



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 21, 2022 – 06:25 PM JST

PDB ID : 7VHR  
Title : Apostichopus japonicus ferritin  
Authors : Wu, Y.; Su, X.R.; Ming, T.H.  
Deposited on : 2021-09-22  
Resolution : 2.76 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

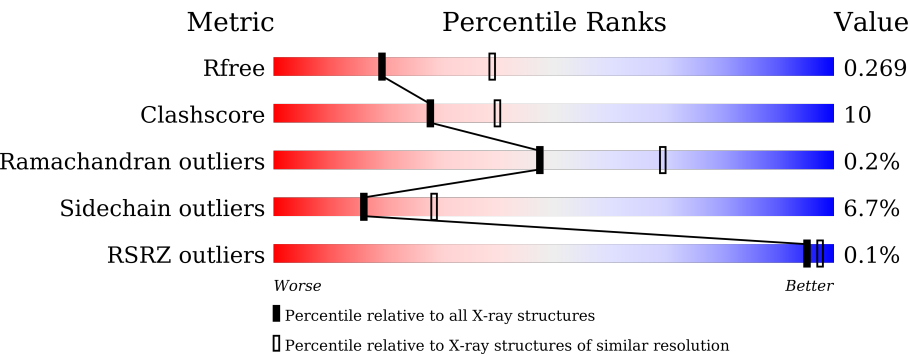
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.76 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.










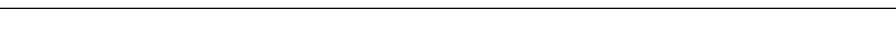
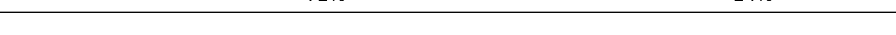
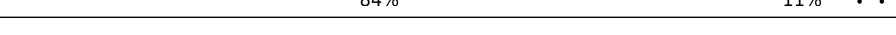
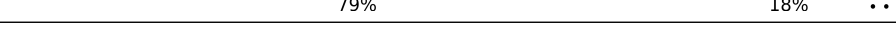







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	173	<div><div></div><div>80%16%..</div></div>
1	B	173	<div><div></div><div>83%15%..</div></div>
1	C	173	<div><div>%</div><div>81%16%..</div></div>
1	D	173	<div><div></div><div>82%15%..</div></div>
1	E	173	<div><div>%</div><div>72%23%..</div></div>
1	F	173	<div><div></div><div>76%20%..</div></div>

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Mol	Chain	Length	Quality of chain
1	G	173	 79% 17% ..
1	H	173	%  76% 17% . ..
1	I	173	 86% 10% ..
1	J	173	 76% 21% ..
1	K	173	%  79% 17% ..
1	L	173	 79% 17% ..
1	M	173	 73% 21% ..
1	N	173	 72% 24% ..
1	O	173	 84% 11% ..
1	P	173	 79% 18% ..
1	Q	173	 82% 13% ...
1	R	173	 73% 23% ..
1	S	173	 83% 12% ..
1	T	173	%  83% 13% ..
1	U	173	 77% 19% ..
1	V	173	 81% 14% ..
1	W	173	 77% 17% . ..
1	X	173	 77% 17% . ..

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33609 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 Ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1318	837	222	255	4			
1	B	171	Total	C	N	O	S	0	0	0
			1334	845	227	258	4			
1	C	168	Total	C	N	O	S	0	0	0
			1341	847	232	258	4			
1	D	169	Total	C	N	O	S	0	0	0
			1339	848	229	258	4			
1	E	169	Total	C	N	O	S	0	0	0
			1338	846	227	261	4			
1	F	169	Total	C	N	O	S	0	0	0
			1334	844	228	258	4			
1	G	169	Total	C	N	O	S	0	0	0
			1323	838	225	256	4			
1	H	168	Total	C	N	O	S	0	0	0
			1332	843	226	259	4			
1	I	169	Total	C	N	O	S	0	0	0
			1326	842	225	255	4			
1	J	170	Total	C	N	O	S	0	0	0
			1345	850	227	264	4			
1	K	169	Total	C	N	O	S	0	0	0
			1334	845	227	258	4			
1	L	168	Total	C	N	O	S	0	0	0
			1323	837	224	258	4			
1	M	168	Total	C	N	O	S	0	0	0
			1330	842	225	259	4			
1	N	168	Total	C	N	O	S	0	0	0
			1325	842	223	256	4			
1	O	168	Total	C	N	O	S	0	0	0
			1334	843	227	260	4			
1	P	169	Total	C	N	O	S	0	0	0
			1340	848	229	259	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	169	Total	C	N	O	S	0	0	0
			1346	854	227	261	4			
1	R	169	Total	C	N	O	S	0	0	0
			1337	846	226	261	4			
1	S	168	Total	C	N	O	S	0	0	0
			1329	844	226	255	4			
1	T	169	Total	C	N	O	S	0	0	0
			1339	848	226	261	4			
1	U	168	Total	C	N	O	S	0	0	0
			1333	841	227	261	4			
1	V	169	Total	C	N	O	S	0	0	0
			1337	845	226	262	4			
1	W	169	Total	C	N	O	S	0	0	0
			1335	845	227	259	4			
1	X	168	Total	C	N	O	S	0	0	0
			1311	836	221	250	4			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	C	1	Total	Mg	0	0
			1	1		
2	D	2	Total	Mg	0	0
			2	2		
2	E	3	Total	Mg	0	0
			3	3		
2	F	1	Total	Mg	0	0
			1	1		
2	G	1	Total	Mg	0	0
			1	1		
2	H	2	Total	Mg	0	0
			2	2		
2	I	1	Total	Mg	0	0
			1	1		
2	J	2	Total	Mg	0	0
			2	2		
2	K	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	1	Total 1	Mg 1	0	0
2	M	1	Total 1	Mg 1	0	0
2	N	4	Total 4	Mg 4	0	0
2	O	2	Total 2	Mg 2	0	0
2	P	2	Total 2	Mg 2	0	0
2	Q	2	Total 2	Mg 2	0	0
2	R	1	Total 1	Mg 1	0	0
2	S	3	Total 3	Mg 3	0	0
2	T	1	Total 1	Mg 1	0	0
2	U	1	Total 1	Mg 1	0	0
2	V	1	Total 1	Mg 1	0	0
2	W	1	Total 1	Mg 1	0	0
2	X	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total 57	O 57	0	0
3	B	24	Total 24	O 24	0	0
3	C	18	Total 18	O 18	0	0
3	D	87	Total 87	O 87	0	0
3	E	71	Total 71	O 71	0	0
3	F	75	Total 75	O 75	0	0

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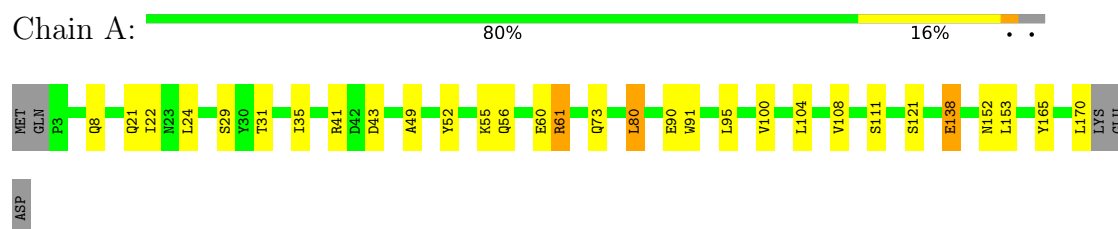
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	69	Total 69	O 69	0	0
3	H	76	Total 76	O 76	0	0
3	I	41	Total 41	O 41	0	0
3	J	73	Total 73	O 73	0	0
3	K	87	Total 87	O 87	0	0
3	L	73	Total 73	O 73	0	0
3	M	86	Total 86	O 86	0	0
3	N	66	Total 66	O 66	0	0
3	O	66	Total 66	O 66	0	0
3	P	62	Total 62	O 62	0	0
3	Q	72	Total 72	O 72	0	0
3	R	83	Total 83	O 83	0	0
3	S	73	Total 73	O 73	0	0
3	T	59	Total 59	O 59	0	0
3	U	73	Total 73	O 73	0	0
3	V	67	Total 67	O 67	0	0
3	W	58	Total 58	O 58	0	0
3	X	70	Total 70	O 70	0	0

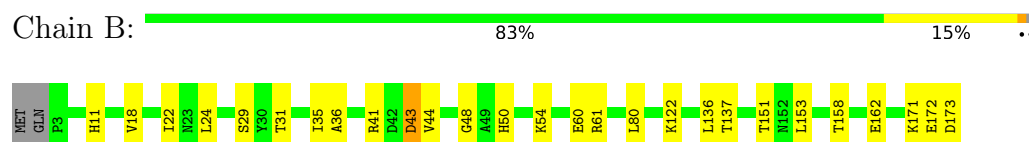
### 3 Residue-property plots [i](#)

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 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.

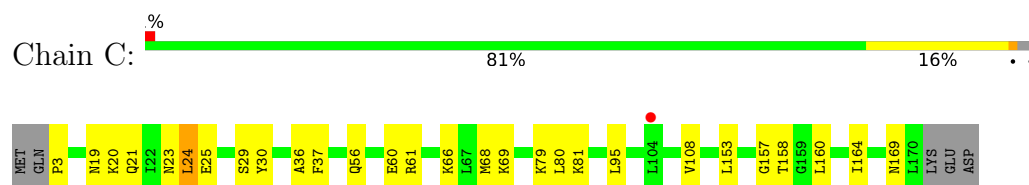
- Molecule 1: Ferritin



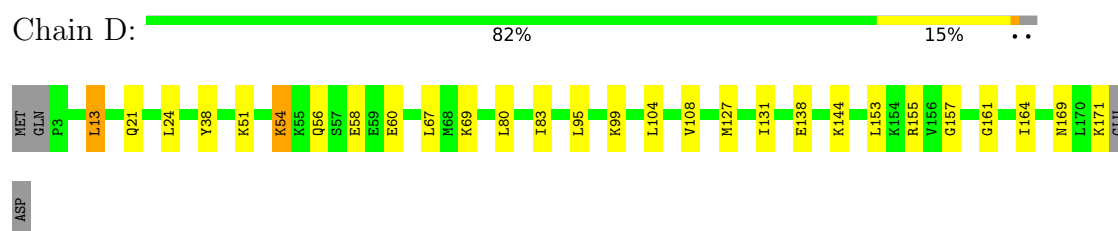
- Molecule 1: Ferritin



- Molecule 1: Ferritin



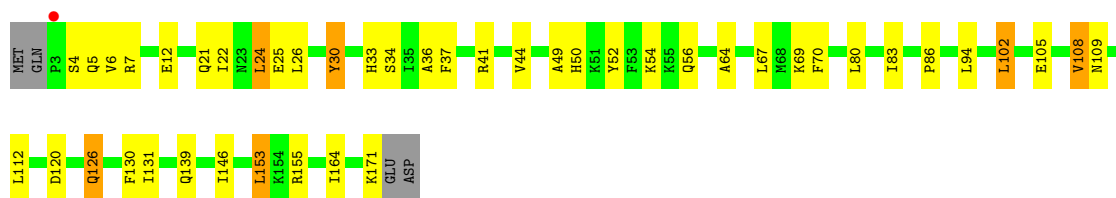
- Molecule 1: Ferritin



- Molecule 1: Ferritin

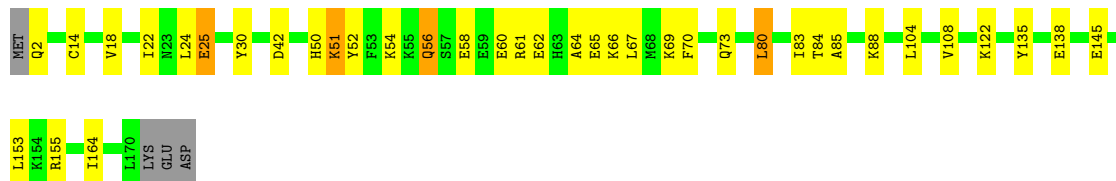






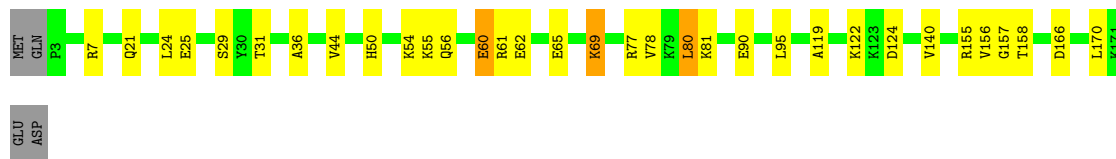
• Molecule 1: Ferritin

Chain F: 76% 20% ..



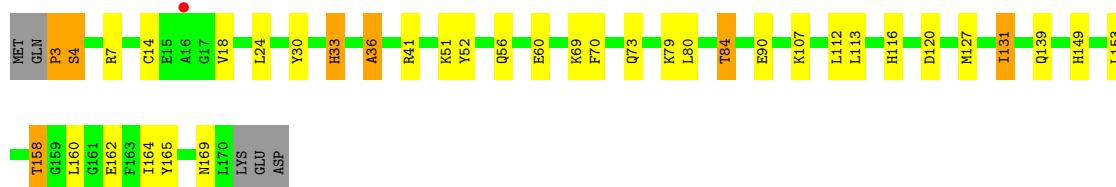
• Molecule 1: Ferritin

Chain G: 79% 17% ..



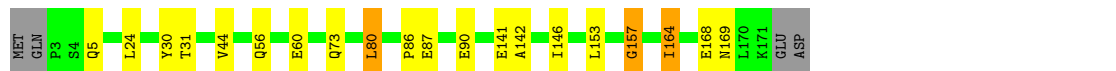
• Molecule 1: Ferritin

Chain H: 76% 17% ..



• Molecule 1: Ferritin

Chain I: 86% 10% ..



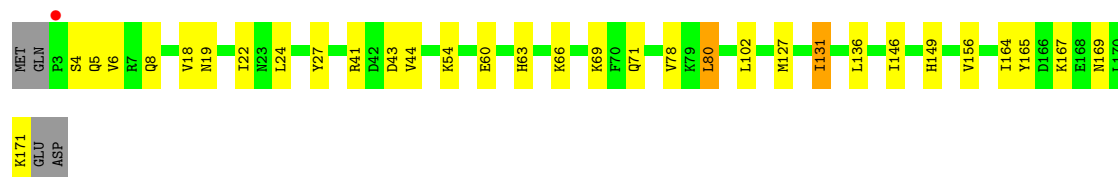
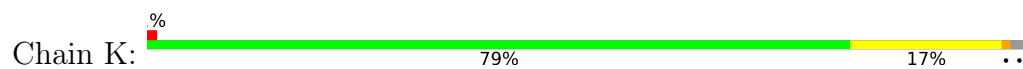
• Molecule 1: Ferritin

Chain J: 76% 21% ..

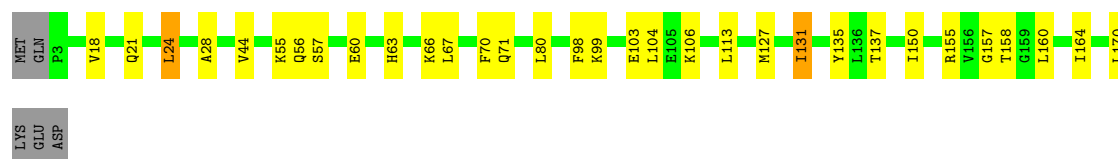
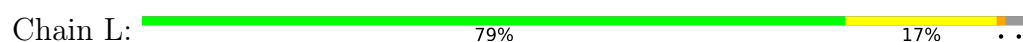




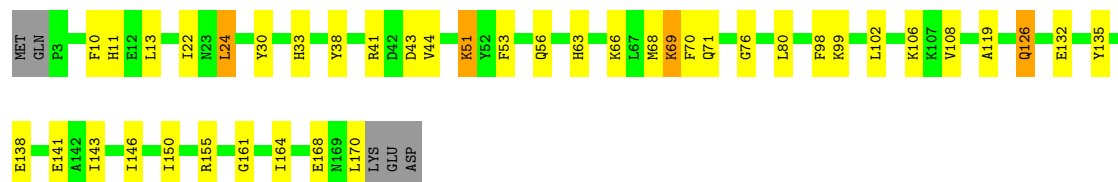
## • Molecule 1: Ferritin



## • Molecule 1: Ferritin



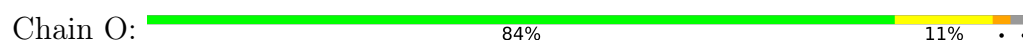
## • Molecule 1: Ferritin




## • Molecule 1: Ferritin

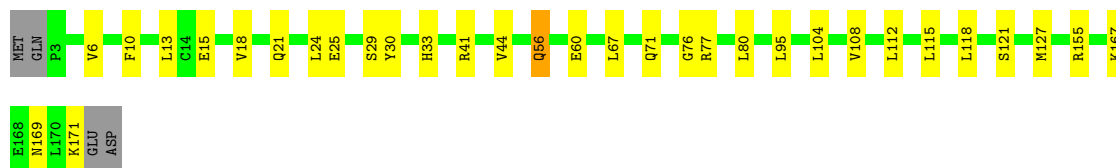


## • Molecule 1: Ferritin




## • Molecule 1: Ferritin

Chain P:  79% 18% ..



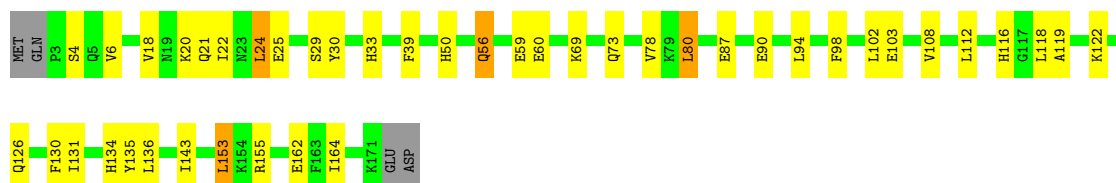
• Molecule 1: Ferritin

Chain Q:  82% 13% ...




• Molecule 1: Ferritin

Chain R:  73% 23% ..




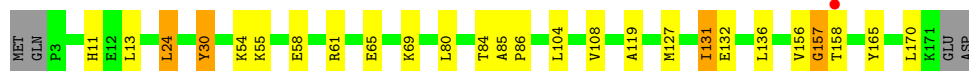
• Molecule 1: Ferritin

Chain S:  83% 12% ..




• Molecule 1: Ferritin

Chain T:  83% 13% ..



• Molecule 1: Ferritin

Chain U:  77% 19% ..



• Molecule 1: Ferritin

Chain V: 

81%

14%

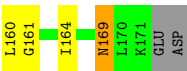
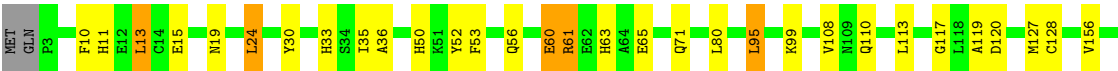


● Molecule 1: Ferritin

Chain W: 

77%

17%



● Molecule 1: Ferritin

Chain X: 

77%

17%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.82Å 178.78Å 126.71Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	49.66 – 2.76 49.66 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.66-2.76) 98.2 (49.66-2.76)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.190 , 0.265 0.198 , 0.269	Depositor DCC
$R_{free}$ test set	6982 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -l,k,h 0.015 for -h,-k,l 0.013 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	33609	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.66	0/1344	0.79	0/1812
1	B	0.67	0/1360	0.77	0/1830
1	C	0.68	0/1367	0.82	0/1831
1	D	0.67	0/1365	0.79	0/1831
1	E	0.67	0/1364	0.77	0/1835
1	F	0.70	0/1360	0.79	0/1829
1	G	0.68	0/1349	0.80	0/1814
1	H	0.67	0/1358	0.81	0/1825
1	I	0.69	0/1352	0.77	0/1818
1	J	0.67	0/1371	0.76	0/1847
1	K	0.69	0/1360	0.81	0/1827
1	L	0.67	0/1349	0.79	0/1814
1	M	0.68	0/1356	0.80	0/1825
1	N	0.68	0/1351	0.78	0/1820
1	O	0.68	0/1360	0.79	0/1827
1	P	0.67	0/1366	0.78	0/1834
1	Q	0.69	0/1372	0.76	0/1846
1	R	0.67	0/1363	0.78	0/1835
1	S	0.68	0/1355	0.78	0/1821
1	T	0.67	0/1365	0.79	0/1836
1	U	0.70	0/1359	0.80	0/1829
1	V	0.70	0/1363	0.80	0/1833
1	W	0.69	1/1361 (0.1%)	0.77	0/1833
1	X	0.70	1/1337 (0.1%)	0.79	0/1800
All	All	0.68	2/32607 (0.0%)	0.79	0/43852

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	C	0	1
1	L	0	1
1	Q	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	60	GLU	CD-OE2	5.15	1.31	1.25
1	W	60	GLU	CD-OE1	-5.13	1.20	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	157	GLY	Peptide
1	L	157	GLY	Peptide
1	Q	157	GLY	Peptide

## 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	1318	0	1203	24	0
1	B	1334	0	1208	13	0
1	C	1341	0	1263	13	0
1	D	1339	0	1245	27	0
1	E	1338	0	1236	42	0
1	F	1334	0	1232	36	0
1	G	1323	0	1207	24	0
1	H	1332	0	1238	24	0
1	I	1326	0	1214	18	0
1	J	1345	0	1239	30	0
1	K	1334	0	1231	26	0
1	L	1323	0	1209	32	0
1	M	1330	0	1230	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1325	0	1225	38	0
1	O	1334	0	1240	22	0
1	P	1340	0	1252	19	0
1	Q	1346	0	1257	17	0
1	R	1337	0	1232	47	0
1	S	1329	0	1237	23	0
1	T	1339	0	1240	20	0
1	U	1333	0	1239	21	0
1	V	1337	0	1232	27	0
1	W	1335	0	1235	30	0
1	X	1311	0	1207	26	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	3	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	4	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	2	0	0	0	0
2	R	1	0	0	0	0
2	S	3	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
3	A	57	0	0	14	0
3	B	24	0	0	5	0
3	C	18	0	0	4	0
3	D	87	0	0	28	0
3	E	71	0	0	23	0
3	F	75	0	0	23	0
3	G	69	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	76	0	0	17	0
3	I	41	0	0	13	0
3	J	73	0	0	23	0
3	K	87	0	0	13	0
3	L	73	0	0	22	0
3	M	86	0	0	24	0
3	N	66	0	0	20	0
3	O	66	0	0	17	0
3	P	62	0	0	9	0
3	Q	72	0	0	5	0
3	R	83	0	0	40	0
3	S	73	0	0	11	0
3	T	59	0	0	12	0
3	U	73	0	0	7	0
3	V	67	0	0	15	0
3	W	58	0	0	14	0
3	X	70	0	0	18	0
All	All	33609	0	29551	609	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 10.

The worst 5 of 609 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:W:169:ASN:HB3	3:W:305:HOH:O	1.29	1.29
1:H:36:ALA:CA	3:H:301:HOH:O	1.71	1.28
1:R:135:TYR:HB3	3:R:376:HOH:O	1.30	1.25
1:A:73:GLN:HB3	3:A:330:HOH:O	1.32	1.22
1:X:165:TYR:HA	3:X:320:HOH:O	1.39	1.21

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 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	166/173 (96%)	162 (98%)	4 (2%)	0	100	100
1	B	169/173 (98%)	161 (95%)	8 (5%)	0	100	100
1	C	166/173 (96%)	157 (95%)	9 (5%)	0	100	100
1	D	167/173 (96%)	162 (97%)	5 (3%)	0	100	100
1	E	167/173 (96%)	162 (97%)	5 (3%)	0	100	100
1	F	167/173 (96%)	161 (96%)	6 (4%)	0	100	100
1	G	167/173 (96%)	161 (96%)	4 (2%)	2 (1%)	13	23
1	H	166/173 (96%)	162 (98%)	3 (2%)	1 (1%)	25	42
1	I	167/173 (96%)	162 (97%)	4 (2%)	1 (1%)	25	42
1	J	168/173 (97%)	164 (98%)	4 (2%)	0	100	100
1	K	167/173 (96%)	161 (96%)	6 (4%)	0	100	100
1	L	166/173 (96%)	161 (97%)	5 (3%)	0	100	100
1	M	166/173 (96%)	162 (98%)	4 (2%)	0	100	100
1	N	166/173 (96%)	161 (97%)	5 (3%)	0	100	100
1	O	166/173 (96%)	163 (98%)	3 (2%)	0	100	100
1	P	167/173 (96%)	163 (98%)	4 (2%)	0	100	100
1	Q	167/173 (96%)	161 (96%)	5 (3%)	1 (1%)	25	42
1	R	167/173 (96%)	163 (98%)	4 (2%)	0	100	100
1	S	166/173 (96%)	161 (97%)	5 (3%)	0	100	100
1	T	167/173 (96%)	160 (96%)	6 (4%)	1 (1%)	25	42
1	U	166/173 (96%)	163 (98%)	3 (2%)	0	100	100
1	V	167/173 (96%)	164 (98%)	3 (2%)	0	100	100
1	W	167/173 (96%)	161 (96%)	6 (4%)	0	100	100
1	X	166/173 (96%)	160 (96%)	5 (3%)	1 (1%)	25	42
All	All	4001/4152 (96%)	3878 (97%)	116 (3%)	7 (0%)	47	69

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	157	GLY
1	Q	157	GLY
1	T	157	GLY

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Mol	Chain	Res	Type
1	X	4	SER
1	G	158	THR

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	126/151 (83%)	119 (94%)	7 (6%)	21	36
1	B	126/151 (83%)	119 (94%)	7 (6%)	21	36
1	C	136/151 (90%)	124 (91%)	12 (9%)	10	17
1	D	132/151 (87%)	125 (95%)	7 (5%)	22	38
1	E	133/151 (88%)	122 (92%)	11 (8%)	11	20
1	F	133/151 (88%)	122 (92%)	11 (8%)	11	20
1	G	129/151 (85%)	120 (93%)	9 (7%)	15	26
1	H	135/151 (89%)	122 (90%)	13 (10%)	8	14
1	I	129/151 (85%)	121 (94%)	8 (6%)	18	32
1	J	135/151 (89%)	125 (93%)	10 (7%)	13	24
1	K	132/151 (87%)	128 (97%)	4 (3%)	41	61
1	L	131/151 (87%)	126 (96%)	5 (4%)	33	53
1	M	133/151 (88%)	124 (93%)	9 (7%)	16	28
1	N	131/151 (87%)	123 (94%)	8 (6%)	18	33
1	O	135/151 (89%)	127 (94%)	8 (6%)	19	34
1	P	137/151 (91%)	126 (92%)	11 (8%)	12	21
1	Q	133/151 (88%)	127 (96%)	6 (4%)	27	46
1	R	131/151 (87%)	121 (92%)	10 (8%)	13	23
1	S	131/151 (87%)	120 (92%)	11 (8%)	11	19
1	T	132/151 (87%)	126 (96%)	6 (4%)	27	46
1	U	135/151 (89%)	123 (91%)	12 (9%)	9	17
1	V	133/151 (88%)	125 (94%)	8 (6%)	19	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	131/151 (87%)	122 (93%)	9 (7%)	15	27
1	X	125/151 (83%)	116 (93%)	9 (7%)	14	25
All	All	3164/3624 (87%)	2953 (93%)	211 (7%)	16	28

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	33	HIS
1	Q	121	SER
1	W	120	ASP
1	N	153	LEU
1	P	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
1	T	56	GLN
1	V	134	HIS
1	T	73	GLN
1	U	63	HIS
1	W	63	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 40 ligands modelled in this entry, 40 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 [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	168/173 (97%)	-0.33	0 100 100	29, 39, 51, 58	0
1	B	171/173 (98%)	-0.25	0 100 100	27, 38, 51, 87	0
1	C	168/173 (97%)	-0.25	1 (0%) 89 92	26, 36, 49, 59	0
1	D	169/173 (97%)	-0.36	0 100 100	27, 35, 46, 65	0
1	E	169/173 (97%)	-0.32	1 (0%) 89 92	30, 37, 49, 71	0
1	F	169/173 (97%)	-0.19	0 100 100	29, 39, 50, 63	0
1	G	169/173 (97%)	-0.31	0 100 100	30, 39, 53, 66	0
1	H	168/173 (97%)	-0.28	1 (0%) 89 92	29, 37, 49, 58	0
1	I	169/173 (97%)	-0.36	0 100 100	29, 37, 48, 67	0
1	J	170/173 (98%)	-0.29	0 100 100	28, 37, 53, 61	0
1	K	169/173 (97%)	-0.36	1 (0%) 89 92	26, 35, 47, 62	0
1	L	168/173 (97%)	-0.35	0 100 100	27, 36, 51, 72	0
1	M	168/173 (97%)	-0.29	0 100 100	26, 36, 48, 61	0
1	N	168/173 (97%)	-0.36	0 100 100	25, 35, 48, 58	0
1	O	168/173 (97%)	-0.28	0 100 100	27, 37, 48, 62	0
1	P	169/173 (97%)	-0.26	0 100 100	29, 39, 53, 79	0
1	Q	169/173 (97%)	-0.28	0 100 100	25, 34, 47, 84	0
1	R	169/173 (97%)	-0.32	0 100 100	27, 35, 48, 65	0
1	S	168/173 (97%)	-0.35	0 100 100	25, 35, 47, 62	0
1	T	169/173 (97%)	-0.23	1 (0%) 89 92	27, 37, 52, 68	0
1	U	168/173 (97%)	-0.33	0 100 100	26, 36, 47, 60	0
1	V	169/173 (97%)	-0.36	0 100 100	27, 36, 49, 58	0
1	W	169/173 (97%)	-0.35	0 100 100	29, 37, 47, 59	0
1	X	168/173 (97%)	-0.32	0 100 100	27, 38, 48, 60	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4049/4152 (97%)	-0.31	5 (0%) 95 97	25, 37, 50, 87	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	158	THR	2.8
1	H	16	ALA	2.5
1	C	104	LEU	2.2
1	K	3	PRO	2.1
1	E	3	PRO	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	202	1/1	0.65	0.24	42,42,42,42	0
2	MG	H	202	1/1	0.77	0.28	54,54,54,54	0
2	MG	P	201	1/1	0.82	0.11	36,36,36,36	0
2	MG	N	202	1/1	0.84	0.12	70,70,70,70	0
2	MG	E	203	1/1	0.88	0.23	49,49,49,49	0
2	MG	B	202	1/1	0.89	0.13	50,50,50,50	0
2	MG	D	202	1/1	0.91	0.18	27,27,27,27	0
2	MG	N	203	1/1	0.91	0.47	2,2,2,2	0
2	MG	E	201	1/1	0.91	0.11	60,60,60,60	0
2	MG	N	204	1/1	0.92	0.23	46,46,46,46	0
2	MG	S	201	1/1	0.93	0.17	49,49,49,49	0
2	MG	V	201	1/1	0.93	0.49	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	H	201	1/1	0.94	0.44	1,1,1,1	0
2	MG	I	201	1/1	0.94	0.42	1,1,1,1	0
2	MG	K	202	1/1	0.94	0.10	37,37,37,37	0
2	MG	Q	202	1/1	0.95	0.26	55,55,55,55	0
2	MG	W	201	1/1	0.95	0.48	1,1,1,1	0
2	MG	K	201	1/1	0.96	0.44	1,1,1,1	0
2	MG	P	202	1/1	0.96	0.43	0,0,0,0	0
2	MG	J	201	1/1	0.96	0.50	2,2,2,2	0
2	MG	N	201	1/1	0.96	0.19	33,33,33,33	0
2	MG	O	201	1/1	0.96	0.50	2,2,2,2	0
2	MG	O	202	1/1	0.96	0.11	33,33,33,33	0
2	MG	F	201	1/1	0.97	0.42	1,1,1,1	0
2	MG	J	202	1/1	0.97	0.16	28,28,28,28	0
2	MG	T	201	1/1	0.97	0.45	3,3,3,3	0
2	MG	B	201	1/1	0.97	0.44	2,2,2,2	0
2	MG	Q	201	1/1	0.97	0.48	1,1,1,1	0
2	MG	C	201	1/1	0.98	0.48	1,1,1,1	0
2	MG	S	202	1/1	0.98	0.45	2,2,2,2	0
2	MG	S	203	1/1	0.98	0.08	33,33,33,33	0
2	MG	M	201	1/1	0.98	0.43	1,1,1,1	0
2	MG	D	201	1/1	0.98	0.50	1,1,1,1	0
2	MG	R	201	1/1	0.98	0.50	1,1,1,1	0
2	MG	X	201	1/1	0.98	0.49	1,1,1,1	0
2	MG	L	201	1/1	0.99	0.42	0,0,0,0	0
2	MG	U	201	1/1	0.99	0.46	1,1,1,1	0
2	MG	E	202	1/1	0.99	0.49	1,1,1,1	0
2	MG	G	201	1/1	0.99	0.52	0,0,0,0	0
2	MG	A	201	1/1	0.99	0.49	2,2,2,2	0

## 6.5 Other polymers

There are no such residues in this entry.