



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2019 – 11:25 AM EDT

PDB ID : 6J4A  
Title : Human H chain ferritin with an extension peptide  
Authors : Zhang, X.; Zang, J.; Zhou, K.; Zhao, G.  
Deposited on : 2019-01-08  
Resolution : 3.99 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.

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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 : 2.4  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

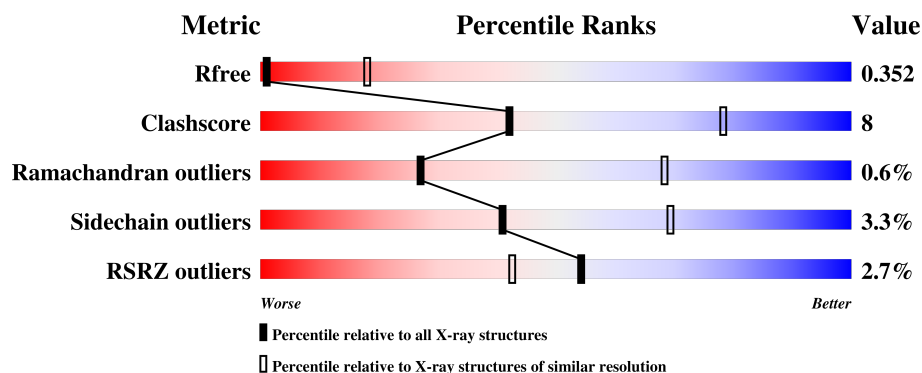
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.99 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))
$R_{free}$	111664	1008 (4.38-3.62)
Clashscore	122126	1012 (4.34-3.66)
Ramachandran outliers	120053	1000 (4.36-3.64)
Sidechain outliers	120020	1023 (4.38-3.62)
RSRZ outliers	108989	1107 (4.40-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	183	
1	B	183	
1	C	183	
1	D	183	
1	E	183	

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Mol	Chain	Length	Quality of chain
1	F	183	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>75%</div><div>18%</div><div>• 6%</div></div></div>
1	G	183	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>79%</div><div>14%</div><div>• 6%</div></div></div>
1	H	183	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>80%</div><div>14%</div><div>• 6%</div></div></div>
1	I	183	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>74%</div><div>19%</div><div>• 6%</div></div></div>
1	J	183	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>69%</div><div>25%</div><div>6%</div></div></div>
1	K	183	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>78%</div><div>16%</div><div>• 6%</div></div></div>
1	L	183	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>84%</div><div>9%</div><div>• 6%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16972 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	B	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	C	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	D	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	E	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	F	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	G	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	H	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	I	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	J	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	K	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			
1	L	172	Total	C	N	O	S	0	0	0
			1413	885	248	273	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	GLN	LYS	conflict	UNP P02794
B	86	GLN	LYS	conflict	UNP P02794
C	86	GLN	LYS	conflict	UNP P02794
D	86	GLN	LYS	conflict	UNP P02794
E	86	GLN	LYS	conflict	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
F	86	GLN	LYS	conflict	UNP P02794
G	86	GLN	LYS	conflict	UNP P02794
H	86	GLN	LYS	conflict	UNP P02794
I	86	GLN	LYS	conflict	UNP P02794
J	86	GLN	LYS	conflict	UNP P02794
K	86	GLN	LYS	conflict	UNP P02794
L	86	GLN	LYS	conflict	UNP P02794

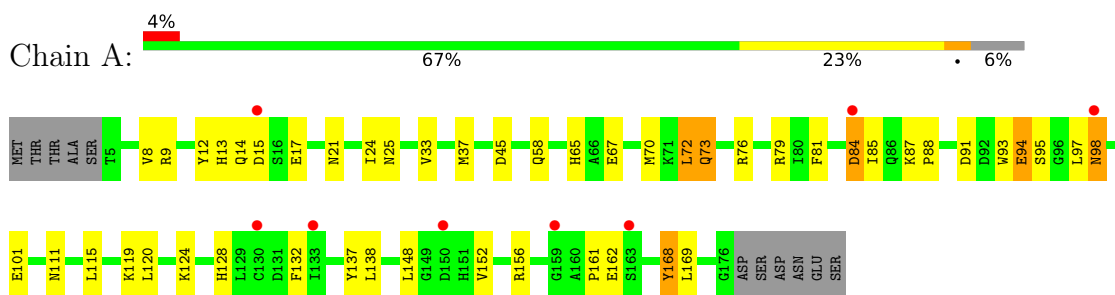
- Molecule 2 is water.

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

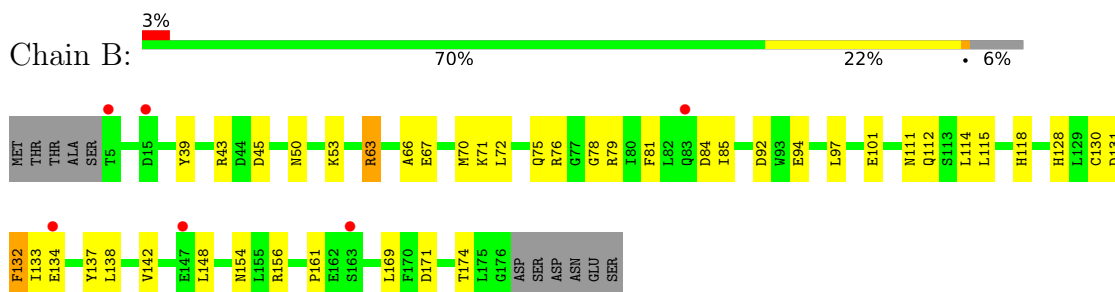
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

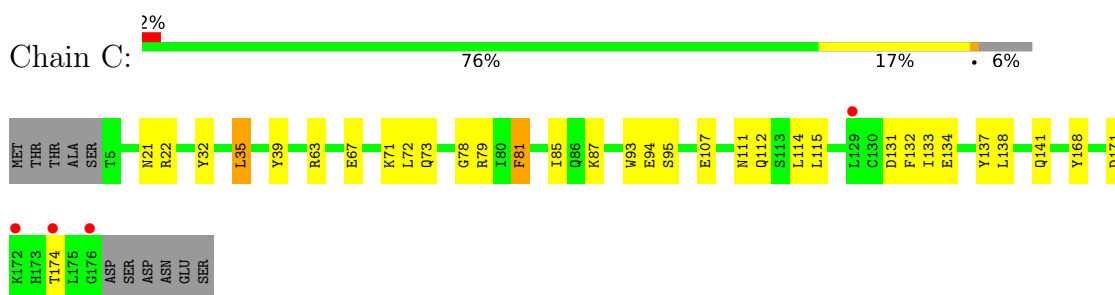
#### • Molecule 1: Ferritin heavy chain



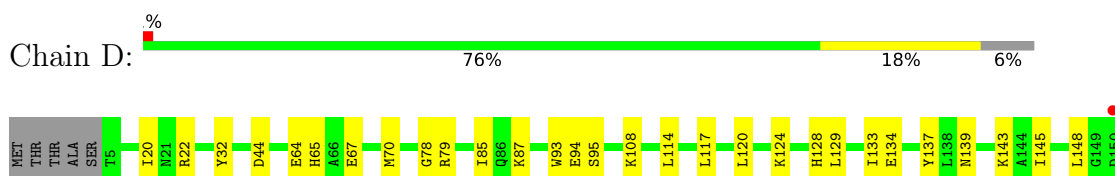
#### • Molecule 1: Ferritin heavy chain



#### • Molecule 1: Ferritin heavy chain

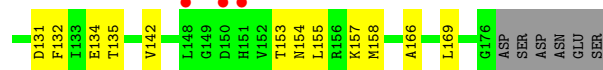
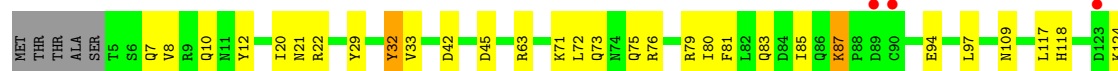


#### • Molecule 1: Ferritin heavy chain

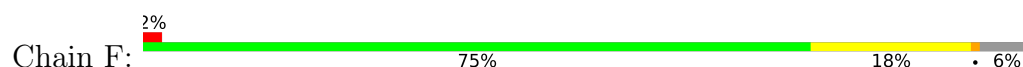




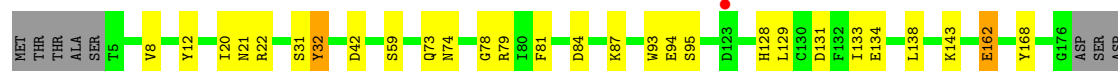
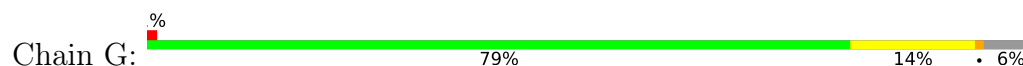
• Molecule 1: Ferritin heavy chain



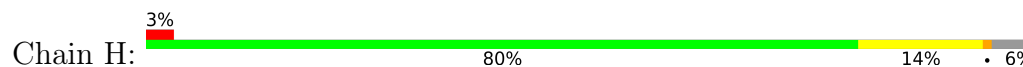
• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain



• Molecule 1: Ferritin heavy chain

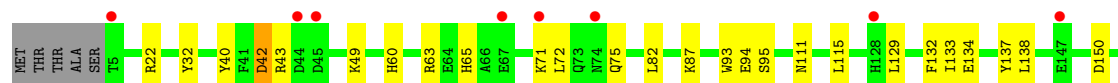
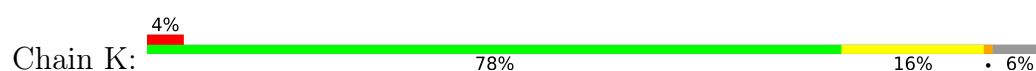




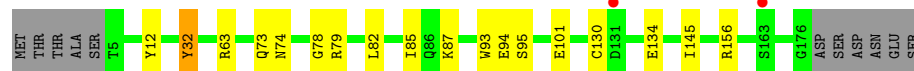
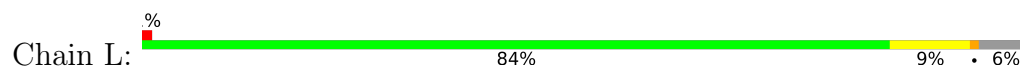
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	219.80Å 219.80Å 148.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.31 – 3.99 107.31 – 3.99	Depositor EDS
% Data completeness (in resolution range)	95.1 (107.31-3.99) 79.5 (107.31-3.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 4.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.283 , 0.351 0.283 , 0.352	Depositor DCC
$R_{free}$ test set	1536 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16972	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2702e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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](#)

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	0.29	0/1442	0.45	0/1943
1	B	0.27	0/1442	0.41	0/1943
1	C	0.27	0/1442	0.40	0/1943
1	D	0.25	0/1442	0.38	0/1943
1	E	0.26	0/1442	0.40	0/1943
1	F	0.26	0/1442	0.37	0/1943
1	G	0.26	0/1442	0.40	0/1943
1	H	0.25	0/1442	0.39	0/1943
1	I	0.26	0/1442	0.39	0/1943
1	J	0.26	0/1442	0.39	0/1943
1	K	0.26	0/1442	0.38	0/1943
1	L	0.26	0/1442	0.38	0/1943
All	All	0.26	0/17304	0.40	0/23316

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1413	0	1352	36	0
1	B	1413	0	1352	35	0
1	C	1413	0	1352	19	0
1	D	1413	0	1352	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1413	0	1352	38	0
1	F	1413	0	1352	27	1
1	G	1413	0	1352	22	1
1	H	1413	0	1352	16	0
1	I	1413	0	1352	25	0
1	J	1413	0	1352	32	0
1	K	1413	0	1352	21	0
1	L	1413	0	1352	12	0
2	A	3	0	0	1	0
2	B	1	0	0	0	0
2	D	2	0	0	1	0
2	E	1	0	0	0	0
2	F	2	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	L	1	0	0	0	0
All	All	16972	0	16224	249	1

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 8.

All (249) 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:33:VAL:HG12	1:A:88:PRO:HB3	1.63	0.80
1:C:21:ASN:HD21	1:C:81:PHE:H	1.30	0.79
1:F:107:GLU:OE1	1:F:141:GLN:NE2	2.18	0.77
1:B:174:THR:HG1	1:J:168:TYR:HH	1.35	0.75
1:B:67:GLU:O	1:B:71:LYS:N	2.16	0.74
1:C:21:ASN:OD1	1:C:73:GLN:NE2	2.24	0.71
1:C:78:GLY:O	1:C:79:ARG:NH1	2.24	0.70
1:D:78:GLY:O	1:D:79:ARG:NH1	2.21	0.70
1:E:63:ARG:HH22	1:F:60:HIS:CD2	2.10	0.69
1:B:78:GLY:O	1:B:79:ARG:NH1	2.26	0.69
1:A:21:ASN:OD1	1:A:73:GLN:NE2	2.27	0.68
1:A:101:GLU:OE1	1:A:156:ARG:NH2	2.29	0.66
1:K:42:ASP:HB3	1:L:74:ASN:HD22	1.61	0.66
1:B:63:ARG:HE	1:B:67:GLU:CD	2.00	0.65
1:D:169:LEU:HD21	1:J:169:LEU:HD13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ILE:HD11	1:B:85:ILE:HD12	1.77	0.65
1:B:174:THR:OG1	1:J:168:TYR:OH	2.08	0.64
1:L:101:GLU:OE1	1:L:156:ARG:NH2	2.30	0.64
1:G:134:GLU:HA	1:G:138:LEU:HB2	1.80	0.64
1:A:79:ARG:NH1	1:B:45:ASP:OD2	2.29	0.64
1:I:74:ASN:HD22	1:J:42:ASP:HB3	1.63	0.64
1:C:21:ASN:ND2	1:C:81:PHE:H	1.95	0.63
1:A:9:ARG:NH2	1:A:17:GLU:OE2	2.32	0.62
1:A:93:TRP:O	1:A:95:SER:N	2.33	0.62
1:C:174:THR:HG1	1:K:168:TYR:HH	1.46	0.62
1:J:65:HIS:O	1:J:137:TYR:OH	2.17	0.62
1:A:21:ASN:ND2	1:A:81:PHE:H	1.98	0.61
1:L:78:GLY:O	1:L:79:ARG:NH1	2.33	0.61
1:A:8:VAL:HG23	1:H:145:ILE:HG22	1.81	0.61
1:B:97:LEU:HD23	1:B:161:PRO:HD3	1.82	0.61
1:F:134:GLU:HA	1:F:138:LEU:HB2	1.82	0.60
1:G:21:ASN:HD21	1:G:81:PHE:HB2	1.66	0.59
1:K:65:HIS:O	1:K:137:TYR:OH	2.20	0.59
1:E:87:LYS:HD3	1:E:87:LYS:H	1.67	0.59
1:A:169:LEU:HD21	1:E:169:LEU:HD13	1.83	0.59
1:E:42:ASP:HB3	1:F:74:ASN:HD22	1.67	0.59
1:K:40:TYR:HD1	1:K:43:ARG:HD3	1.67	0.58
1:J:154:ASN:O	1:J:158:MET:HG2	2.03	0.58
1:G:131:ASP:HA	1:G:134:GLU:HG2	1.86	0.58
1:I:12:TYR:OH	1:I:73:GLN:OE1	2.22	0.57
1:E:118:HIS:NE2	1:E:134:GLU:OE2	2.37	0.57
1:F:31:SER:HB2	1:F:62:GLU:HB2	1.86	0.57
1:I:35:LEU:HD11	1:J:70:MET:SD	2.45	0.57
1:B:101:GLU:OE1	1:B:156:ARG:NH2	2.38	0.56
1:E:131:ASP:O	1:E:135:THR:N	2.39	0.56
1:I:24:ILE:HD13	1:I:70:MET:HG3	1.88	0.56
1:J:130:CYS:O	1:J:134:GLU:HG3	2.06	0.56
1:G:31:SER:O	1:G:59:SER:OG	2.23	0.56
1:B:72:LEU:HB2	1:B:132:PHE:HE2	1.71	0.55
1:E:131:ASP:HA	1:E:134:GLU:HB2	1.87	0.55
1:I:97:LEU:HD13	1:I:155:LEU:HB2	1.89	0.55
1:E:12:TYR:OH	1:E:73:GLN:OE1	2.23	0.55
1:I:107:GLU:OE1	1:I:141:GLN:NE2	2.34	0.55
1:I:45:ASP:N	1:I:45:ASP:OD1	2.37	0.55
1:A:12:TYR:HD1	1:A:76:ARG:HE	1.53	0.54
1:I:130:CYS:O	1:I:134:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:GLU:HG3	1:F:138:LEU:HD12	1.90	0.54
1:C:131:ASP:HA	1:C:134:GLU:HB2	1.90	0.54
1:E:10:GLN:HE21	1:I:112:GLN:HE22	1.56	0.54
1:H:118:HIS:NE2	1:H:134:GLU:OE2	2.37	0.54
1:J:20:ILE:HG23	1:J:69:LEU:HD22	1.90	0.54
1:K:150:ASP:O	1:K:154:ASN:ND2	2.41	0.53
1:G:12:TYR:OH	1:G:73:GLN:OE1	2.23	0.53
1:J:63:ARG:HG2	1:J:63:ARG:HH11	1.72	0.53
1:C:114:LEU:HD13	1:C:137:TYR:HB3	1.91	0.53
1:A:65:HIS:O	1:A:137:TYR:OH	2.26	0.53
1:C:133:ILE:HG22	1:C:138:LEU:HG	1.90	0.52
1:C:174:THR:OG1	1:K:168:TYR:OH	2.21	0.52
1:B:114:LEU:HD13	1:B:137:TYR:HB3	1.91	0.52
1:F:50:ASN:ND2	1:F:171:ASP:OD1	2.43	0.52
1:D:20:ILE:HD13	1:D:117:LEU:HD11	1.90	0.52
1:A:79:ARG:HH22	1:B:43:ARG:CZ	2.23	0.52
1:D:134:GLU:OE1	2:D:201:HOH:O	2.19	0.51
1:E:87:LYS:H	1:E:87:LYS:CD	2.22	0.51
1:K:72:LEU:HD22	1:K:132:PHE:CD2	2.46	0.51
1:A:120:LEU:O	1:A:124:LYS:HG2	2.10	0.51
1:L:130:CYS:O	1:L:134:GLU:HG3	2.10	0.51
1:D:139:ASN:O	1:D:143:LYS:HG3	2.10	0.51
1:A:58:GLN:NE2	2:A:201:HOH:O	2.35	0.51
1:F:43:ARG:NH2	1:F:45:ASP:OD2	2.44	0.51
1:I:29:TYR:O	1:I:33:VAL:HG23	2.10	0.51
1:K:71:LYS:O	1:K:75:GLN:HG3	2.11	0.51
1:D:129:LEU:O	1:D:133:ILE:HG12	2.11	0.51
1:E:8:VAL:HB	1:I:145:ILE:HG22	1.92	0.51
1:G:133:ILE:HG22	1:G:138:LEU:HG	1.93	0.50
1:I:87:LYS:N	1:J:84:ASP:OD1	2.44	0.50
1:J:70:MET:HE3	1:J:80:ILE:HG21	1.92	0.50
1:F:47:ALA:HB1	1:I:150:ASP:OD1	2.11	0.50
1:A:98:ASN:ND2	1:A:98:ASN:O	2.26	0.50
1:G:20:ILE:HD11	1:G:129:LEU:HD11	1.94	0.50
1:J:66:ALA:O	1:J:70:MET:HG3	2.11	0.50
1:A:25:ASN:ND2	1:A:84:ASP:O	2.41	0.50
1:B:154:ASN:ND2	1:J:47:ALA:O	2.45	0.50
1:B:66:ALA:O	1:B:70:MET:HG3	2.12	0.50
1:G:21:ASN:ND2	1:G:81:PHE:HB2	2.26	0.49
1:A:13:HIS:CE1	1:A:15:ASP:HB2	2.47	0.49
1:D:108:LYS:HG3	1:D:145:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASP:C	1:E:153:THR:HG21	2.32	0.49
1:B:133:ILE:HG22	1:B:138:LEU:HG	1.94	0.49
1:K:63:ARG:HH11	1:L:63:ARG:HH11	1.61	0.49
1:I:76:ARG:HH22	1:I:126:ASP:CG	2.14	0.49
1:I:105:HIS:ND1	1:I:105:HIS:O	2.44	0.48
1:D:93:TRP:O	1:D:95:SER:N	2.47	0.48
1:F:78:GLY:O	1:F:79:ARG:NH1	2.46	0.48
1:A:168:TYR:CE2	1:E:158:MET:SD	3.07	0.48
1:G:21:ASN:HD21	1:G:81:PHE:H	1.61	0.48
1:I:78:GLY:O	1:I:79:ARG:NH1	2.47	0.48
1:A:94:GLU:HG2	1:A:95:SER:H	1.78	0.48
1:B:118:HIS:NE2	1:B:134:GLU:OE2	2.47	0.48
1:C:85:ILE:HD12	1:D:85:ILE:HD12	1.95	0.48
1:F:45:ASP:N	1:F:45:ASP:OD1	2.40	0.48
1:K:82:LEU:HD13	1:L:32:TYR:CE1	2.49	0.48
1:C:79:ARG:HD3	1:C:79:ARG:HA	1.70	0.48
1:K:133:ILE:HG22	1:K:138:LEU:HG	1.95	0.48
1:K:72:LEU:HD21	1:K:129:LEU:HD13	1.95	0.48
1:G:42:ASP:HB3	1:H:74:ASN:HD22	1.79	0.47
1:L:12:TYR:OH	1:L:73:GLN:OE1	2.30	0.47
1:E:83:GLN:HA	1:F:87:LYS:HD2	1.95	0.47
1:A:94:GLU:HG2	1:A:95:SER:N	2.30	0.47
1:E:154:ASN:O	1:E:157:LYS:N	2.48	0.47
1:A:37:MET:HG2	1:A:93:TRP:CE2	2.50	0.47
1:J:89:ASP:N	1:J:89:ASP:OD1	2.44	0.47
1:D:65:HIS:O	1:D:137:TYR:OH	2.32	0.47
1:B:169:LEU:HD21	1:H:169:LEU:HD13	1.97	0.47
1:B:76:ARG:HD2	1:E:142:VAL:HG11	1.96	0.47
1:E:32:TYR:HE2	1:F:85:ILE:HG13	1.80	0.47
1:F:24:ILE:HD13	1:F:70:MET:HG2	1.97	0.47
1:J:71:LYS:O	1:J:75:GLN:HG3	2.14	0.47
1:C:72:LEU:HD22	1:C:132:PHE:CD2	2.50	0.46
1:A:97:LEU:HD23	1:A:161:PRO:HD3	1.97	0.46
1:A:67:GLU:HG2	1:B:39:TYR:OH	2.14	0.46
1:C:107:GLU:OE1	1:C:141:GLN:NE2	2.38	0.46
1:J:72:LEU:HD21	1:J:129:LEU:HD13	1.97	0.46
1:A:111:ASN:O	1:A:115:LEU:HG	2.14	0.46
1:E:72:LEU:HD22	1:E:132:PHE:CD2	2.51	0.46
1:F:50:ASN:HA	1:F:53:LYS:HB2	1.97	0.46
1:G:78:GLY:O	1:G:79:ARG:NH1	2.40	0.46
1:J:8:VAL:HB	1:L:145:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ASP:HA	1:B:134:GLU:HG3	1.97	0.46
1:B:134:GLU:HB3	1:I:131:ASP:HB2	1.97	0.46
1:A:24:ILE:HD13	1:A:70:MET:HG3	1.98	0.46
1:D:65:HIS:HB3	1:D:137:TYR:HE2	1.81	0.46
1:E:154:ASN:O	1:E:158:MET:HG3	2.16	0.46
1:E:21:ASN:ND2	1:E:81:PHE:O	2.49	0.45
1:A:128:HIS:HD1	1:H:142:VAL:HG21	1.81	0.45
1:B:63:ARG:NE	1:B:67:GLU:OE2	2.43	0.45
1:J:29:TYR:O	1:J:33:VAL:HG23	2.16	0.45
1:E:158:MET:HB2	1:E:166:ALA:HB1	1.99	0.45
1:E:71:LYS:O	1:E:75:GLN:HG3	2.17	0.45
1:I:37:MET:HA	1:I:93:TRP:CD1	2.51	0.45
1:B:71:LYS:O	1:B:75:GLN:HG3	2.16	0.45
1:G:162:GLU:HG3	1:G:162:GLU:H	1.58	0.45
1:E:45:ASP:OD2	1:F:79:ARG:NH2	2.47	0.45
1:E:10:GLN:NE2	1:I:112:GLN:HE22	2.14	0.45
1:J:141:GLN:O	1:J:145:ILE:HG13	2.17	0.45
1:A:72:LEU:HD13	1:A:132:PHE:CD2	2.52	0.45
1:A:21:ASN:HD21	1:A:81:PHE:H	1.64	0.44
1:E:10:GLN:O	1:E:76:ARG:NH2	2.46	0.44
1:E:79:ARG:HD2	1:F:43:ARG:HD2	1.99	0.44
1:K:129:LEU:O	1:K:133:ILE:HG12	2.18	0.44
1:F:28:LEU:HB3	1:F:85:ILE:HD13	1.99	0.44
1:B:111:ASN:O	1:B:115:LEU:HG	2.16	0.44
1:E:79:ARG:HD3	1:E:79:ARG:HA	1.73	0.44
1:D:79:ARG:HD3	1:D:79:ARG:HA	1.77	0.44
1:E:20:ILE:HD13	1:E:117:LEU:HD11	2.00	0.44
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.87	0.44
1:A:148:LEU:O	1:A:152:VAL:HG23	2.17	0.44
1:C:93:TRP:O	1:C:95:SER:N	2.51	0.44
1:E:63:ARG:HH22	1:F:60:HIS:HD2	1.63	0.43
1:H:153:THR:O	1:H:157:LYS:HG2	2.18	0.43
1:J:108:LYS:HG3	1:J:145:ILE:HD13	2.00	0.43
1:L:93:TRP:O	1:L:95:SER:N	2.51	0.43
1:G:32:TYR:CE1	1:H:82:LEU:HD13	2.54	0.43
1:J:111:ASN:O	1:J:115:LEU:HG	2.18	0.43
1:J:23:GLN:OE1	1:J:113:SER:OG	2.36	0.43
1:J:63:ARG:NH1	1:J:63:ARG:HG2	2.33	0.43
1:L:79:ARG:HD3	1:L:79:ARG:HA	1.73	0.43
1:K:154:ASN:O	1:K:158:MET:HG3	2.19	0.43
1:F:114:LEU:HD22	1:F:133:ILE:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:149:GLY:O	1:I:153:THR:OG1	2.35	0.43
1:J:20:ILE:HD13	1:J:117:LEU:HD11	1.99	0.43
1:K:32:TYR:CZ	1:L:82:LEU:HD13	2.53	0.43
1:B:76:ARG:HD3	1:B:128:HIS:HD1	1.84	0.43
1:B:79:ARG:HD3	1:B:79:ARG:HA	1.82	0.43
1:A:87:LYS:N	1:B:84:ASP:OD1	2.47	0.43
1:H:76:ARG:HG3	1:H:76:ARG:HH11	1.83	0.43
1:J:72:LEU:HD22	1:J:132:PHE:CD2	2.54	0.43
1:B:53:LYS:HB2	1:B:53:LYS:HE3	1.91	0.43
1:D:139:ASN:HA	1:G:128:HIS:CD2	2.54	0.43
1:H:141:GLN:O	1:H:145:ILE:HG13	2.19	0.42
1:J:135:THR:HB	1:J:136:HIS:CD2	2.53	0.42
1:C:67:GLU:O	1:C:71:LYS:N	2.36	0.42
1:D:120:LEU:O	1:D:124:LYS:HG2	2.19	0.42
1:F:105:HIS:ND1	1:F:105:HIS:O	2.53	0.42
1:G:79:ARG:HA	1:G:79:ARG:HD3	1.73	0.42
1:G:93:TRP:O	1:G:95:SER:N	2.51	0.42
1:J:124:LYS:N	1:J:124:LYS:HD2	2.33	0.42
1:K:134:GLU:HA	1:K:138:LEU:HD12	2.01	0.42
1:K:111:ASN:O	1:K:115:LEU:HG	2.18	0.42
1:A:84:ASP:OD1	1:A:84:ASP:N	2.53	0.42
1:J:134:GLU:HA	1:J:138:LEU:HD12	2.01	0.42
1:J:13:HIS:CG	1:J:124:LYS:HG2	2.54	0.42
1:C:39:TYR:OH	1:D:67:GLU:HB3	2.18	0.42
1:D:148:LEU:HA	1:D:148:LEU:HD23	1.92	0.42
1:E:29:TYR:O	1:E:33:VAL:HG23	2.20	0.42
1:F:72:LEU:HD22	1:F:132:PHE:CD2	2.55	0.42
1:G:129:LEU:O	1:G:133:ILE:HG12	2.20	0.42
1:D:145:ILE:HG22	1:G:8:VAL:HB	2.02	0.42
1:K:93:TRP:O	1:K:95:SER:N	2.53	0.42
1:K:32:TYR:CE1	1:L:85:ILE:HD11	2.55	0.42
1:A:162:GLU:HA	1:A:162:GLU:OE1	2.20	0.41
1:B:50:ASN:HB2	1:B:171:ASP:OD1	2.20	0.41
1:E:73:GLN:HG2	1:E:80:ILE:HG12	2.02	0.41
1:E:7:GLN:HG3	1:E:8:VAL:HG13	2.01	0.41
1:C:72:LEU:HD22	1:C:132:PHE:CE2	2.55	0.41
1:I:113:SER:O	1:I:117:LEU:HB2	2.20	0.41
1:K:134:GLU:HA	1:K:138:LEU:HB2	2.01	0.41
1:D:114:LEU:HD13	1:D:137:TYR:HB3	2.02	0.41
1:D:159:GLY:O	1:D:162:GLU:HG2	2.20	0.41
1:E:21:ASN:ND2	1:E:81:PHE:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:71:LYS:O	1:H:75:GLN:HG3	2.20	0.41
1:I:120:LEU:O	1:I:124:LYS:HG2	2.20	0.41
1:E:97:LEU:HD13	1:E:155:LEU:HB3	2.03	0.41
1:E:87:LYS:HD2	1:F:84:ASP:OD1	2.21	0.41
1:G:21:ASN:HD21	1:G:81:PHE:N	2.18	0.41
1:H:133:ILE:O	1:H:138:LEU:HG	2.21	0.41
1:J:72:LEU:HD22	1:J:132:PHE:CE2	2.55	0.41
1:A:138:LEU:HA	1:A:138:LEU:HD23	1.95	0.41
1:F:45:ASP:HA	1:I:153:THR:HG21	2.02	0.41
1:H:29:TYR:O	1:H:33:VAL:HG23	2.20	0.41
1:C:35:LEU:HD21	1:D:70:MET:SD	2.61	0.41
1:K:60:HIS:O	1:K:63:ARG:HB3	2.21	0.41
1:B:138:LEU:HA	1:B:138:LEU:HD23	1.84	0.40
1:E:124:LYS:HA	1:E:124:LYS:HD3	1.82	0.40
1:I:124:LYS:HD2	1:I:124:LYS:HA	1.89	0.40
1:H:79:ARG:HD3	1:H:79:ARG:HA	1.81	0.40
1:B:72:LEU:HD13	1:B:132:PHE:CE2	2.56	0.40
1:G:143:LYS:HD3	1:G:143:LYS:N	2.37	0.40
1:H:114:LEU:HD12	1:H:141:GLN:HG3	2.04	0.40
1:B:130:CYS:O	1:B:134:GLU:HG3	2.21	0.40
1:E:85:ILE:HG13	1:F:32:TYR:CE2	2.57	0.40
1:E:79:ARG:NH2	1:F:44:ASP:OD1	2.51	0.40
1:D:165:LEU:HD11	1:J:169:LEU:HD12	2.04	0.40
1:B:142:VAL:HG21	1:I:76:ARG:HD3	2.03	0.40
1:A:85:ILE:CD1	1:B:85:ILE:HD12	2.49	0.40
1:C:111:ASN:O	1:C:115:LEU:HG	2.22	0.40
1:F:29:TYR:O	1:F:33:VAL:HG23	2.21	0.40
1:G:74:ASN:HD22	1:H:42:ASP:HB3	1.86	0.40
1:G:84:ASP:OD1	1:H:87:LYS:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:THR:OG1	1:G:168:TYR:OH[8_777]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	170/183 (93%)	158 (93%)	11 (6%)	1 (1%)	27	68
1	B	170/183 (93%)	161 (95%)	8 (5%)	1 (1%)	27	68
1	C	170/183 (93%)	165 (97%)	4 (2%)	1 (1%)	27	68
1	D	170/183 (93%)	164 (96%)	5 (3%)	1 (1%)	27	68
1	E	170/183 (93%)	160 (94%)	9 (5%)	1 (1%)	27	68
1	F	170/183 (93%)	164 (96%)	5 (3%)	1 (1%)	27	68
1	G	170/183 (93%)	164 (96%)	5 (3%)	1 (1%)	27	68
1	H	170/183 (93%)	165 (97%)	4 (2%)	1 (1%)	27	68
1	I	170/183 (93%)	168 (99%)	1 (1%)	1 (1%)	27	68
1	J	170/183 (93%)	163 (96%)	5 (3%)	2 (1%)	14	55
1	K	170/183 (93%)	161 (95%)	8 (5%)	1 (1%)	27	68
1	L	170/183 (93%)	165 (97%)	4 (2%)	1 (1%)	27	68
All	All	2040/2196 (93%)	1958 (96%)	69 (3%)	13 (1%)	27	68

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	GLU
1	D	94	GLU
1	H	94	GLU
1	B	94	GLU
1	E	94	GLU
1	G	94	GLU
1	I	94	GLU
1	K	94	GLU
1	C	94	GLU
1	F	94	GLU
1	L	94	GLU
1	J	159	GLY

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Mol	Chain	Res	Type
1	J	94	GLU

### 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	153/163 (94%)	145 (95%)	8 (5%)	25	59
1	B	153/163 (94%)	148 (97%)	5 (3%)	41	69
1	C	153/163 (94%)	144 (94%)	9 (6%)	21	55
1	D	153/163 (94%)	147 (96%)	6 (4%)	35	65
1	E	153/163 (94%)	149 (97%)	4 (3%)	49	74
1	F	153/163 (94%)	149 (97%)	4 (3%)	49	74
1	G	153/163 (94%)	149 (97%)	4 (3%)	49	74
1	H	153/163 (94%)	148 (97%)	5 (3%)	41	69
1	I	153/163 (94%)	148 (97%)	5 (3%)	41	69
1	J	153/163 (94%)	149 (97%)	4 (3%)	49	74
1	K	153/163 (94%)	148 (97%)	5 (3%)	41	69
1	L	153/163 (94%)	151 (99%)	2 (1%)	71	86
All	All	1836/1956 (94%)	1775 (97%)	61 (3%)	41	69

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	72	LEU
1	A	73	GLN
1	A	84	ASP
1	A	91	ASP
1	A	98	ASN
1	A	119	LYS
1	A	168	TYR
1	B	63	ARG

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Mol	Chain	Res	Type
1	B	81	PHE
1	B	92	ASP
1	B	112	GLN
1	B	132	PHE
1	C	22	ARG
1	C	32	TYR
1	C	35	LEU
1	C	63	ARG
1	C	81	PHE
1	C	87	LYS
1	C	112	GLN
1	C	168	TYR
1	C	171	ASP
1	D	22	ARG
1	D	32	TYR
1	D	44	ASP
1	D	64	GLU
1	D	87	LYS
1	D	128	HIS
1	E	22	ARG
1	E	32	TYR
1	E	87	LYS
1	E	109	ASN
1	F	32	TYR
1	F	87	LYS
1	F	112	GLN
1	F	162	GLU
1	G	22	ARG
1	G	32	TYR
1	G	87	LYS
1	G	162	GLU
1	H	32	TYR
1	H	87	LYS
1	H	125	ASN
1	H	140	GLU
1	H	172	LYS
1	I	32	TYR
1	I	87	LYS
1	I	105	HIS
1	I	119	LYS
1	I	136	HIS
1	J	21	ASN

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Mol	Chain	Res	Type
1	J	32	TYR
1	J	45	ASP
1	J	87	LYS
1	K	22	ARG
1	K	42	ASP
1	K	49	LYS
1	K	87	LYS
1	K	171	ASP
1	L	32	TYR
1	L	87	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	10	GLN
1	F	60	HIS
1	G	21	ASN
1	I	111	ASN
1	J	154	ASN
1	L	74	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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 ⓘ

### 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(Å²)	Q<0.9	
1	A	172/183 (93%)	0.48	8 (4%)	31	23	27, 44, 61, 77	0
1	B	172/183 (93%)	0.57	6 (3%)	44	33	28, 44, 65, 75	0
1	C	172/183 (93%)	0.38	4 (2%)	60	49	28, 44, 66, 91	0
1	D	172/183 (93%)	0.38	1 (0%)	89	83	27, 43, 64, 78	0
1	E	172/183 (93%)	0.46	6 (3%)	44	33	23, 42, 63, 83	0
1	F	172/183 (93%)	0.33	4 (2%)	60	49	21, 40, 59, 68	0
1	G	172/183 (93%)	0.28	1 (0%)	89	83	21, 40, 60, 70	0
1	H	172/183 (93%)	0.47	6 (3%)	44	33	21, 41, 62, 84	0
1	I	172/183 (93%)	0.38	5 (2%)	51	39	23, 39, 57, 71	0
1	J	172/183 (93%)	0.45	4 (2%)	60	49	21, 40, 59, 75	0
1	K	172/183 (93%)	0.45	8 (4%)	31	23	20, 41, 59, 68	0
1	L	172/183 (93%)	0.37	2 (1%)	79	69	20, 41, 60, 70	0
All	All	2064/2196 (93%)	0.42	55 (2%)	54	42	20, 42, 62, 91	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	150	ASP	3.2
1	I	158	MET	3.2
1	H	161	PRO	3.1
1	I	131	ASP	2.8
1	E	89	ASP	2.8
1	C	176	GLY	2.8
1	C	174	THR	2.8
1	K	128	HIS	2.8
1	K	147	GLU	2.7
1	K	45	ASP	2.6
1	F	158	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	147	GLU	2.5
1	B	15	ASP	2.5
1	D	150	ASP	2.5
1	J	96	GLY	2.5
1	A	163	SER	2.5
1	F	154	ASN	2.5
1	E	90	CYS	2.5
1	K	67	GLU	2.5
1	C	172	LYS	2.4
1	A	84	ASP	2.4
1	I	154	ASN	2.4
1	A	159	GLY	2.4
1	L	131	ASP	2.4
1	J	125	ASN	2.4
1	F	81	PHE	2.3
1	E	123	ASP	2.3
1	B	163	SER	2.3
1	G	123	ASP	2.3
1	A	15	ASP	2.3
1	C	129	LEU	2.3
1	K	5	THR	2.3
1	B	83	GLN	2.2
1	H	128	HIS	2.2
1	B	5	THR	2.2
1	A	98	ASN	2.2
1	K	44	ASP	2.2
1	K	71	LYS	2.2
1	J	147	GLU	2.2
1	A	150	ASP	2.2
1	A	133	ILE	2.2
1	I	94	GLU	2.2
1	A	130	CYS	2.1
1	H	131	ASP	2.1
1	J	150	ASP	2.1
1	H	151	HIS	2.1
1	L	163	SER	2.1
1	F	21	ASN	2.1
1	K	74	ASN	2.1
1	I	130	CYS	2.1
1	E	151	HIS	2.0
1	B	147	GLU	2.0
1	H	127	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	134	GLU	2.0
1	E	148	LEU	2.0

## 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 carbohydrates 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.