



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2025 – 02:21 AM JST

PDB ID : 7DQP / pdb_00007dqp
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

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) : 2.0rc1
EDS : **FAILED**
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

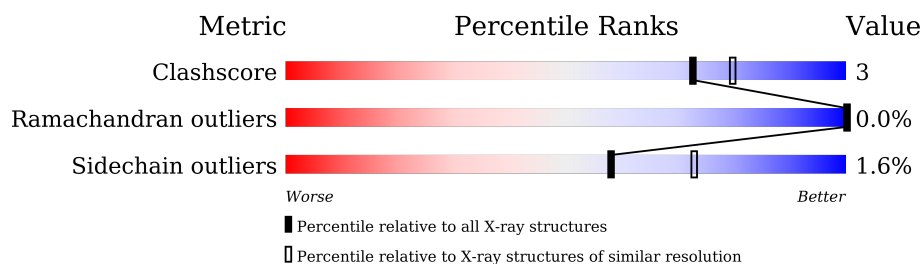
1 Overall quality at a glance

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))
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)

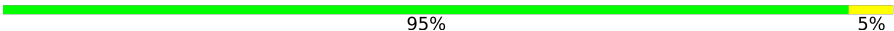
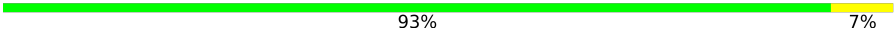
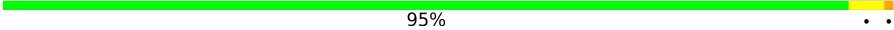

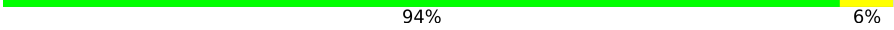
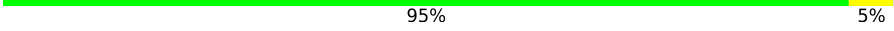
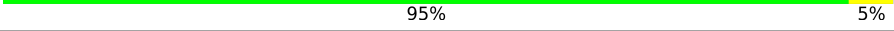
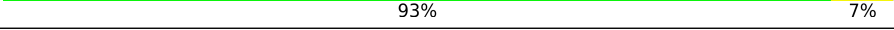
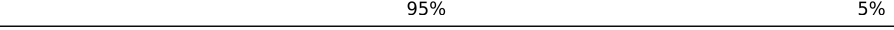


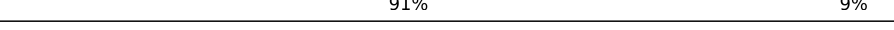
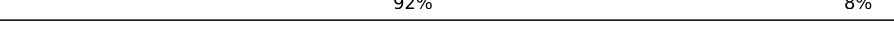
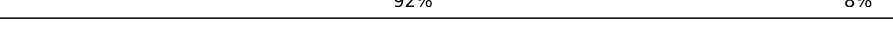
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	169	90% 10%
1	B	169	93% 7%
1	C	169	85% 14% .
1	D	169	95% 5%
1	E	169	89% 11% .
1	F	169	89% 11%
1	G	169	87% 13%
1	H	169	89% 10% .

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Mol	Chain	Length	Quality of chain
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

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
1	C	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	F	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	A	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	B	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	D	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	E	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	G	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	H	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	I	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	J	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	K	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	L	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	M	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	N	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	O	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			
1	P	169	Total	C	N	O	S	0	0	0
			1359	852	228	272	7			

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

- Molecule 2 is water.

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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. 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.


Note EDS failed to run properly.

- 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

Chain G: 87% 13%



- Molecule 1: Ferritin

Chain H: 89% 10%



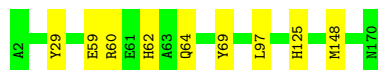
- Molecule 1: Ferritin

Chain I: 91% 9%



- Molecule 1: Ferritin

Chain J: 95% 5%



- Molecule 1: Ferritin

Chain K: 93% 7%



- Molecule 1: Ferritin

Chain L: 95% 5%



- Molecule 1: Ferritin

Chain M: 93% 7%



- Molecule 1: Ferritin

Chain N: 94% 6%



- Molecule 1: Ferritin

Chain O: 95% 5%



- Molecule 1: Ferritin

Chain P: 95% 5%



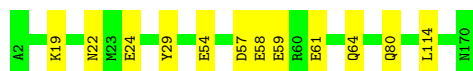
- Molecule 1: Ferritin

Chain Q: 93% 7%



- Molecule 1: Ferritin

Chain R: 93% 7%



- Molecule 1: Ferritin

Chain S: 95% 5%



- Molecule 1: Ferritin

Chain T: 91% 9%



- Molecule 1: Ferritin

Chain U: 91% 8%



- Molecule 1: Ferritin

Chain V: 91% 9%



- Molecule 1: Ferritin

Chain W: 92% 8%



- Molecule 1: Ferritin

Chain X: 92% 8%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	124.62Å 124.60Å 124.89Å 90.42° 119.79° 119.67°	Depositor
Resolution (Å)	40.62 – 2.20	Depositor
% Data completeness (in resolution range)	96.2 (40.62-2.20)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.173 , 0.179	Depositor
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.438	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.426 for -k,h+k+l,-h 0.426 for -l,-h,h+k+l 0.036 for h+l,-l,k 0.036 for h+k,l,-k 0.035 for -h-k-l,h+k,h+l 0.035 for h+k+l,-h-l,-h-k 0.036 for -k,-h-l,h+k 0.036 for h+l,-h,-h-k-l 0.038 for l,h+k,-h-l 0.038 for -h-l,h+k+l,h 0.036 for -h-k,h,h+k+l 0.036 for k,-h-k,h+l 0.036 for -l,h+l,-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+l,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+l,-k,-l 0.037 for -h-l,-k,l 0.096 for -h,-l,-k	Xtriage

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¹Intensities estimated from amplitudes.

²Theoretical 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.

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Property	Value	Source
Total number of atoms	33319	wwPDB-VP
Average B, all atoms (\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 ⓘ

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

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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

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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

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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

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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

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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

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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%)	22	23
1	D	167/169 (99%)	164 (98%)	3 (2%)	0	100	100

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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 ⓘ

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%)	62	77
1	B	145/145 (100%)	143 (99%)	2 (1%)	62	77
1	C	145/145 (100%)	143 (99%)	2 (1%)	62	77
1	D	145/145 (100%)	145 (100%)	0	100	100
1	E	145/145 (100%)	142 (98%)	3 (2%)	48	63
1	F	145/145 (100%)	141 (97%)	4 (3%)	38	51
1	G	145/145 (100%)	142 (98%)	3 (2%)	48	63
1	H	145/145 (100%)	140 (97%)	5 (3%)	32	42
1	I	145/145 (100%)	142 (98%)	3 (2%)	48	63
1	J	145/145 (100%)	144 (99%)	1 (1%)	81	90
1	K	145/145 (100%)	142 (98%)	3 (2%)	48	63
1	L	145/145 (100%)	141 (97%)	4 (3%)	38	51
1	M	145/145 (100%)	143 (99%)	2 (1%)	62	77
1	N	145/145 (100%)	143 (99%)	2 (1%)	62	77
1	O	145/145 (100%)	144 (99%)	1 (1%)	81	90
1	P	145/145 (100%)	144 (99%)	1 (1%)	81	90
1	Q	145/145 (100%)	142 (98%)	3 (2%)	48	63
1	R	145/145 (100%)	143 (99%)	2 (1%)	62	77
1	S	145/145 (100%)	143 (99%)	2 (1%)	62	77
1	T	145/145 (100%)	144 (99%)	1 (1%)	81	90
1	U	145/145 (100%)	143 (99%)	2 (1%)	62	77
1	V	145/145 (100%)	142 (98%)	3 (2%)	48	63
1	W	145/145 (100%)	143 (99%)	2 (1%)	62	77
1	X	145/145 (100%)	143 (99%)	2 (1%)	62	77
All	All	3480/3480 (100%)	3425 (98%)	55 (2%)	58	73

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

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Mol	Chain	Res	Type
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

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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 oligosaccharides 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](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.