
1	A	25	HIS
1	A	61	GLN
1	A	63	HIS
1	A	77	GLN

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

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
3	HEM	A	155	1,2	30,50,50	4.71	24 (80%)	24,82,82	2.82	13 (54%)

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	155	1,2	-	0/10/54/54	0/0/8/8

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	HEM	C2D-C3D	-5.57	1.37	1.54
3	A	155	HEM	C2C-C1C	-3.20	1.46	1.52
3	A	155	HEM	CBB-CAB	2.49	1.43	1.29
3	A	155	HEM	CMB-C2B	2.49	1.58	1.53
3	A	155	HEM	C3D-C4D	2.61	1.55	1.51
3	A	155	HEM	C2D-C1D	2.81	1.61	1.51
3	A	155	HEM	CMC-C2C	2.99	1.60	1.53
3	A	155	HEM	CMA-C3A	3.07	1.58	1.51
3	A	155	HEM	C1A-CHA	3.28	1.48	1.39
3	A	155	HEM	CMD-C2D	3.29	1.60	1.53
3	A	155	HEM	C3C-CAC	3.29	1.57	1.51
3	A	155	HEM	C2A-C3A	3.80	1.48	1.37
3	A	155	HEM	CHC-C1C	4.66	1.47	1.36
3	A	155	HEM	C4A-CHB	4.93	1.53	1.39
3	A	155	HEM	FE-ND	4.94	2.23	1.97
3	A	155	HEM	CAD-C3D	4.99	1.64	1.54
3	A	155	HEM	CAA-C2A	5.05	1.60	1.52
3	A	155	HEM	FE-NC	6.11	2.19	1.95
3	A	155	HEM	CHD-C4C	6.75	1.52	1.36
3	A	155	HEM	C4C-NC	6.88	1.44	1.36
3	A	155	HEM	FE-NB	7.33	2.36	1.97
3	A	155	HEM	C3B-CAB	8.00	1.66	1.51
3	A	155	HEM	C3B-C4B	8.06	1.59	1.51
3	A	155	HEM	C1C-NC	9.41	1.47	1.36

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	155	HEM	CAA-C2A-C1A	-5.50	121.03	127.01
3	A	155	HEM	CMA-C3A-C4A	-4.76	120.50	128.36
3	A	155	HEM	CBA-CAA-C2A	-3.22	106.76	112.53
3	A	155	HEM	CAA-CBA-CGA	-2.78	107.66	112.75
3	A	155	HEM	CBD-CAD-C3D	-2.72	105.64	113.55
3	A	155	HEM	C2C-C1C-NC	-2.22	106.46	110.21
3	A	155	HEM	C1D-CHD-C4C	2.27	129.61	125.82
3	A	155	HEM	C2D-C3D-C4D	2.37	105.52	101.50
3	A	155	HEM	CMD-C2D-C3D	2.78	126.64	114.35
3	A	155	HEM	CMC-C2C-C3C	4.18	126.97	116.53
3	A	155	HEM	CAD-C3D-C4D	4.22	127.36	112.47
3	A	155	HEM	CMB-C2B-C3B	4.23	127.10	116.53
3	A	155	HEM	CAD-C3D-C2D	4.83	127.12	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	155	HEM	3	0

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	153/153 (100%)	4.92	143 (93%)	0 0	8, 17, 47, 65	19 (12%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	LEU	24.3
1	A	2	ALA	23.3
1	A	51	SER	16.1
1	A	1	GLY	13.7
1	A	47	LEU	10.7
1	A	19	ASN	10.3
1	A	153	ALA	9.7
1	A	50	THR	9.5
1	A	49	GLY	9.2
1	A	124	ALA	9.1
1	A	46	PHE	9.1
1	A	136	ILE	9.1
1	A	130	LEU	8.9
1	A	83	VAL	8.7
1	A	20	ALA	8.3
1	A	45	SER	8.0
1	A	82	GLY	7.9
1	A	101	GLY	7.8
1	A	48	LYS	7.8
1	A	44	PHE	7.7
1	A	144	VAL	7.6
1	A	60	LEU	7.4
1	A	42	ASP	7.1
1	A	53	VAL	7.1
1	A	90	LEU	6.9
1	A	15	TRP	6.8
1	A	58	PRO	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	152	ALA	6.7
1	A	26	THR	6.4
1	A	89	THR	6.4
1	A	145	ILE	6.4
1	A	32	LEU	6.4
1	A	138	TYR	6.2
1	A	150	ASP	6.1
1	A	151	ASP	6.1
1	A	88	ALA	6.0
1	A	40	ALA	5.9
1	A	56	ASN	5.8
1	A	122	VAL	5.8
1	A	116	LYS	5.7
1	A	80	VAL	5.7
1	A	10	LEU	5.6
1	A	81	THR	5.4
1	A	11	VAL	5.3
1	A	108	PRO	5.3
1	A	5	GLU	5.3
1	A	87	ASP	5.3
1	A	149	MET	5.3
1	A	93	LEU	5.1
1	A	96	VAL	5.1
1	A	123	GLY	5.0
1	A	107	PHE	5.0
1	A	22	ILE	4.9
1	A	55	GLN	4.9
1	A	67	VAL	4.9
1	A	140	GLU	4.9
1	A	36	ILE	4.9
1	A	54	PRO	4.8
1	A	69	LYS	4.7
1	A	23	PRO	4.7
1	A	18	PHE	4.7
1	A	126	TRP	4.6
1	A	137	ALA	4.6
1	A	84	VAL	4.6
1	A	99	SER	4.6
1	A	64	ALA	4.6
1	A	59	GLU	4.4
1	A	143	ILE	4.4
1	A	114	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	98	VAL	4.4
1	A	115	LEU	4.3
1	A	16	GLU	4.3
1	A	43	LEU	4.2
1	A	76	ILE	4.2
1	A	102	VAL	4.2
1	A	118	ILE	4.2
1	A	70	LEU	4.1
1	A	57	ASN	4.1
1	A	110	VAL	4.1
1	A	72	TYR	4.1
1	A	92	ASN	4.0
1	A	8	ALA	4.0
1	A	78	LEU	4.0
1	A	117	THR	3.9
1	A	147	LYS	3.9
1	A	63	HIS	3.9
1	A	97	HIS	3.9
1	A	105	ALA	3.8
1	A	135	THR	3.8
1	A	129	GLU	3.8
1	A	142	ALA	3.8
1	A	127	SER	3.8
1	A	104	ASP	3.8
1	A	30	PHE	3.6
1	A	131	ASN	3.6
1	A	68	PHE	3.6
1	A	12	LYS	3.6
1	A	95	SER	3.6
1	A	121	VAL	3.5
1	A	41	LYS	3.5
1	A	7	GLN	3.5
1	A	9	ALA	3.5
1	A	39	ALA	3.4
1	A	113	ALA	3.4
1	A	61	GLN	3.4
1	A	71	VAL	3.3
1	A	74	ALA	3.3
1	A	24	LYS	3.2
1	A	75	ALA	3.2
1	A	31	ILE	3.2
1	A	86	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	6	SER	3.2
1	A	103	ALA	3.2
1	A	73	GLU	3.1
1	A	79	GLU	3.1
1	A	34	LEU	3.0
1	A	139	ASP	3.0
1	A	27	HIS	3.0
1	A	38	PRO	3.0
1	A	14	SER	3.0
1	A	146	LYS	2.9
1	A	62	ALA	2.9
1	A	125	LYS	2.9
1	A	29	PHE	2.9
1	A	141	LEU	2.9
1	A	148	GLU	2.9
1	A	77	GLN	2.8
1	A	100	LYS	2.8
1	A	33	VAL	2.7
1	A	35	GLU	2.7
1	A	134	TRP	2.7
1	A	109	VAL	2.7
1	A	13	SER	2.7
1	A	66	LYS	2.7
1	A	94	GLY	2.6
1	A	65	GLY	2.5
1	A	133	ALA	2.5
1	A	4	THR	2.5
1	A	21	ASN	2.4
1	A	52	GLU	2.3
1	A	91	LYS	2.2
1	A	128	GLU	2.1
1	A	28	ARG	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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
3	HEM	A	155	43/43	0.75	0.29	-0.94	0,13,39,47	3
2	F	A	154	1/1	0.62	0.38	-	20,20,20,20	0

6.5 Other polymers

There are no such residues in this entry.