



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:53 AM GMT

PDB ID : 2LH2  
Title : X-RAY STRUCTURAL INVESTIGATION OF LEGHEMOGLOBIN. VI. STRUCTURE OF ACETATE-FERRILEGHEMOGLOBIN AT A RESOLUTION OF 2.0 ANGSTROMS (RUSSIAN)  
Authors : Vainshtein, B.K.; Harutyunyan, E.H.; Kuranova, I.P.; Borisov, V.V.; Sosfenov, N.I.; Pavlovsky, A.G.; Grebenko, A.I.; Konareva, N.V.  
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](mailto: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

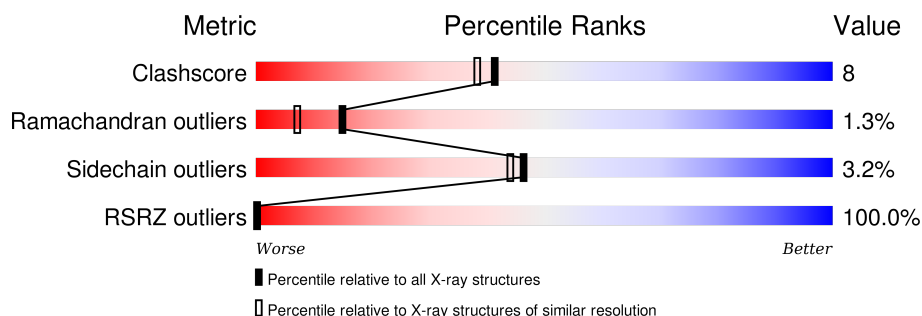
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	153	

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
2	HEM	A	154	-	-	-	X

## 2 Entry composition [i](#)

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.

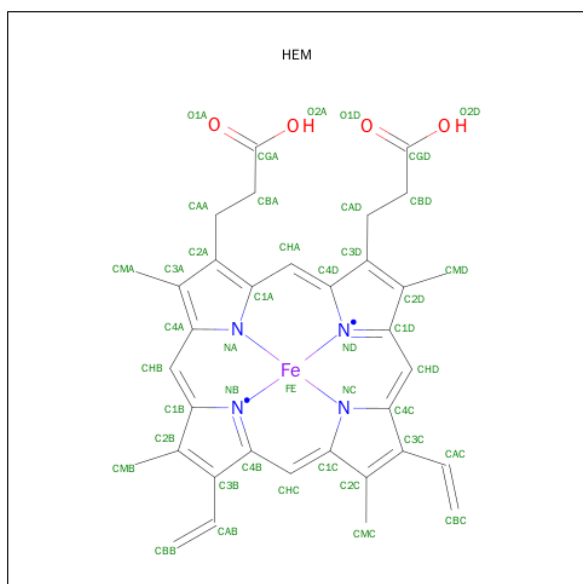
- Molecule 1 is a protein called LEGHEMOGLOBIN (AQUO MET).

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



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

- Molecule 3 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		

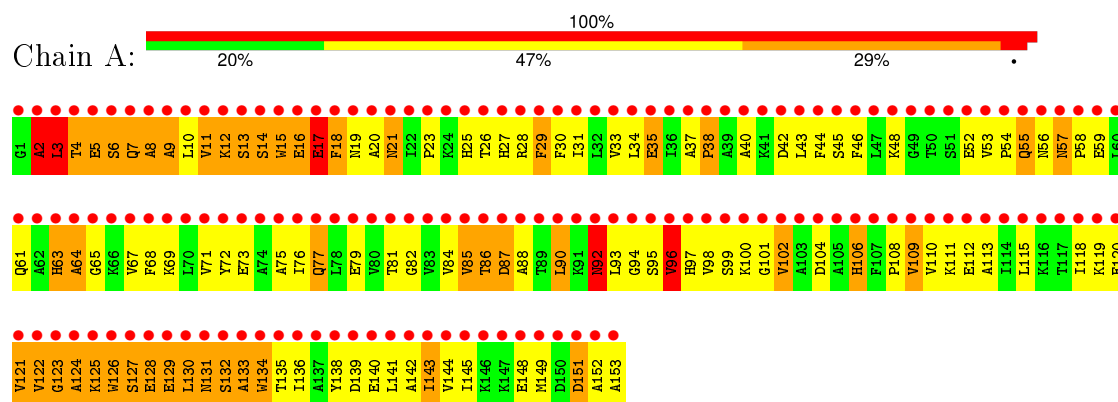
- Molecule 4 is water.

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

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: LEGHEMOGLOBIN (AQUO MET)



## 4 Data and refinement statistics

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.22Å 38.26Å 52.01Å 90.00° 90.00° 98.80°	Depositor
Resolution (Å)	(Not available) – 2.00 9.93 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 96.4 (9.93-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	unknown	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.502 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 11861 reflections	Xtriage
$F_o, F_c$ correlation	0.36	EDS
Total number of atoms	1291	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Theoretical 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: HEM, O

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	3.25	138/1214 (11.4%)	2.13	39/1648 (2.4%)

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	8

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	SER	CB-OG	10.60	1.56	1.42
1	A	138	TYR	CB-CG	9.88	1.66	1.51
1	A	15	TRP	CD2-CE2	9.48	1.52	1.41
1	A	138	TYR	CZ-OH	9.47	1.53	1.37
1	A	112	GLU	CG-CD	9.30	1.65	1.51
1	A	132[A]	SER	CA-CB	9.09	1.66	1.52
1	A	132[B]	SER	CA-CB	9.09	1.66	1.52
1	A	132[C]	SER	CA-CB	9.09	1.66	1.52
1	A	120	GLU	CG-CD	8.72	1.65	1.51
1	A	106	HIS	CB-CG	8.58	1.65	1.50
1	A	72	TYR	CE1-CZ	8.49	1.49	1.38
1	A	123	GLY	CA-C	8.48	1.65	1.51
1	A	15	TRP	CB-CG	8.37	1.65	1.50
1	A	5	GLU	CD-OE2	8.26	1.34	1.25
1	A	94	GLY	CA-C	8.13	1.64	1.51
1	A	18	PHE	CB-CG	8.06	1.65	1.51
1	A	65	GLY	C-O	8.02	1.36	1.23
1	A	13	SER	CA-CB	7.94	1.64	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	GLU	CD-OE2	7.69	1.34	1.25
1	A	72	TYR	CG-CD2	7.61	1.49	1.39
1	A	44	PHE	CB-CG	7.49	1.64	1.51
1	A	128	GLU	CD-OE2	-7.40	1.17	1.25
1	A	46	PHE	CB-CG	7.30	1.63	1.51
1	A	138	TYR	CD2-CE2	7.18	1.50	1.39
1	A	140	GLU	CB-CG	7.15	1.65	1.52
1	A	129	GLU	CD-OE1	7.07	1.33	1.25
1	A	15	TRP	CZ3-CH2	7.06	1.51	1.40
1	A	144	VAL	CB-CG2	7.06	1.67	1.52
1	A	110	VAL	CB-CG2	7.05	1.67	1.52
1	A	11	VAL	CB-CG1	7.03	1.67	1.52
1	A	121	VAL	CB-CG2	7.03	1.67	1.52
1	A	35	GLU	CD-OE1	-6.99	1.18	1.25
1	A	134	TRP	N-CA	6.96	1.60	1.46
1	A	72	TYR	C-O	6.94	1.36	1.23
1	A	101	GLY	CA-C	6.90	1.62	1.51
1	A	111	LYS	N-CA	6.88	1.60	1.46
1	A	85	VAL	CB-CG2	6.87	1.67	1.52
1	A	113	ALA	CA-CB	6.85	1.66	1.52
1	A	102	VAL	CB-CG1	6.84	1.67	1.52
1	A	88	ALA	N-CA	6.83	1.60	1.46
1	A	104	ASP	N-CA	6.79	1.59	1.46
1	A	13	SER	CB-OG	-6.76	1.33	1.42
1	A	40	ALA	CA-CB	6.75	1.66	1.52
1	A	68	PHE	C-O	6.74	1.36	1.23
1	A	27	HIS	CE1-NE2	6.71	1.48	1.32
1	A	152	ALA	C-O	6.64	1.35	1.23
1	A	79	GLU	CB-CG	6.62	1.64	1.52
1	A	138	TYR	CD1-CE1	6.59	1.49	1.39
1	A	124	ALA	N-CA	6.57	1.59	1.46
1	A	109	VAL	CA-CB	6.48	1.68	1.54
1	A	124	ALA	C-O	6.44	1.35	1.23
1	A	95	SER	N-CA	6.41	1.59	1.46
1	A	6	SER	CA-CB	6.40	1.62	1.52
1	A	11	VAL	N-CA	6.38	1.59	1.46
1	A	111	LYS	CD-CE	6.37	1.67	1.51
1	A	14	SER	CB-OG	-6.36	1.33	1.42
1	A	61	GLN	C-O	6.36	1.35	1.23
1	A	86	THR	N-CA	6.33	1.59	1.46
1	A	145	ILE	N-CA	6.33	1.58	1.46
1	A	15	TRP	NE1-CE2	-6.31	1.29	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	SER	CB-OG	6.31	1.50	1.42
1	A	67	VAL	CB-CG2	6.31	1.66	1.52
1	A	28	ARG	CZ-NH1	6.29	1.41	1.33
1	A	99	SER	C-O	6.28	1.35	1.23
1	A	149	MET	C-O	6.26	1.35	1.23
1	A	68	PHE	CG-CD2	6.22	1.48	1.38
1	A	73	GLU	CG-CD	6.20	1.61	1.51
1	A	15	TRP	C-O	6.18	1.35	1.23
1	A	15	TRP	CD1-NE1	6.18	1.48	1.38
1	A	16	GLU	CG-CD	6.17	1.61	1.51
1	A	148	GLU	CB-CG	6.16	1.63	1.52
1	A	148	GLU	CD-OE2	6.09	1.32	1.25
1	A	79	GLU	C-O	6.07	1.34	1.23
1	A	97	HIS	CA-CB	6.07	1.67	1.53
1	A	102	VAL	N-CA	6.05	1.58	1.46
1	A	122	VAL	N-CA	6.05	1.58	1.46
1	A	68	PHE	CE1-CZ	6.03	1.48	1.37
1	A	55	GLN	C-O	6.03	1.34	1.23
1	A	2	ALA	CA-CB	6.01	1.65	1.52
1	A	106	HIS	ND1-CE1	5.99	1.49	1.34
1	A	9	ALA	CA-CB	5.96	1.65	1.52
1	A	97	HIS	CG-CD2	-5.90	1.25	1.35
1	A	63	HIS	CE1-NE2	5.90	1.46	1.32
1	A	98	VAL	CB-CG2	5.88	1.65	1.52
1	A	99	SER	N-CA	5.86	1.58	1.46
1	A	27	HIS	CG-ND1	5.83	1.51	1.38
1	A	76	ILE	C-O	5.82	1.34	1.23
1	A	75	ALA	N-CA	5.80	1.57	1.46
1	A	79	GLU	CD-OE2	5.80	1.32	1.25
1	A	53	VAL	CA-CB	5.79	1.66	1.54
1	A	75	ALA	C-O	5.78	1.34	1.23
1	A	90	LEU	CA-CB	5.77	1.67	1.53
1	A	77	GLN	CG-CD	5.76	1.64	1.51
1	A	8	ALA	C-O	5.72	1.34	1.23
1	A	18	PHE	N-CA	5.71	1.57	1.46
1	A	152	ALA	N-CA	5.69	1.57	1.46
1	A	111	LYS	CB-CG	5.66	1.67	1.52
1	A	58	PRO	N-CD	5.66	1.55	1.47
1	A	59	GLU	CD-OE2	5.64	1.31	1.25
1	A	4	THR	C-O	5.64	1.34	1.23
1	A	52	GLU	CG-CD	-5.62	1.43	1.51
1	A	84	VAL	CB-CG1	5.61	1.64	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	GLU	CA-CB	5.60	1.66	1.53
1	A	96	VAL	CB-CG1	5.60	1.64	1.52
1	A	71	VAL	CB-CG1	5.51	1.64	1.52
1	A	125	LYS	CD-CE	5.50	1.65	1.51
1	A	68	PHE	N-CA	5.48	1.57	1.46
1	A	69	LYS	C-O	5.48	1.33	1.23
1	A	92	ASN	CB-CG	5.43	1.63	1.51
1	A	140	GLU	CD-OE2	5.42	1.31	1.25
1	A	153	ALA	C-OXT	5.41	1.33	1.23
1	A	92	ASN	C-O	5.39	1.33	1.23
1	A	30	PHE	CG-CD2	-5.38	1.30	1.38
1	A	127	SER	C-O	5.38	1.33	1.23
1	A	141	LEU	N-CA	5.37	1.57	1.46
1	A	82	GLY	CA-C	5.35	1.60	1.51
1	A	45	SER	N-CA	5.34	1.57	1.46
1	A	130	LEU	N-CA	5.33	1.57	1.46
1	A	52	GLU	N-CA	5.31	1.56	1.46
1	A	143	ILE	CA-CB	5.29	1.67	1.54
1	A	3	LEU	CA-CB	5.24	1.65	1.53
1	A	115	LEU	N-CA	5.20	1.56	1.46
1	A	58	PRO	CA-C	-5.20	1.42	1.52
1	A	148	GLU	CG-CD	-5.19	1.44	1.51
1	A	15	TRP	CG-CD1	5.17	1.44	1.36
1	A	133	ALA	CA-C	5.16	1.66	1.52
1	A	15	TRP	N-CA	5.14	1.56	1.46
1	A	134	TRP	CD2-CE2	-5.14	1.35	1.41
1	A	81	THR	CA-CB	5.12	1.66	1.53
1	A	79	GLU	CD-OE1	5.12	1.31	1.25
1	A	64	ALA	N-CA	5.11	1.56	1.46
1	A	57	ASN	C-O	5.09	1.33	1.23
1	A	138	TYR	N-CA	5.08	1.56	1.46
1	A	144	VAL	CA-C	5.08	1.66	1.52
1	A	38	PRO	N-CA	5.06	1.55	1.47
1	A	43	LEU	CA-CB	5.06	1.65	1.53
1	A	17	GLU	CB-CG	5.05	1.61	1.52
1	A	20	ALA	CA-CB	5.01	1.62	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	TYR	CB-CG-CD1	-9.86	115.09	121.00
1	A	112	GLU	OE1-CD-OE2	-9.81	111.52	123.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	GLU	OE1-CD-OE2	-8.52	113.07	123.30
1	A	16	GLU	OE1-CD-OE2	-8.04	113.66	123.30
1	A	28	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	A	15	TRP	CG-CD2-CE3	-7.64	127.03	133.90
1	A	138	TYR	CB-CG-CD2	7.04	125.22	121.00
1	A	46	PHE	CB-CG-CD2	6.99	125.69	120.80
1	A	87	ASP	CB-CG-OD2	-6.77	112.20	118.30
1	A	108	PRO	N-CA-CB	6.77	111.43	103.30
1	A	17	GLU	OE1-CD-OE2	-6.72	115.24	123.30
1	A	29	PHE	CB-CG-CD1	-6.70	116.11	120.80
1	A	128	GLU	OE1-CD-OE2	-6.52	115.47	123.30
1	A	120	GLU	OE1-CD-OE2	-6.52	115.47	123.30
1	A	54	PRO	N-CA-CB	6.46	111.05	103.30
1	A	126	TRP	CE2-CD2-CG	-6.41	102.17	107.30
1	A	29	PHE	CD1-CG-CD2	6.38	126.60	118.30
1	A	30	PHE	CB-CG-CD2	-6.28	116.41	120.80
1	A	72	TYR	CG-CD1-CE1	-6.24	116.31	121.30
1	A	134	TRP	CG-CD1-NE1	-6.17	103.93	110.10
1	A	23	PRO	N-CA-CB	6.14	110.67	103.30
1	A	48	LYS	CB-CA-C	-5.87	98.66	110.40
1	A	68	PHE	CB-CG-CD1	-5.84	116.71	120.80
1	A	126	TRP	NE1-CE2-CD2	5.79	113.09	107.30
1	A	138	TYR	CD1-CE1-CZ	5.79	125.01	119.80
1	A	15	TRP	CH2-CZ2-CE2	-5.79	111.61	117.40
1	A	15	TRP	CD2-CE3-CZ3	-5.53	111.61	118.80
1	A	15	TRP	CD1-NE1-CE2	-5.53	104.03	109.00
1	A	131	ASN	O-C-N	5.50	131.51	122.70
1	A	142	ALA	O-C-N	5.44	131.40	122.70
1	A	8	ALA	O-C-N	5.35	131.26	122.70
1	A	124	ALA	CB-CA-C	-5.30	102.14	110.10
1	A	15	TRP	NE1-CE2-CZ2	-5.18	124.70	130.40
1	A	76	ILE	O-C-N	5.17	130.98	122.70
1	A	149	MET	O-C-N	5.14	130.92	122.70
1	A	12	LYS	O-C-N	5.13	130.91	122.70
1	A	138	TYR	O-C-N	5.08	130.83	122.70
1	A	3	LEU	N-CA-CB	5.06	120.52	110.40
1	A	29	PHE	CB-CG-CD2	-5.02	117.29	120.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	ASP	Sidechain
1	A	17	GLU	Sidechain
1	A	19	ASN	Sidechain
1	A	42	ASP	Sidechain
1	A	57	ASN	Sidechain
1	A	7	GLN	Sidechain
1	A	87	ASP	Sidechain
1	A	92	ASN	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	1180	0	1200	20	209
2	A	43	0	30	3	0
3	A	1	0	0	0	0
4	A	67	0	0	0	31
All	All	1291	0	1230	20	210

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 8.

All (20) 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	2.01	0.61
1:A:139:ASP:O	1:A:143:ILE:HG13	2.06	0.55
1:A:77:GLN:NE2	1:A:85:VAL:H	2.05	0.54
1:A:21:ASN:C	1:A:21:ASN:HD22	2.12	0.52
1:A:2:ALA:O	1:A:3:LEU:HB2	2.14	0.48
1:A:106:HIS:O	1:A:109:VAL:HB	2.14	0.48
1:A:63:HIS:HE1	2:A:154:HEM:C4D	2.32	0.47
1:A:93:LEU:HA	1:A:93:LEU:HD23	1.56	0.46
1:A:21:ASN:C	1:A:21:ASN:ND2	2.69	0.46
1:A:126:TRP:CZ2	1:A:131:ASN:HB2	2.52	0.45
1:A:18:PHE:CE1	1:A:25:HIS:HB3	2.53	0.44
1:A:100:LYS:HG3	2:A:154:HEM:HAD2	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PHE:O	1:A:33:VAL:HG23	2.18	0.44
1:A:17:GLU:OE2	1:A:122:VAL:HG12	2.18	0.42
1:A:26:THR:HB	1:A:64:ALA:HB3	2.01	0.42
1:A:31:ILE:O	1:A:35:GLU:HG3	2.20	0.41
1:A:102:VAL:HG13	2:A:154:HEM:HAC	2.02	0.41
1:A:86:THR:HA	1:A:90:LEU:HD12	2.01	0.41
1:A:37:ALA:HA	1:A:38:PRO:HD2	1.94	0.41

All (210) 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]	0.08	2.12
1:A:126:TRP:CD1	1:A:128:GLU:C[2_675]	0.40	1.80
1:A:9:ALA:CB	1:A:12:LYS:C[2_675]	0.42	1.78
1:A:127:SER:N	1:A:131:ASN:CA[2_675]	0.47	1.73
1:A:8:ALA:CA	1:A:13:SER:OG[2_675]	0.51	1.69
1:A:6:SER:O	1:A:14:SER:N[2_675]	0.58	1.62
1:A:126:TRP:NE1	1:A:128:GLU:CA[2_675]	0.64	1.56
1:A:6:SER:OG	1:A:14:SER:O[2_675]	0.72	1.48
1:A:119:LYS:CD	1:A:128:GLU:OE2[2_675]	0.73	1.47
1:A:9:ALA:N	1:A:13:SER:CA[2_675]	0.75	1.45
1:A:126:TRP:C	1:A:131:ASN:C[2_675]	0.75	1.45
1:A:10:LEU:CA	1:A:10:LEU:C[2_675]	0.76	1.44
1:A:126:TRP:C	1:A:131:ASN:CA[2_675]	0.79	1.41
1:A:119:LYS:CE	1:A:128:GLU:CG[2_675]	0.82	1.38
1:A:119:LYS:O	4:A:182:HOH:O[2_675]	0.83	1.37
1:A:8:ALA:C	1:A:13:SER:CB[2_675]	0.85	1.35
1:A:9:ALA:CA	1:A:13:SER:N[2_675]	0.88	1.32
1:A:10:LEU:CA	1:A:10:LEU:O[2_675]	0.96	1.24
1:A:126:TRP:CG	1:A:128:GLU:O[2_675]	0.97	1.23
1:A:10:LEU:O	1:A:10:LEU:CB[2_675]	1.02	1.18
1:A:126:TRP:NE1	1:A:128:GLU:N[2_675]	1.04	1.16
1:A:130:LEU:N	1:A:130:LEU:CD2[2_675]	1.07	1.13
1:A:130:LEU:O	4:A:192:HOH:O[2_675]	1.12	1.08
1:A:7:GLN:CA	4:A:203:HOH:O[2_675]	1.15	1.05
1:A:126:TRP:CD1	1:A:128:GLU:O[2_675]	1.15	1.05
1:A:134:TRP:N	4:A:219:HOH:O[2_675]	1.16	1.04
1:A:7:GLN:CG	1:A:17:GLU:OE2[2_675]	1.17	1.03
1:A:125:LYS:CB	1:A:133:ALA:CA[2_675]	1.17	1.03

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLN:NE2	1:A:122:VAL:CA[2_675]	1.17	1.03
1:A:127:SER:N	1:A:131:ASN:N[2_675]	1.19	1.01
1:A:7:GLN:C	4:A:203:HOH:O[2_675]	1.20	1.00
1:A:9:ALA:O	1:A:9:ALA:O[2_675]	1.23	0.97
1:A:125:LYS:C	1:A:133:ALA:N[2_675]	1.24	0.96
1:A:8:ALA:N	1:A:13:SER:OG[2_675]	1.25	0.95
1:A:9:ALA:CB	1:A:13:SER:N[2_675]	1.27	0.93
1:A:126:TRP:O	1:A:131:ASN:O[2_675]	1.27	0.93
1:A:119:LYS:CD	1:A:128:GLU:CD[2_675]	1.28	0.92
1:A:7:GLN:OE1	1:A:17:GLU:OE1[2_675]	1.28	0.92
1:A:126:TRP:O	1:A:131:ASN:C[2_675]	1.29	0.91
1:A:9:ALA:N	1:A:13:SER:CB[2_675]	1.29	0.91
1:A:7:GLN:CB	4:A:203:HOH:O[2_675]	1.32	0.88
1:A:6:SER:CB	1:A:14:SER:O[2_675]	1.33	0.87
1:A:123:GLY:O	1:A:132[B]:SER:OG[2_675]	1.33	0.87
1:A:6:SER:O	1:A:14:SER:CA[2_675]	1.33	0.87
1:A:6:SER:N	1:A:17:GLU:N[2_675]	1.34	0.86
1:A:4:THR:CB	1:A:17:GLU:CB[2_675]	1.35	0.85
1:A:126:TRP:CD1	1:A:128:GLU:CA[2_675]	1.37	0.83
1:A:122:VAL:N	1:A:129:GLU:OE2[2_675]	1.37	0.83
1:A:126:TRP:CE2	1:A:128:GLU:CA[2_675]	1.40	0.80
1:A:6:SER:C	1:A:14:SER:CA[2_675]	1.40	0.80
1:A:7:GLN:CB	1:A:17:GLU:OE2[2_675]	1.44	0.76
1:A:9:ALA:N	1:A:13:SER:N[2_675]	1.45	0.75
1:A:9:ALA:CB	1:A:12:LYS:CA[2_675]	1.45	0.75
1:A:130:LEU:CA	1:A:130:LEU:CD2[2_675]	1.45	0.75
1:A:7:GLN:CD	1:A:17:GLU:OE2[2_675]	1.47	0.73
1:A:6:SER:O	1:A:13:SER:C[2_675]	1.48	0.72
1:A:8:ALA:C	1:A:13:SER:OG[2_675]	1.48	0.72
1:A:126:TRP:CA	1:A:131:ASN:C[2_675]	1.49	0.71
1:A:126:TRP:CB	1:A:128:GLU:O[2_675]	1.51	0.69
1:A:6:SER:C	1:A:13:SER:O[2_675]	1.52	0.68
1:A:126:TRP:NE1	1:A:128:GLU:C[2_675]	1.52	0.68
1:A:130:LEU:CB	1:A:130:LEU:CG[2_675]	1.52	0.68
1:A:17:GLU:O	4:A:222:HOH:O[2_675]	1.52	0.68
1:A:4:THR:N	1:A:17:GLU:CG[2_675]	1.52	0.68
1:A:6:SER:C	1:A:14:SER:N[2_675]	1.52	0.68
1:A:7:GLN:OE1	1:A:17:GLU:OE2[2_675]	1.53	0.67
1:A:4:THR:OG1	1:A:17:GLU:CA[2_675]	1.54	0.66
1:A:125:LYS:O	1:A:133:ALA:N[2_675]	1.54	0.66
1:A:4:THR:CB	1:A:17:GLU:CA[2_675]	1.55	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ALA:CB	1:A:12:LYS:O[2_675]	1.56	0.64
1:A:126:TRP:CH2	1:A:126:TRP:CH2[2_675]	1.57	0.63
1:A:8:ALA:CA	1:A:13:SER:CB[2_675]	1.57	0.63
1:A:10:LEU:CG	1:A:14:SER:OG[2_675]	1.58	0.62
1:A:4:THR:CA	1:A:17:GLU:CG[2_675]	1.59	0.61
1:A:7:GLN:OE1	1:A:17:GLU:CD[2_675]	1.59	0.61
1:A:15:TRP:CB	4:A:221:HOH:O[2_675]	1.59	0.61
1:A:10:LEU:N	1:A:10:LEU:O[2_675]	1.60	0.60
1:A:10:LEU:CD1	1:A:14:SER:OG[2_675]	1.60	0.60
1:A:56:ASN:OD1	4:A:171:HOH:O[1_545]	1.61	0.59
1:A:123:GLY:C	1:A:132[C]:SER:OG[2_675]	1.62	0.58
1:A:122:VAL:CG2	1:A:132[A]:SER:OG[2_675]	1.62	0.58
1:A:134:TRP:CA	4:A:219:HOH:O[2_675]	1.62	0.58
1:A:17:GLU:C	4:A:222:HOH:O[2_675]	1.63	0.57
1:A:118:ILE:O	1:A:129:GLU:OE2[2_675]	1.63	0.57
1:A:6:SER:C	1:A:13:SER:C[2_675]	1.63	0.57
1:A:7:GLN:N	1:A:13:SER:O[2_675]	1.64	0.56
1:A:10:LEU:CD2	1:A:11:VAL:CA[2_675]	1.64	0.56
1:A:118:ILE:CG2	1:A:129:GLU:CB[2_675]	1.64	0.56
1:A:125:LYS:CA	1:A:133:ALA:N[2_675]	1.65	0.55
1:A:10:LEU:CA	1:A:10:LEU:CA[2_675]	1.65	0.55
1:A:4:THR:OG1	1:A:17:GLU:CG[2_675]	1.68	0.52
1:A:129:GLU:C	1:A:130:LEU:CD2[2_675]	1.68	0.52
1:A:126:TRP:CG	1:A:128:GLU:C[2_675]	1.68	0.52
1:A:5:GLU:C	1:A:16:GLU:CB[2_675]	1.68	0.52
1:A:126:TRP:C	1:A:131:ASN:CB[2_675]	1.69	0.51
1:A:6:SER:CB	1:A:14:SER:C[2_675]	1.69	0.51
1:A:124:ALA:O	1:A:135:THR:CB[2_675]	1.69	0.51
1:A:130:LEU:CA	1:A:130:LEU:CB[2_675]	1.69	0.51
1:A:125:LYS:CB	1:A:133:ALA:N[2_675]	1.70	0.50
1:A:126:TRP:CD1	1:A:129:GLU:N[2_675]	1.70	0.50
1:A:127:SER:CA	1:A:131:ASN:CA[2_675]	1.70	0.50
1:A:127:SER:N	1:A:131:ASN:CB[2_675]	1.71	0.49
1:A:9:ALA:CA	1:A:13:SER:CA[2_675]	1.72	0.48
1:A:6:SER:CB	1:A:15:TRP:CA[2_675]	1.72	0.48
1:A:56:ASN:N	4:A:170:HOH:O[1_545]	1.72	0.48
1:A:9:ALA:C	1:A:9:ALA:O[2_675]	1.72	0.48
1:A:126:TRP:NE1	1:A:127:SER:C[2_675]	1.72	0.48
1:A:9:ALA:C	1:A:13:SER:N[2_675]	1.73	0.47
1:A:6:SER:C	1:A:14:SER:C[2_675]	1.73	0.47
1:A:4:THR:O	4:A:206:HOH:O[2_675]	1.73	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TRP:O	1:A:131:ASN:CA[2_675]	1.74	0.46
1:A:7:GLN:N	1:A:14:SER:CA[2_675]	1.74	0.46
1:A:6:SER:CA	1:A:16:GLU:N[2_675]	1.75	0.45
1:A:5:GLU:CB	1:A:16:GLU:CB[2_675]	1.75	0.45
1:A:130:LEU:CA	1:A:130:LEU:CG[2_675]	1.77	0.43
1:A:10:LEU:C	1:A:10:LEU:CB[2_675]	1.79	0.41
4:A:159:HOH:O	4:A:177:HOH:O[2_675]	1.80	0.40
1:A:119:LYS:CG	1:A:128:GLU:CB[2_675]	1.80	0.40
1:A:10:LEU:O	1:A:10:LEU:CG[2_675]	1.81	0.39
1:A:118:ILE:O	1:A:129:GLU:CD[2_675]	1.81	0.39
1:A:6:SER:CB	1:A:15:TRP:N[2_675]	1.81	0.39
1:A:6:SER:N	1:A:16:GLU:N[2_675]	1.82	0.38
1:A:4:THR:N	1:A:17:GLU:CD[2_675]	1.82	0.38
1:A:6:SER:CB	1:A:15:TRP:C[2_675]	1.82	0.38
1:A:127:SER:N	1:A:131:ASN:C[2_675]	1.82	0.38
1:A:6:SER:CA	1:A:15:TRP:N[2_675]	1.82	0.38
1:A:119:LYS:C	4:A:182:HOH:O[2_675]	1.82	0.38
1:A:7:GLN:NE2	1:A:122:VAL:CB[2_675]	1.83	0.37
1:A:126:TRP:N	1:A:131:ASN:C[2_675]	1.83	0.37
1:A:7:GLN:NE2	1:A:122:VAL:C[2_675]	1.83	0.37
1:A:15:TRP:N	4:A:221:HOH:O[2_675]	1.84	0.36
1:A:126:TRP:C	1:A:131:ASN:O[2_675]	1.84	0.36
1:A:123:GLY:O	1:A:132[C]:SER:OG[2_675]	1.84	0.36
1:A:5:GLU:CG	1:A:16:GLU:CB[2_675]	1.84	0.36
1:A:122:VAL:O	1:A:132[C]:SER:OG[2_675]	1.85	0.35
1:A:8:ALA:O	1:A:13:SER:CB[2_675]	1.86	0.34
1:A:125:LYS:O	1:A:130:LEU:O[2_675]	1.86	0.34
1:A:5:GLU:CA	1:A:16:GLU:CB[2_675]	1.88	0.32
1:A:135:THR:OG1	4:A:159:HOH:O[2_675]	1.88	0.32
1:A:122:VAL:CG2	1:A:129:GLU:O[2_675]	1.88	0.32
1:A:4:THR:C	1:A:17:GLU:CG[2_675]	1.88	0.32
1:A:6:SER:CA	1:A:14:SER:C[2_675]	1.89	0.31
1:A:56:ASN:CB	4:A:189:HOH:O[1_545]	1.89	0.31
1:A:119:LYS:CG	1:A:128:GLU:OE2[2_675]	1.90	0.30
1:A:6:SER:OG	1:A:14:SER:C[2_675]	1.91	0.29
1:A:119:LYS:CD	1:A:128:GLU:CG[2_675]	1.91	0.29
1:A:9:ALA:CA	1:A:12:LYS:C[2_675]	1.92	0.28
1:A:56:ASN:OD1	4:A:170:HOH:O[1_545]	1.92	0.28
1:A:10:LEU:CD1	1:A:14:SER:CB[2_675]	1.92	0.28
1:A:6:SER:N	1:A:16:GLU:C[2_675]	1.92	0.28
1:A:126:TRP:C	1:A:131:ASN:N[2_675]	1.93	0.27

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:N	4:A:212:HOH:O[2_675]	1.93	0.27
1:A:126:TRP:CE2	1:A:128:GLU:N[2_675]	1.93	0.27
1:A:11:VAL:O	4:A:221:HOH:O[2_675]	1.95	0.25
1:A:10:LEU:N	1:A:10:LEU:C[2_675]	1.95	0.25
1:A:10:LEU:C	1:A:10:LEU:C[2_675]	1.95	0.25
1:A:126:TRP:O	1:A:131:ASN:CG[2_675]	1.96	0.24
1:A:7:GLN:CG	1:A:122:VAL:CG1[2_675]	1.97	0.23
1:A:8:ALA:C	1:A:13:SER:CA[2_675]	1.97	0.23
1:A:130:LEU:N	1:A:130:LEU:CG[2_675]	1.98	0.22
1:A:8:ALA:CB	1:A:13:SER:OG[2_675]	1.98	0.22
1:A:4:THR:N	1:A:17:GLU:OE1[2_675]	1.99	0.21
1:A:6:SER:N	1:A:16:GLU:CA[2_675]	1.99	0.21
1:A:7:GLN:C	1:A:13:SER:OG[2_675]	2.00	0.20
1:A:4:THR:CB	1:A:17:GLU:CG[2_675]	2.00	0.20
1:A:15:TRP:CA	4:A:221:HOH:O[2_675]	2.01	0.19
1:A:7:GLN:O	4:A:203:HOH:O[2_675]	2.02	0.18
1:A:122:VAL:CG2	1:A:129:GLU:CA[2_675]	2.03	0.17
1:A:126:TRP:CB	4:A:191:HOH:O[2_675]	2.03	0.17
1:A:126:TRP:CB	1:A:132[B]:SER:OG[2_675]	2.04	0.16
1:A:130:LEU:C	4:A:192:HOH:O[2_675]	2.05	0.15
1:A:4:THR:O	1:A:17:GLU:CG[2_675]	2.05	0.15
1:A:121:VAL:CB	1:A:129:GLU:OE1[2_675]	2.06	0.14
1:A:126:TRP:CZ3	1:A:126:TRP:CH2[2_675]	2.06	0.14
1:A:8:ALA:N	1:A:13:SER:CB[2_675]	2.08	0.12
1:A:56:ASN:CB	4:A:170:HOH:O[1_545]	2.08	0.12
1:A:5:GLU:O	1:A:16:GLU:CB[2_675]	2.08	0.12
1:A:125:LYS:CB	1:A:133:ALA:C[2_675]	2.08	0.12
1:A:8:ALA:N	4:A:203:HOH:O[2_675]	2.08	0.12
1:A:5:GLU:O	1:A:13:SER:O[2_675]	2.08	0.12
1:A:7:GLN:NE2	1:A:122:VAL:O[2_675]	2.10	0.10
1:A:133:ALA:C	4:A:219:HOH:O[2_675]	2.11	0.09
1:A:126:TRP:CG	1:A:128:GLU:CA[2_675]	2.11	0.09
1:A:119:LYS:NZ	1:A:128:GLU:CG[2_675]	2.11	0.09
1:A:122:VAL:CG1	1:A:129:GLU:CG[2_675]	2.11	0.09
1:A:5:GLU:C	1:A:16:GLU:CA[2_675]	2.12	0.08
1:A:7:GLN:N	1:A:13:SER:C[2_675]	2.12	0.08
1:A:122:VAL:CG2	1:A:129:GLU:C[2_675]	2.12	0.08
1:A:126:TRP:CA	1:A:131:ASN:CA[2_675]	2.13	0.07
1:A:7:GLN:N	1:A:14:SER:N[2_675]	2.13	0.07
1:A:55:GLN:OE1	4:A:172:HOH:O[1_545]	2.14	0.06
1:A:122:VAL:C	1:A:132[C]:SER:OG[2_675]	2.14	0.06

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TRP:N	1:A:133:ALA:N[2_675]	2.14	0.06
1:A:119:LYS:CE	1:A:128:GLU:CB[2_675]	2.14	0.06
1:A:119:LYS:CB	1:A:128:GLU:CB[2_675]	2.15	0.05
1:A:18:PHE:N	4:A:222:HOH:O[2_675]	2.16	0.04
1:A:5:GLU:CG	1:A:16:GLU:CG[2_675]	2.16	0.04
1:A:125:LYS:CA	1:A:133:ALA:CA[2_675]	2.16	0.04
1:A:5:GLU:N	1:A:17:GLU:N[2_675]	2.17	0.03
1:A:16:GLU:O	4:A:222:HOH:O[2_675]	2.17	0.03
1:A:6:SER:O	1:A:14:SER:C[2_675]	2.18	0.02
1:A:125:LYS:O	1:A:134:TRP:N[2_675]	2.18	0.02
1:A:3:LEU:CG	1:A:125:LYS:CE[2_675]	2.18	0.02
1:A:127:SER:N	1:A:130:LEU:C[2_675]	2.18	0.02
1:A:125:LYS:O	1:A:133:ALA:CA[2_675]	2.19	0.01
1:A:126:TRP:O	1:A:131:ASN:CB[2_675]	2.19	0.01
1:A:7:GLN:CA	1:A:14:SER:CA[2_675]	2.19	0.01
1:A:126:TRP:NE1	1:A:128:GLU:CB[2_675]	2.19	0.01
1:A:6:SER:C	1:A:15:TRP:N[2_675]	2.19	0.01
1:A:126:TRP:CD2	1:A:128:GLU:CA[2_675]	2.19	0.01

## 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	153/153 (100%)	148 (97%)	3 (2%)	2 (1%)	<b>15</b> <b>7</b>

All (2) Ramachandran outliers are listed below:

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

### 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	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 [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

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	$\# Z  > 2$
2	HEM	A	154	1,3	30,50,50	4.32	22 (73%)	24,82,82	2.70	11 (45%)

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
2	HEM	A	154	1,3	-	0/10/54/54	0/0/8/8

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	C2D-C3D	-6.10	1.36	1.54
2	A	154	HEM	C2C-C1C	-3.11	1.46	1.52
2	A	154	HEM	C2D-C1D	2.21	1.59	1.51
2	A	154	HEM	CMA-C3A	2.77	1.57	1.51
2	A	154	HEM	CMB-C2B	3.11	1.60	1.53
2	A	154	HEM	CMD-C2D	3.18	1.60	1.53
2	A	154	HEM	CMC-C2C	3.19	1.60	1.53
2	A	154	HEM	C3C-CAC	3.20	1.57	1.51
2	A	154	HEM	C2A-C3A	3.28	1.47	1.37
2	A	154	HEM	C1A-CHA	3.47	1.49	1.39
2	A	154	HEM	FE-ND	3.57	2.16	1.97
2	A	154	HEM	C4A-CHB	4.09	1.51	1.39
2	A	154	HEM	C3D-C4D	4.11	1.56	1.51
2	A	154	HEM	CAA-C2A	5.21	1.60	1.52
2	A	154	HEM	CAD-C3D	5.31	1.64	1.54
2	A	154	HEM	CHC-C1C	5.36	1.48	1.36
2	A	154	HEM	CHD-C4C	6.17	1.50	1.36
2	A	154	HEM	C3B-C4B	6.37	1.57	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	C4C-NC	6.42	1.44	1.36
2	A	154	HEM	FE-NB	6.61	2.32	1.97
2	A	154	HEM	C3B-CAB	7.23	1.64	1.51
2	A	154	HEM	C1C-NC	8.76	1.46	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	154	HEM	CMA-C3A-C4A	-4.70	120.58	128.36
2	A	154	HEM	CAA-C2A-C1A	-4.49	122.13	127.01
2	A	154	HEM	C2C-C1C-NC	-2.56	105.90	110.21
2	A	154	HEM	CBA-CAA-C2A	-2.36	108.31	112.53
2	A	154	HEM	C3C-CAC-CBC	-2.09	121.25	124.46
2	A	154	HEM	CMA-C3A-C2A	2.01	129.44	125.24
2	A	154	HEM	CMD-C2D-C3D	2.28	124.42	114.35
2	A	154	HEM	CMB-C2B-C3B	3.77	125.93	116.53
2	A	154	HEM	CAD-C3D-C2D	4.41	125.91	113.22
2	A	154	HEM	CAD-C3D-C4D	4.84	129.55	112.47
2	A	154	HEM	CMC-C2C-C3C	5.51	130.28	116.53

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
2	A	154	HEM	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	153/153 (100%)	16.12	153 (100%) 0 0	7, 17, 49, 66	19 (12%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	LEU	37.8
1	A	93	LEU	34.9
1	A	143	ILE	31.5
1	A	75	ALA	29.2
1	A	60	LEU	28.3
1	A	109	VAL	27.6
1	A	85	VAL	26.4
1	A	67	VAL	25.7
1	A	36	ILE	25.6
1	A	97	HIS	24.6
1	A	47	LEU	24.6
1	A	84	VAL	24.3
1	A	30	PHE	24.2
1	A	4	THR	24.2
1	A	34	LEU	24.1
1	A	53	VAL	24.1
1	A	38	PRO	23.9
1	A	145	ILE	23.7
1	A	72	TYR	23.5
1	A	113	ALA	23.0
1	A	107	PHE	22.9
1	A	11	VAL	22.8
1	A	46	PHE	22.7
1	A	96	VAL	22.7
1	A	89	THR	22.6
1	A	65	GLY	22.5
1	A	25	HIS	22.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	64	ALA	22.1
1	A	114	ILE	21.6
1	A	126	TRP	21.4
1	A	149	MET	20.7
1	A	110	VAL	20.5
1	A	43	LEU	20.2
1	A	6	SER	20.2
1	A	134	TRP	20.1
1	A	29	PHE	20.1
1	A	138	TYR	20.0
1	A	102	VAL	20.0
1	A	63	HIS	19.1
1	A	140	GLU	18.7
1	A	141	LEU	18.5
1	A	13	SER	18.2
1	A	86	THR	18.1
1	A	18	PHE	18.0
1	A	105	ALA	17.9
1	A	122	VAL	17.7
1	A	90	LEU	17.6
1	A	44	PHE	17.6
1	A	135	THR	17.5
1	A	45	SER	17.4
1	A	118	ILE	17.4
1	A	37	ALA	17.3
1	A	2	ALA	17.1
1	A	31	ILE	17.0
1	A	57	ASN	16.9
1	A	16	GLU	16.9
1	A	21	ASN	16.9
1	A	68	PHE	16.8
1	A	133	ALA	16.8
1	A	99	SER	16.7
1	A	78	LEU	16.6
1	A	40	ALA	16.6
1	A	136	ILE	16.6
1	A	14	SER	16.1
1	A	49	GLY	16.1
1	A	142	ALA	16.0
1	A	144	VAL	16.0
1	A	26	THR	15.9
1	A	12	LYS	15.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	119	LYS	15.8
1	A	3	LEU	15.8
1	A	61	GLN	15.7
1	A	42	ASP	15.5
1	A	19	ASN	15.4
1	A	33	VAL	15.3
1	A	23	PRO	15.0
1	A	152	ALA	14.8
1	A	1	GLY	14.8
1	A	132[A]	SER	14.6
1	A	124	ALA	14.6
1	A	9	ALA	14.5
1	A	70	LEU	14.3
1	A	91	LYS	14.2
1	A	115	LEU	14.1
1	A	20	ALA	14.1
1	A	71	VAL	14.0
1	A	8	ALA	14.0
1	A	77	GLN	13.8
1	A	10	LEU	13.8
1	A	56	ASN	13.7
1	A	121	VAL	13.7
1	A	15	TRP	13.5
1	A	69	LYS	13.5
1	A	41	LYS	13.4
1	A	5	GLU	13.4
1	A	48	LYS	13.3
1	A	111	LYS	13.2
1	A	88	ALA	13.2
1	A	98	VAL	13.2
1	A	7	GLN	13.1
1	A	51	SER	13.0
1	A	95	SER	13.0
1	A	74	ALA	12.9
1	A	35	GLU	12.8
1	A	130	LEU	12.7
1	A	73	GLU	12.7
1	A	80	VAL	12.7
1	A	127	SER	12.4
1	A	55	GLN	12.0
1	A	83	VAL	11.9
1	A	58	PRO	11.9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	150	ASP	11.9
1	A	129	GLU	11.9
1	A	117	THR	11.8
1	A	79	GLU	11.8
1	A	128	GLU	11.8
1	A	123	GLY	11.7
1	A	22	ILE	11.6
1	A	146	LYS	11.6
1	A	116	LYS	11.6
1	A	66	LYS	11.5
1	A	81	THR	11.5
1	A	82	GLY	11.4
1	A	27	HIS	11.2
1	A	139	ASP	11.2
1	A	112	GLU	11.1
1	A	147	LYS	11.0
1	A	76	ILE	10.9
1	A	104	ASP	10.8
1	A	24	LYS	10.7
1	A	59	GLU	10.7
1	A	151	ASP	10.7
1	A	120	GLU	10.4
1	A	125	LYS	10.4
1	A	62	ALA	10.4
1	A	17	GLU	10.3
1	A	131	ASN	10.1
1	A	100	LYS	10.1
1	A	28	ARG	10.0
1	A	101	GLY	9.9
1	A	50	THR	9.7
1	A	103	ALA	9.7
1	A	54	PRO	9.6
1	A	39	ALA	9.5
1	A	148	GLU	9.5
1	A	108	PRO	9.3
1	A	137	ALA	9.3
1	A	94	GLY	9.2
1	A	106	HIS	9.1
1	A	92	ASN	8.9
1	A	87	ASP	8.5
1	A	153	ALA	8.5
1	A	52	GLU	7.6

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	154	43/43	-0.06	1.04	-0.19	0,15,37,45	3
3	O	A	155	1/1	0.00	1.90	-	8,8,8,8	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.