



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 01:24 AM EST

PDB ID : 7K3V
EMDB ID : EMD-22657
Title : Apoferritin structure at 1.34 angstrom resolution determined from a 300 kV Titan Krios G3i electron microscope with K3 detector
Authors : Zhang, K.; Pintilie, G.; Li, S.; Schmid, M.; Chiu, W.
Deposited on : 2020-09-14
Resolution : 1.34 Å(reported)
Based on initial model : 3AJ0

This is a Full wwPDB EM Validation Report for a publicly released PDB 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

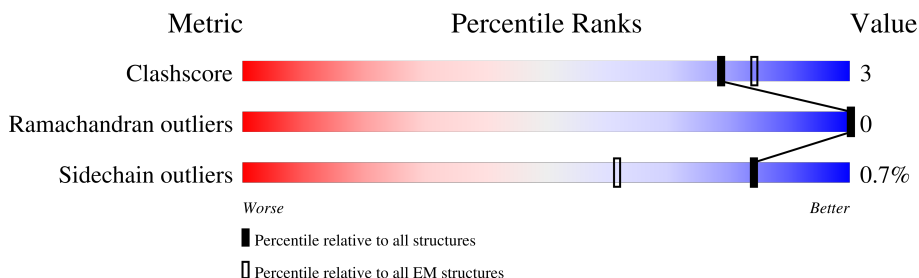
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.34 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)	EM structures (#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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	172	95% 5%
1	B	172	95% 5%
1	C	172	94% 6%
1	D	172	94% 6%
1	E	172	94% 6%
1	F	172	95% 5%
1	G	172	94% 6%
1	H	172	93% 7%
1	I	172	95% 5%

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Mol	Chain	Length	Quality of chain
1	J	172	 96% .
1	K	172	 94% 6%
1	L	172	 94% 6%
1	M	172	 94% 6%
1	N	172	 95% 5%
1	O	172	 94% 6%
1	P	172	 94% 6%
1	Q	172	 95% 5%
1	R	172	 94% 6%
1	S	172	 95% 5%
1	T	172	 94% 6%
1	U	172	 94% 6%
1	V	172	 94% 6%
1	W	172	 94% 6%
1	X	172	 95% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 38406 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.

- Molecule 1 is a protein called Ferritin heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	B	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	C	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	D	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	E	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	F	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	G	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	H	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	I	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	J	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	K	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	L	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	M	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	N	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	O	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	P	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	Q	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	S	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	T	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	U	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	V	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	W	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		
1	X	172	Total	C	N	O	S	10	0
			1475	927	254	286	8		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	12	Total	Zn	0
			12	12	
2	B	12	Total	Zn	0
			12	12	
2	C	12	Total	Zn	0
			12	12	
2	D	12	Total	Zn	0
			12	12	
2	E	11	Total	Zn	0
			11	11	
2	F	11	Total	Zn	0
			11	11	
2	G	10	Total	Zn	0
			10	10	
2	H	12	Total	Zn	0
			12	12	
2	I	11	Total	Zn	0
			11	11	
2	J	10	Total	Zn	0
			10	10	
2	K	10	Total	Zn	0
			10	10	
2	L	11	Total	Zn	0
			11	11	

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Mol	Chain	Residues	Atoms		AltConf
2	M	10	Total 10	Zn 10	0
2	N	10	Total 10	Zn 10	0
2	O	10	Total 10	Zn 10	0
2	P	10	Total 10	Zn 10	0
2	Q	10	Total 10	Zn 10	0
2	R	10	Total 10	Zn 10	0
2	S	10	Total 10	Zn 10	0
2	T	10	Total 10	Zn 10	0
2	U	10	Total 10	Zn 10	0
2	V	10	Total 10	Zn 10	0
2	W	10	Total 10	Zn 10	0
2	X	10	Total 10	Zn 10	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
3	A	3	Total 3	Na 3	0
3	B	3	Total 3	Na 3	0
3	C	3	Total 3	Na 3	0
3	D	3	Total 3	Na 3	0
3	E	3	Total 3	Na 3	0
3	F	3	Total 3	Na 3	0
3	G	4	Total 4	Na 4	0

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Mol	Chain	Residues	Atoms		AltConf
3	H	3	Total 3	Na 3	0
3	I	3	Total 3	Na 3	0
3	J	3	Total 3	Na 3	0
3	K	4	Total 4	Na 4	0
3	L	3	Total 3	Na 3	0
3	M	4	Total 4	Na 4	0
3	N	3	Total 3	Na 3	0
3	O	4	Total 4	Na 4	0
3	P	3	Total 3	Na 3	0
3	Q	4	Total 4	Na 4	0
3	R	4	Total 4	Na 4	0
3	S	3	Total 3	Na 3	0
3	T	4	Total 4	Na 4	0
3	U	3	Total 3	Na 3	0
3	V	4	Total 4	Na 4	0
3	W	3	Total 3	Na 3	0
3	X	3	Total 3	Na 3	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	111	Total 111	O 111	0
4	B	111	Total 111	O 111	0

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Mol	Chain	Residues	Atoms		AltConf
4	C	112	Total 112	O 112	0
4	D	111	Total 111	O 111	0
4	E	111	Total 111	O 111	0
4	F	112	Total 112	O 112	0
4	G	111	Total 111	O 111	0
4	H	112	Total 112	O 112	0
4	I	111	Total 111	O 111	0
4	J	112	Total 112	O 112	0
4	K	110	Total 110	O 110	0
4	L	111	Total 111	O 111	0
4	M	110	Total 110	O 110	0
4	N	113	Total 113	O 113	0
4	O	110	Total 110	O 110	0
4	P	112	Total 112	O 112	0
4	Q	111	Total 111	O 111	0
4	R	110	Total 110	O 110	0
4	S	113	Total 113	O 113	0
4	T	111	Total 111	O 111	0
4	U	112	Total 112	O 112	0
4	V	110	Total 110	O 110	0
4	W	113	Total 113	O 113	0

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Mol	Chain	Residues	Atoms		AltConf
4	X	112	Total	O	0
			112	112	

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.

- Molecule 1: Ferritin heavy chain

Chain A:  95% 5%



- Molecule 1: Ferritin heavy chain

Chain B:  95% 5%



- Molecule 1: Ferritin heavy chain

Chain C:  94% 6%



- Molecule 1: Ferritin heavy chain

Chain D:  94% 6%



- Molecule 1: Ferritin heavy chain

Chain E:  94% 6%



- Molecule 1: Ferritin heavy chain

Chain F:  95% 5%



- Molecule 1: Ferritin heavy chain

Chain G:  94% 6%



- Molecule 1: Ferritin heavy chain

Chain H:  93% 7%



- Molecule 1: Ferritin heavy chain

Chain I:  95% 5%



- Molecule 1: Ferritin heavy chain

Chain J:  96% .



- Molecule 1: Ferritin heavy chain

Chain K:  94% 6%



- Molecule 1: Ferritin heavy chain

Chain L:  94% 6%



- Molecule 1: Ferritin heavy chain

Chain M:  94% 6%



- Molecule 1: Ferritin heavy chain

Chain N: 95% 5%



- Molecule 1: Ferritin heavy chain

Chain O: 94% 6%



- Molecule 1: Ferritin heavy chain

Chain P: 94% 6%



- Molecule 1: Ferritin heavy chain

Chain Q: 95% 5%



- Molecule 1: Ferritin heavy chain

Chain R: 94% 6%



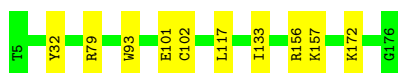
- Molecule 1: Ferritin heavy chain

Chain S: 95% 5%



- Molecule 1: Ferritin heavy chain

Chain T: 94% 6%



- Molecule 1: Ferritin heavy chain

Chain U:  94% 6%



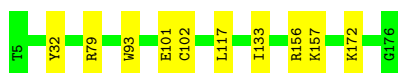
- Molecule 1: Ferritin heavy chain

Chain V:  94% 6%



- Molecule 1: Ferritin heavy chain

Chain W:  94% 6%



- Molecule 1: Ferritin heavy chain

Chain X:  95% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, O	Depositor
Number of particles used	902455	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	100	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ZN

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	0.31	0/1553	0.49	0/2088
1	B	0.31	0/1553	0.49	0/2088
1	C	0.31	0/1553	0.49	0/2088
1	D	0.31	0/1553	0.49	0/2088
1	E	0.31	0/1553	0.49	0/2088
1	F	0.31	0/1553	0.49	0/2088
1	G	0.31	0/1553	0.49	0/2088
1	H	0.31	0/1553	0.49	0/2088
1	I	0.31	0/1553	0.49	0/2088
1	J	0.31	0/1553	0.49	0/2088
1	K	0.31	0/1553	0.49	0/2088
1	L	0.31	0/1553	0.49	0/2088
1	M	0.31	0/1553	0.49	0/2088
1	N	0.31	0/1553	0.49	0/2088
1	O	0.31	0/1553	0.49	0/2088
1	P	0.31	0/1553	0.49	0/2088
1	Q	0.31	0/1553	0.49	0/2088
1	R	0.31	0/1553	0.49	0/2088
1	S	0.31	0/1553	0.49	0/2088
1	T	0.31	0/1553	0.49	0/2088
1	U	0.31	0/1553	0.49	0/2088
1	V	0.31	0/1553	0.49	0/2088
1	W	0.31	0/1553	0.49	0/2088
1	X	0.31	0/1553	0.49	0/2088
All	All	0.31	0/37272	0.49	0/50112

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

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	1475	0	1407	7	0
1	B	1475	0	1407	7	0
1	C	1475	0	1407	8	0
1	D	1475	0	1407	9	0
1	E	1475	0	1407	9	0
1	F	1475	0	1407	7	0
1	G	1475	0	1407	9	0
1	H	1475	0	1407	10	0
1	I	1475	0	1407	7	0
1	J	1475	0	1407	6	0
1	K	1475	0	1407	8	0
1	L	1475	0	1407	9	0
1	M	1475	0	1407	9	0
1	N	1475	0	1407	7	0
1	O	1475	0	1407	9	0
1	P	1475	0	1407	9	0
1	Q	1475	0	1407	8	0
1	R	1475	0	1407	8	0
1	S	1475	0	1407	8	0
1	T	1475	0	1407	8	0
1	U	1475	0	1407	9	0
1	V	1475	0	1407	8	0
1	W	1475	0	1407	8	0
1	X	1475	0	1407	7	0
2	A	12	0	0	0	0
2	B	12	0	0	0	0
2	C	12	0	0	0	0
2	D	12	0	0	0	0
2	E	11	0	0	0	0
2	F	11	0	0	0	0
2	G	10	0	0	0	0
2	H	12	0	0	0	0
2	I	11	0	0	0	0
2	J	10	0	0	0	0
2	K	10	0	0	0	0
2	L	11	0	0	0	0
2	M	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	10	0	0	0	0
2	O	10	0	0	0	0
2	P	10	0	0	0	0
2	Q	10	0	0	0	0
2	R	10	0	0	0	0
2	S	10	0	0	0	0
2	T	10	0	0	0	0
2	U	10	0	0	0	0
2	V	10	0	0	0	0
2	W	10	0	0	0	0
2	X	10	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	4	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
3	K	4	0	0	0	0
3	L	3	0	0	0	0
3	M	4	0	0	0	0
3	N	3	0	0	0	0
3	O	4	0	0	0	0
3	P	3	0	0	0	0
3	Q	4	0	0	0	0
3	R	4	0	0	0	0
3	S	3	0	0	0	0
3	T	4	0	0	0	0
3	U	3	0	0	0	0
3	V	4	0	0	0	0
3	W	3	0	0	0	0
3	X	3	0	0	0	0
4	A	111	0	0	4	0
4	B	111	0	0	4	0
4	C	112	0	0	4	0
4	D	111	0	0	4	0
4	E	111	0	0	4	0
4	F	112	0	0	3	0
4	G	111	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	112	0	0	4	0
4	I	111	0	0	4	0
4	J	112	0	0	3	0
4	K	110	0	0	4	0
4	L	111	0	0	4	0
4	M	110	0	0	4	0
4	N	113	0	0	3	0
4	O	110	0	0	4	0
4	P	112	0	0	3	0
4	Q	111	0	0	3	0
4	R	110	0	0	3	0
4	S	113	0	0	3	0
4	T	111	0	0	3	0
4	U	112	0	0	3	0
4	V	110	0	0	3	0
4	W	113	0	0	3	0
4	X	112	0	0	3	0
All	All	38406	0	33768	194	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 3.

All (194) 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:101:GLU:OE2	1:A:156[B]:ARG:NH2	2.18	0.77
1:I:101:GLU:OE2	1:I:156[B]:ARG:NH2	2.18	0.77
1:W:101:GLU:OE2	1:W:156[B]:ARG:NH2	2.18	0.77
1:V:101:GLU:OE2	1:V:156[B]:ARG:NH2	2.18	0.77
1:X:101:GLU:OE2	1:X:156[B]:ARG:NH2	2.18	0.77
1:C:101:GLU:OE2	1:C:156[B]:ARG:NH2	2.18	0.77
1:J:101:GLU:OE2	1:J:156[B]:ARG:NH2	2.18	0.77
1:K:101:GLU:OE2	1:K:156[B]:ARG:NH2	2.18	0.77
1:P:101:GLU:OE2	1:P:156[B]:ARG:NH2	2.18	0.77
1:B:101:GLU:OE2	1:B:156[B]:ARG:NH2	2.18	0.76
1:D:101:GLU:OE2	1:D:156[B]:ARG:NH2	2.18	0.76
1:H:101:GLU:OE2	1:H:156[B]:ARG:NH2	2.18	0.76
1:L:101:GLU:OE2	1:L:156[B]:ARG:NH2	2.18	0.76
1:Q:101:GLU:OE2	1:Q:156[B]:ARG:NH2	2.18	0.76
1:S:101:GLU:OE2	1:S:156[B]:ARG:NH2	2.18	0.76
1:T:101:GLU:OE2	1:T:156[B]:ARG:NH2	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:101:GLU:OE2	1:U:156[B]:ARG:NH2	2.18	0.76
1:R:101:GLU:OE2	1:R:156[B]:ARG:NH2	2.18	0.76
1:F:101:GLU:OE2	1:F:156[B]:ARG:NH2	2.18	0.76
1:N:101:GLU:OE2	1:N:156[B]:ARG:NH2	2.18	0.76
1:E:101:GLU:OE2	1:E:156[B]:ARG:NH2	2.18	0.75
1:M:101:GLU:OE2	1:M:156[B]:ARG:NH2	2.18	0.75
1:G:101:GLU:OE2	1:G:156[B]:ARG:NH2	2.18	0.75
1:O:101:GLU:OE2	1:O:156[B]:ARG:NH2	2.18	0.75
1:B:172:LYS:HE2	4:B:337:HOH:O	2.03	0.59
1:J:172:LYS:HE2	4:J:337:HOH:O	2.03	0.59
1:R:93:TRP:HZ3	1:R:102[B]:CYS:HG	1.49	0.59
1:T:93:TRP:HZ3	1:T:102[B]:CYS:HG	1.49	0.59
1:R:172:LYS:HE2	4:R:337:HOH:O	2.03	0.59
1:T:172:LYS:HE2	4:T:338:HOH:O	2.03	0.59
1:W:172:LYS:HE2	4:W:338:HOH:O	2.03	0.59
1:A:172:LYS:HE2	4:A:337:HOH:O	2.03	0.58
1:C:172:LYS:HE2	4:C:338:HOH:O	2.03	0.58
1:I:172:LYS:HE2	4:I:337:HOH:O	2.03	0.58
1:U:172:LYS:HE2	4:U:337:HOH:O	2.03	0.58
1:K:172:LYS:HE2	4:K:337:HOH:O	2.03	0.58
1:V:172:LYS:HE2	4:V:337:HOH:O	2.03	0.58
1:E:172:LYS:HE2	4:E:337:HOH:O	2.03	0.58
1:M:172:LYS:HE2	4:M:337:HOH:O	2.03	0.58
1:X:172:LYS:HE2	4:X:337:HOH:O	2.03	0.58
1:G:172:LYS:HE2	4:G:338:HOH:O	2.03	0.57
1:L:172:LYS:HE2	4:L:337:HOH:O	2.03	0.57
1:N:172:LYS:HE2	4:N:338:HOH:O	2.03	0.57
1:O:172:LYS:HE2	4:O:337:HOH:O	2.03	0.57
1:D:172:LYS:HE2	4:D:337:HOH:O	2.03	0.57
1:F:172:LYS:HE2	4:F:337:HOH:O	2.03	0.57
1:Q:172:LYS:HE2	4:Q:338:HOH:O	2.03	0.57
1:S:172:LYS:HE2	4:S:338:HOH:O	2.03	0.57
1:H:172:LYS:HE2	4:H:338:HOH:O	2.03	0.57
1:P:172:LYS:HE2	4:P:337:HOH:O	2.03	0.56
1:U:93:TRP:HZ3	1:U:102[B]:CYS:HG	1.54	0.55
1:W:93:TRP:HZ3	1:W:102[B]:CYS:HG	1.54	0.54
1:C:93:TRP:HZ3	1:C:102[B]:CYS:HG	1.52	0.54
1:K:93:TRP:HZ3	1:K:102[B]:CYS:HG	1.52	0.54
1:D:157:LYS:HG3	4:D:374:HOH:O	2.09	0.53
1:L:157:LYS:HG3	4:L:374:HOH:O	2.09	0.53
1:E:157:LYS:HG3	4:E:374:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:157:LYS:HG3	4:M:373:HOH:O	2.09	0.52
1:R:157:LYS:HG3	4:R:373:HOH:O	2.09	0.52
1:A:157:LYS:HG3	4:A:374:HOH:O	2.09	0.52
1:C:157:LYS:HG3	4:C:375:HOH:O	2.09	0.52
1:D:172:LYS:HG2	4:D:337:HOH:O	2.10	0.52
1:N:157:LYS:HG3	4:N:375:HOH:O	2.09	0.52
1:T:157:LYS:HG3	4:T:374:HOH:O	2.09	0.52
1:I:157:LYS:HG3	4:I:374:HOH:O	2.09	0.52
1:K:157:LYS:HG3	4:K:373:HOH:O	2.09	0.52
1:L:172:LYS:HG2	4:L:337:HOH:O	2.10	0.52
1:X:157:LYS:HG3	4:X:374:HOH:O	2.09	0.52
1:F:157:LYS:HG3	4:F:374:HOH:O	2.09	0.52
1:F:172:LYS:HG2	4:F:337:HOH:O	2.10	0.52
1:V:157:LYS:HG3	4:V:373:HOH:O	2.09	0.52
1:N:172:LYS:HG2	4:N:338:HOH:O	2.10	0.51
1:Q:157:LYS:HG3	4:Q:374:HOH:O	2.09	0.51
1:W:157:LYS:HG3	4:W:375:HOH:O	2.09	0.51
1:E:93:TRP:HZ3	1:E:102[B]:CYS:HG	1.57	0.51
1:S:157:LYS:HG3	4:S:375:HOH:O	2.09	0.51
1:S:172:LYS:HG2	4:S:338:HOH:O	2.10	0.51
1:B:157:LYS:HG3	4:B:374:HOH:O	2.09	0.51
1:M:93:TRP:HZ3	1:M:102[B]:CYS:HG	1.57	0.51
1:P:93:TRP:HZ3	1:P:102[B]:CYS:HG	1.59	0.51
1:Q:172:LYS:HG2	4:Q:338:HOH:O	2.10	0.51
1:U:157:LYS:HG3	4:U:374:HOH:O	2.09	0.51
1:J:157:LYS:HG3	4:J:374:HOH:O	2.09	0.51
1:K:172:LYS:HG2	4:K:337:HOH:O	2.10	0.51
1:O:157:LYS:HG3	4:O:373:HOH:O	2.09	0.51
1:C:172:LYS:HG2	4:C:338:HOH:O	2.10	0.51
1:G:157:LYS:HG3	4:G:374:HOH:O	2.09	0.51
1:B:172:LYS:HG2	4:B:337:HOH:O	2.10	0.51
1:J:172:LYS:HG2	4:J:337:HOH:O	2.10	0.51
1:O:172:LYS:HG2	4:O:337:HOH:O	2.10	0.51
1:Q:93:TRP:HZ3	1:Q:102[B]:CYS:HG	1.59	0.51
1:R:172:LYS:HG2	4:R:337:HOH:O	2.10	0.51
1:A:172:LYS:HG2	4:A:337:HOH:O	2.10	0.51
1:S:93:TRP:HZ3	1:S:102[B]:CYS:HG	1.59	0.51
1:T:172:LYS:HG2	4:T:338:HOH:O	2.10	0.51
1:G:172:LYS:HG2	4:G:338:HOH:O	2.10	0.51
1:H:157:LYS:HG3	4:H:375:HOH:O	2.09	0.51
1:I:172:LYS:HG2	4:I:337:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:157:LYS:HG3	4:P:374:HOH:O	2.09	0.50
1:U:172:LYS:HG2	4:U:337:HOH:O	2.10	0.50
1:W:172:LYS:HG2	4:W:338:HOH:O	2.10	0.50
1:P:172:LYS:HG2	4:P:337:HOH:O	2.10	0.50
1:V:172:LYS:HG2	4:V:337:HOH:O	2.10	0.50
1:X:172:LYS:HG2	4:X:337:HOH:O	2.10	0.50
1:H:172:LYS:HG2	4:H:338:HOH:O	2.10	0.50
1:I:93:TRP:HZ3	1:I:102[B]:CYS:HG	1.59	0.50
1:E:172:LYS:HG2	4:E:337:HOH:O	2.10	0.50
1:M:172:LYS:HG2	4:M:337:HOH:O	2.10	0.50
1:H:93:TRP:HZ3	1:H:102[B]:CYS:HG	1.60	0.49
1:B:93:TRP:HZ3	1:B:102[B]:CYS:HG	1.59	0.49
1:J:93:TRP:HZ3	1:J:102[B]:CYS:HG	1.59	0.49
1:O:93:TRP:HZ3	1:O:102[B]:CYS:HG	1.59	0.49
1:D:93:TRP:HZ3	1:D:102[B]:CYS:HG	1.55	0.49
1:L:93:TRP:HZ3	1:L:102[B]:CYS:HG	1.55	0.49
1:F:93:TRP:HZ3	1:F:102[B]:CYS:HG	1.60	0.48
1:N:93:TRP:HZ3	1:N:102[B]:CYS:HG	1.60	0.48
1:G:93:TRP:HZ3	1:G:102[B]:CYS:HG	1.60	0.47
1:X:93:TRP:HZ3	1:X:102[B]:CYS:HG	1.59	0.46
1:V:93:TRP:HZ3	1:V:102[B]:CYS:HG	1.60	0.45
1:A:93:TRP:HZ3	1:A:102[B]:CYS:HG	1.60	0.44
1:W:79:ARG:HA	1:W:79:ARG:HD3	1.84	0.44
1:P:79:ARG:HA	1:P:79:ARG:HD3	1.84	0.44
1:U:79:ARG:HD3	1:U:79:ARG:HA	1.84	0.44
1:H:79:ARG:HD3	1:H:79:ARG:HA	1.84	0.44
1:L:93:TRP:HZ3	1:L:102[B]:CYS:SG	2.42	0.43
1:R:93:TRP:HZ3	1:R:102[B]:CYS:SG	2.42	0.43
1:T:93:TRP:HZ3	1:T:102[B]:CYS:SG	2.42	0.43
1:D:93:TRP:HZ3	1:D:102[B]:CYS:SG	2.42	0.43
1:H:93:TRP:HZ3	1:H:102[B]:CYS:SG	2.42	0.43
1:P:93:TRP:HZ3	1:P:102[B]:CYS:SG	2.42	0.43
1:U:68:LYS:HB2	1:U:68:LYS:HE2	1.75	0.43
1:U:93:TRP:HZ3	1:U:102[B]:CYS:SG	2.42	0.43
1:O:93:TRP:HZ3	1:O:102[B]:CYS:SG	2.42	0.43
1:Q:68:LYS:HB2	1:Q:68:LYS:HE2	1.75	0.43
1:W:93:TRP:HZ3	1:W:102[B]:CYS:SG	2.42	0.43
1:A:93:TRP:HZ3	1:A:102[B]:CYS:SG	2.42	0.43
1:G:93:TRP:HZ3	1:G:102[B]:CYS:SG	2.42	0.43
1:I:93:TRP:HZ3	1:I:102[B]:CYS:SG	2.42	0.43
1:N:93:TRP:HZ3	1:N:102[B]:CYS:SG	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:79:ARG:HD3	1:M:79:ARG:HA	1.84	0.42
1:O:79:ARG:HA	1:O:79:ARG:HD3	1.84	0.42
1:S:68:LYS:HB2	1:S:68:LYS:HE2	1.75	0.42
1:V:93:TRP:HZ3	1:V:102[B]:CYS:SG	2.42	0.42
1:X:93:TRP:HZ3	1:X:102[B]:CYS:SG	2.42	0.42
1:F:93:TRP:HZ3	1:F:102[B]:CYS:SG	2.42	0.42
1:B:93:TRP:HZ3	1:B:102[B]:CYS:SG	2.42	0.42
1:E:79:ARG:HD3	1:E:79:ARG:HA	1.84	0.42
1:H:68:LYS:HB2	1:H:68:LYS:HE2	1.75	0.42
1:K:93:TRP:HZ3	1:K:102[B]:CYS:SG	2.42	0.42
1:C:93:TRP:HZ3	1:C:102[B]:CYS:SG	2.42	0.42
1:J:93:TRP:HZ3	1:J:102[B]:CYS:SG	2.42	0.42
1:Q:93:TRP:HZ3	1:Q:102[B]:CYS:SG	2.42	0.42
1:R:79:ARG:HA	1:R:79:ARG:HD3	1.84	0.42
1:M:93:TRP:HZ3	1:M:102[B]:CYS:SG	2.42	0.42
1:S:93:TRP:HZ3	1:S:102[B]:CYS:SG	2.42	0.42
1:E:93:TRP:HZ3	1:E:102[B]:CYS:SG	2.42	0.42
1:G:79:ARG:HA	1:G:79:ARG:HD3	1.84	0.42
1:L:79:ARG:HD3	1:L:79:ARG:HA	1.84	0.42
1:P:68:LYS:HB2	1:P:68:LYS:HE2	1.75	0.42
1:M:64[B]:GLU:HG3	4:M:367:HOH:O	2.20	0.42
1:E:64[B]:GLU:HG3	4:E:368:HOH:O	2.20	0.42
1:Q:79:ARG:HD3	1:Q:79:ARG:HA	1.84	0.42
1:T:79:ARG:HA	1:T:79:ARG:HD3	1.84	0.41
1:D:79:ARG:HD3	1:D:79:ARG:HA	1.84	0.41
1:S:79:ARG:HD3	1:S:79:ARG:HA	1.84	0.41
1:A:64[B]:GLU:HG3	4:A:368:HOH:O	2.20	0.41
1:H:64[B]:GLU:HG3	4:H:369:HOH:O	2.20	0.41
1:I:64[B]:GLU:HG3	4:I:368:HOH:O	2.20	0.41
1:C:64[B]:GLU:HG3	4:C:369:HOH:O	2.20	0.41
1:K:64[B]:GLU:HG3	4:K:367:HOH:O	2.20	0.41
1:O:64[B]:GLU:HG3	4:O:367:HOH:O	2.20	0.41
1:G:64[B]:GLU:HG3	4:G:368:HOH:O	2.20	0.41
1:G:117:LEU:HG	1:G:133:ILE:HD11	2.03	0.41
1:H:117:LEU:HG	1:H:133:ILE:HD11	2.03	0.41
1:N:79:ARG:HD3	1:N:79:ARG:HA	1.84	0.41
1:P:117:LEU:HG	1:P:133:ILE:HD11	2.03	0.41
1:R:117:LEU:HG	1:R:133:ILE:HD11	2.03	0.41
1:T:117:LEU:HG	1:T:133:ILE:HD11	2.03	0.41
1:L:64[B]:GLU:HG3	4:L:368:HOH:O	2.20	0.41
1:O:117:LEU:HG	1:O:133:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:117:LEU:HG	1:U:133:ILE:HD11	2.03	0.41
1:V:143:LYS:HB2	1:V:143:LYS:HE3	1.88	0.41
1:W:117:LEU:HG	1:W:133:ILE:HD11	2.03	0.41
1:X:143:LYS:HB2	1:X:143:LYS:HE3	1.88	0.41
1:D:64[B]:GLU:HG3	4:D:368:HOH:O	2.20	0.40
1:E:117:LEU:HG	1:E:133:ILE:HD11	2.03	0.40
1:F:79:ARG:HD3	1:F:79:ARG:HA	1.84	0.40
1:M:117:LEU:HG	1:M:133:ILE:HD11	2.03	0.40
1:L:117:LEU:HG	1:L:133:ILE:HD11	2.03	0.40
1:D:117:LEU:HG	1:D:133:ILE:HD11	2.03	0.40
1:B:64[B]:GLU:HG3	4:B:368:HOH:O	2.20	0.40
1:C:117:LEU:HG	1:C:133:ILE:HD11	2.03	0.40
1:K:117:LEU:HG	1:K:133:ILE:HD11	2.03	0.40
1:V:117:LEU:HG	1:V:133:ILE:HD11	2.03	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	A	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	B	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	C	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	D	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	E	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	F	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	G	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	H	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	I	182/172 (106%)	179 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	K	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	L	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	M	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	N	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	O	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	P	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	Q	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	R	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	S	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	T	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	U	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	V	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	W	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
1	X	182/172 (106%)	179 (98%)	3 (2%)	0	100	100
All	All	4368/4128 (106%)	4296 (98%)	72 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	Percentiles	
1	A	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	B	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	C	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	D	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	E	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	F	165/153 (108%)	164 (99%)	1 (1%)	86	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	H	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	I	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	J	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	K	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	L	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	M	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	N	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	O	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	P	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	Q	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	R	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	S	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	T	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	U	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	V	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	W	165/153 (108%)	164 (99%)	1 (1%)	86	67
1	X	165/153 (108%)	164 (99%)	1 (1%)	86	67
All	All	3960/3672 (108%)	3936 (99%)	24 (1%)	84	67

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	B	32	TYR
1	C	32	TYR
1	D	32	TYR
1	E	32	TYR
1	F	32	TYR
1	G	32	TYR
1	H	32	TYR
1	I	32	TYR
1	J	32	TYR
1	K	32	TYR
1	L	32	TYR
1	M	32	TYR

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Mol	Chain	Res	Type
1	N	32	TYR
1	O	32	TYR
1	P	32	TYR
1	Q	32	TYR
1	R	32	TYR
1	S	32	TYR
1	T	32	TYR
1	U	32	TYR
1	V	32	TYR
1	W	32	TYR
1	X	32	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	105	HIS
1	B	60	HIS
1	B	105	HIS
1	C	60	HIS
1	C	105	HIS
1	D	60	HIS
1	D	105	HIS
1	E	60	HIS
1	E	105	HIS
1	F	60	HIS
1	F	105	HIS
1	G	60	HIS
1	G	105	HIS
1	H	60	HIS
1	H	105	HIS
1	I	60	HIS
1	I	105	HIS
1	J	60	HIS
1	J	105	HIS
1	K	60	HIS
1	K	105	HIS
1	L	60	HIS
1	L	105	HIS
1	M	60	HIS
1	M	105	HIS
1	N	60	HIS

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Mol	Chain	Res	Type
1	N	105	HIS
1	O	60	HIS
1	O	105	HIS
1	P	60	HIS
1	P	105	HIS
1	Q	60	HIS
1	Q	105	HIS
1	R	60	HIS
1	R	105	HIS
1	S	60	HIS
1	S	105	HIS
1	T	60	HIS
1	T	105	HIS
1	U	60	HIS
1	U	105	HIS
1	V	60	HIS
1	V	105	HIS
1	W	60	HIS
1	W	105	HIS
1	X	60	HIS
1	X	105	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 334 ligands modelled in this entry, 334 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22657. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.