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PDB ID	:	8F49
EMDB ID	:	EMD-32695
Title	:	1.8 angstrom structure of apoferritin embedded in crystalline ice
Authors	:	Shi, H.; Wu, C.; Zhang, X.
Deposited on	:	2022-11-10
Resolution	:	1.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 1.80 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.



Motria	Whole archive	EM structures		
wietric	$(\# {\rm Entries})$	$(\# {\rm Entries})$		
Clashscore	158937	4297		
Ramachandran outliers	154571	4023		
Sidechain outliers	154315	3826		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Mol	Chain	Length	Quality of chain	
1	А	172	90%	10%
1	В	172	93%	7%
1	С	172	92%	8%
1	D	172	92%	8%
1	Е	172	92%	8%
1	F	172	92%	8%
1	G	172	92%	8%
1	Н	172	94%	6%
1	Ι	172	92%	8%



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Mol	Chain	Length	Quality of chain	
1	J	172	92%	8%
1	K	172	92%	8%
1	L	172	92%	8%
1	М	172	93%	7%
1	Ν	172	94%	6%
1	0	172	94%	6%
1	Р	172	92%	8%
1	Q	172	92%	8%
1	B	172	02%	8%
1	S	172	0.2%	7%
1	T	172	95%	770
1	1	172	92%	8%
1	U	172	91%	9%
1	V	172	93%	7%
1	W	172	91%	9%
1	Х	172	92%	8%



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 33216 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues		At	oms			AltConf	Trace
1	I	172	Total	С	Ν	0	S	0	0
	0	112	1384	871	242	264	7	0	0
1	Δ	172	Total	С	Ν	Ο	\mathbf{S}	0	0
		112	1384	871	242	264	7	0	0
1	В	172	Total	С	Ν	Ο	\mathbf{S}	0	0
		112	1384	871	242	264	7	0	0
1	С	172	Total	С	Ν	Ο	\mathbf{S}	0	0
		112	1384	871	242	264	7	0	0
1	Л	172	Total	С	Ν	Ο	\mathbf{S}	0	0
		112	1384	871	242	264	7	0	0
1	E	172	Total	С	Ν	Ο	\mathbf{S}	0	0
	L	112	1384	871	242	264	7	Ŭ	
1	F	172	Total	С	Ν	Ο	\mathbf{S}	0	0
-	1	112	1384	871	242	264	7	0	0
1	G	172	Total	С	Ν	Ο	\mathbf{S}	0	0
		112	1384	871	242	264	7	Ŭ	
1	Н	172	Total	С	Ν	Ο	\mathbf{S}	0	0
-			1384	871	242	264	7		
1	T	I 172	Total	С	Ν	Ο	\mathbf{S}	0	0
-	-	112	1384	871	242	264	7	0	
1	I	I 172	Total	С	Ν	Ο	\mathbf{S}	0	0
		112	1384	871	242	264	7	Ŭ	
1	K	172	Total	С	Ν	Ο	\mathbf{S}	0	0
		112	1384	871	242	264	7	Ŭ	
1	L	172	Total	С	Ν	Ο	\mathbf{S}	0	0
		112	1384	871	242	264	7	Ŭ	
1	М	172	Total	С	Ν	Ο	\mathbf{S}	0	0
1 1/1	112	1384	871	242	264	7	Ŭ		
1	Ν	172	Total	С	Ν	Ο	\mathbf{S}	0	0
	T 11		1384	871	242	264	7	Ŭ	
1	0	172	Total	С	Ν	Ο	\mathbf{S}	0	0
		112	1384	871	242	264	7		
1	Р	172	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
	L 114	1384	871	242	264	7			

• Molecule 1 is a protein called Ferritin heavy chain.



Mol	Chain	Residues		At	oms			AltConf	Trace
1	0	179	Total	С	Ν	0	S	0	0
1	Q	172	1384	871	242	264	7	0	0
1	В	179	Total	С	Ν	Ο	\mathbf{S}	0	0
1	π	172	1384	871	242	264	7	0	0
1	C	179	Total	С	Ν	0	\mathbf{S}	0	0
	172	1384	871	242	264	7	0	0	
1	т	179	Total	С	Ν	0	\mathbf{S}	0	0
	112	1384	871	242	264	7	0	0	
1	V	179	Total	С	Ν	0	\mathbf{S}	0	0
1	v	112	1384	871	242	264	7	0	0
1	W	179	Total	С	Ν	0	S	0	0
1	vv	112	1384	871	242	264	7	0	0
1	v	179	Total	С	Ν	0	S	0	0
	172	1384	871	242	264	7		0	

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3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.



Chain F:	92%	8%
T1 H9 010 111 113 113 113 113 113 113 113 113	11 40 11 71 40 11 72 11 72 11 72	
• Molecule 1: Ferritin h	neavy chain	
Chain G:	92%	8%
11 H9 010 111 111 111 1115 1115 1116 1116 111	1148 K153 1148 1144 K168 C172 C172	
• Molecule 1: Ferritin h	eavy chain	
Chain H:	94%	6%
11 H9 010 111 114 K120 K120 K153 P157	Y164 6172 6172	
• Molecule 1: Ferritin h	neavy chain	
Chain I:	92%	8%
H1 H9 010 011 11 11 11 11 11 11 11 11 11 11 1	EI 30 71 49 71 68 71 68 71 68 72 68	
• Molecule 1: Ferritin h	eavy chain	
Chain J:	92%	8%
11 19 111 111 111 111 113 114 1114 1114	E130 1149 1149 1164 1164 0172	
• Molecule 1: Ferritin h	eavy chain	
Chain K:	92%	8%
T1 H9 H9 D11 D11 L93 E97 E97 E97 K115 K116 K120	E130 1149 1145 1164 1168 1172	
• Molecule 1: Ferritin h	leavy chain	
Chain L:	92%	8%



Chain M:	93%	7%
T1 H9 H1 11 11 11 11 14 11 11 14 15 71 14 15 71 14 15 71 14 15 71 14 15 71 14 15 71 14 15 71 71 72 81 72 81 72 81 72 81 73 81 74 81 75 81 81 81 81 81 81 81 81 81 81 81 81 81		
• Molecule 1: Ferritin heavy chain		
Chain N:	94%	6%
11 H9 H9 D11 L93 L93 L93 L93 K120 K120 K153 K153 Y164 Y164 Y164 K153 R153 R153 R153 R157 R157 R157 R157 R157 R157 R157 R157		
• Molecule 1: Ferritin heavy chain		
Chain O:	94%	6%
11 H9 H9 H1 11 K7 K7 K1 K1 K1 K1 K1 K1 K1 K1 K1 K1 K1 K1 K1		
• Molecule 1: Ferritin heavy chain		
Chain P:	92%	8%
11 19 11 11 11 11 11 11 11 11 11 11 11 1	6 <mark>112</mark>	
• Molecule 1: Ferritin heavy chain		
Chain Q:	92%	8%
11 H9 110 111 193 193 193 114 1116 1116 1116 1116 1116 1116 1116	<mark>8</mark>	
• Molecule 1: Ferritin heavy chain		
Chain R:	92%	8%
11 H9 H9 H10 H10 H11 E97 E97 E97 K15 K115 K115 K115 K120 K120 K153 K153 Y164	<mark>K108</mark> 617 2	
• Molecule 1: Ferritin heavy chain		
Chain S:	93%	7%



Chain T:	92%	8%
11 19 10 11 11 11 11 11 11 11 11 11 11 11 11	1149 1149 1157 1149 1157 1149 1157 1149 1172	
• Molecule 1: Ferritin h	eavy chain	
Chain V:	93%	7%
11 H9 H9 H10 D11 L13 E97 E97 E97 K120 K120 K120	K153 P157 Y164 K168 G172	
• Molecule 1: Ferritin h	eavy chain	
Chain W:	91%	9%
11 19 11 11 11 11 11 11 11 11 11 11 11 1	E130 1149 1149 1163 1163 1164 1164 1164 1164 1164 1172	
• Molecule 1: Ferritin h	eavy chain	
Chain X:	92%	8%
11 H9 Q10 D11 E93 E97 H114 K116 K116 K120	E1 30 71 49 71 57 71 64 61 72 61 72	



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94792	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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	
IVIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.26	0/1413	0.45	0/1908
1	В	0.26	0/1413	0.44	0/1908
1	С	0.26	0/1413	0.45	0/1908
1	D	0.26	0/1413	0.44	0/1908
1	Е	0.26	0/1413	0.45	0/1908
1	F	0.26	0/1413	0.45	0/1908
1	G	0.26	0/1413	0.45	0/1908
1	Н	0.26	0/1413	0.45	0/1908
1	Ι	0.26	0/1413	0.45	0/1908
1	J	0.26	0/1413	0.45	0/1908
1	Κ	0.27	0/1413	0.45	0/1908
1	L	0.26	0/1413	0.45	0/1908
1	М	0.26	0/1413	0.45	0/1908
1	Ν	0.26	0/1413	0.45	0/1908
1	0	0.26	0/1413	0.45	0/1908
1	Р	0.26	0/1413	0.45	0/1908
1	Q	0.26	0/1413	0.45	0/1908
1	R	0.26	0/1413	0.45	0/1908
1	S	0.26	0/1413	0.45	0/1908
1	Т	0.26	0/1413	0.45	0/1908
1	U	0.26	0/1413	0.45	0/1908
1	V	0.26	0/1413	0.45	0/1908
1	W	0.26	0/1413	0.45	0/1908
1	X	0.26	0/1413	0.44	0/1908
All	All	0.26	0/33912	0.45	0/45792

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.



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	А	1384	0	1310	12	0
1	В	1384	0	1310	9	0
1	С	1384	0	1310	10	0
1	D	1384	0	1310	11	0
1	Е	1384	0	1310	10	0
1	F	1384	0	1310	10	0
1	G	1384	0	1310	10	0
1	Н	1384	0	1310	8	0
1	Ι	1384	0	1310	12	0
1	J	1384	0	1310	12	0
1	Κ	1384	0	1310	12	0
1	L	1384	0	1310	10	0
1	М	1384	0	1310	9	0
1	Ν	1384	0	1310	10	0
1	0	1384	0	1310	9	0
1	Р	1384	0	1310	10	0
1	Q	1384	0	1310	10	0
1	R	1384	0	1310	11	0
1	S	1384	0	1310	9	0
1	Т	1384	0	1310	10	0
1	U	1384	0	1310	11	0
1	V	1384	0	1310	10	0
1	W	1384	0	1310	11	0
1	Х	1384	0	1310	11	0
All	All	33216	0	31440	247	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (247) 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:E:9:HIS:CE1	1:E:11:ASP:OD2	2.51	0.64
1:U:93:LEU:HD23	1:U:157:PRO:HG3	1.80	0.64
1:C:9:HIS:CE1	1:C:11:ASP:OD2	2.51	0.64



	Interatomic Clash						
Atom-1	Atom-2	distance (Å)	overlap (Å)				
1:W:9:HIS:CE1	1:W:11:ASP:OD2	2.51	0.64				
1:Q:9:HIS:CE1	1:Q:11:ASP:OD2	2.51	0.64				
1:R:9:HIS:CE1	1:R:11:ASP:OD2	2.51	0.64				
1:V:9:HIS:CE1	1:V:11:ASP:OD2	2.51	0.64				
1:U:9:HIS:CE1	1:U:11:ASP:OD2	2.51	0.63				
1:T:9:HIS:CE1	1:T:11:ASP:OD2	2.51	0.63				
1:P:9:HIS:CE1	1:P:11:ASP:OD1	2.52	0.63				
1:F:9:HIS:CE1	1:F:11:ASP:OD2	2.51	0.63				
1:M:9:HIS:CE1	1:M:11:ASP:OD1	2.52	0.63				
1:S:9:HIS:CE1	1:S:11:ASP:OD2	2.51	0.63				
1:I:9:HIS:CE1	1:I:11:ASP:OD2	2.52	0.63				
1:J:9:HIS:CE1	1:J:11:ASP:OD2	2.52	0.63				
1:G:9:HIS:CE1	1:G:11:ASP:OD2	2.52	0.63				
1:L:9:HIS:CE1	1:L:11:ASP:OD2	2.51	0.63				
1:O:9:HIS:CE1	1:0:11:ASP:OD2	2.51	0.63				
1:D:9:HIS:CE1	1:D:11:ASP:OD2	2.51	0.63				
1:A:9:HIS:CE1	1:A:11:ASP:OD1	2.52	0.63				
1:H:9:HIS:CE1	1:H:11:ASP:OD2	2.51	0.62				
1:X:93:LEU:HD23	1:X:157:PRO:HG3	1.81	0.62				
1:D:93:LEU:HD23	1:D:157:PRO:HG3	1.80	0.62				
1:B:9:HIS:CE1	1:B:11:ASP:OD1	2.52	0.62				
1:N:9:HIS:CE1	1:N:11:ASP:OD2	2.51	0.62				
1:E:93:LEU:HD23	1:E:157:PRO:HG3	1.80	0.62				
1:J:149:THR:O	1:J:153:LYS:HG2	1.99	0.62				
1:T:149:THR:O	1:T:153:LYS:HG2	2.00	0.62				
1:A:149:THR:O	1:A:153:LYS:HG2	2.00	0.62				
1:L:149:THR:O	1:L:153:LYS:HG2	2.00	0.62				
1:H:93:LEU:HD23	1:H:157:PRO:HG3	1.81	0.62				
1:K:9:HIS:CE1	1:K:11:ASP:OD1	2.53	0.62				
1:X:149:THR:O	1:X:153:LYS:HG2	2.00	0.62				
1:S:93:LEU:HD23	1:S:157:PRO:HG3	1.81	0.62				
1:D:149:THR:O	1:D:153:LYS:HG2	2.00	0.62				
1:E:149:THR:O	1:E:153:LYS:HG2	2.00	0.62				
1:O:93:LEU:HD23	1:O:157:PRO:HG3	1.81	0.62				
1:W:149:THR:O	1:W:153:LYS:HG2	2.00	0.62				
1:A:93:LEU:HD23	1:A:157:PRO:HG3	1.82	0.61				
1:I:149:THR:O	1:I:153:LYS:HG2	2.00	0.61				
1:P:149:THR:O	1:P:153:LYS:HG2	2.00	0.61				
1:Q:93:LEU:HD23	1:Q:157:PRO:HG3	1.82	0.61				
1:T:93:LEU:HD23	1:T:157:PRO:HG3	1.81	0.61				
1:X:9:HIS:CE1	1:X:11:ASP:OD1	2.52	0.61				



Interatomic Clash						
Atom-1	Atom-2	distance $(Å)$	overlan (Å)			
1·B·149·THB·O	1.B.153.LVS.HG2	2.00	0.61			
1.V.93.LEU.HD23	1.V.157.PRO.HG3	1.82	0.61			
1.U.149.THB.O	1.U.153.LVS.HG2	2.00	0.61			
1·B·93·LEU·HD23	1·B·157·PRO·HG3	1.82	0.61			
1:C:149:THR:O	1:C:153:LYS:HG2	2.00	0.61			
1:M:149:THR:O	1:M:153:LYS:HG2	2.00	0.61			
1:R:93:LEU:HD23	1:B:157:PRO:HG3	1.82	0.61			
1:Q:149:THR:O	1:Q:153:LYS:HG2	2.00	0.61			
1:F:93:LEU:HD23	1:F:157:PRO:HG3	1.82	0.61			
1:N:93:LEU:HD23	1:N:157:PRO:HG3	1.82	0.61			
1:M:93:LEU:HD23	1:M:157:PRO:HG3	1.82	0.61			
1:P:93:LEU:HD23	1:P:157:PRO:HG3	1.82	0.61			
1:B:149:THR:O	1:B:153:LYS:HG2	2.00	0.61			
1:F:149:THR:O	1:F:153:LYS:HG2	2.00	0.61			
1:K:149:THR:O	1:K:153:LYS:HG2	1.99	0.61			
1:L:93:LEU:HD23	1:L:157:PRO:HG3	1.81	0.61			
1:C:93:LEU:HD23	1:C:157:PRO:HG3	1.82	0.60			
1:S:149:THR:O	1:S:153:LYS:HG2	2.00	0.60			
1:V:149:THR:O	1:V:153:LYS:HG2	2.00	0.60			
1:G:93:LEU:HD23	1:G:157:PRO:HG3	1.82	0.60			
1:I:93:LEU:HD23	1:I:157:PRO:HG3	1.83	0.60			
1:J:93:LEU:HD23	1:J:157:PRO:HG3	1.82	0.60			
1:A:127:ASP:O	1:A:131:THR:HG23	2.02	0.60			
1:K:93:LEU:HD23	1:K:157:PRO:HG3	1.83	0.60			
1:O:149:THR:O	1:O:153:LYS:HG2	2.04	0.58			
1:G:149:THR:O	1:G:153:LYS:HG2	2.04	0.58			
1:N:149:THR:O	1:N:153:LYS:HG2	2.04	0.58			
1:H:149:THR:O	1:H:153:LYS:HG2	2.04	0.58			
1:T:64:LYS:HE3	1:T:132:HIS:HB3	1.87	0.56			
1:A:9:HIS:CE1	1:A:11:ASP:CG	2.83	0.52			
1:R:9:HIS:CE1	1:R:11:ASP:CG	2.84	0.52			
1:B:9:HIS:CE1	1:B:11:ASP:CG	2.84	0.51			
1:C:9:HIS:HE1	1:C:11:ASP:OD2	1.94	0.51			
1:S:9:HIS:HE1	1:S:11:ASP:OD2	1.93	0.51			
1:S:9:HIS:CE1	1:S:11:ASP:CG	2.84	0.51			
1:T:9:HIS:CE1	1:T:11:ASP:CG	2.84	0.51			
1:H:9:HIS:CE1	1:H:11:ASP:CG	2.84	0.51			
1:M:9:HIS:CE1	1:M:11:ASP:CG	2.84	0.51			
1:T:9:HIS:HE1	1:T:11:ASP:OD2	1.93	0.51			
1:W:9:HIS:CE1	1:W:11:ASP:CG	2.84	0.51			
1:U:9:HIS:CE1	1:U:11:ASP:CG	2.84	0.51			



Interatomic Clash						
Atom-1	Atom-2	distance (Å)	overlap (Å)			
1:Q:9:HIS:CE1	1:Q:11:ASP:CG	2.84	0.51			
1:Q:9:HIS:HE1	1:Q:11:ASP:OD2	1.94	0.51			
1:V:9:HIS:CE1	1:V:11:ASP:CG	2.84	0.51			
1:C:9:HIS:CE1	1:C:11:ASP:CG	2.84	0.51			
1:X:9:HIS:CE1	1:X:11:ASP:CG	2.84	0.51			
1:N:9:HIS:CE1	1:N:11:ASP:CG	2.84	0.51			
1:P:9:HIS:CE1	1:P:11:ASP:CG	2.84	0.51			
1:E:9:HIS:CE1	1:E:11:ASP:CG	2.84	0.51			
1:F:9:HIS:HE1	1:F:11:ASP:OD2	1.94	0.51			
1:G:9:HIS:CE1	1:G:11:ASP:CG	2.84	0.51			
1:0:9:HIS:CE1	1:0:11:ASP:CG	2.84	0.51			
1:O:9:HIS:HE1	1:0:11:ASP:OD2	1.93	0.51			
1:U:9:HIS:HE1	1:U:11:ASP:OD2	1.94	0.51			
1:H:9:HIS:HE1	1:H:11:ASP:OD2	1.93	0.51			
1:I:9:HIS:CE1	1:I:11:ASP:CG	2.84	0.51			
1:J:9:HIS:CE1	1:J:11:ASP:CG	2.84	0.51			
1:B:9:HIS:HE1	1:B:11:ASP:OD1	1.94	0.50			
1:D:9:HIS:CE1	1:D:11:ASP:CG	2.84	0.50			
1:F:9:HIS:CE1	1:F:11:ASP:CG	2.84	0.50			
1:K:9:HIS:CE1	1:K:11:ASP:CG	2.84	0.50			
1:M:9:HIS:HE1	1:M:11:ASP:OD1	1.95	0.50			
1:A:116:LEU:O	1:A:120:LYS:HG2	2.12	0.50			
1:L:9:HIS:CE1	1:L:11:ASP:CG	2.84	0.50			
1:X:116:LEU:O	1:X:120:LYS:HG2	2.12	0.50			
1:0:116:LEU:O	1:O:120:LYS:HG2	2.12	0.50			
1:R:116:LEU:O	1:R:120:LYS:HG2	2.12	0.50			
1:D:116:LEU:O	1:D:120:LYS:HG2	2.12	0.50			
1:W:114:HIS:NE2	1:W:130:GLU:OE2	2.34	0.50			
1:W:116:LEU:O	1:W:120:LYS:HG2	2.12	0.50			
1:B:116:LEU:O	1:B:120:LYS:HG2	2.12	0.50			
1:K:114:HIS:NE2	1:K:130:GLU:OE2	2.34	0.50			
1:Q:116:LEU:O	1:Q:120:LYS:HG2	2.12	0.50			
1:A:64:LYS:HE3	1:A:132:HIS:HB3	1.94	0.50			
1:L:116:LEU:O	1:L:120:LYS:HG2	2.12	0.50			
1:S:116:LEU:O	1:S:120:LYS:HG2	2.12	0.50			
1:J:114:HIS:NE2	1:J:130:GLU:OE2	2.34	0.49			
1:N:9:HIS:HE1	1:N:11:ASP:OD2	1.94	0.49			
1:V:116:LEU:O	1:V:120:LYS:HG2	2.12	0.49			
1:X:9:HIS:HE1	1:X:11:ASP:OD1	1.95	0.49			
1:T:116:LEU:O	1:T:120:LYS:HG2	2.12	0.49			
1:K:9:HIS:HE1	1:K:11:ASP:OD1	1.95	0.49			



	Interatomic Clash						
Atom-1	Atom-2	distance (Å)	overlap (Å)				
1:F:116:LEU:O	1:F:120:LYS:HG2	2.12	0.49				
1:R:9:HIS:HE1	1:R:11:ASP:OD2	1.94	0.49				
1:M:116:LEU:O	1:M:120:LYS:HG2	2.12	0.49				
1:W:9:HIS:HE1	1:W:11:ASP:OD2	1.93	0.49				
1:C:116:LEU:O	1:C:120:LYS:HG2	2.12	0.49				
1:E:9:HIS:HE1	1:E:11:ASP:OD2	1.93	0.49				
1:H:116:LEU:O	1:H:120:LYS:HG2	2.12	0.49				
1:S:114:HIS:NE2	1:S:130:GLU:OE1	2.34	0.49				
1:E:116:LEU:O	1:E:120:LYS:HG2	2.12	0.48				
1:I:114:HIS:NE2	1:I:130:GLU:OE2	2.34	0.48				
1:P:116:LEU:O	1:P:120:LYS:HG2	2.12	0.48				
1:A:9:HIS:HE1	1:A:11:ASP:OD1	1.95	0.48				
1:L:9:HIS:HE1	1:L:11:ASP:OD2	1.93	0.48				
1:P:9:HIS:HE1	1:P:11:ASP:OD1	1.94	0.48				
1:V:9:HIS:HE1	1:V:11:ASP:OD2	1.94	0.48				
1:D:9:HIS:HE1	1:D:11:ASP:OD2	1.94	0.48				
1:B:114:HIS:NE2	1:B:130:GLU:OE2	2.33	0.47				
1:J:9:HIS:HE1	1:J:11:ASP:OD2	1.95	0.47				
1:I:9:HIS:HE1	1:I:11:ASP:OD2	1.95	0.47				
1:A:9:HIS:HE1	1:A:11:ASP:CG	2.18	0.47				
1:E:114:HIS:NE2	1:E:130:GLU:OE1	2.34	0.47				
1:H:164:TYR:O	1:H:168:LYS:HG2	2.15	0.47				
1:W:93:LEU:O	1:W:97:GLU:HG3	2.15	0.47				
1:K:164:TYR:O	1:K:168:LYS:HG2	2.15	0.47				
1:S:164:TYR:O	1:S:168:LYS:HG2	2.15	0.47				
1:V:164:TYR:O	1:V:168:LYS:HG2	2.15	0.47				
1:C:164:TYR:O	1:C:168:LYS:HG2	2.16	0.46				
1:D:164:TYR:O	1:D:168:LYS:HG2	2.16	0.46				
1:E:164:TYR:O	1:E:168:LYS:HG2	2.16	0.46				
1:I:164:TYR:O	1:I:168:LYS:HG2	2.16	0.46				
1:L:164:TYR:O	1:L:168:LYS:HG2	2.16	0.46				
1:N:164:TYR:O	1:N:168:LYS:HG2	2.16	0.46				
1:R:164:TYR:O	1:R:168:LYS:HG2	2.16	0.46				
1:A:164:TYR:O	1:A:168:LYS:HG2	2.16	0.46				
1:M:164:TYR:O	1:M:168:LYS:HG2	2.16	0.46				
1:P:164:TYR:O	1:P:168:LYS:HG2	2.16	0.46				
1:R:9:HIS:HE1	1:R:11:ASP:CG	2.19	0.46				
1:B:164:TYR:O	1:B:168:LYS:HG2	2.16	0.46				
1:F:164:TYR:O	1:F:168:LYS:HG2	2.16	0.46				
1:Q:9:HIS:HE1	1:Q:11:ASP:CG	2.19	0.46				
1:S:9:HIS:HE1	1:S:11:ASP:CG	2.19	0.46				



	Interatomic Clash					
Atom-1	Atom-2	distance (Å)	overlap (Å)			
1:H:9:HIS:HE1	1:H:11:ASP:CG	2.19	0.46			
1:V:9:HIS:HE1	1:V:11:ASP:CG	2.19	0.46			
1:B:9:HIS:HE1	1:B:11:ASP:CG	2.19	0.46			
1:W:9:HIS:HE1	1:W:11:ASP:CG	2.19	0.46			
1:U:9:HIS:HE1	1:U:11:ASP:CG	2.19	0.46			
1:C:9:HIS:HE1	1:C:11:ASP:CG	2.19	0.46			
1:J:164:TYR:O	1:J:168:LYS:HG2	2.15	0.46			
1:M:9:HIS:HE1	1:M:11:ASP:CG	2.19	0.46			
1:U:164:TYR:O	1:U:168:LYS:HG2	2.15	0.46			
1:0:164:TYR:0	1:O:168:LYS:HG2	2.15	0.46			
1:P:9:HIS:HE1	1:P:11:ASP:CG	2.19	0.46			
1:Q:164:TYR:O	1:Q:168:LYS:HG2	2.16	0.46			
1:E:9:HIS:HE1	1:E:11:ASP:CG	2.19	0.45			
1:F:114:HIS:NE2	1:F:130:GLU:OE1	2.34	0.45			
1:M:114:HIS:NE2	1:M:130:GLU:OE1	2.34	0.45			
1:N:9:HIS:HE1	1:N:11:ASP:CG	2.20	0.45			
1:W:164:TYR:O	1:W:168:LYS:HG2	2.16	0.45			
1:G:164:TYR:O	1:G:168:LYS:HG2	2.15	0.45			
1:I:9:HIS:HE1	1:I:11:ASP:CG	2.20	0.45			
1:P:114:HIS:NE2	1:P:130:GLU:OE2	2.34	0.45			
1:X:9:HIS:HE1	1:X:11:ASP:CG	2.19	0.45			
1:X:164:TYR:O	1:X:168:LYS:HG2	2.15	0.45			
1:L:9:HIS:HE1	1:L:11:ASP:CG	2.19	0.45			
1:O:9:HIS:HE1	1:0:11:ASP:CG	2.19	0.45			
1:D:9:HIS:HE1	1:D:11:ASP:CG	2.19	0.45			
1:T:9:HIS:HE1	1:T:11:ASP:CG	2.19	0.45			
1:I:120:LYS:HA	1:I:120:LYS:HD2	1.90	0.45			
1:J:9:HIS:HE1	1:J:11:ASP:CG	2.20	0.45			
1:G:9:HIS:HE1	1:G:11:ASP:OD2	1.95	0.45			
1:F:9:HIS:HE1	1:F:11:ASP:CG	2.19	0.45			
1:U:93:LEU:O	1:U:97:GLU:HG3	2.17	0.45			
1:C:114:HIS:NE2	1:C:130:GLU:OE2	2.34	0.45			
1:U:5:ARG:NH2	1:U:10:GLN:OE1	2.50	0.44			
1:K:9:HIS:HE1	1:K:11:ASP:CG	2.19	0.44			
1:T:164:TYR:O	1:T:168:LYS:HG2	2.16	0.44			
1:G:9:HIS:HE1	1:G:11:ASP:CG	2.20	0.44			
1:D:114:HIS:NE2	1:D:130:GLU:OE1	2.34	0.44			
1:W:156:ALA:HA	1:W:162:ALA:HB3	2.00	0.44			
1:Q:93:LEU:O	1:Q:97:GLU:HG3	2.18	0.43			
1:G:93:LEU:O	1:G:97:GLU:HG3	2.18	0.43			
1:J:116:LEU:O	1:J:120:LYS:HG2	2.18	0.43			



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:R:114:HIS:NE2	1:R:130:GLU:OE1	2.34	0.43
1:U:116:LEU:O	1:U:120:LYS:HG2	2.18	0.43
1:W:75:ARG:HA	1:W:75:ARG:HD3	1.86	0.43
1:C:93:LEU:O	1:C:97:GLU:HG3	2.18	0.43
1:L:114:HIS:NE2	1:L:130:GLU:OE1	2.34	0.43
1:N:93:LEU:O	1:N:97:GLU:HG3	2.18	0.43
1:Q:114:HIS:NE2	1:Q:130:GLU:OE2	2.34	0.43
1:U:114:HIS:NE2	1:U:130:GLU:OE2	2.33	0.43
1:J:120:LYS:HA	1:J:120:LYS:HD2	1.90	0.43
1:K:93:LEU:O	1:K:97:GLU:HG3	2.18	0.43
1:K:116:LEU:O	1:K:120:LYS:HG2	2.18	0.43
1:P:75:ARG:HA	1:P:75:ARG:HD3	1.78	0.43
1:A:75:ARG:HD3	1:A:75:ARG:HA	1.86	0.43
1:X:93:LEU:O	1:X:97:GLU:HG3	2.18	0.43
1:J:93:LEU:O	1:J:97:GLU:HG3	2.18	0.43
1:D:93:LEU:O	1:D:97:GLU:HG3	2.18	0.43
1:N:116:LEU:O	1:N:120:LYS:HG2	2.18	0.43
1:V:93:LEU:O	1:V:97:GLU:HG3	2.18	0.43
1:A:5:ARG:NH2	1:A:10:GLN:OE1	2.51	0.42
1:I:93:LEU:O	1:I:97:GLU:HG3	2.18	0.42
1:K:120:LYS:HA	1:K:120:LYS:HD2	1.89	0.42
1:R:75:ARG:HD3	1:R:75:ARG:HA	1.86	0.42
1:F:75:ARG:HA	1:F:75:ARG:HD3	1.86	0.42
1:T:114:HIS:NE2	1:T:130:GLU:OE1	2.34	0.42
1:G:116:LEU:O	1:G:120:LYS:HG2	2.18	0.42
1:K:75:ARG:HA	1:K:75:ARG:HD3	1.86	0.42
1:X:75:ARG:HD3	1:X:75:ARG:HA	1.86	0.42
1:R:93:LEU:O	1:R:97:GLU:HG3	2.18	0.42
1:D:75:ARG:HD3	1:D:75:ARG:HA	1.86	0.42
1:I:116:LEU:O	1:I:120:LYS:HG2	2.18	0.42
1:E:75:ARG:HD3	1:E:75:ARG:HA	1.86	0.42
1:L:75:ARG:HD3	1:L:75:ARG:HA	1.86	0.42
1:N:120:LYS:HA	1:N:120:LYS:HD2	1.90	0.42
1:O:75:ARG:HD3	1:O:75:ARG:HA	1.86	0.42
1:G:114:HIS:NE2	1:G:130:GLU:OE2	2.34	0.41
1:V:75:ARG:HA	1:V:75:ARG:HD3	1.86	0.41
1:I:75:ARG:HA	1:I:75:ARG:HD3	1.86	0.40
1:J:75:ARG:HA	1:J:75:ARG:HD3	1.86	0.40
1:X:114:HIS:NE2	1:X:130:GLU:OE2	2.34	0.40

There are no symmetry-related clashes.



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 PDB entries followed by that with respect to all EM entries.

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	А	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	В	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	С	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	D	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	Е	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	F	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	G	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	Η	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	Ι	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	J	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	Κ	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	L	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	М	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	Ν	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	Ο	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	Р	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	Q	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	R	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	S	170/172~(99%)	167~(98%)	3~(2%)	0	100 100
1	Т	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	U	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	V	170/172~(99%)	168 (99%)	2(1%)	0	100 100
1	W	170/172~(99%)	168 (99%)	2 (1%)	0	100 100
1	X	$\overline{170/172}~(99\%)$	168 (99%)	2 (1%)	0	100 100
All	All	4080/4128 (99%)	4031 (99%)	49 (1%)	0	100 100



There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	Perce	ntiles
1	А	145/153~(95%)	145 (100%)	0	100	100
1	В	145/153~(95%)	145 (100%)	0	100	100
1	С	145/153~(95%)	145 (100%)	0	100	100
1	D	145/153~(95%)	145 (100%)	0	100	100
1	Ε	145/153~(95%)	145 (100%)	0	100	100
1	F	145/153~(95%)	145 (100%)	0	100	100
1	G	145/153~(95%)	145 (100%)	0	100	100
1	Н	145/153~(95%)	145 (100%)	0	100	100
1	Ι	145/153~(95%)	145 (100%)	0	100	100
1	J	145/153~(95%)	145 (100%)	0	100	100
1	K	145/153~(95%)	145 (100%)	0	100	100
1	L	145/153~(95%)	145 (100%)	0	100	100
1	М	145/153~(95%)	145 (100%)	0	100	100
1	Ν	145/153~(95%)	145 (100%)	0	100	100
1	О	145/153~(95%)	145 (100%)	0	100	100
1	Р	145/153~(95%)	145 (100%)	0	100	100
1	Q	145/153~(95%)	145 (100%)	0	100	100
1	R	145/153~(95%)	145 (100%)	0	100	100
1	S	145/153~(95%)	145 (100%)	0	100	100
1	Т	145/153~(95%)	145 (100%)	0	100	100
1	U	145/153~(95%)	145 (100%)	0	100	100
1	V	145/153~(95%)	145 (100%)	0	100	100
1	W	145/153~(95%)	145 (100%)	0	100	100
1	Х	145/153~(95%)	145 (100%)	0	100	100



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3480/3672~(95%)	3480 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

