



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 10:51 PM JST

PDB ID : 7DQP  
Title : Thermal treated Marsupinaeus japonicus ferritin  
Authors : Tan, X.; Liu, Y.; Zang, J.; Zhang, T.; Zhao, G.  
Deposited on : 2020-12-24  
Resolution : 2.20 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

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

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:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

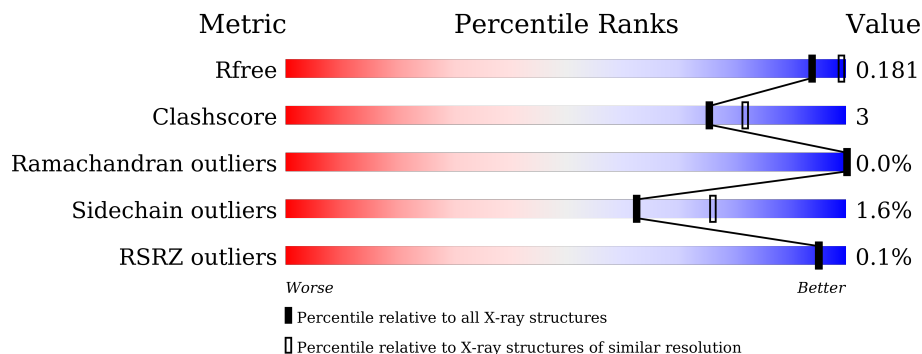
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	169	
1	B	169	
1	C	169	
1	D	169	
1	E	169	
1	F	169	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	169	87% 13%
1	H	169	89% 10% .
1	I	169	91% 9%
1	J	169	95% 5%
1	K	169	93% 7%
1	L	169	95% . .
1	M	169	93% 7%
1	N	169	94% 6%
1	O	169	95% 5%
1	P	169	95% 5%
1	Q	169	93% 7% .
1	R	169	93% 7%
1	S	169	95% 5%
1	T	169	91% 9%
1	U	169	% 91% 8% .
1	V	169	91% 9%
1	W	169	92% 8%
1	X	169	% 92% 8%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 33319 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
			Total	C	N	O	S			
1	C	169	1359	852	228	272	7	0	0	0
1	F	169	1359	852	228	272	7	0	0	0
1	A	169	1359	852	228	272	7	0	0	0
1	B	169	1359	852	228	272	7	0	0	0
1	D	169	1359	852	228	272	7	0	0	0
1	E	169	1359	852	228	272	7	0	0	0
1	G	169	1359	852	228	272	7	0	0	0
1	H	169	1359	852	228	272	7	0	0	0
1	I	169	1359	852	228	272	7	0	0	0
1	J	169	1359	852	228	272	7	0	0	0
1	K	169	1359	852	228	272	7	0	0	0
1	L	169	1359	852	228	272	7	0	0	0
1	M	169	1359	852	228	272	7	0	0	0
1	N	169	1359	852	228	272	7	0	0	0
1	O	169	1359	852	228	272	7	0	0	0
1	P	169	1359	852	228	272	7	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	169	Total 1359	C 852	N 228	O 272	S 7	0	0	0
1	R	169	Total 1359	C 852	N 228	O 272	S 7	0	0	0
1	S	169	Total 1359	C 852	N 228	O 272	S 7	0	0	0
1	T	169	Total 1359	C 852	N 228	O 272	S 7	0	0	0
1	U	169	Total 1359	C 852	N 228	O 272	S 7	0	0	0
1	V	169	Total 1359	C 852	N 228	O 272	S 7	0	0	0
1	W	169	Total 1359	C 852	N 228	O 272	S 7	0	0	0
1	X	169	Total 1359	C 852	N 228	O 272	S 7	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	34	Total 34	O 34	0	0
2	F	28	Total 28	O 28	0	0
2	A	26	Total 26	O 26	0	0
2	B	27	Total 27	O 27	0	0
2	D	34	Total 34	O 34	0	0
2	E	27	Total 27	O 27	0	0
2	G	36	Total 36	O 36	0	0
2	H	29	Total 29	O 29	0	0
2	I	26	Total 26	O 26	0	0
2	J	32	Total 32	O 32	0	0
2	K	36	Total 36	O 36	0	0

Continued on next page...


*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	L	22	Total 22	O 22	0	0
2	M	29	Total 29	O 29	0	0
2	N	28	Total 28	O 28	0	0
2	O	29	Total 29	O 29	0	0
2	P	29	Total 29	O 29	0	0
2	Q	26	Total 26	O 26	0	0
2	R	29	Total 29	O 29	0	0
2	S	26	Total 26	O 26	0	0
2	T	31	Total 31	O 31	0	0
2	U	31	Total 31	O 31	0	0
2	V	31	Total 31	O 31	0	0
2	W	30	Total 30	O 30	0	0
2	X	27	Total 27	O 27	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

Chain C:  85% 14%



- Molecule 1: Ferritin

Chain F:  89% 11%



- Molecule 1: Ferritin

Chain A:  90% 10%



- Molecule 1: Ferritin

Chain B:  93% 7%



- Molecule 1: Ferritin

Chain D:  95% 5%



- Molecule 1: Ferritin

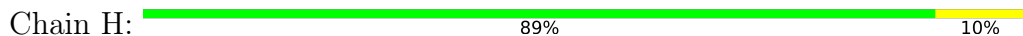
Chain E:  89% 11%



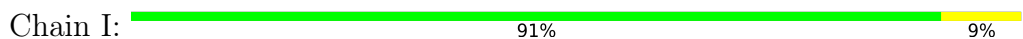
- Molecule 1: Ferritin



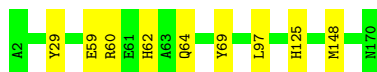
- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin







- Molecule 1: Ferritin



- Molecule 1: Ferritin



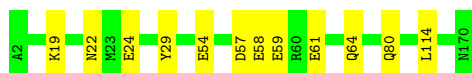
- Molecule 1: Ferritin



- Molecule 1: Ferritin



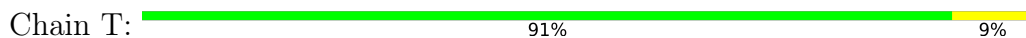
- Molecule 1: Ferritin



- Molecule 1: Ferritin

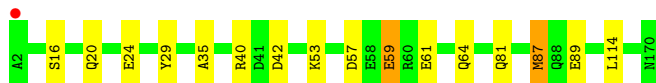
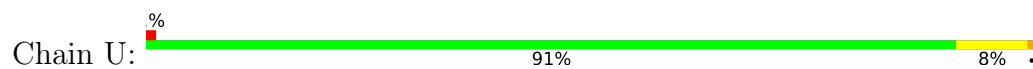


- Molecule 1: Ferritin

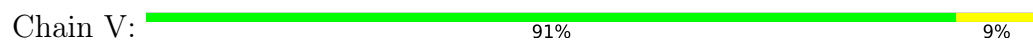




- Molecule 1: Ferritin



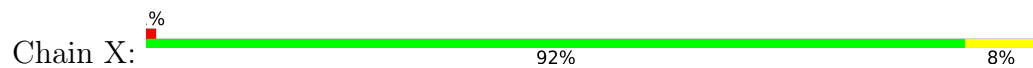
- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.62Å 124.60Å 124.89Å 90.42° 119.79° 119.67°	Depositor
Resolution (Å)	40.62 – 2.20 40.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (40.62-2.20) 95.9 (40.62-2.20)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.173 , 0.179 0.174 , 0.181	Depositor DCC
$R_{free}$ test set	1961 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , -18.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage

*Continued on next page...*

<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.

Continued from previous page...

Property	Value	Source
Estimated twinning fraction	0.426 for $-k, h+k+1, -h$ 0.426 for $-l, -h, h+k+1$ 0.036 for $h+1, -l, k$ 0.036 for $h+k, l, -k$ 0.035 for $-h-k-l, h+k, h+1$ 0.035 for $h+k+1, -h-l, -h-k$ 0.036 for $-k, -h-l, h+k$ 0.036 for $h+1, -h, -h-k-l$ 0.038 for $l, h+k, -h-l$ 0.038 for $-h-l, h+k+1, h$ 0.036 for $-h-k, h, h+k+1$ 0.036 for $k, -h-k, h+1$ 0.036 for $-l, h+1, -h-k$ 0.036 for $h+k, -h-k-l, -h$ 0.037 for $-h-k, k, -l$ 0.038 for $h, -h-k, -h-l$ 0.036 for $-h, h+1, h+k$ 0.096 for $k, h, -h-k-l$ 0.099 for $l, -h-k-l, h$ 0.436 for $-h-k-l, l, k$ 0.095 for $h+k+1, -k, -l$ 0.037 for $-h-l, -k, l$ 0.096 for $-h, -l, -k$	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	33319	wwPDB-VP
Average B, all atoms ( $\text{\AA}^2$ )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

## 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	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.39	0/1383	0.52	0/1859
1	B	0.43	0/1383	0.53	0/1859
1	C	0.42	0/1383	0.54	1/1859 (0.1%)
1	D	0.42	0/1383	0.50	0/1859
1	E	0.41	0/1383	0.52	0/1859
1	F	0.39	0/1383	0.49	0/1859
1	G	0.41	0/1383	0.48	0/1859
1	H	0.41	0/1383	0.50	0/1859
1	I	0.39	0/1383	0.49	0/1859
1	J	0.42	0/1383	0.49	0/1859
1	K	0.42	0/1383	0.50	0/1859
1	L	0.38	0/1383	0.49	0/1859
1	M	0.40	0/1383	0.49	0/1859
1	N	0.47	2/1383 (0.1%)	0.50	0/1859
1	O	0.40	0/1383	0.48	0/1859
1	P	0.39	0/1383	0.49	0/1859
1	Q	0.41	0/1383	0.50	0/1859
1	R	0.41	0/1383	0.50	0/1859
1	S	0.40	0/1383	0.51	0/1859
1	T	0.42	0/1383	0.50	0/1859
1	U	0.50	2/1383 (0.1%)	0.57	0/1859
1	V	0.42	0/1383	0.51	0/1859
1	W	0.39	0/1383	0.50	0/1859
1	X	0.44	0/1383	0.51	0/1859
All	All	0.41	4/33192 (0.0%)	0.50	1/44616 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	59	GLU	CB-CG	7.92	1.67	1.52
1	N	168	GLU	CD-OE2	-6.27	1.18	1.25
1	U	59	GLU	CG-CD	5.74	1.60	1.51
1	N	168	GLU	CD-OE1	-5.58	1.19	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	87	MET	C-N-CA	6.50	137.96	121.70

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	A	1359	0	1311	12	0
1	B	1359	0	1311	17	0
1	C	1359	0	1311	18	0
1	D	1359	0	1311	8	0
1	E	1359	0	1311	14	0
1	F	1359	0	1311	9	0
1	G	1359	0	1311	11	0
1	H	1359	0	1311	11	0
1	I	1359	0	1311	9	0
1	J	1359	0	1311	6	0
1	K	1359	0	1311	5	0
1	L	1359	0	1311	5	0
1	M	1359	0	1311	7	0
1	N	1359	0	1311	5	0
1	O	1359	0	1311	5	0
1	P	1359	0	1311	6	0
1	Q	1359	0	1311	7	0
1	R	1359	0	1311	7	0
1	S	1359	0	1311	9	0
1	T	1359	0	1311	12	0
1	U	1359	0	1311	13	0
1	V	1359	0	1311	10	0
1	W	1359	0	1311	9	0
1	X	1359	0	1311	8	0
2	A	26	0	0	0	0
2	B	27	0	0	4	0
2	C	34	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	34	0	0	0	0
2	E	27	0	0	0	0
2	F	28	0	0	0	0
2	G	36	0	0	2	0
2	H	29	0	0	1	0
2	I	26	0	0	1	0
2	J	32	0	0	0	0
2	K	36	0	0	0	0
2	L	22	0	0	0	0
2	M	29	0	0	0	0
2	N	28	0	0	0	0
2	O	29	0	0	0	0
2	P	29	0	0	0	0
2	Q	26	0	0	1	0
2	R	29	0	0	2	0
2	S	26	0	0	3	0
2	T	31	0	0	0	0
2	U	31	0	0	0	0
2	V	31	0	0	0	0
2	W	30	0	0	0	0
2	X	27	0	0	0	0
All	All	33319	0	31464	197	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 (197) 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:P:114:LEU:HD22	1:P:130:LEU:HD11	1.27	1.09
1:P:114:LEU:CD2	1:P:130:LEU:HD11	2.04	0.88
1:U:87:MET:CE	1:U:89:GLU:HB2	2.08	0.83
1:U:40:ARG:NH1	1:U:42:ASP:OD1	2.13	0.82
1:F:50:LYS:NZ	1:F:169:LEU:O	2.14	0.81
1:H:80:GLN:HG2	1:I:80:GLN:HG2	1.63	0.80
1:U:87:MET:HE2	1:U:89:GLU:HB2	1.63	0.79
1:H:60:ARG:NH2	2:H:201:HOH:O	2.15	0.79
1:B:76:ARG:HE	1:B:77:ILE:N	1.82	0.78
1:S:76:ARG:NH2	2:S:201:HOH:O	2.19	0.76
1:G:137:GLU:OE2	2:G:201:HOH:O	2.04	0.76
1:X:59:GLU:OE1	1:X:62:HIS:ND1	2.19	0.75

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:24:GLU:OE1	2:R:201:HOH:O	2.03	0.75
1:U:35:ALA:HB1	1:U:53:LYS:HG3	1.70	0.73
1:A:35:ALA:HB1	1:A:53:LYS:HG3	1.71	0.72
1:B:71:ASN:OD1	2:B:201:HOH:O	2.07	0.72
1:R:59:GLU:OE1	2:R:201:HOH:O	2.07	0.71
1:G:35:ALA:HB1	1:G:53:LYS:HG3	1.73	0.70
1:E:24:GLU:OE1	1:E:59:GLU:OE1	2.10	0.70
1:A:81:GLN:H	1:A:81:GLN:CD	1.95	0.70
1:C:23:MET:HE1	1:C:107:VAL:HA	1.75	0.68
1:P:114:LEU:HD22	1:P:130:LEU:CD1	2.14	0.67
1:B:76:ARG:NH2	2:B:202:HOH:O	2.27	0.67
1:B:76:ARG:NH2	2:B:201:HOH:O	2.28	0.67
1:U:40:ARG:HH21	1:V:76:ARG:HG2	1.60	0.67
1:C:87:MET:HA	1:C:88:GLN:HB2	1.76	0.66
1:S:71:ASN:OD1	2:S:201:HOH:O	2.13	0.65
1:K:59:GLU:OE1	1:K:62:HIS:ND1	2.30	0.64
1:Q:102:ASP:OD2	1:Q:106:GLN:NE2	2.31	0.64
1:A:79:LEU:H	1:B:88:GLN:NE2	1.96	0.63
1:U:87:MET:HE1	1:U:89:GLU:HB2	1.80	0.63
1:A:78:VAL:HA	1:B:88:GLN:HE22	1.63	0.62
1:I:35:ALA:HB1	1:I:53:LYS:HG3	1.82	0.62
1:S:76:ARG:NE	1:S:76:ARG:HA	2.13	0.61
1:C:94:LEU:O	1:C:98:GLN:HG3	1.99	0.61
1:D:76:ARG:NH2	1:E:40:ARG:HG2	2.14	0.61
1:C:35:ALA:HB1	1:C:53:LYS:HG3	1.83	0.61
1:V:163:TYR:CD2	1:V:164:MET:HE3	2.36	0.61
1:S:50:LYS:NZ	1:S:169:LEU:O	2.33	0.60
1:C:17:ILE:O	1:C:21:ILE:HG12	2.01	0.60
1:M:50:LYS:NZ	1:M:54:GLU:OE2	2.35	0.60
1:W:94:LEU:O	1:W:98:GLN:HG3	2.01	0.60
1:L:20:GLN:HG2	1:L:114:LEU:HD12	1.83	0.59
1:A:78:VAL:HA	1:B:88:GLN:NE2	2.18	0.59
1:I:102:ASP:OD2	1:I:106:GLN:NE2	2.35	0.58
1:W:40:ARG:NH1	1:X:76:ARG:HG3	2.18	0.58
1:P:141:SER:O	1:P:145:ILE:HG22	2.04	0.58
1:O:94:LEU:O	1:O:98:GLN:HG3	2.03	0.58
1:V:114:LEU:HD22	1:V:130:LEU:HD11	1.85	0.57
1:S:76:ARG:HA	1:S:76:ARG:CZ	2.36	0.56
1:M:35:ALA:HB1	1:M:53:LYS:HG3	1.88	0.56
1:X:50:LYS:HZ1	1:X:170:ASN:C	2.09	0.56
1:F:60:ARG:O	1:F:64:GLN:HG3	2.05	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:19:LYS:NZ	1:G:110:SER:OG	2.38	0.56
1:F:114:LEU:HD22	1:F:130:LEU:HD11	1.88	0.55
1:S:76:ARG:HD3	1:T:40:ARG:CZ	2.35	0.55
1:U:20:GLN:O	1:U:24:GLU:HG2	2.06	0.55
1:F:57:ASP:O	1:F:61:GLU:HG2	2.07	0.55
1:G:57:ASP:O	1:G:61:GLU:HG2	2.06	0.55
1:S:76:ARG:CZ	1:T:40:ARG:HD2	2.37	0.55
1:C:20:GLN:HE22	1:C:23:MET:CE	2.20	0.55
1:S:77:ILE:HG13	2:S:201:HOH:O	2.06	0.55
1:Q:11:GLU:H	1:Q:11:GLU:CD	2.09	0.55
1:I:60:ARG:HD2	1:J:60:ARG:NH2	2.22	0.54
1:B:76:ARG:HE	1:B:77:ILE:H	1.52	0.54
1:Q:128:LYS:NZ	2:Q:201:HOH:O	2.40	0.54
1:D:76:ARG:NH1	1:E:42:ASP:OD2	2.42	0.53
1:C:20:GLN:HE22	1:C:23:MET:HE2	1.73	0.53
1:Q:114:LEU:HG	1:Q:130:LEU:HD11	1.89	0.53
1:D:76:ARG:HH21	1:E:40:ARG:HG2	1.74	0.53
1:L:87:MET:HE2	1:L:89:GLU:H	1.73	0.53
1:U:81:GLN:H	1:U:81:GLN:CD	2.13	0.52
1:W:60:ARG:O	1:W:64:GLN:HG3	2.09	0.52
1:A:40:ARG:NH1	1:A:42:ASP:OD1	2.42	0.52
1:W:128:LYS:NZ	1:W:132:ASP:OD2	2.38	0.52
1:J:59:GLU:O	1:J:62:HIS:HB2	2.09	0.52
1:A:36:TYR:HE1	1:B:68:LYS:HG3	1.75	0.51
1:C:20:GLN:NE2	1:C:23:MET:HE2	2.26	0.51
1:B:11:GLU:H	1:B:11:GLU:CD	2.15	0.51
1:D:114:LEU:HG	1:D:130:LEU:HD11	1.94	0.50
1:C:68:LYS:HE3	1:C:72:LYS:HE3	1.93	0.50
1:T:27:ALA:HB3	1:T:59:GLU:HG2	1.94	0.50
1:C:20:GLN:O	1:C:24:GLU:HG2	2.12	0.50
1:N:114:LEU:HD22	1:N:130:LEU:HD11	1.93	0.49
1:C:69:TYR:CD1	1:C:129:LEU:HD22	2.48	0.49
1:H:58:GLU:HA	1:H:58:GLU:OE1	2.12	0.49
1:G:64:GLN:HB3	1:H:36:TYR:OH	2.13	0.49
1:G:31:TYR:OH	1:G:104:GLU:OE2	2.21	0.49
1:T:20:GLN:O	1:T:24:GLU:HG2	2.13	0.49
1:T:69:TYR:CD1	1:T:129:LEU:HD22	2.48	0.49
1:I:69:TYR:CD1	1:I:129:LEU:HD22	2.48	0.49
1:E:87:MET:HE2	1:E:89:GLU:HB3	1.94	0.48
1:P:97:LEU:HB3	1:P:145:ILE:HD11	1.94	0.48
1:W:16:SER:OG	1:W:114:LEU:HD13	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:LEU:HG	1:G:130:LEU:HD11	1.95	0.48
1:D:16:SER:HB3	1:D:114:LEU:HD13	1.95	0.48
1:D:102:ASP:OD2	1:D:106:GLN:NE2	2.46	0.48
1:V:101:LEU:O	1:V:105:LYS:HG3	2.14	0.48
1:V:164:MET:HA	1:V:164:MET:CE	2.44	0.47
1:R:57:ASP:O	1:R:61:GLU:HG2	2.14	0.47
1:U:57:ASP:O	1:U:61:GLU:HG2	2.14	0.47
1:C:163:TYR:CZ	1:C:167:LYS:HE2	2.49	0.47
1:M:20:GLN:O	1:M:24:GLU:HG2	2.14	0.47
1:K:76:ARG:HD3	1:K:76:ARG:HA	1.61	0.47
1:M:80:GLN:OE1	1:Q:80:GLN:HG2	2.15	0.47
1:C:163:TYR:CE2	1:C:167:LYS:HE2	2.50	0.46
1:A:16:SER:OG	1:A:114:LEU:HD13	2.15	0.46
1:C:21:ILE:HD13	1:C:66:PHE:HB3	1.97	0.46
1:I:36:TYR:OH	1:J:64:GLN:HB3	2.16	0.46
1:W:69:TYR:CD1	1:W:129:LEU:HD22	2.50	0.46
1:C:41:ASP:HA	1:T:147:ASP:OD1	2.16	0.46
1:T:40:ARG:HH21	1:T:40:ARG:HG2	1.81	0.46
1:U:24:GLU:OE1	1:U:59:GLU:OE1	2.32	0.46
1:X:114:LEU:HD22	1:X:130:LEU:HD11	1.98	0.46
1:K:128:LYS:NZ	1:K:132:ASP:OD2	2.46	0.46
1:N:53:LYS:HE2	1:N:53:LYS:HB2	1.66	0.46
1:E:69:TYR:CD1	1:E:129:LEU:HD22	2.51	0.45
1:F:59:GLU:O	1:F:62:HIS:HB2	2.17	0.45
1:W:76:ARG:HD3	1:W:76:ARG:HA	1.78	0.45
1:E:37:TYR:HA	1:E:40:ARG:HD3	1.99	0.45
1:B:76:ARG:HH21	1:B:77:ILE:H	1.64	0.44
1:E:69:TYR:HE1	1:E:125:HIS:CE1	2.35	0.44
1:C:21:ILE:CD1	1:C:66:PHE:HB3	2.47	0.44
1:V:164:MET:HE2	1:V:167:LYS:HD2	1.99	0.44
1:I:20:GLN:O	1:I:24:GLU:HG2	2.17	0.44
1:C:129:LEU:HD12	1:C:133:GLU:HG3	1.99	0.44
1:Q:57:ASP:O	1:Q:61:GLU:HG2	2.18	0.44
1:B:76:ARG:HE	1:B:76:ARG:CA	2.31	0.44
1:V:20:GLN:O	1:V:24:GLU:HG2	2.18	0.44
1:E:20:GLN:O	1:E:24:GLU:HG2	2.18	0.44
1:U:64:GLN:HB3	1:V:36:TYR:OH	2.18	0.44
1:D:20:GLN:O	1:D:24:GLU:HG2	2.18	0.43
1:T:76:ARG:HD3	1:T:76:ARG:HA	1.80	0.43
1:T:104:GLU:OE1	1:T:138:GLN:NE2	2.51	0.43
1:K:20:GLN:O	1:K:24:GLU:HG2	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:137:GLU:H	1:V:137:GLU:CD	2.20	0.43
1:J:69:TYR:HE1	1:J:125:HIS:CE1	2.36	0.43
1:U:16:SER:HB3	1:U:114:LEU:HD13	2.01	0.43
1:P:109:GLN:NE2	1:P:113:GLU:OE2	2.49	0.43
1:X:102:ASP:OD2	1:X:106:GLN:NE2	2.52	0.43
1:F:4:GLN:O	1:T:105:LYS:NZ	2.38	0.43
1:A:79:LEU:HD12	1:B:33:SER:HB2	2.00	0.43
1:H:53:LYS:HE2	1:H:53:LYS:HB2	1.93	0.43
1:H:102:ASP:OD1	1:H:106:GLN:NE2	2.42	0.43
1:T:163:TYR:CE2	1:T:167:LYS:HE2	2.54	0.43
1:F:40:ARG:HH12	1:F:89:GLU:HG2	1.84	0.43
1:G:129:LEU:HD12	1:G:133:GLU:HG3	2.00	0.43
1:H:69:TYR:CD1	1:H:129:LEU:HD22	2.54	0.43
1:J:97:LEU:HD21	1:J:148:MET:HE2	2.01	0.43
1:F:69:TYR:CD1	1:F:129:LEU:HD22	2.54	0.42
1:B:87:MET:O	1:B:88:GLN:HG3	2.18	0.42
1:H:11:GLU:CD	1:H:11:GLU:H	2.22	0.42
1:E:114:LEU:HD13	1:E:130:LEU:HD21	2.01	0.42
1:L:53:LYS:HE3	1:L:53:LYS:HB2	1.73	0.42
1:K:144:LYS:HB3	1:K:144:LYS:HE2	1.85	0.42
1:B:76:ARG:NE	1:B:76:ARG:HA	2.34	0.42
1:E:76:ARG:HD3	1:E:76:ARG:HA	1.81	0.42
1:M:36:TYR:OH	1:N:64:GLN:HB3	2.17	0.42
1:A:69:TYR:HE1	1:A:125:HIS:CE1	2.38	0.42
1:W:40:ARG:HH12	1:X:76:ARG:HG3	1.84	0.42
1:X:109:GLN:NE2	1:X:113:GLU:OE2	2.50	0.42
1:L:114:LEU:HD13	1:L:130:LEU:HD21	2.01	0.42
1:W:64:GLN:HB3	1:X:36:TYR:OH	2.19	0.42
1:G:54:GLU:O	1:G:58:GLU:HG3	2.20	0.42
1:O:95:GLU:HA	1:O:98:GLN:HE21	1.85	0.42
1:R:54:GLU:O	1:R:58:GLU:HG3	2.20	0.42
1:B:114:LEU:HD22	1:B:130:LEU:HD11	2.01	0.42
1:T:24:GLU:OE1	1:T:59:GLU:OE2	2.37	0.42
1:I:11:GLU:HG3	2:I:219:HOH:O	2.19	0.41
1:O:69:TYR:CD1	1:O:129:LEU:HD22	2.55	0.41
1:A:20:GLN:O	1:A:24:GLU:HG2	2.20	0.41
1:A:69:TYR:CD1	1:A:129:LEU:HD22	2.56	0.41
1:E:57:ASP:OD1	1:E:60:ARG:NH1	2.54	0.41
1:M:20:GLN:OE1	1:M:110:SER:OG	2.33	0.41
1:Q:36:TYR:OH	1:R:64:GLN:HB3	2.20	0.41
1:G:136:GLU:HB3	2:G:201:HOH:O	2.19	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:163:TYR:CZ	1:S:167:LYS:HE3	2.54	0.41
1:C:16:SER:HB3	1:C:114:LEU:HD13	2.01	0.41
1:E:37:TYR:O	1:E:40:ARG:HD3	2.21	0.41
1:F:40:ARG:NH1	1:F:89:GLU:HG2	2.35	0.41
1:E:53:LYS:HB2	1:E:53:LYS:HE2	1.53	0.41
1:D:137:GLU:H	1:D:137:GLU:CD	2.24	0.41
1:H:19:LYS:HA	1:H:19:LYS:HD2	1.93	0.41
1:U:40:ARG:NH2	1:V:76:ARG:HG2	2.33	0.41
1:O:76:ARG:HA	1:O:76:ARG:HD3	1.76	0.41
1:B:76:ARG:CZ	2:B:202:HOH:O	2.64	0.41
1:I:76:ARG:HD3	1:I:76:ARG:HA	1.89	0.41
1:J:69:TYR:CE1	1:J:125:HIS:CE1	3.09	0.41
1:O:163:TYR:CZ	1:O:167:LYS:HE3	2.55	0.41
1:G:97:LEU:HD21	1:G:148:MET:HE2	2.03	0.41
1:L:76:ARG:HA	1:L:76:ARG:HD3	1.83	0.40
1:R:22:ASN:ND2	1:R:80:GLN:HG3	2.36	0.40
1:H:57:ASP:O	1:H:61:GLU:HG2	2.21	0.40
1:H:76:ARG:HA	1:H:76:ARG:HD3	1.93	0.40
1:M:64:GLN:HB3	1:N:36:TYR:OH	2.22	0.40
1:N:97:LEU:HD21	1:N:148:MET:HE2	2.02	0.40
1:R:19:LYS:HA	1:R:19:LYS:HD2	1.97	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 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	167/169 (99%)	163 (98%)	4 (2%)	0	100	100
1	B	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	C	167/169 (99%)	162 (97%)	4 (2%)	1 (1%)	25	26
1	D	167/169 (99%)	164 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	F	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	G	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	H	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	I	167/169 (99%)	163 (98%)	4 (2%)	0	100	100
1	J	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	K	167/169 (99%)	163 (98%)	4 (2%)	0	100	100
1	L	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	M	167/169 (99%)	163 (98%)	4 (2%)	0	100	100
1	N	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	O	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	P	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	Q	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	R	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	S	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	T	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	U	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	V	167/169 (99%)	166 (99%)	1 (1%)	0	100	100
1	W	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
1	X	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
All	All	4008/4056 (99%)	3932 (98%)	75 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	88	GLN

### 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	145/145 (100%)	143 (99%)	2 (1%)	67	80
1	B	145/145 (100%)	143 (99%)	2 (1%)	67	80
1	C	145/145 (100%)	143 (99%)	2 (1%)	67	80
1	D	145/145 (100%)	145 (100%)	0	100	100
1	E	145/145 (100%)	142 (98%)	3 (2%)	53	67
1	F	145/145 (100%)	141 (97%)	4 (3%)	43	56
1	G	145/145 (100%)	142 (98%)	3 (2%)	53	67
1	H	145/145 (100%)	140 (97%)	5 (3%)	37	47
1	I	145/145 (100%)	142 (98%)	3 (2%)	53	67
1	J	145/145 (100%)	144 (99%)	1 (1%)	84	91
1	K	145/145 (100%)	142 (98%)	3 (2%)	53	67
1	L	145/145 (100%)	141 (97%)	4 (3%)	43	56
1	M	145/145 (100%)	143 (99%)	2 (1%)	67	80
1	N	145/145 (100%)	143 (99%)	2 (1%)	67	80
1	O	145/145 (100%)	144 (99%)	1 (1%)	84	91
1	P	145/145 (100%)	144 (99%)	1 (1%)	84	91
1	Q	145/145 (100%)	142 (98%)	3 (2%)	53	67
1	R	145/145 (100%)	143 (99%)	2 (1%)	67	80
1	S	145/145 (100%)	143 (99%)	2 (1%)	67	80
1	T	145/145 (100%)	144 (99%)	1 (1%)	84	91
1	U	145/145 (100%)	143 (99%)	2 (1%)	67	80
1	V	145/145 (100%)	142 (98%)	3 (2%)	53	67
1	W	145/145 (100%)	143 (99%)	2 (1%)	67	80
1	X	145/145 (100%)	143 (99%)	2 (1%)	67	80
All	All	3480/3480 (100%)	3425 (98%)	55 (2%)	62	76

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	29	TYR
1	C	81	GLN
1	F	29	TYR
1	F	53	LYS
1	F	119	SER
1	F	170	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	29	TYR
1	A	168	GLU
1	B	53	LYS
1	B	169	LEU
1	E	29	TYR
1	E	114	LEU
1	E	170	ASN
1	G	29	TYR
1	G	141	SER
1	G	170	ASN
1	H	29	TYR
1	H	53	LYS
1	H	114	LEU
1	H	119	SER
1	H	170	ASN
1	I	29	TYR
1	I	169	LEU
1	I	170	ASN
1	J	29	TYR
1	K	17	ILE
1	K	29	TYR
1	K	114	LEU
1	L	20	GLN
1	L	29	TYR
1	L	81	GLN
1	L	114	LEU
1	M	29	TYR
1	M	114	LEU
1	N	29	TYR
1	N	170	ASN
1	O	29	TYR
1	P	29	TYR
1	Q	29	TYR
1	Q	128	LYS
1	Q	170	ASN
1	R	29	TYR
1	R	114	LEU
1	S	29	TYR
1	S	114	LEU
1	T	29	TYR
1	U	29	TYR
1	U	87	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	V	3	SER
1	V	29	TYR
1	V	169	LEU
1	W	29	TYR
1	W	168	GLU
1	X	29	TYR
1	X	86	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	20	GLN
1	C	81	GLN
1	C	170	ASN
1	B	88	GLN
1	I	109	GLN
1	O	98	GLN
1	V	106	GLN
1	W	109	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 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.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	169/169 (100%)	-0.70	0 100 100	16, 22, 33, 49	0
1	B	169/169 (100%)	-0.71	0 100 100	17, 22, 35, 43	0
1	C	169/169 (100%)	-0.77	0 100 100	16, 22, 32, 41	0
1	D	169/169 (100%)	-0.73	0 100 100	16, 22, 33, 43	0
1	E	169/169 (100%)	-0.69	0 100 100	15, 22, 33, 50	0
1	F	169/169 (100%)	-0.71	1 (0%) 89 88	17, 22, 33, 47	0
1	G	169/169 (100%)	-0.71	0 100 100	17, 22, 32, 44	0
1	H	169/169 (100%)	-0.76	0 100 100	16, 22, 31, 40	0
1	I	169/169 (100%)	-0.80	0 100 100	17, 22, 31, 42	0
1	J	169/169 (100%)	-0.74	0 100 100	17, 22, 31, 43	0
1	K	169/169 (100%)	-0.73	0 100 100	16, 22, 34, 42	0
1	L	169/169 (100%)	-0.75	0 100 100	16, 22, 33, 46	0
1	M	169/169 (100%)	-0.74	0 100 100	18, 22, 31, 41	0
1	N	169/169 (100%)	-0.70	0 100 100	17, 22, 31, 44	0
1	O	169/169 (100%)	-0.74	0 100 100	16, 22, 32, 45	0
1	P	169/169 (100%)	-0.76	0 100 100	15, 21, 33, 42	0
1	Q	169/169 (100%)	-0.75	0 100 100	16, 22, 31, 42	0
1	R	169/169 (100%)	-0.76	0 100 100	17, 22, 31, 45	0
1	S	169/169 (100%)	-0.70	0 100 100	15, 21, 33, 43	0
1	T	169/169 (100%)	-0.77	0 100 100	15, 22, 31, 44	0
1	U	169/169 (100%)	-0.69	1 (0%) 89 88	17, 22, 33, 46	0
1	V	169/169 (100%)	-0.74	0 100 100	16, 22, 34, 43	0
1	W	169/169 (100%)	-0.74	0 100 100	15, 22, 31, 45	0
1	X	169/169 (100%)	-0.72	1 (0%) 89 88	16, 21, 33, 44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4056/4056 (100%)	-0.73	3 (0%) 95   95	15, 22, 33, 50	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	2	ALA	2.7
1	U	2	ALA	2.5
1	F	2	ALA	2.5

## 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.