



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:40 PM GMT

PDB ID : 1LH6  
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

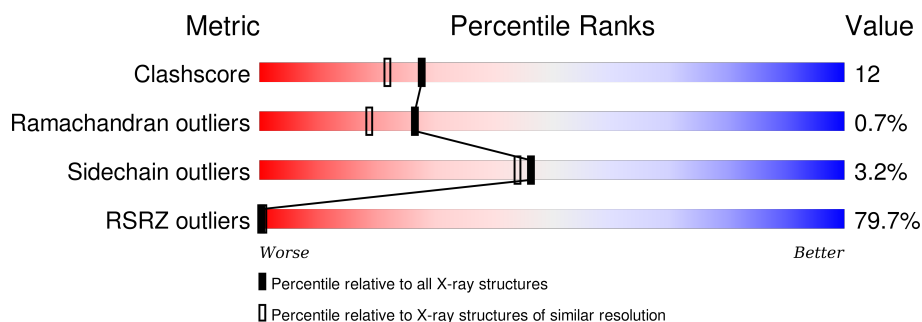
# 1 Overall quality at a glance

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	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1297 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.

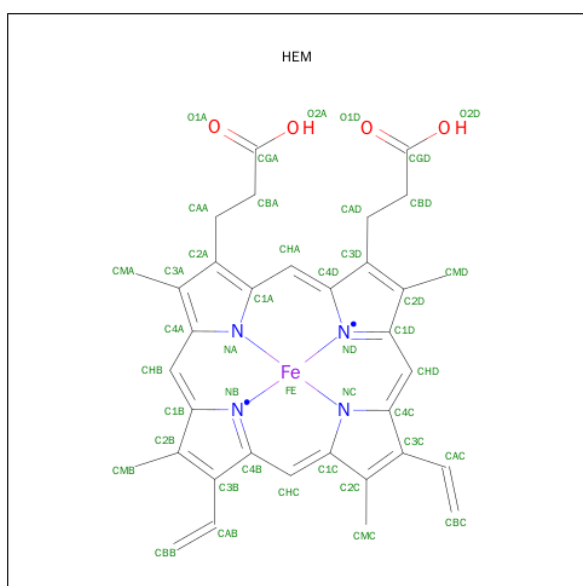
- Molecule 1 is a protein called LEGHEMOGLOBIN A (NICOTINATE MET).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	35	1	0
			1180	761	193	225	1			

There are 2 discrepancies between the modelled and reference sequences:

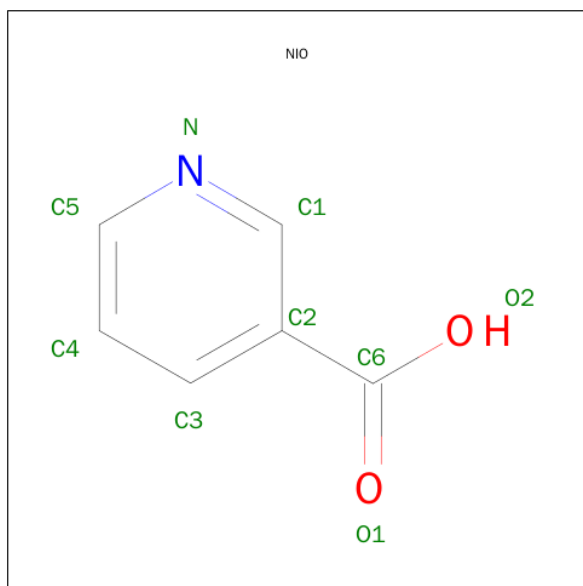
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLU	GLN	CONFLICT	UNP P02240
A	150	ASP	ASN	CONFLICT	UNP P02240

- 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 NICOTINIC ACID (three-letter code: NIO) (formula:  $C_6H_5NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		

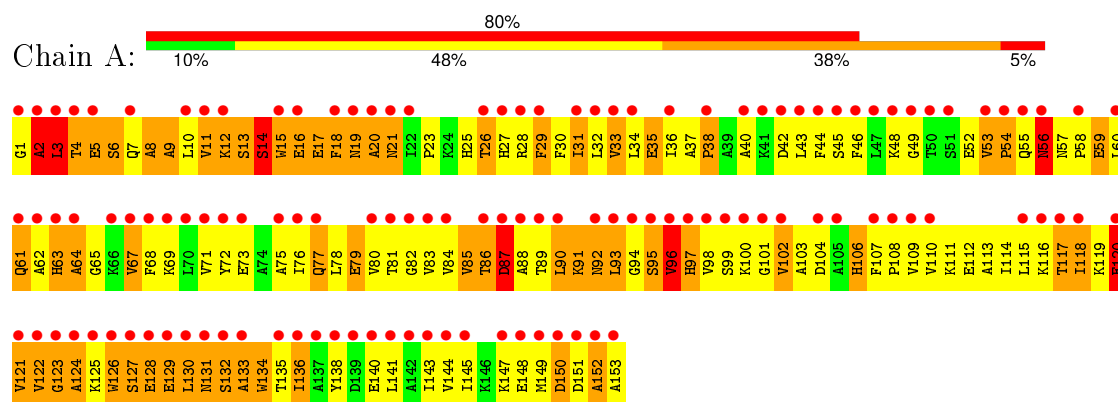
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total	O	0	0
			65	65		

### 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 A (NICOTINATE MET)



## 4 Data and refinement statistics

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.92Å 38.64Å 52.36Å 90.00° 90.00° 99.60°	Depositor
Resolution (Å)	(Not available) – 2.00 9.99 – 1.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 91.9 (9.99-1.99)	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) 0.485 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.214	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>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 11555 reflections	Xtriage
$F_o, F_c$ correlation	0.52	EDS
Total number of atoms	1297	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 11.51% 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, NIO

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	3.52	190/1214 (15.7%)	2.42	66/1648 (4.0%)

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	12

All (190) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	TYR	CB-CG	12.03	1.69	1.51
1	A	95	SER	CB-OG	11.30	1.56	1.42
1	A	112	GLU	CG-CD	11.20	1.68	1.51
1	A	15	TRP	CD2-CE2	10.60	1.54	1.41
1	A	132[A]	SER	CA-CB	9.88	1.67	1.52
1	A	132[B]	SER	CA-CB	9.88	1.67	1.52
1	A	132[C]	SER	CA-CB	9.88	1.67	1.52
1	A	148	GLU	CD-OE2	9.45	1.36	1.25
1	A	101	GLY	CA-C	9.44	1.67	1.51
1	A	138	TYR	CZ-OH	9.22	1.53	1.37
1	A	120	GLU	CG-CD	9.15	1.65	1.51
1	A	45	SER	CB-OG	8.95	1.53	1.42
1	A	121	VAL	CB-CG2	8.70	1.71	1.52
1	A	106	HIS	CB-CG	8.69	1.65	1.50
1	A	27	HIS	CE1-NE2	8.60	1.52	1.32
1	A	123	GLY	CA-C	8.59	1.65	1.51
1	A	94	GLY	CA-C	8.57	1.65	1.51
1	A	129	GLU	CD-OE1	8.56	1.35	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	VAL	CB-CG2	8.56	1.70	1.52
1	A	15	TRP	CD1-NE1	8.50	1.52	1.38
1	A	11	VAL	CB-CG1	8.49	1.70	1.52
1	A	44	PHE	CB-CG	8.48	1.65	1.51
1	A	16	GLU	CG-CD	8.47	1.64	1.51
1	A	72	TYR	CE1-CZ	8.41	1.49	1.38
1	A	35	GLU	CD-OE2	8.40	1.34	1.25
1	A	45	SER	N-CA	8.34	1.63	1.46
1	A	13	SER	CA-CB	8.15	1.65	1.52
1	A	111	LYS	N-CA	8.12	1.62	1.46
1	A	124	ALA	N-CA	8.09	1.62	1.46
1	A	73	GLU	CG-CD	8.02	1.64	1.51
1	A	15	TRP	CZ3-CH2	7.96	1.52	1.40
1	A	99	SER	N-CA	7.96	1.62	1.46
1	A	15	TRP	CB-CG	7.94	1.64	1.50
1	A	6	SER	CA-CB	7.92	1.64	1.52
1	A	59	GLU	CD-OE1	-7.92	1.17	1.25
1	A	18	PHE	CB-CG	7.91	1.64	1.51
1	A	27	HIS	CG-ND1	7.91	1.56	1.38
1	A	68	PHE	CG-CD2	7.81	1.50	1.38
1	A	113	ALA	CA-CB	7.80	1.68	1.52
1	A	46	PHE	CB-CG	7.74	1.64	1.51
1	A	140	GLU	CB-CG	7.54	1.66	1.52
1	A	79	GLU	CB-CG	7.51	1.66	1.52
1	A	40	ALA	CA-CB	7.50	1.68	1.52
1	A	65	GLY	C-O	7.41	1.35	1.23
1	A	138	TYR	CD2-CE2	7.38	1.50	1.39
1	A	85	VAL	CB-CG2	7.38	1.68	1.52
1	A	68	PHE	CE1-CZ	7.32	1.51	1.37
1	A	102	VAL	CB-CG1	7.30	1.68	1.52
1	A	15	TRP	CG-CD1	7.28	1.47	1.36
1	A	122	VAL	N-CA	7.27	1.60	1.46
1	A	124	ALA	C-O	7.25	1.37	1.23
1	A	84	VAL	CB-CG1	7.18	1.68	1.52
1	A	72	TYR	C-O	7.15	1.36	1.23
1	A	9	ALA	CA-CB	7.13	1.67	1.52
1	A	138	TYR	CD1-CE1	7.09	1.50	1.39
1	A	18	PHE	N-CA	7.08	1.60	1.46
1	A	28	ARG	CZ-NH1	7.00	1.42	1.33
1	A	90	LEU	CA-CB	6.97	1.69	1.53
1	A	128	GLU	CG-CD	6.94	1.62	1.51
1	A	88	ALA	N-CA	6.90	1.60	1.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	ASP	N-CA	6.87	1.60	1.46
1	A	15	TRP	C-O	6.82	1.36	1.23
1	A	110	VAL	CB-CG2	6.79	1.67	1.52
1	A	95	SER	N-CA	6.79	1.59	1.46
1	A	133	ALA	CA-C	6.79	1.70	1.52
1	A	86	THR	N-CA	6.74	1.59	1.46
1	A	61	GLN	C-O	6.72	1.36	1.23
1	A	68	PHE	C-O	6.72	1.36	1.23
1	A	109	VAL	CA-CB	6.70	1.68	1.54
1	A	11	VAL	N-CA	6.68	1.59	1.46
1	A	148	GLU	CB-CG	6.68	1.64	1.52
1	A	81	THR	CA-CB	6.67	1.70	1.53
1	A	128	GLU	CD-OE2	-6.63	1.18	1.25
1	A	82	GLY	CA-C	6.62	1.62	1.51
1	A	13	SER	N-CA	-6.62	1.33	1.46
1	A	149	MET	N-CA	6.61	1.59	1.46
1	A	18	PHE	CD2-CE2	6.61	1.52	1.39
1	A	117	THR	CB-OG1	6.57	1.56	1.43
1	A	134	TRP	N-CA	6.55	1.59	1.46
1	A	72	TYR	CG-CD2	6.53	1.47	1.39
1	A	75	ALA	C-O	6.52	1.35	1.23
1	A	53	VAL	CA-CB	6.49	1.68	1.54
1	A	83	VAL	N-CA	6.46	1.59	1.46
1	A	106	HIS	ND1-CE1	6.45	1.50	1.34
1	A	99	SER	C-O	6.44	1.35	1.23
1	A	152	ALA	C-O	6.41	1.35	1.23
1	A	61	GLN	N-CA	6.41	1.59	1.46
1	A	55	GLN	C-O	6.41	1.35	1.23
1	A	97	HIS	CG-CD2	-6.38	1.25	1.35
1	A	4	THR	C-O	6.35	1.35	1.23
1	A	145	ILE	N-CA	6.34	1.59	1.46
1	A	97	HIS	CA-CB	6.32	1.67	1.53
1	A	127	SER	CA-CB	6.29	1.62	1.52
1	A	136	ILE	CA-CB	6.28	1.69	1.54
1	A	35	GLU	CD-OE1	-6.27	1.18	1.25
1	A	5	GLU	CD-OE2	6.25	1.32	1.25
1	A	85	VAL	CA-C	6.25	1.69	1.52
1	A	67	VAL	CB-CG2	6.20	1.65	1.52
1	A	140	GLU	CD-OE2	6.20	1.32	1.25
1	A	75	ALA	N-CA	6.19	1.58	1.46
1	A	120	GLU	CA-CB	6.18	1.67	1.53
1	A	91	LYS	CD-CE	6.17	1.66	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	PHE	CG-CD2	-6.17	1.29	1.38
1	A	138	TYR	N-CA	6.17	1.58	1.46
1	A	111	LYS	CD-CE	6.16	1.66	1.51
1	A	5	GLU	CD-OE1	-6.15	1.18	1.25
1	A	13	SER	CB-OG	-6.14	1.34	1.42
1	A	29	PHE	CG-CD2	6.14	1.48	1.38
1	A	77	GLN	CG-CD	6.09	1.65	1.51
1	A	130	LEU	N-CA	6.04	1.58	1.46
1	A	11	VAL	CA-CB	-5.97	1.42	1.54
1	A	52	GLU	CG-CD	-5.97	1.43	1.51
1	A	115	LEU	N-CA	5.96	1.58	1.46
1	A	110	VAL	CA-C	5.90	1.68	1.52
1	A	8	ALA	C-O	5.88	1.34	1.23
1	A	79	GLU	CD-OE2	5.83	1.32	1.25
1	A	92	ASN	C-O	5.82	1.34	1.23
1	A	111	LYS	CB-CG	5.78	1.68	1.52
1	A	71	VAL	CB-CG1	5.77	1.65	1.52
1	A	140	GLU	CG-CD	-5.75	1.43	1.51
1	A	30	PHE	CA-CB	5.72	1.66	1.53
1	A	5	GLU	CG-CD	5.61	1.60	1.51
1	A	58	PRO	CA-C	-5.59	1.41	1.52
1	A	147	LYS	CA-CB	5.58	1.66	1.53
1	A	141	LEU	N-CA	5.58	1.57	1.46
1	A	107	PHE	N-CA	5.57	1.57	1.46
1	A	9	ALA	N-CA	-5.57	1.35	1.46
1	A	46	PHE	N-CA	-5.56	1.35	1.46
1	A	52	GLU	N-CA	5.55	1.57	1.46
1	A	98	VAL	CA-C	5.53	1.67	1.52
1	A	67	VAL	CA-C	5.52	1.67	1.52
1	A	79	GLU	C-O	5.51	1.33	1.23
1	A	68	PHE	N-CA	5.50	1.57	1.46
1	A	108	PRO	C-N	5.47	1.46	1.34
1	A	20	ALA	CA-CB	5.46	1.64	1.52
1	A	97	HIS	C-N	-5.43	1.21	1.34
1	A	148	GLU	CD-OE1	5.43	1.31	1.25
1	A	143	ILE	CA-CB	5.42	1.67	1.54
1	A	127	SER	C-O	5.42	1.33	1.23
1	A	55	GLN	N-CA	5.40	1.57	1.46
1	A	147	LYS	N-CA	-5.39	1.35	1.46
1	A	20	ALA	N-CA	-5.38	1.35	1.46
1	A	152	ALA	N-CA	5.37	1.57	1.46
1	A	96	VAL	CB-CG1	5.36	1.64	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	TYR	CZ-OH	5.35	1.47	1.37
1	A	149	MET	C-O	5.33	1.33	1.23
1	A	148	GLU	C-O	5.33	1.33	1.23
1	A	28	ARG	CZ-NH2	5.31	1.40	1.33
1	A	87	ASP	CA-C	5.30	1.66	1.52
1	A	29	PHE	CE1-CZ	5.30	1.47	1.37
1	A	63	HIS	CB-CG	5.30	1.59	1.50
1	A	65	GLY	N-CA	5.29	1.53	1.46
1	A	126	TRP	N-CA	-5.29	1.35	1.46
1	A	8	ALA	N-CA	5.28	1.56	1.46
1	A	43	LEU	CA-CB	5.28	1.65	1.53
1	A	64	ALA	N-CA	5.26	1.56	1.46
1	A	141	LEU	CB-CG	5.25	1.67	1.52
1	A	76	ILE	C-O	5.24	1.33	1.23
1	A	29	PHE	CE2-CZ	5.23	1.47	1.37
1	A	32	LEU	N-CA	5.23	1.56	1.46
1	A	26	THR	C-N	-5.23	1.22	1.34
1	A	63	HIS	CA-C	5.22	1.66	1.52
1	A	118	ILE	CB-CG2	5.21	1.69	1.52
1	A	44	PHE	CD2-CE2	5.19	1.49	1.39
1	A	23	PRO	N-CA	5.18	1.56	1.47
1	A	102	VAL	N-CA	5.18	1.56	1.46
1	A	3	LEU	CA-CB	5.17	1.65	1.53
1	A	14	SER	CA-C	5.17	1.66	1.52
1	A	18	PHE	CD1-CE1	5.17	1.49	1.39
1	A	58	PRO	N-CD	5.16	1.55	1.47
1	A	144	VAL	CA-C	5.16	1.66	1.52
1	A	44	PHE	CD1-CE1	5.15	1.49	1.39
1	A	69	LYS	C-O	5.14	1.33	1.23
1	A	2	ALA	CA-CB	5.14	1.63	1.52
1	A	55	GLN	CD-OE1	5.13	1.35	1.24
1	A	153	ALA	C-OXT	5.13	1.33	1.23
1	A	118	ILE	N-CA	5.12	1.56	1.46
1	A	93	LEU	C-N	-5.11	1.23	1.33
1	A	15	TRP	NE1-CE2	-5.10	1.30	1.37
1	A	48	LYS	N-CA	5.10	1.56	1.46
1	A	38	PRO	N-CA	5.08	1.55	1.47
1	A	28	ARG	CA-CB	5.07	1.65	1.53
1	A	152	ALA	CA-CB	-5.07	1.41	1.52
1	A	92	ASN	CB-CG	5.07	1.62	1.51
1	A	54	PRO	C-N	-5.06	1.22	1.34
1	A	71	VAL	N-CA	5.06	1.56	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	PHE	N-CA	-5.05	1.36	1.46
1	A	68	PHE	CE2-CZ	5.05	1.47	1.37
1	A	131	ASN	CA-C	-5.03	1.39	1.52
1	A	52	GLU	CA-CB	-5.01	1.43	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ARG	NE-CZ-NH2	-10.96	114.82	120.30
1	A	16	GLU	OE1-CD-OE2	-10.38	110.85	123.30
1	A	112	GLU	OE1-CD-OE2	-10.23	111.02	123.30
1	A	15	TRP	CG-CD2-CE3	-10.15	124.77	133.90
1	A	73	GLU	OE1-CD-OE2	-8.73	112.82	123.30
1	A	138	TYR	CB-CG-CD2	8.70	126.22	121.00
1	A	124	ALA	CB-CA-C	-8.46	97.41	110.10
1	A	128	GLU	OE1-CD-OE2	-8.30	113.34	123.30
1	A	30	PHE	CB-CG-CD2	-8.07	115.15	120.80
1	A	29	PHE	CB-CG-CD1	-7.84	115.31	120.80
1	A	87	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	A	126	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	A	15	TRP	CD1-NE1-CE2	-7.33	102.40	109.00
1	A	59	GLU	OE1-CD-OE2	-7.19	114.67	123.30
1	A	134	TRP	CG-CD1-NE1	-7.11	102.99	110.10
1	A	54	PRO	N-CA-CB	6.89	111.56	103.30
1	A	5	GLU	OE1-CD-OE2	-6.88	115.04	123.30
1	A	15	TRP	CH2-CZ2-CE2	-6.81	110.59	117.40
1	A	68	PHE	CB-CG-CD1	-6.81	116.03	120.80
1	A	31	ILE	CB-CA-C	-6.80	97.99	111.60
1	A	15	TRP	CB-CG-CD1	6.79	135.83	127.00
1	A	108	PRO	N-CA-CB	6.64	111.27	103.30
1	A	72	TYR	CG-CD1-CE1	-6.57	116.05	121.30
1	A	29	PHE	CD1-CG-CD2	6.55	126.82	118.30
1	A	15	TRP	CD2-CE3-CZ3	-6.48	110.37	118.80
1	A	23	PRO	N-CA-CB	6.45	111.03	103.30
1	A	134	TRP	CD1-CG-CD2	6.34	111.37	106.30
1	A	36	ILE	CG1-CB-CG2	-6.28	97.59	111.40
1	A	80	VAL	CA-CB-CG2	-6.26	101.51	110.90
1	A	138	TYR	CG-CD2-CE2	6.25	126.30	121.30
1	A	48	LYS	CB-CA-C	-6.18	98.05	110.40
1	A	19	ASN	N-CA-CB	-6.07	99.67	110.60
1	A	15	TRP	CE2-CD2-CE3	6.05	125.96	118.70
1	A	15	TRP	NE1-CE2-CZ2	-6.05	123.75	130.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ASN	O-C-N	6.04	132.36	122.70
1	A	138	TYR	CD1-CE1-CZ	6.00	125.20	119.80
1	A	46	PHE	CB-CG-CD2	5.97	124.98	120.80
1	A	83	VAL	CB-CA-C	-5.92	100.15	111.40
1	A	152	ALA	CB-CA-C	-5.84	101.33	110.10
1	A	133	ALA	O-C-N	-5.83	113.38	122.70
1	A	3	LEU	CB-CA-C	5.73	121.08	110.20
1	A	49	GLY	CA-C-O	-5.66	110.41	120.60
1	A	78	LEU	CB-CG-CD2	-5.65	101.40	111.00
1	A	102	VAL	CA-CB-CG2	-5.57	102.54	110.90
1	A	83	VAL	CA-CB-CG1	-5.52	102.62	110.90
1	A	17	GLU	OE1-CD-OE2	-5.51	116.69	123.30
1	A	33	VAL	CB-CA-C	-5.46	101.02	111.40
1	A	126	TRP	CD1-CG-CD2	5.43	110.65	106.30
1	A	72	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	A	118	ILE	CB-CA-C	-5.41	100.78	111.60
1	A	85	VAL	O-C-N	-5.39	114.08	122.70
1	A	126	TRP	NE1-CE2-CD2	5.38	112.67	107.30
1	A	43	LEU	CB-CG-CD2	-5.31	101.98	111.00
1	A	15	TRP	NE1-CE2-CD2	5.30	112.60	107.30
1	A	96	VAL	CA-CB-CG2	-5.28	102.99	110.90
1	A	56	ASN	CB-CA-C	-5.26	99.87	110.40
1	A	17	GLU	O-C-N	-5.26	114.28	122.70
1	A	68	PHE	CD1-CG-CD2	5.17	125.03	118.30
1	A	89	THR	N-CA-CB	-5.11	100.60	110.30
1	A	150	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	A	90	LEU	CB-CG-CD1	5.09	119.66	111.00
1	A	60	LEU	CB-CG-CD1	-5.07	102.39	111.00
1	A	114	ILE	CB-CA-C	-5.04	101.51	111.60
1	A	5	GLU	N-CA-CB	-5.02	101.56	110.60
1	A	12	LYS	O-C-N	5.02	130.73	122.70
1	A	46	PHE	CG-CD2-CE2	5.02	126.32	120.80

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	GLU	Sidechain
1	A	14	SER	Mainchain
1	A	150	ASP	Mainchain
1	A	2	ALA	Mainchain
1	A	20	ALA	Mainchain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	42	ASP	Sidechain
1	A	56	ASN	Sidechain
1	A	57	ASN	Sidechain
1	A	59	GLU	Sidechain
1	A	61	GLN	Sidechain
1	A	62	ALA	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	27	267
2	A	43	0	30	6	0
3	A	9	0	4	2	0
4	A	65	0	0	0	39
All	All	1297	0	1234	28	268

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 12.

All (28) 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:95:SER:HA	1:A:152:ALA:HB1	1.72	0.71
1:A:21:ASN:C	1:A:21:ASN:HD22	2.02	0.61
1:A:77:GLN:NE2	1:A:85:VAL:H	1.99	0.60
1:A:102:VAL:HG13	2:A:154:HEM:HAC	1.84	0.60
1:A:87:ASP:O	1:A:91:LYS:HG3	2.03	0.58
1:A:18:PHE:CE1	1:A:25:HIS:HB3	2.42	0.55
1:A:26:THR:HB	1:A:64:ALA:HB3	1.89	0.53
1:A:31:ILE:O	1:A:35:GLU:HG3	2.11	0.51
1:A:103:ALA:O	1:A:106:HIS:HB2	2.10	0.51
1:A:21:ASN:C	1:A:21:ASN:ND2	2.66	0.49
1:A:86:THR:HA	1:A:90:LEU:HD12	1.96	0.48
1:A:116:LYS:O	1:A:120:GLU:HG3	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.60	0.45
1:A:92:ASN:O	1:A:96:VAL:HG12	2.17	0.44
2:A:154:HEM:C1A	3:A:155:NIO:H1	2.52	0.44
1:A:67:VAL:HG22	2:A:154:HEM:CHB	2.49	0.43
1:A:29:PHE:O	1:A:33:VAL:HG23	2.20	0.42
1:A:100:LYS:HB3	2:A:154:HEM:HMD1	2.00	0.42
1:A:1:GLY:HA3	1:A:7:GLN:HE22	1.84	0.42
1:A:100:LYS:HG3	2:A:154:HEM:HAD2	2.01	0.42
1:A:63:HIS:HB3	3:A:155:NIO:O2	2.20	0.42
1:A:95:SER:HA	1:A:152:ALA:CB	2.47	0.41
1:A:97:HIS:CE1	2:A:154:HEM:NA	2.88	0.41
1:A:117:THR:O	1:A:121:VAL:HG23	2.21	0.41
1:A:7:GLN:O	1:A:10:LEU:HB2	2.21	0.40
1:A:53:VAL:HA	1:A:54:PRO:HD2	1.93	0.40
1:A:37:ALA:HA	1:A:38:PRO:HD2	1.94	0.40

All (268) 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:126:TRP:C	1:A:131:ASN:O[2_675]	0.48	1.72
1:A:9:ALA:N	1:A:13:SER:N[2_675]	0.56	1.64
1:A:118:ILE:CG2	1:A:129:GLU:CB[2_675]	0.58	1.62
1:A:130:LEU:CA	1:A:130:LEU:CG[2_675]	0.62	1.58
1:A:10:LEU:C	1:A:10:LEU:C[2_675]	0.65	1.55
1:A:126:TRP:CD1	1:A:128:GLU:O[2_675]	0.72	1.48
1:A:128:GLU:N	4:A:210:HOH:O[2_675]	0.72	1.48
1:A:4:THR:N	1:A:17:GLU:CG[2_675]	0.74	1.46
1:A:8:ALA:N	1:A:13:SER:C[2_675]	0.81	1.39
1:A:56:ASN:OD1	4:A:170:HOH:O[1_545]	0.83	1.37
1:A:7:GLN:CA	1:A:14:SER:CA[2_675]	0.87	1.33
1:A:134:TRP:CA	4:A:217:HOH:O[2_675]	0.88	1.32
1:A:6:SER:C	1:A:15:TRP:N[2_675]	0.88	1.32
1:A:4:THR:CB	1:A:17:GLU:CA[2_675]	0.91	1.29
1:A:9:ALA:CA	1:A:12:LYS:CA[2_675]	0.92	1.28
1:A:9:ALA:N	1:A:12:LYS:C[2_675]	0.94	1.26
1:A:6:SER:C	1:A:14:SER:C[2_675]	0.95	1.25
1:A:19:ASN:N	4:A:220:HOH:O[2_675]	0.95	1.25
1:A:9:ALA:CA	1:A:12:LYS:C[2_675]	0.96	1.24
1:A:5:GLU:C	1:A:16:GLU:N[2_675]	0.97	1.23

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:VAL:CG2	1:A:132[A]:SER:OG[2_675]	0.98	1.22
1:A:8:ALA:CA	1:A:13:SER:CA[2_675]	0.98	1.22
1:A:7:GLN:NE2	1:A:122:VAL:CA[2_675]	0.98	1.22
1:A:130:LEU:CA	1:A:130:LEU:CD2[2_675]	0.99	1.21
1:A:8:ALA:C	1:A:13:SER:CA[2_675]	0.99	1.21
1:A:8:ALA:C	1:A:13:SER:N[2_675]	1.00	1.20
1:A:8:ALA:CA	1:A:13:SER:CB[2_675]	1.00	1.20
1:A:118:ILE:O	1:A:129:GLU:OE2[2_675]	1.01	1.19
1:A:5:GLU:CA	1:A:16:GLU:CB[2_675]	1.01	1.19
1:A:126:TRP:C	1:A:131:ASN:C[2_675]	1.01	1.19
1:A:10:LEU:CA	1:A:10:LEU:C[2_675]	1.02	1.18
1:A:9:ALA:C	1:A:12:LYS:N[2_675]	1.03	1.17
1:A:4:THR:CB	1:A:17:GLU:C[2_675]	1.03	1.17
1:A:9:ALA:CB	1:A:12:LYS:CA[2_675]	1.05	1.15
1:A:127:SER:N	1:A:131:ASN:CA[2_675]	1.06	1.14
1:A:4:THR:CA	1:A:17:GLU:CA[2_675]	1.06	1.14
1:A:10:LEU:CA	1:A:11:VAL:N[2_675]	1.06	1.14
1:A:6:SER:N	1:A:16:GLU:N[2_675]	1.09	1.11
1:A:6:SER:CA	1:A:15:TRP:CA[2_675]	1.09	1.11
1:A:5:GLU:N	1:A:16:GLU:C[2_675]	1.11	1.09
1:A:119:LYS:C	4:A:181:HOH:O[2_675]	1.11	1.09
1:A:119:LYS:CA	4:A:181:HOH:O[2_675]	1.13	1.07
1:A:3:LEU:N	1:A:17:GLU:OE1[2_675]	1.13	1.07
1:A:7:GLN:N	1:A:14:SER:C[2_675]	1.14	1.06
1:A:7:GLN:C	1:A:14:SER:N[2_675]	1.16	1.04
1:A:126:TRP:CA	1:A:131:ASN:C[2_675]	1.19	1.01
1:A:126:TRP:CE3	1:A:131:ASN:OD1[2_675]	1.19	1.01
1:A:10:LEU:CA	1:A:10:LEU:O[2_675]	1.19	1.01
1:A:130:LEU:CB	1:A:130:LEU:CG[2_675]	1.20	1.00
1:A:125:LYS:CG	1:A:136:ILE:CB[2_675]	1.20	1.00
1:A:5:GLU:CA	1:A:16:GLU:CA[2_675]	1.21	0.99
1:A:5:GLU:C	1:A:16:GLU:CA[2_675]	1.21	0.99
1:A:7:GLN:N	1:A:14:SER:CA[2_675]	1.22	0.98
1:A:4:THR:C	1:A:17:GLU:N[2_675]	1.24	0.96
1:A:126:TRP:O	1:A:131:ASN:O[2_675]	1.25	0.95
1:A:130:LEU:CB	1:A:130:LEU:CB[2_675]	1.25	0.95
1:A:6:SER:CA	1:A:15:TRP:C[2_675]	1.26	0.94
1:A:10:LEU:CD1	1:A:134:TRP:NE1[2_675]	1.28	0.92
1:A:7:GLN:OE1	1:A:17:GLU:OE2[2_675]	1.28	0.92
1:A:127:SER:N	1:A:131:ASN:C[2_675]	1.29	0.91
1:A:135:THR:OG1	4:A:159:HOH:O[2_675]	1.33	0.87

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:C	1:A:17:GLU:CG[2_675]	1.34	0.86
1:A:126:TRP:NE1	1:A:128:GLU:O[2_675]	1.37	0.83
1:A:6:SER:O	1:A:15:TRP:N[2_675]	1.37	0.83
1:A:8:ALA:CA	1:A:13:SER:OG[2_675]	1.37	0.83
1:A:9:ALA:O	1:A:12:LYS:N[2_675]	1.38	0.82
1:A:130:LEU:N	1:A:130:LEU:CD2[2_675]	1.39	0.81
1:A:6:SER:CA	1:A:15:TRP:N[2_675]	1.39	0.81
1:A:6:SER:N	1:A:15:TRP:C[2_675]	1.39	0.81
1:A:4:THR:OG1	1:A:17:GLU:CA[2_675]	1.39	0.81
1:A:9:ALA:N	1:A:13:SER:CA[2_675]	1.39	0.81
1:A:6:SER:OG	1:A:14:SER:O[2_675]	1.39	0.81
1:A:6:SER:CB	1:A:15:TRP:CA[2_675]	1.40	0.80
1:A:128:GLU:CA	4:A:210:HOH:O[2_675]	1.41	0.79
1:A:127:SER:N	1:A:131:ASN:O[2_675]	1.42	0.78
1:A:122:VAL:O	1:A:136:ILE:CD1[2_675]	1.43	0.77
1:A:8:ALA:N	1:A:13:SER:O[2_675]	1.44	0.76
1:A:118:ILE:CG2	1:A:129:GLU:CG[2_675]	1.44	0.76
1:A:4:THR:N	1:A:17:GLU:CB[2_675]	1.45	0.75
1:A:9:ALA:CA	1:A:13:SER:N[2_675]	1.45	0.75
1:A:5:GLU:N	1:A:17:GLU:N[2_675]	1.45	0.75
1:A:7:GLN:CG	1:A:122:VAL:CG1[2_675]	1.46	0.74
1:A:124:ALA:O	1:A:135:THR:CB[2_675]	1.48	0.72
1:A:8:ALA:C	1:A:13:SER:CB[2_675]	1.49	0.71
1:A:126:TRP:NE1	1:A:128:GLU:C[2_675]	1.50	0.70
1:A:124:ALA:O	1:A:135:THR:CG2[2_675]	1.50	0.70
1:A:9:ALA:CB	1:A:12:LYS:C[2_675]	1.50	0.70
1:A:79:GLU:CG	4:A:204:HOH:O[2_675]	1.51	0.69
1:A:3:LEU:CA	1:A:17:GLU:CD[2_675]	1.52	0.68
1:A:7:GLN:NE2	1:A:122:VAL:CB[2_675]	1.54	0.66
1:A:18:PHE:C	4:A:220:HOH:O[2_675]	1.56	0.64
1:A:10:LEU:C	1:A:11:VAL:N[2_675]	1.56	0.64
1:A:10:LEU:O	1:A:10:LEU:CB[2_675]	1.57	0.63
1:A:10:LEU:CD1	1:A:14:SER:OG[2_675]	1.57	0.63
1:A:5:GLU:O	1:A:16:GLU:N[2_675]	1.58	0.62
1:A:56:ASN:CG	4:A:170:HOH:O[1_545]	1.59	0.61
1:A:10:LEU:CA	1:A:11:VAL:CA[2_675]	1.59	0.61
1:A:5:GLU:CB	1:A:16:GLU:CA[2_675]	1.60	0.60
1:A:8:ALA:N	1:A:14:SER:N[2_675]	1.60	0.60
1:A:119:LYS:O	4:A:181:HOH:O[2_675]	1.61	0.59
1:A:7:GLN:OE1	1:A:17:GLU:CD[2_675]	1.62	0.58
1:A:122:VAL:C	1:A:132[C]:SER:OG[2_675]	1.62	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLN:C	1:A:13:SER:C[2_675]	1.62	0.58
1:A:125:LYS:O	1:A:134:TRP:N[2_675]	1.62	0.58
1:A:134:TRP:N	4:A:217:HOH:O[2_675]	1.64	0.56
1:A:3:LEU:CG	1:A:125:LYS:CE[2_675]	1.64	0.56
1:A:1:GLY:CA	1:A:121:VAL:O[2_675]	1.66	0.54
1:A:4:THR:OG1	1:A:17:GLU:C[2_675]	1.66	0.54
1:A:8:ALA:N	1:A:13:SER:CA[2_675]	1.66	0.54
1:A:10:LEU:CG	1:A:14:SER:OG[2_675]	1.66	0.54
1:A:130:LEU:CA	1:A:130:LEU:CB[2_675]	1.66	0.54
1:A:4:THR:OG1	1:A:17:GLU:CB[2_675]	1.67	0.53
1:A:10:LEU:N	1:A:10:LEU:O[2_675]	1.67	0.53
1:A:6:SER:CA	1:A:16:GLU:N[2_675]	1.68	0.52
1:A:126:TRP:O	1:A:135:THR:OG1[2_675]	1.68	0.52
1:A:5:GLU:CA	1:A:16: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:3:LEU:N	1:A:17:GLU:CD[2_675]	1.69	0.51
1:A:126:TRP:NE1	1:A:128:GLU:CA[2_675]	1.69	0.51
1:A:118:ILE:C	1:A:129:GLU:OE2[2_675]	1.69	0.51
1:A:9:ALA:CA	1:A:12:LYS:N[2_675]	1.70	0.50
1:A:134:TRP:N	4:A:190:HOH:O[2_675]	1.70	0.50
1:A:7:GLN:N	1:A:14:SER:O[2_675]	1.70	0.50
1:A:126:TRP:CE3	1:A:131:ASN:CG[2_675]	1.71	0.49
1:A:7:GLN:CA	1:A:14:SER:N[2_675]	1.71	0.49
1:A:126:TRP:CA	1:A:131:ASN:O[2_675]	1.71	0.49
1:A:9:ALA:CB	1:A:12:LYS:O[2_675]	1.71	0.49
1:A:4:THR:C	1:A:17:GLU:CA[2_675]	1.71	0.49
1:A:130:LEU:C	1:A:130:LEU:CD2[2_675]	1.72	0.48
1:A:4:THR:CA	1:A:17:GLU:CB[2_675]	1.72	0.48
1:A:130:LEU:C	1:A:130:LEU:CB[2_675]	1.73	0.47
1:A:8:ALA:CB	1:A:13:SER:OG[2_675]	1.73	0.47
1:A:7:GLN:CD	1:A:17:GLU:OE2[2_675]	1.73	0.47
1:A:10:LEU:N	1:A:11:VAL:C[2_675]	1.73	0.47
1:A:129:GLU:O	1:A:130:LEU:CD2[2_675]	1.74	0.46
1:A:8:ALA:O	1:A:9:ALA:O[2_675]	1.75	0.45
1:A:6:SER:C	1:A:14:SER:CA[2_675]	1.75	0.45
1:A:6:SER:N	1:A:16:GLU:CA[2_675]	1.76	0.44
1:A:127:SER:C	4:A:210:HOH:O[2_675]	1.76	0.44
1:A:6:SER:N	1:A:17:GLU:N[2_675]	1.76	0.44
1:A:7:GLN:NE2	1:A:122:VAL:CG1[2_675]	1.76	0.44
1:A:118:ILE:CB	1:A:129:GLU:CB[2_675]	1.76	0.44
1:A:10:LEU:C	1:A:10:LEU:O[2_675]	1.76	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:THR:O	1:A:13:SER:O[2_675]	1.76	0.44
1:A:126:TRP:CD2	1:A:131:ASN:CB[2_675]	1.77	0.43
1:A:126:TRP:CD1	1:A:128:GLU:C[2_675]	1.78	0.42
1:A:9:ALA:CA	1:A:12:LYS:CB[2_675]	1.78	0.42
1:A:5:GLU:O	1:A:12:LYS:O[2_675]	1.78	0.42
1:A:7:GLN:CA	1:A:14:SER:CB[2_675]	1.80	0.40
1:A:4:THR:OG1	1:A:18:PHE:N[2_675]	1.80	0.40
1:A:4:THR:CB	1:A:17:GLU:CB[2_675]	1.80	0.40
1:A:7:GLN:CD	1:A:122:VAL:CG1[2_675]	1.81	0.39
1:A:123:GLY:N	1:A:132[C]:SER:OG[2_675]	1.81	0.39
1:A:6:SER:O	1:A:14:SER:N[2_675]	1.81	0.39
4:A:159:HOH:O	4:A:176:HOH:O[2_675]	1.82	0.38
1:A:8:ALA:O	1:A:13:SER:CB[2_675]	1.82	0.38
1:A:5:GLU:CB	1:A:16:GLU:CB[2_675]	1.82	0.38
1:A:6:SER:O	1:A:14:SER:C[2_675]	1.83	0.37
1:A:5:GLU:N	1:A:16:GLU:O[2_675]	1.83	0.37
1:A:3:LEU:CD1	1:A:125:LYS:CE[2_675]	1.83	0.37
1:A:6:SER:N	1:A:16:GLU:C[2_675]	1.84	0.36
1:A:6:SER:CB	1:A:15:TRP:C[2_675]	1.85	0.35
1:A:9:ALA:C	1:A:12:LYS:CA[2_675]	1.85	0.35
1:A:126:TRP:CD2	4:A:189:HOH:O[2_675]	1.85	0.35
1:A:125:LYS:O	1:A:133:ALA:C[2_675]	1.85	0.35
1:A:130:LEU:N	1:A:130:LEU:CG[2_675]	1.86	0.34
1:A:4:THR:CB	1:A:17:GLU:O[2_675]	1.86	0.34
1:A:125:LYS:CA	1:A:136:ILE:N[2_675]	1.87	0.33
1:A:6:SER:O	1:A:14:SER:CA[2_675]	1.88	0.32
1:A:9:ALA:C	1:A:11:VAL:C[2_675]	1.88	0.32
1:A:119:LYS:N	4:A:181:HOH:O[2_675]	1.88	0.32
1:A:9:ALA:N	1:A:12:LYS:O[2_675]	1.88	0.32
1:A:10:LEU:N	1:A:12:LYS:N[2_675]	1.89	0.31
1:A:7:GLN:NE2	1:A:122:VAL:N[2_675]	1.89	0.31
1:A:15:TRP:CB	4:A:219:HOH:O[2_675]	1.89	0.31
1:A:3:LEU:CD2	4:A:201:HOH:O[2_675]	1.90	0.30
1:A:5:GLU:CG	1:A:16:GLU:CG[2_675]	1.90	0.30
1:A:56:ASN:CB	4:A:187:HOH:O[1_545]	1.90	0.30
1:A:7:GLN:OE1	1:A:17:GLU:OE1[2_675]	1.90	0.30
1:A:16:GLU:OE1	1:A:79:GLU:OE1[2_675]	1.91	0.29
1:A:126:TRP:C	1:A:131:ASN:CA[2_675]	1.91	0.29
1:A:3:LEU:CA	1:A:17:GLU:OE1[2_675]	1.92	0.28
1:A:119:LYS:CE	1:A:128:GLU:CG[2_675]	1.92	0.28
1:A:126:TRP:CG	1:A:128:GLU:O[2_675]	1.92	0.28

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:SER:CA	1:A:131:ASN:ND2[2_675]	1.93	0.27
1:A:5:GLU:O	1:A:16:GLU:CB[2_675]	1.93	0.27
1:A:4:THR:OG1	1:A:17:GLU:N[2_675]	1.94	0.26
1:A:124:ALA:O	1:A:135:THR:C[2_675]	1.95	0.25
1:A:6:SER:O	1:A:11:VAL:O[2_675]	1.95	0.25
1:A:122:VAL:CG2	1:A:129:GLU:O[2_675]	1.95	0.25
1:A:3:LEU:CD1	1:A:125:LYS:CD[2_675]	1.95	0.25
1:A:128:GLU:C	4:A:210:HOH:O[2_675]	1.96	0.24
1:A:6:SER:CA	1:A:14:SER:C[2_675]	1.96	0.24
1:A:118:ILE:O	4:A:181:HOH:O[2_675]	1.96	0.24
1:A:7:GLN:C	1:A:14:SER:CA[2_675]	1.96	0.24
1:A:8:ALA:CA	1:A:13:SER:C[2_675]	1.97	0.23
1:A:6:SER:C	1:A:14:SER:O[2_675]	1.97	0.23
1:A:8:ALA:O	1:A:13:SER:N[2_675]	1.97	0.23
1:A:4:THR:CA	1:A:17:GLU:N[2_675]	1.98	0.22
1:A:134:TRP:C	4:A:217:HOH:O[2_675]	1.98	0.22
1:A:7:GLN:O	1:A:14:SER:N[2_675]	1.98	0.22
1:A:135:THR:CG2	4:A:159:HOH:O[2_675]	1.98	0.22
1:A:4:THR:CG2	1:A:17:GLU:C[2_675]	1.99	0.21
1:A:126:TRP:CZ3	1:A:131:ASN:OD1[2_675]	1.99	0.21
1:A:8:ALA:CB	1:A:13:SER:CA[2_675]	1.99	0.21
1:A:5:GLU:N	1:A:16:GLU:CA[2_675]	2.01	0.19
1:A:135:THR:CB	4:A:159:HOH:O[2_675]	2.01	0.19
1:A:127:SER:O	1:A:131:ASN:CA[2_675]	2.02	0.18
1:A:1:GLY:C	1:A:121:VAL:O[2_675]	2.02	0.18
1:A:4:THR:N	1:A:17:GLU:CD[2_675]	2.02	0.18
1:A:5:GLU:C	1:A:16:GLU:C[2_675]	2.03	0.17
1:A:18:PHE:CA	4:A:220:HOH:O[2_675]	2.03	0.17
1:A:124:ALA:CB	4:A:188:HOH:O[2_675]	2.04	0.16
1:A:118:ILE:O	1:A:129:GLU:CD[2_675]	2.04	0.16
1:A:129:GLU:N	4:A:210:HOH:O[2_675]	2.04	0.16
1:A:125:LYS:CB	1:A:133:ALA:O[2_675]	2.04	0.16
1:A:3:LEU:C	1:A:17:GLU:CD[2_675]	2.05	0.15
1:A:118:ILE:CG2	1:A:129:GLU:CA[2_675]	2.05	0.15
1:A:7:GLN:N	1:A:15:TRP:N[2_675]	2.05	0.15
1:A:4:THR:C	1:A:16:GLU:C[2_675]	2.05	0.15
1:A:130:LEU:CA	1:A:130:LEU:CD1[2_675]	2.05	0.15
1:A:1:GLY:O	1:A:121:VAL:O[2_675]	2.05	0.15
1:A:9:ALA:C	1:A:13:SER:N[2_675]	2.06	0.14
1:A:4:THR:CB	1:A:18:PHE:N[2_675]	2.06	0.14
1:A:3:LEU:CA	1:A:17:GLU:CG[2_675]	2.06	0.14

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:C	1:A:130:LEU:CG[2_675]	2.06	0.14
1:A:7:GLN:O	1:A:10:LEU:O[2_675]	2.07	0.13
1:A:10:LEU:N	1:A:10:LEU:C[2_675]	2.08	0.12
1:A:130:LEU:O	4:A:190:HOH:O[2_675]	2.08	0.12
1:A:4:THR:CA	1:A:17:GLU:CG[2_675]	2.08	0.12
1:A:126:TRP:CE3	1:A:131:ASN:CB[2_675]	2.09	0.11
1:A:6:SER:CA	1:A:14:SER:O[2_675]	2.09	0.11
1:A:124:ALA:O	1:A:135:THR:CA[2_675]	2.09	0.11
1:A:127:SER:CA	1:A:131:ASN:CA[2_675]	2.09	0.11
1:A:4:THR:O	1:A:17:GLU:N[2_675]	2.09	0.11
1:A:10:LEU:C	1:A:10:LEU:CB[2_675]	2.10	0.10
1:A:6:SER:CB	1:A:14:SER:O[2_675]	2.10	0.10
1:A:125:LYS:N	1:A:136:ILE:CG1[2_675]	2.11	0.09
1:A:56:ASN:CB	4:A:170:HOH:O[1_545]	2.11	0.09
1:A:127:SER:O	1:A:131:ASN:CB[2_675]	2.11	0.09
1:A:118:ILE:CD1	1:A:129:GLU:OE1[2_675]	2.11	0.09
1:A:4:THR:CG2	1:A:17:GLU:O[2_675]	2.12	0.08
1:A:6:SER:CB	1:A:15:TRP:O[2_675]	2.12	0.08
1:A:18:PHE:N	4:A:220:HOH:O[2_675]	2.12	0.08
1:A:2:ALA:C	1:A:17:GLU:OE1[2_675]	2.12	0.08
1:A:8:ALA:CB	1:A:13:SER:CB[2_675]	2.12	0.08
1:A:127:SER:C	1:A:131:ASN:ND2[2_675]	2.13	0.07
1:A:126:TRP:CG	4:A:189:HOH:O[2_675]	2.13	0.07
1:A:56:ASN:CG	4:A:187:HOH:O[1_545]	2.13	0.07
1:A:7:GLN:N	1:A:14:SER:N[2_675]	2.14	0.06
1:A:122:VAL:CG2	1:A:132[C]:SER:OG[2_675]	2.14	0.06
1:A:9:ALA:N	1:A:12:LYS:CA[2_675]	2.14	0.06
1:A:124:ALA:O	1:A:136:ILE:N[2_675]	2.15	0.05
1:A:5:GLU:CG	1:A:16:GLU:CB[2_675]	2.15	0.05
1:A:8:ALA:CA	1:A:13:SER:N[2_675]	2.16	0.04
1:A:118:ILE:CA	1:A:129:GLU:OE2[2_675]	2.16	0.04
1:A:56:ASN:OD1	4:A:171:HOH:O[1_545]	2.16	0.04
1:A:125:LYS:CG	1:A:136:ILE:CG2[2_675]	2.17	0.03
1:A:118:ILE:C	4:A:181:HOH:O[2_675]	2.17	0.03
1:A:133:ALA:O	4:A:217:HOH:O[2_675]	2.17	0.03
1:A:12:LYS:CB	4:A:203:HOH:O[2_675]	2.17	0.03
1:A:9:ALA:CA	1:A:12:LYS:O[2_675]	2.18	0.02
1:A:4:THR:OG1	1:A:14:SER:O[2_675]	2.18	0.02
1:A:7:GLN:CB	1:A:17:GLU:OE2[2_675]	2.18	0.02
1:A:7:GLN:CB	4:A:201:HOH:O[2_675]	2.19	0.01
1:A:6:SER:C	1:A:14:SER:N[2_675]	2.19	0.01

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TRP:CB	1:A:131:ASN:C[2_675]	2.19	0.01
1:A:5:GLU:O	1:A:16: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%)	4 (3%)	1 (1%)	26 19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	151	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	25	HIS
1	A	61	GLN
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 [i](#)

2 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
2	HEM	A	154	1,3	30,50,50	5.10	25 (83%)	24,82,82	3.21	12 (50%)
3	NIO	A	155	2	6,9,9	3.03	3 (50%)	8,11,11	3.35	4 (50%)

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
3	NIO	A	155	2	-	0/0/4/4	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	C2D-C3D	-5.94	1.36	1.54
3	A	155	NIO	C1-C2	-4.85	1.30	1.39
3	A	155	NIO	C4-C5	-3.75	1.26	1.37
2	A	154	HEM	C2C-C1C	-3.25	1.46	1.52
2	A	154	HEM	CAD-CBD	-2.25	1.41	1.52
2	A	154	HEM	C2B-C1B	2.39	1.59	1.51
2	A	154	HEM	CMB-C2B	2.54	1.59	1.53
2	A	154	HEM	CBB-CAB	2.56	1.44	1.29
2	A	154	HEM	C2D-C1D	3.05	1.61	1.51
2	A	154	HEM	CMA-C3A	3.12	1.58	1.51
2	A	154	HEM	C3C-CAC	3.27	1.57	1.51
2	A	154	HEM	CMC-C2C	3.37	1.61	1.53
2	A	154	HEM	CMD-C2D	3.84	1.62	1.53
2	A	154	HEM	C1A-CHA	3.91	1.50	1.39
3	A	155	NIO	C1-N	4.01	1.43	1.34
2	A	154	HEM	C2A-C3A	4.49	1.51	1.37
2	A	154	HEM	C4A-CHB	5.16	1.54	1.39
2	A	154	HEM	C3D-C4D	5.30	1.58	1.51
2	A	154	HEM	CAD-C3D	5.36	1.64	1.54
2	A	154	HEM	CHC-C1C	5.49	1.49	1.36
2	A	154	HEM	FE-ND	5.64	2.27	1.97
2	A	154	HEM	FE-NB	6.31	2.30	1.97
2	A	154	HEM	C4C-NC	6.72	1.44	1.36
2	A	154	HEM	CHD-C4C	6.76	1.52	1.36
2	A	154	HEM	CAA-C2A	6.96	1.63	1.52
2	A	154	HEM	C3B-CAB	7.73	1.65	1.51
2	A	154	HEM	C3B-C4B	9.69	1.60	1.51
2	A	154	HEM	C1C-NC	11.77	1.50	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	154	HEM	CMA-C3A-C4A	-7.49	115.97	128.36

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	154	HEM	CAA-C2A-C1A	-6.64	119.80	127.01
2	A	154	HEM	C2C-C1C-NC	-2.71	105.64	110.21
3	A	155	NIO	C4-C5-N	-2.60	115.02	122.51
2	A	154	HEM	C3C-CAC-CBC	-2.55	120.55	124.46
2	A	154	HEM	CAD-CBD-CGD	-2.29	103.66	113.02
2	A	154	HEM	C2D-C3D-C4D	2.24	105.29	101.50
2	A	154	HEM	CMD-C2D-C3D	2.97	127.48	114.35
2	A	154	HEM	CMA-C3A-C2A	3.52	132.59	125.24
2	A	154	HEM	CAD-C3D-C4D	4.09	126.91	112.47
3	A	155	NIO	C3-C2-C6	4.28	126.20	120.45
2	A	154	HEM	CMC-C2C-C3C	4.49	127.74	116.53
2	A	154	HEM	CMB-C2B-C3B	4.53	127.83	116.53
3	A	155	NIO	C4-C3-C2	4.70	126.77	120.56
2	A	154	HEM	CAD-C3D-C2D	4.99	127.57	113.22
3	A	155	NIO	C5-N-C1	6.13	128.13	116.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	154	HEM	6	0
3	A	155	NIO	2	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%)	4.18	122 (79%) 0 1	6, 17, 50, 67	18 (11%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	19.3
1	A	153	ALA	16.8
1	A	45	SER	13.4
1	A	124	ALA	10.0
1	A	1	GLY	9.9
1	A	47	LEU	9.8
1	A	51	SER	8.7
1	A	101	GLY	8.5
1	A	40	ALA	8.4
1	A	60	LEU	8.3
1	A	46	PHE	8.2
1	A	151	ASP	8.1
1	A	49	GLY	8.1
1	A	80	VAL	7.6
1	A	136	ILE	7.3
1	A	107	PHE	7.3
1	A	88	ALA	7.1
1	A	48	LYS	7.1
1	A	152	ALA	6.9
1	A	144	VAL	6.9
1	A	50	THR	6.5
1	A	150	ASP	6.5
1	A	90	LEU	6.5
1	A	100	LYS	6.4
1	A	133	ALA	6.4
1	A	130	LEU	6.2
1	A	105	ALA	6.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	99	SER	6.1
1	A	108	PRO	6.1
1	A	87	ASP	5.8
1	A	19	ASN	5.8
1	A	95	SER	5.6
1	A	69	LYS	5.6
1	A	138	TYR	5.5
1	A	89	THR	5.5
1	A	70	LEU	5.5
1	A	31	ILE	5.4
1	A	41	LYS	5.4
1	A	116	LYS	5.3
1	A	93	LEU	5.3
1	A	3	LEU	5.2
1	A	43	LEU	5.2
1	A	18	PHE	5.2
1	A	44	PHE	5.1
1	A	123	GLY	5.0
1	A	54	PRO	4.9
1	A	5	GLU	4.8
1	A	33	VAL	4.7
1	A	129	GLU	4.7
1	A	92	ASN	4.5
1	A	145	ILE	4.5
1	A	62	ALA	4.5
1	A	109	VAL	4.4
1	A	143	ILE	4.4
1	A	26	THR	4.4
1	A	71	VAL	4.3
1	A	20	ALA	4.3
1	A	127	SER	4.3
1	A	15	TRP	4.3
1	A	75	ALA	4.3
1	A	135	THR	4.2
1	A	126	TRP	4.2
1	A	29	PHE	4.1
1	A	148	GLU	4.1
1	A	55	GLN	4.0
1	A	122	VAL	4.0
1	A	56	ASN	4.0
1	A	63	HIS	3.9
1	A	10	LEU	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	141	LEU	3.9
1	A	42	ASP	3.8
1	A	117	THR	3.8
1	A	21	ASN	3.8
1	A	121	VAL	3.8
1	A	28	ARG	3.7
1	A	67	VAL	3.7
1	A	22	ILE	3.7
1	A	72	TYR	3.7
1	A	137	ALA	3.7
1	A	58	PRO	3.6
1	A	32	LEU	3.5
1	A	125	LYS	3.4
1	A	11	VAL	3.4
1	A	110	VAL	3.4
1	A	131	ASN	3.4
1	A	147	LYS	3.4
1	A	83	VAL	3.3
1	A	102	VAL	3.3
1	A	86	THR	3.3
1	A	27	HIS	3.2
1	A	115	LEU	3.2
1	A	64	ALA	3.2
1	A	76	ILE	3.2
1	A	38	PRO	3.1
1	A	73	GLU	3.1
1	A	98	VAL	3.0
1	A	96	VAL	3.0
1	A	36	ILE	2.9
1	A	16	GLU	2.9
1	A	132[A]	SER	2.9
1	A	68	PHE	2.8
1	A	34	LEU	2.8
1	A	82	GLY	2.6
1	A	149	MET	2.6
1	A	120	GLU	2.6
1	A	7	GLN	2.6
1	A	66	LYS	2.5
1	A	142	ALA	2.5
1	A	139	ASP	2.4
1	A	140	GLU	2.4
1	A	118	ILE	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	94	GLY	2.3
1	A	4	THR	2.3
1	A	104	ASP	2.3
1	A	77	GLN	2.3
1	A	12	LYS	2.2
1	A	81	THR	2.1
1	A	61	GLN	2.1
1	A	128	GLU	2.1
1	A	97	HIS	2.1
1	A	53	VAL	2.1
1	A	84	VAL	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 [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(Å <sup>2</sup> )	Q<0.9
3	NIO	A	155	9/9	0.64	0.37	0.38	7,12,19,21	0
2	HEM	A	154	43/43	0.75	0.28	-0.59	0,17,44,50	3

## 6.5 Other polymers [i](#)

There are no such residues in this entry.