



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:49 AM GMT

PDB ID : 2BKC  
Title : THE X-RAY STRUCTURE OF THE H43G LISTERIA INNOCUA DPS MUTANT  
Authors : Ilari, A.; Stefanini, S.; Chiancone, E.  
Deposited on : 2005-02-15  
Resolution : 2.30 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

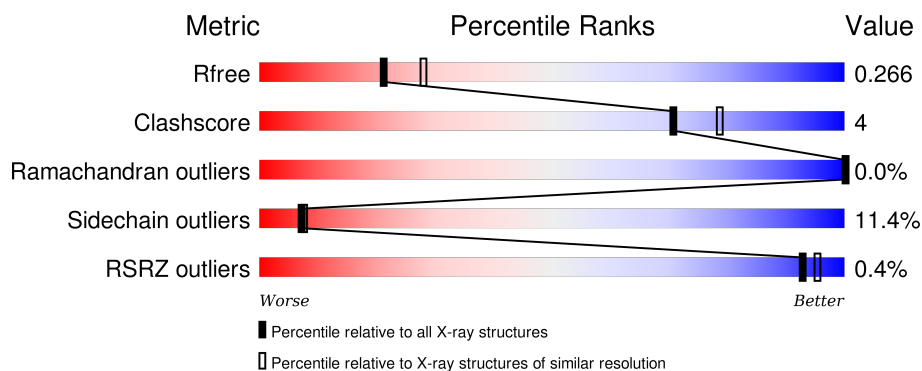
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	156	<div> <div>82%</div> <div>12%</div> <div>• •</div> </div>
1	B	156	<div> <div>%</div> <div>79%</div> <div>13%</div> <div>• •</div> </div>
1	C	156	<div> <div>79%</div> <div>14%</div> <div>• •</div> </div>
1	D	156	<div> <div>74%</div> <div>20%</div> <div>• •</div> </div>
1	E	156	<div> <div>%</div> <div>79%</div> <div>12%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	156	
1	G	156	
1	H	156	
1	I	156	
1	J	156	
1	K	156	
1	L	156	
1	M	156	
1	N	156	
1	O	156	
1	P	156	
1	Q	156	
1	R	156	
1	S	156	
1	T	156	
1	U	156	
1	V	156	
1	X	156	
1	Y	156	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29380 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 NON-HEME IRON-CONTAINING FERRITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	B	150	Total	C	N	O	S	0	1	0
			1220	782	194	237	7			
1	C	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	D	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	E	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	F	150	Total	C	N	O	S	0	1	0
			1220	782	194	237	7			
1	G	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	H	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	I	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	J	150	Total	C	N	O	S	0	1	0
			1220	782	194	237	7			
1	K	150	Total	C	N	O	S	0	1	0
			1220	782	194	237	7			
1	L	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	M	150	Total	C	N	O	S	0	1	0
			1220	782	194	237	7			
1	N	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	O	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	P	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	R	149	Total	C	N	O	S	0	1	0
			1213	777	193	236	7			
1	S	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	T	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	U	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	V	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	X	150	Total	C	N	O	S	0	0	0
			1216	780	194	235	7			
1	Y	150	Total	C	N	O	S	0	0	0
			1213	778	193	235	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
B	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
C	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
D	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
E	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
F	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
G	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
H	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
I	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
J	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
K	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
L	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
M	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
N	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
O	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
P	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
Q	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
R	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
S	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
T	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
U	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
V	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725
X	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	43	GLY	HIS	ENGINEERED MUTATION	UNP P80725

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total O 12 12	0	0
2	B	8	Total O 8 8	0	0
2	C	14	Total O 14 14	0	0
2	D	9	Total O 9 9	0	0
2	E	10	Total O 10 10	0	0
2	F	7	Total O 7 7	0	0
2	G	6	Total O 6 6	0	0
2	H	10	Total O 10 10	0	0
2	I	7	Total O 7 7	0	0
2	J	7	Total O 7 7	0	0
2	K	16	Total O 16 16	0	0
2	L	7	Total O 7 7	0	0
2	M	9	Total O 9 9	0	0
2	N	5	Total O 5 5	0	0
2	O	5	Total O 5 5	0	0
2	P	3	Total O 3 3	0	0
2	Q	3	Total O 3 3	0	0
2	R	13	Total O 13 13	0	0
2	S	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	T	9	Total	O	0	0
			9	9		
2	U	4	Total	O	0	0
			4	4		
2	V	5	Total	O	0	0
			5	5		
2	X	5	Total	O	0	0
			5	5		
2	Y	4	Total	O	0	0
			4	4		

### 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 errors 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: NON-HEME IRON-CONTAINING FERRITIN

Chain A: 




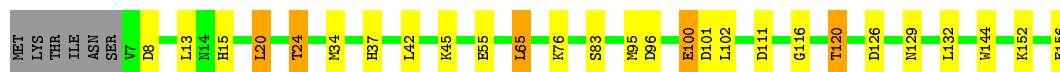
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain B: 



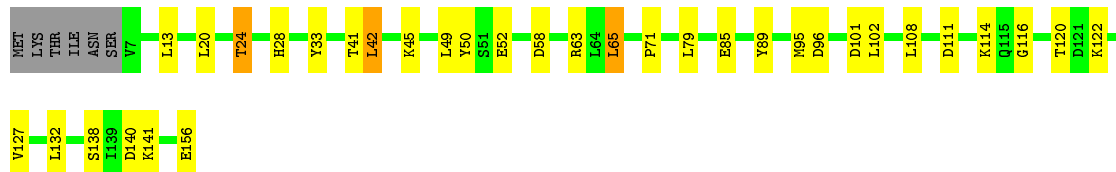
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain C: 




- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain D: 



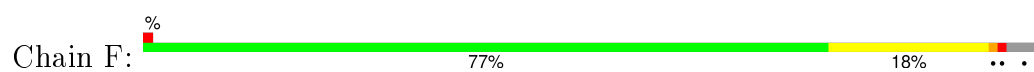
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain E: 

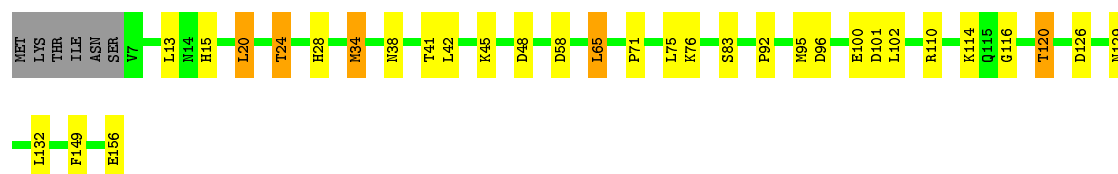
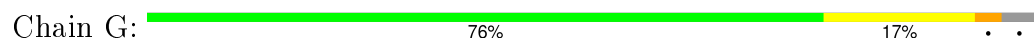


- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

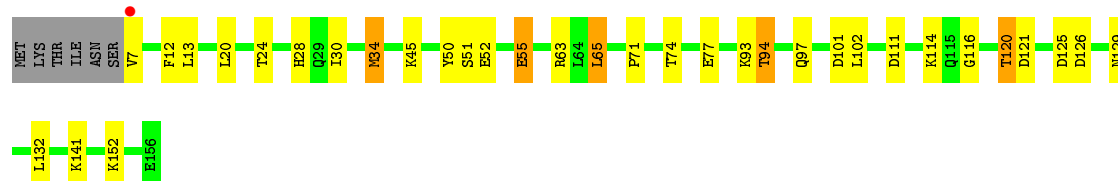




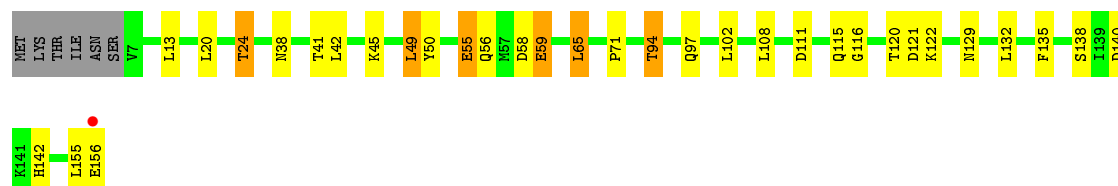
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



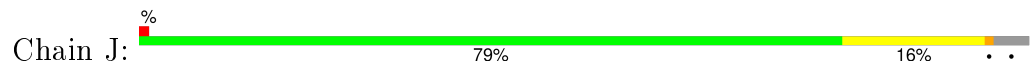
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



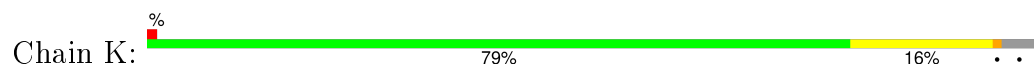
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



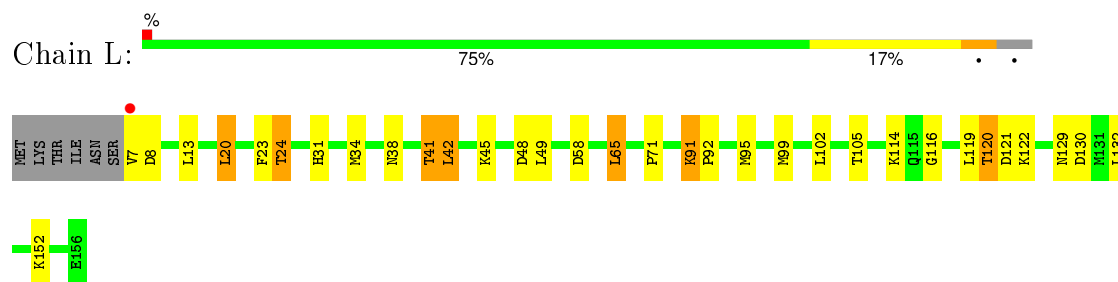
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



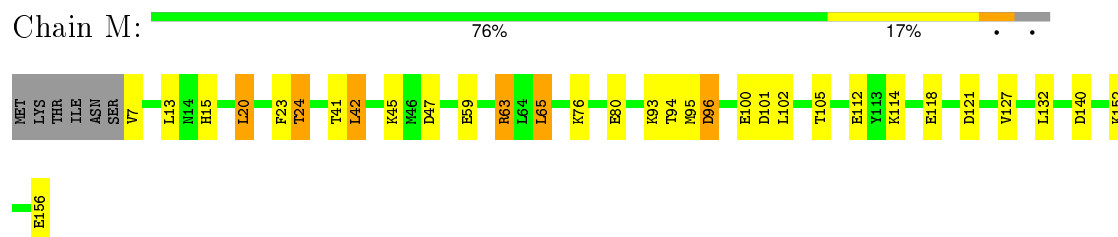
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



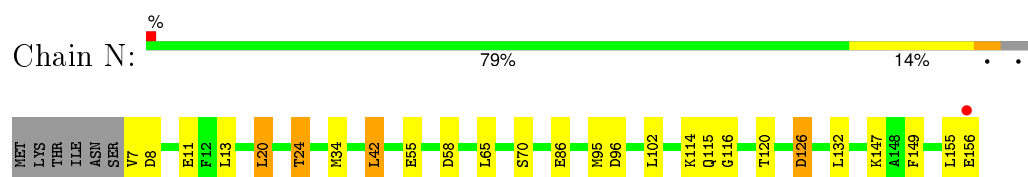
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



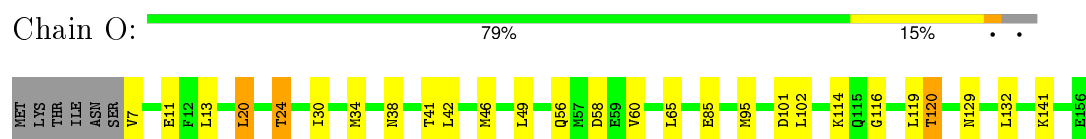
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



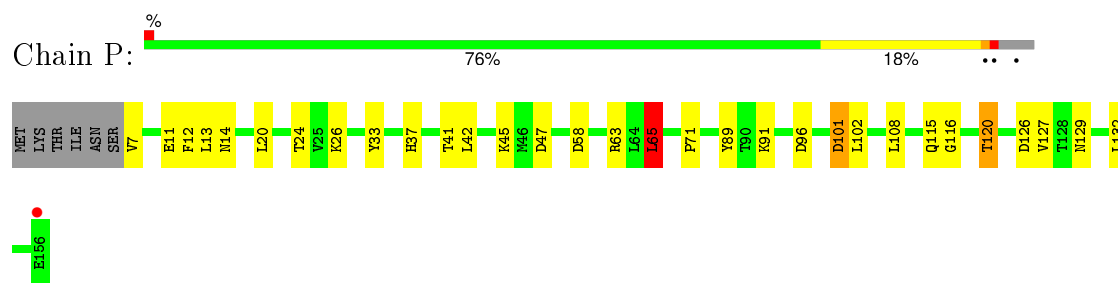
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



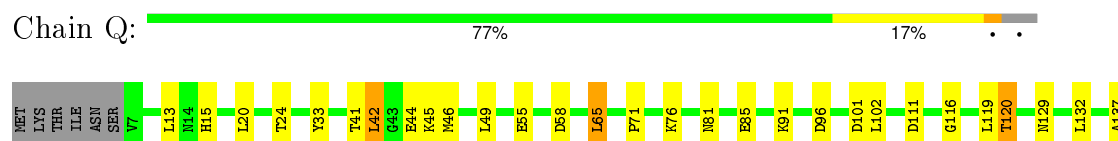
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

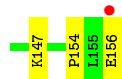
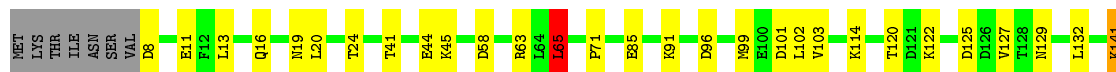
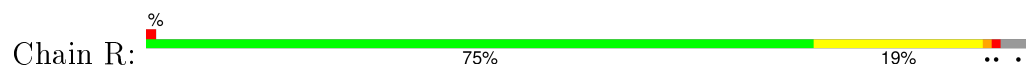


- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

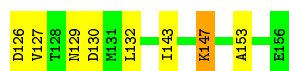




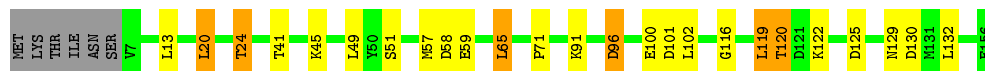
• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



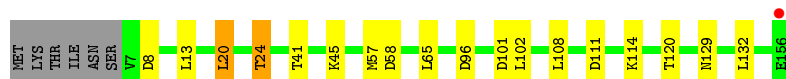
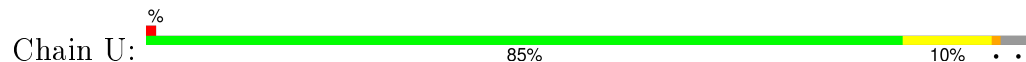
• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



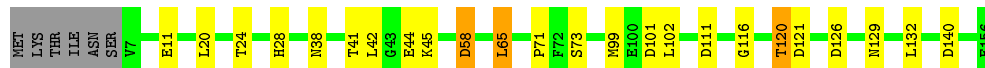
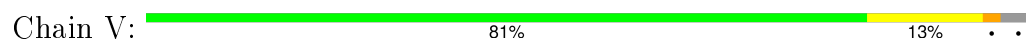
• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



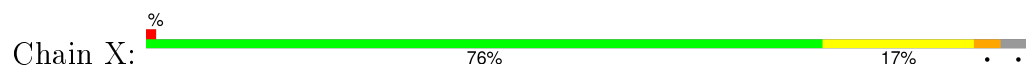
• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



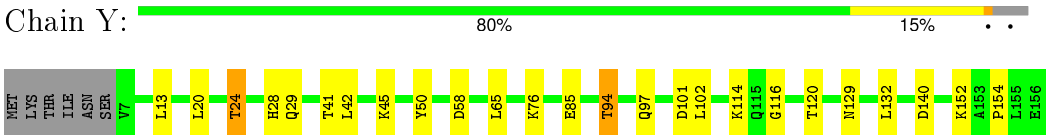
• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.73 Å 175.65 Å 135.96 Å 90.00° 92.53° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 49.18 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.5 (25.00-2.30) 91.5 (49.18-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.209 , 0.266 0.212 , 0.266	Depositor DCC
$R_{free}$ test set	8690 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 26.9	EDS
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 172118 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	29380	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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	0.81	0/1242	0.93	3/1674 (0.2%)
1	B	0.81	0/1250	0.94	6/1685 (0.4%)
1	C	0.83	0/1242	0.91	5/1674 (0.3%)
1	D	0.82	0/1242	0.94	5/1674 (0.3%)
1	E	0.80	0/1242	0.92	6/1674 (0.4%)
1	F	0.83	0/1250	0.94	8/1685 (0.5%)
1	G	0.79	0/1242	0.91	6/1674 (0.4%)
1	H	0.84	1/1242 (0.1%)	0.96	6/1674 (0.4%)
1	I	0.84	1/1242 (0.1%)	0.92	3/1674 (0.2%)
1	J	0.77	0/1250	0.94	5/1685 (0.3%)
1	K	0.82	0/1250	0.97	5/1685 (0.3%)
1	L	0.82	0/1242	0.96	4/1674 (0.2%)
1	M	0.79	0/1250	0.99	8/1685 (0.5%)
1	N	0.78	0/1242	0.92	4/1674 (0.2%)
1	O	0.81	0/1242	0.91	2/1674 (0.1%)
1	P	0.77	0/1242	0.92	6/1674 (0.4%)
1	Q	0.77	0/1242	0.91	3/1674 (0.2%)
1	R	0.81	1/1243 (0.1%)	0.93	7/1675 (0.4%)
1	S	0.82	0/1242	0.95	7/1674 (0.4%)
1	T	0.81	0/1242	0.94	4/1674 (0.2%)
1	U	0.81	0/1242	0.91	4/1674 (0.2%)
1	V	0.76	0/1242	0.90	6/1674 (0.4%)
1	X	0.80	0/1242	0.97	9/1674 (0.5%)
1	Y	0.80	0/1239	0.88	2/1671 (0.1%)
All	All	0.81	3/29846 (0.0%)	0.93	124/40229 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	141	LYS	CD-CE	6.84	1.68	1.51
1	H	55	GLU	CG-CD	6.07	1.61	1.51
1	I	55	GLU	CD-OE2	5.16	1.31	1.25

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	58	ASP	CB-CG-OD2	10.00	127.30	118.30
1	X	111	ASP	CB-CG-OD2	9.32	126.69	118.30
1	D	58	ASP	CB-CG-OD2	8.80	126.22	118.30
1	D	101	ASP	CB-CG-OD2	8.71	126.14	118.30
1	J	111	ASP	CB-CG-OD2	8.55	126.00	118.30
1	U	58	ASP	CB-CG-OD2	8.44	125.90	118.30
1	B	101	ASP	CB-CG-OD2	7.65	125.19	118.30
1	N	96	ASP	CB-CG-OD2	7.58	125.12	118.30
1	A	126	ASP	CB-CG-OD2	7.57	125.12	118.30
1	J	58[A]	ASP	CB-CG-OD2	7.43	124.99	118.30
1	J	58[B]	ASP	CB-CG-OD2	7.43	124.99	118.30
1	I	111	ASP	CB-CG-OD2	7.43	124.98	118.30
1	C	8	ASP	CB-CG-OD2	7.33	124.90	118.30
1	L	48	ASP	CB-CG-OD2	7.32	124.89	118.30
1	H	125	ASP	CB-CG-OD2	7.20	124.78	118.30
1	M	63	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	H	111	ASP	CB-CG-OD2	7.18	124.77	118.30
1	G	101	ASP	CB-CG-OD2	7.12	124.71	118.30
1	G	96	ASP	CB-CG-OD2	7.12	124.70	118.30
1	R	58[A]	ASP	CB-CG-OD2	7.03	124.62	118.30
1	R	58[B]	ASP	CB-CG-OD2	7.03	124.62	118.30
1	F	101	ASP	CB-CG-OD2	7.02	124.62	118.30
1	G	110	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	X	47	ASP	CB-CG-OD2	6.97	124.58	118.30
1	M	121	ASP	CB-CG-OD2	6.93	124.53	118.30
1	P	47	ASP	CB-CG-OD2	6.82	124.44	118.30
1	M	65	LEU	CA-CB-CG	6.81	130.97	115.30
1	T	130	ASP	CB-CG-OD2	6.73	124.35	118.30
1	P	58	ASP	CB-CG-OD2	6.60	124.24	118.30
1	M	96	ASP	CB-CG-OD2	6.55	124.20	118.30
1	J	101	ASP	CB-CG-OD2	6.54	124.19	118.30
1	O	101	ASP	CB-CG-OD2	6.53	124.18	118.30
1	Q	96	ASP	CB-CG-OD2	6.53	124.17	118.30
1	F	125	ASP	CB-CG-OD2	6.47	124.12	118.30
1	B	121	ASP	CB-CG-OD2	6.47	124.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	96	ASP	CB-CG-OD2	6.40	124.06	118.30
1	E	96	ASP	CB-CG-OD2	6.39	124.05	118.30
1	H	121	ASP	CB-CG-OD2	6.37	124.03	118.30
1	R	8	ASP	CB-CG-OD2	6.36	124.03	118.30
1	S	96	ASP	CB-CG-OD2	6.35	124.02	118.30
1	M	101	ASP	CB-CG-OD2	6.32	123.99	118.30
1	X	121	ASP	CB-CG-OD2	6.31	123.98	118.30
1	Y	101	ASP	CB-CG-OD2	6.31	123.98	118.30
1	M	47	ASP	CB-CG-OD2	6.28	123.95	118.30
1	T	125	ASP	CB-CG-OD2	6.26	123.94	118.30
1	U	96	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	8	ASP	CB-CG-OD2	6.21	123.89	118.30
1	S	65	LEU	CA-CB-CG	6.21	129.57	115.30
1	L	130	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	96	ASP	CB-CG-OD2	6.16	123.84	118.30
1	I	140	ASP	CB-CG-OD1	6.15	123.83	118.30
1	S	101	ASP	CB-CG-OD2	6.14	123.83	118.30
1	D	111	ASP	CB-CG-OD2	6.10	123.79	118.30
1	H	126	ASP	CB-CG-OD2	6.09	123.78	118.30
1	V	126	ASP	CB-CG-OD2	6.07	123.76	118.30
1	M	63	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	Q	101	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	126	ASP	CB-CG-OD2	6.00	123.70	118.30
1	N	8	ASP	CB-CG-OD2	5.98	123.68	118.30
1	M	140	ASP	CB-CG-OD1	5.94	123.65	118.30
1	X	65	LEU	CA-CB-CG	5.93	128.94	115.30
1	D	140	ASP	CB-CG-OD2	5.90	123.61	118.30
1	I	121	ASP	CB-CG-OD2	5.88	123.60	118.30
1	H	101	ASP	CB-CG-OD2	5.87	123.59	118.30
1	K	47	ASP	CB-CG-OD2	5.87	123.58	118.30
1	E	121	ASP	CB-CG-OD2	5.87	123.58	118.30
1	X	125	ASP	CB-CG-OD2	5.85	123.57	118.30
1	F	119	LEU	CA-CB-CG	5.84	128.74	115.30
1	Y	140	ASP	CB-CG-OD2	5.82	123.54	118.30
1	S	125	ASP	CB-CG-OD2	5.81	123.53	118.30
1	O	58	ASP	CB-CG-OD2	5.79	123.51	118.30
1	G	126	ASP	CB-CG-OD2	5.77	123.49	118.30
1	X	130	ASP	CB-CG-OD2	5.74	123.47	118.30
1	X	126	ASP	CB-CG-OD2	5.74	123.46	118.30
1	L	121	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	125	ASP	CB-CG-OD2	5.66	123.39	118.30
1	G	48	ASP	CB-CG-OD2	5.65	123.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	111	ASP	CB-CG-OD2	5.64	123.37	118.30
1	G	110	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	U	101	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	101	ASP	CB-CG-OD2	5.58	123.32	118.30
1	E	111	ASP	CB-CG-OD2	5.53	123.28	118.30
1	V	140	ASP	CB-CG-OD2	5.53	123.27	118.30
1	A	58	ASP	CB-CG-OD2	5.53	123.27	118.30
1	R	101	ASP	CB-CG-OD2	5.52	123.26	118.30
1	E	8	ASP	CB-CG-OD2	5.51	123.26	118.30
1	E	140	ASP	CB-CG-OD2	5.50	123.25	118.30
1	N	126	ASP	CB-CG-OD2	5.48	123.23	118.30
1	F	8	ASP	CB-CG-OD2	5.47	123.22	118.30
1	K	126	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	126	ASP	CB-CG-OD2	5.42	123.18	118.30
1	F	126	ASP	CB-CG-OD2	5.38	123.14	118.30
1	F	111	ASP	CB-CG-OD2	5.37	123.13	118.30
1	N	58	ASP	CB-CG-OD2	5.35	123.11	118.30
1	S	130	ASP	CB-CG-OD2	5.30	123.07	118.30
1	S	63	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	R	96	ASP	CB-CG-OD2	5.29	123.06	118.30
1	V	101	ASP	CB-CG-OD2	5.27	123.05	118.30
1	D	96	ASP	CB-CG-OD2	5.27	123.04	118.30
1	C	101	ASP	CB-CG-OD2	5.24	123.01	118.30
1	S	126	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	65	LEU	CA-CB-CG	5.20	127.25	115.30
1	V	58	ASP	CB-CG-OD2	5.18	122.97	118.30
1	X	65	LEU	CB-CG-CD1	5.15	119.76	111.00
1	E	65	LEU	CA-CB-CG	5.13	127.11	115.30
1	T	101	ASP	CB-CG-OD2	5.13	122.92	118.30
1	R	141	LYS	CD-CE-NZ	5.13	123.49	111.70
1	V	121	ASP	CB-CG-OD2	5.12	122.91	118.30
1	J	96	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	111	ASP	CB-CG-OD2	5.10	122.89	118.30
1	F	65	LEU	CA-CB-CG	5.09	127.02	115.30
1	P	65	LEU	CA-CB-CG	5.08	126.99	115.30
1	P	126	ASP	CB-CG-OD2	5.08	122.87	118.30
1	Q	111	ASP	CB-CG-OD2	5.07	122.86	118.30
1	K	101	ASP	CB-CG-OD1	5.06	122.86	118.30
1	P	101	ASP	CB-CG-OD2	5.06	122.85	118.30
1	R	65	LEU	CA-CB-CG	5.05	126.93	115.30
1	T	96	ASP	CB-CG-OD2	5.04	122.84	118.30
1	F	121	ASP	CB-CG-OD2	5.04	122.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	101	ASP	CB-CG-OD2	5.03	122.83	118.30
1	H	63	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	U	111	ASP	CB-CG-OD2	5.01	122.81	118.30
1	K	58[A]	ASP	CB-CG-OD2	5.00	122.80	118.30
1	K	58[B]	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	7	VAL	Peptide

## 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	1216	0	1182	9	0
1	B	1220	0	1182	7	0
1	C	1216	0	1182	11	0
1	D	1216	0	1182	10	0
1	E	1216	0	1182	16	0
1	F	1220	0	1182	9	0
1	G	1216	0	1182	14	0
1	H	1216	0	1182	16	0
1	I	1216	0	1182	15	0
1	J	1220	0	1182	6	0
1	K	1220	0	1182	16	0
1	L	1216	0	1182	19	0
1	M	1220	0	1182	12	0
1	N	1216	0	1182	6	0
1	O	1216	0	1182	14	0
1	P	1216	0	1182	12	0
1	Q	1216	0	1182	10	0
1	R	1213	0	1173	9	0
1	S	1216	0	1182	18	0
1	T	1216	0	1182	10	0
1	U	1216	0	1182	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	1216	0	1182	9	0
1	X	1216	0	1182	7	0
1	Y	1213	0	1173	10	0
2	A	12	0	0	2	0
2	B	8	0	0	0	0
2	C	14	0	0	0	0
2	D	9	0	0	0	0
2	E	10	0	0	0	0
2	F	7	0	0	0	0
2	G	6	0	0	0	0
2	H	10	0	0	0	0
2	I	7	0	0	0	0
2	J	7	0	0	0	0
2	K	16	0	0	0	0
2	L	7	0	0	0	0
2	M	9	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	3	0	0	0	0
2	Q	3	0	0	0	0
2	R	13	0	0	0	0
2	S	4	0	0	0	0
2	T	9	0	0	0	0
2	U	4	0	0	0	0
2	V	5	0	0	0	0
2	X	5	0	0	0	0
2	Y	4	0	0	0	0
All	All	29380	0	28350	255	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 4.

All (255) 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:F:120:THR:HG22	1:F:129:ASN:HB2	1.55	0.87
1:A:37:HIS:NE2	1:K:37:HIS:ND1	2.21	0.86
1:D:42:LEU:HD23	1:D:95:MET:SD	2.17	0.85
1:C:116:GLY:O	1:C:120:THR:HB	1.80	0.81
1:L:34:MET:HB2	1:L:95:MET:SD	2.21	0.80
1:Q:116:GLY:O	1:Q:120:THR:HB	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:94:THR:H	1:I:97:GLN:HE21	1.30	0.80
1:A:37:HIS:HE2	1:K:37:HIS:HD1	0.83	0.80
1:I:38:ASN:HB3	1:I:42:LEU:HD23	1.63	0.80
1:T:116:GLY:O	1:T:120:THR:HG22	1.82	0.78
1:G:38:ASN:HB3	1:G:42:LEU:HD23	1.65	0.77
1:A:37:HIS:CE1	1:K:37:HIS:HD1	2.05	0.75
1:V:116:GLY:O	1:V:120:THR:HB	1.88	0.74
1:L:120:THR:CG2	1:L:129:ASN:HB2	2.16	0.74
1:C:100:GLU:OE1	1:C:152:LYS:NZ	2.21	0.73
1:H:28:HIS:CD2	1:H:50:TYR:CE2	2.76	0.73
2:A:2003:HOH:O	1:K:37:HIS:HE1	1.72	0.72
1:R:120:THR:HG22	1:R:129:ASN:HB2	1.72	0.71
1:S:118:GLU:O	1:S:122:LYS:HG2	1.90	0.70
1:P:116:GLY:O	1:P:120:THR:HB	1.92	0.70
1:I:94:THR:HG22	1:I:97:GLN:H	1.57	0.70
1:S:26:LYS:NZ	1:S:101:ASP:OD2	2.22	0.69
1:Q:120:THR:HG23	1:Q:129:ASN:HB2	1.75	0.69
1:O:116:GLY:O	1:O:120:THR:HB	1.92	0.69
1:T:119:LEU:HD23	1:T:119:LEU:C	2.14	0.68
1:T:119:LEU:HD23	1:T:120:THR:N	2.09	0.68
1:L:120:THR:HG21	1:L:129:ASN:CA	2.24	0.67
1:R:147:LYS:NZ	1:R:154:PRO:O	2.26	0.67
1:Y:116:GLY:O	1:Y:120:THR:HG22	1.95	0.67
1:N:147:LYS:NZ	1:N:156:GLU:HB2	2.10	0.67
1:F:120:THR:CG2	1:F:129:ASN:HB2	2.25	0.67
1:H:116:GLY:O	1:H:120:THR:HB	1.95	0.66
1:K:94:THR:H	1:K:97:GLN:HE21	1.44	0.65
1:E:116:GLY:O	1:E:120:THR:HB	1.96	0.65
1:O:120:THR:HG23	1:O:129:ASN:HB2	1.79	0.65
1:G:116:GLY:O	1:G:120:THR:HB	1.95	0.65
1:P:120:THR:HG22	1:P:129:ASN:HD22	1.60	0.65
1:C:42:LEU:HD23	1:C:95:MET:SD	2.37	0.64
1:E:37:HIS:HB3	1:L:38:ASN:HD21	1.63	0.64
1:X:120:THR:HG22	1:X:129:ASN:HB2	1.79	0.64
1:X:120:THR:HG21	1:X:129:ASN:N	2.13	0.63
1:B:116:GLY:O	1:B:120:THR:HB	1.97	0.63
1:T:20:LEU:O	1:T:24:THR:HB	1.98	0.63
1:H:120:THR:HG23	1:H:129:ASN:HB2	1.83	0.60
1:G:120:THR:HG21	1:G:129:ASN:HA	1.84	0.60
1:U:120:THR:HG21	1:U:129:ASN:HA	1.84	0.60
1:Y:120:THR:HG23	1:Y:129:ASN:HD22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:THR:HG23	1:C:129:ASN:HB2	1.84	0.59
1:O:34:MET:HB2	1:O:95:MET:SD	2.43	0.59
1:E:120:THR:HG22	1:E:129:ASN:HD22	1.69	0.58
1:C:37:HIS:HE1	1:E:96:ASP:OD1	1.86	0.58
1:R:65:LEU:HD13	1:R:71:PRO:HD3	1.85	0.58
1:I:24:THR:HG23	1:I:50:TYR:CE2	2.39	0.58
1:C:120:THR:HG22	1:C:129:ASN:HD22	1.68	0.58
1:E:120:THR:HG21	1:E:129:ASN:HA	1.86	0.58
1:S:94:THR:HG23	1:S:97:GLN:H	1.67	0.57
1:F:96:ASP:O	1:F:100:GLU:HG3	2.05	0.57
1:O:120:THR:CG2	1:O:129:ASN:HD22	2.18	0.57
1:L:120:THR:HG22	1:L:129:ASN:HB2	1.84	0.57
1:H:120:THR:HG21	1:H:129:ASN:HA	1.85	0.57
1:S:65:LEU:HD13	1:S:71:PRO:HD3	1.86	0.57
1:I:116:GLY:O	1:I:120:THR:HG22	2.05	0.57
1:Y:120:THR:HG21	1:Y:129:ASN:HA	1.87	0.56
1:E:147:LYS:NZ	1:E:156:GLU:O	2.37	0.56
1:L:116:GLY:O	1:L:120:THR:HB	2.06	0.56
1:H:30:ILE:O	1:H:34:MET:HB3	2.05	0.56
1:F:65:LEU:HD13	1:F:71:PRO:HD3	1.88	0.55
1:T:65:LEU:HD13	1:T:71:PRO:HD3	1.87	0.55
1:S:63:ARG:NH2	1:S:127:VAL:HB	2.21	0.55
1:Y:94:THR:HG22	1:Y:97:GLN:HG3	1.88	0.55
1:T:96:ASP:O	1:T:100:GLU:HG3	2.08	0.54
1:N:116:GLY:O	1:N:120:THR:HG23	2.07	0.54
1:A:38:ASN:HD21	1:K:37:HIS:HB3	1.72	0.54
1:H:28:HIS:NE2	1:H:50:TYR:CZ	2.75	0.54
1:L:7:VAL:HG23	1:L:119:LEU:HD22	1.90	0.53
1:L:65:LEU:HD13	1:L:71:PRO:HD3	1.89	0.53
1:C:20:LEU:O	1:C:24:THR:HB	2.08	0.53
1:H:94:THR:HB	1:H:97:GLN:H	1.73	0.53
1:M:76:LYS:O	1:M:80:GLU:HG3	2.08	0.53
1:H:74:THR:OG1	1:H:77:GLU:OE1	2.19	0.53
1:L:120:THR:HG21	1:L:129:ASN:HA	1.89	0.53
1:G:120:THR:HG23	1:G:129:ASN:HB2	1.91	0.53
1:C:120:THR:HG21	1:C:129:ASN:HA	1.89	0.53
1:P:120:THR:HG21	1:P:129:ASN:HA	1.91	0.53
1:M:127:VAL:HG13	1:Q:137:ALA:HB2	1.89	0.53
1:E:41:THR:CG2	1:L:41:THR:HG21	2.39	0.52
1:H:120:THR:HG22	1:H:129:ASN:HD22	1.74	0.52
1:I:120:THR:HG21	1:I:129:ASN:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:120:THR:HG22	1:S:129:ASN:HB2	1.90	0.52
1:S:147:LYS:HG2	1:S:153:ALA:O	2.10	0.52
1:J:20:LEU:O	1:J:24:THR:HB	2.10	0.51
1:S:120:THR:HG23	1:S:125:ASP:HB3	1.93	0.51
1:V:120:THR:HG21	1:V:129:ASN:HA	1.92	0.51
1:J:120:THR:HG23	1:J:129:ASN:HB2	1.93	0.51
1:E:41:THR:HG21	1:L:41:THR:HG21	1.93	0.51
1:L:120:THR:HG21	1:L:129:ASN:N	2.26	0.51
1:O:120:THR:HG21	1:O:129:ASN:HA	1.93	0.51
1:M:42:LEU:HD23	1:M:95:MET:SD	2.51	0.51
1:U:20:LEU:HD23	1:U:57:MET:HA	1.93	0.51
1:X:42:LEU:HD23	1:X:95:MET:SD	2.51	0.51
1:Y:94:THR:HG22	1:Y:97:GLN:H	1.76	0.50
1:M:15:HIS:HE1	1:M:112:GLU:OE1	1.93	0.50
1:P:14:ASN:OD1	1:P:71:PRO:HA	2.12	0.50
1:O:38:ASN:HB3	1:O:42:LEU:HD23	1.93	0.50
1:Q:42:LEU:HD21	1:Q:149:PHE:CZ	2.46	0.50
1:F:58[A]:ASP:OD2	1:H:28:HIS:HE1	1.95	0.50
1:P:37:HIS:HE1	1:S:96:ASP:OD1	1.94	0.50
1:X:15:HIS:HE1	1:X:83:SER:OG	1.95	0.50
1:K:120:THR:HG23	1:K:129:ASN:HB2	1.94	0.50
1:K:155:LEU:O	1:K:156:GLU:HB2	2.12	0.50
1:P:26:LYS:NZ	1:P:101:ASP:OD2	2.33	0.49
1:L:20:LEU:O	1:L:24:THR:HB	2.12	0.49
1:C:42:LEU:CD2	1:C:95:MET:SD	3.01	0.49
1:L:120:THR:CG2	1:L:129:ASN:CB	2.90	0.49
1:S:120:THR:HG21	1:S:129:ASN:N	2.27	0.49
2:A:2003:HOH:O	1:K:37:HIS:CE1	2.55	0.49
1:V:120:THR:HG23	1:V:129:ASN:HB2	1.95	0.48
1:R:63:ARG:NH2	1:R:127:VAL:HB	2.28	0.48
1:J:108:LEU:HD23	1:J:108:LEU:C	2.34	0.48
1:M:94:THR:HG22	1:M:96:ASP:H	1.78	0.48
1:O:20:LEU:O	1:O:24:THR:HB	2.14	0.48
1:D:63:ARG:NH2	1:D:127:VAL:HB	2.29	0.48
1:D:28:HIS:CD2	1:D:50:TYR:CE2	3.01	0.48
1:F:120:THR:HG21	1:F:129:ASN:N	2.28	0.48
1:I:155:LEU:O	1:I:156:GLU:C	2.51	0.48
1:E:120:THR:CG2	1:E:129:ASN:HD22	2.27	0.48
1:H:65:LEU:HD13	1:H:71:PRO:HD3	1.95	0.48
1:T:20:LEU:HD23	1:T:57:MET:HA	1.96	0.47
1:U:120:THR:HG23	1:U:129:ASN:HD22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:94:THR:H	1:K:97:GLN:NE2	2.11	0.47
1:F:108:LEU:C	1:F:108:LEU:HD23	2.35	0.47
1:T:65:LEU:HD13	1:T:71:PRO:CD	2.44	0.47
1:E:37:HIS:HB3	1:L:38:ASN:ND2	2.28	0.47
1:S:143:ILE:O	1:S:147:LYS:HB2	2.15	0.47
1:V:73:SER:HB2	1:Y:29:GLN:HB2	1.97	0.47
1:D:65:LEU:HD13	1:D:71:PRO:HD3	1.97	0.47
1:H:52:GLU:O	1:H:55:GLU:HG3	2.15	0.47
1:L:42:LEU:HA	1:L:42:LEU:HD12	1.81	0.47
1:X:120:THR:HG23	1:X:125:ASP:HB3	1.97	0.46
1:N:147:LYS:HZ1	1:N:156:GLU:HB2	1.78	0.46
1:M:76:LYS:O	1:M:80:GLU:CG	2.63	0.46
1:U:120:THR:CG2	1:U:129:ASN:HD22	2.29	0.46
1:P:33:TYR:CD2	1:P:89:TYR:CD2	3.03	0.46
1:J:52:GLU:OE2	1:J:138:SER:OG	2.20	0.46
1:R:120:THR:HG21	1:R:129:ASN:N	2.29	0.46
1:O:42:LEU:O	1:O:46:MET:HG2	2.16	0.46
1:E:120:THR:HG23	1:E:129:ASN:HB2	1.98	0.46
1:M:63:ARG:NH2	1:M:127:VAL:HB	2.30	0.46
1:N:42:LEU:HD21	1:N:149:PHE:CZ	2.51	0.46
1:K:15:HIS:HE1	1:K:83:SER:OG	1.99	0.46
1:L:95:MET:O	1:L:99:MET:HG2	2.16	0.46
1:Q:120:THR:CG2	1:Q:129:ASN:HB2	2.45	0.46
1:I:55:GLU:OE1	1:I:59:GLU:OE1	2.33	0.46
1:G:120:THR:HG22	1:G:129:ASN:HD22	1.81	0.46
1:D:108:LEU:HD23	1:D:108:LEU:C	2.36	0.46
1:S:42:LEU:N	1:S:42:LEU:HD12	2.30	0.46
1:I:56:GLN:HG3	1:I:135:PHE:CE2	2.51	0.45
1:O:120:THR:HG22	1:O:129:ASN:HD22	1.81	0.45
1:A:65:LEU:HD13	1:A:71:PRO:CD	2.47	0.45
1:B:24:THR:HG23	1:B:50:TYR:CE2	2.51	0.45
1:I:138:SER:O	1:I:142:HIS:HD2	1.99	0.45
1:I:49:LEU:HD11	1:I:142:HIS:ND1	2.30	0.45
1:M:15:HIS:CE1	1:M:112:GLU:OE1	2.68	0.45
1:B:120:THR:HG23	1:B:129:ASN:HB2	1.97	0.45
1:I:156:GLU:OE1	1:I:156:GLU:HA	2.14	0.45
1:E:108:LEU:HD23	1:E:108:LEU:C	2.37	0.45
1:O:34:MET:HB2	1:O:95:MET:CE	2.46	0.45
1:Q:120:THR:HG21	1:Q:129:ASN:HA	1.99	0.45
1:K:94:THR:N	1:K:97:GLN:HE21	2.10	0.45
1:D:79:LEU:HA	1:D:79:LEU:HD23	1.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:23:PHE:CD1	1:L:105:THR:HG21	2.51	0.45
1:P:65:LEU:O	1:R:154:PRO:HG2	2.17	0.45
1:A:24:THR:HG23	1:A:50:TYR:CE2	2.53	0.44
1:O:120:THR:HG23	1:O:129:ASN:CB	2.46	0.44
1:G:65:LEU:HD13	1:G:71:PRO:HD3	1.99	0.44
1:X:155:LEU:O	1:X:156:GLU:HB2	2.18	0.44
1:M:20:LEU:O	1:M:24:THR:HB	2.17	0.44
1:G:120:THR:CG2	1:G:129:ASN:HA	2.48	0.44
1:U:108:LEU:HD23	1:U:108:LEU:C	2.37	0.44
1:E:20:LEU:HD23	1:E:57:MET:HA	1.99	0.44
1:V:120:THR:CG2	1:V:129:ASN:HA	2.47	0.43
1:D:116:GLY:O	1:D:120:THR:HG22	2.18	0.43
1:S:75:LEU:HD12	1:S:75:LEU:N	2.33	0.43
1:P:63:ARG:NH2	1:P:127:VAL:HB	2.33	0.43
1:M:42:LEU:HA	1:M:42:LEU:HD12	1.85	0.43
1:V:120:THR:HG22	1:V:129:ASN:HD22	1.83	0.43
1:I:65:LEU:HD13	1:I:71:PRO:HD3	2.00	0.43
1:Y:24:THR:HG23	1:Y:50:TYR:CE2	2.53	0.43
1:P:12:PHE:CZ	1:P:116:GLY:HA3	2.54	0.43
1:S:42:LEU:O	1:S:46:MET:HG2	2.19	0.43
1:A:95:MET:C	1:A:95:MET:SD	2.96	0.43
1:E:120:THR:CG2	1:E:129:ASN:HA	2.47	0.43
1:B:120:THR:HG22	1:B:129:ASN:HD22	1.84	0.43
1:U:20:LEU:O	1:U:24:THR:HB	2.19	0.43
1:R:16:GLN:HA	1:R:19:ASN:HB2	2.01	0.43
1:D:33:TYR:CD2	1:D:89:TYR:CD2	3.07	0.42
1:O:56:GLN:O	1:O:60:VAL:HG23	2.19	0.42
1:J:112:GLU:HA	1:J:115:GLN:HE21	1.84	0.42
1:I:120:THR:HG23	1:I:129:ASN:HB2	2.01	0.42
1:T:96:ASP:O	1:T:100:GLU:CG	2.67	0.42
1:K:94:THR:HB	1:K:97:GLN:HE21	1.84	0.42
1:M:94:THR:HG22	1:M:96:ASP:N	2.33	0.42
1:F:141:LYS:O	1:F:145:MET:HG3	2.19	0.42
1:P:120:THR:HG23	1:P:129:ASN:HB2	2.01	0.42
1:X:42:LEU:O	1:X:46:MET:HG2	2.20	0.42
1:Y:120:THR:CG2	1:Y:129:ASN:HD22	2.32	0.42
1:H:120:THR:HG21	1:H:129:ASN:CA	2.50	0.42
1:G:65:LEU:HD13	1:G:71:PRO:CD	2.49	0.42
1:A:20:LEU:HD23	1:A:57:MET:HA	2.01	0.42
1:J:28:HIS:CD2	1:J:50:TYR:CE2	3.08	0.42
1:G:42:LEU:HD21	1:G:149:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:20:LEU:O	1:S:24:THR:HB	2.19	0.42
1:O:120:THR:HG23	1:O:129:ASN:HD22	1.85	0.42
1:P:108:LEU:C	1:P:108:LEU:HD23	2.40	0.42
1:K:42:LEU:HA	1:K:42:LEU:HD12	1.82	0.42
1:D:52:GLU:OE2	1:D:138:SER:OG	2.23	0.42
1:N:20:LEU:O	1:N:24:THR:HB	2.20	0.42
1:H:28:HIS:NE2	1:H:50:TYR:CE2	2.87	0.42
1:R:120:THR:HG23	1:R:125:ASP:HB3	2.01	0.42
1:D:24:THR:HG23	1:D:50:TYR:CE2	2.55	0.42
1:E:20:LEU:O	1:E:24:THR:HB	2.19	0.42
1:G:75:LEU:HD12	1:G:75:LEU:N	2.34	0.42
1:U:120:THR:HG23	1:U:129:ASN:HB2	2.02	0.41
1:G:20:LEU:O	1:G:24:THR:HB	2.20	0.41
1:C:37:HIS:CE1	1:E:96:ASP:OD1	2.69	0.41
1:S:65:LEU:O	1:Y:154:PRO:HG2	2.20	0.41
1:B:42:LEU:HA	1:B:45:LYS:HB2	2.02	0.41
1:I:108:LEU:HD23	1:I:108:LEU:O	2.20	0.41
1:L:91:LYS:O	1:L:92:PRO:C	2.58	0.41
1:Q:42:LEU:O	1:Q:46:MET:HG2	2.20	0.41
1:M:23:PHE:CD1	1:M:105:THR:HG21	2.56	0.41
1:G:42:LEU:HD22	1:G:42:LEU:N	2.35	0.41
1:Y:24:THR:HG23	1:Y:50:TYR:HE2	1.85	0.41
1:V:38:ASN:HB3	1:V:42:LEU:HD23	2.03	0.41
1:V:65:LEU:HD13	1:V:71:PRO:HD3	2.03	0.41
1:R:99:MET:O	1:R:103:VAL:HG23	2.21	0.41
1:Q:15:HIS:CD2	1:Q:81:ASN:O	2.73	0.41
1:N:34:MET:HB2	1:N:95:MET:SD	2.61	0.41
1:K:94:THR:HB	1:K:97:GLN:NE2	2.35	0.41
1:G:15:HIS:HE1	1:G:83:SER:OG	2.03	0.41
1:O:30:ILE:HG22	1:O:34:MET:HE3	2.02	0.41
1:Q:65:LEU:HD13	1:Q:71:PRO:HD3	2.03	0.41
1:B:49:LEU:HA	1:B:49:LEU:HD12	1.91	0.41
1:T:120:THR:HG23	1:T:129:ASN:HD22	1.84	0.40
1:H:12:PHE:CD2	1:H:12:PHE:C	2.94	0.40
1:V:42:LEU:HD12	1:V:99:MET:SD	2.60	0.40
1:B:52:GLU:OE2	1:B:138:SER:OG	2.24	0.40
1:S:15:HIS:HE1	1:S:83:SER:OG	2.04	0.40
1:Q:33:TYR:OH	1:S:71:PRO:O	2.28	0.40
1:C:15:HIS:HE1	1:C:83:SER:OG	2.04	0.40
1:A:38:ASN:HB3	1:A:42:LEU:HD22	2.03	0.40
1:H:120:THR:CG2	1:H:129:ASN:HD22	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:116:GLY:O	1:K:120:THR:HB	2.22	0.40
1:F:75:LEU:HD12	1:F:75:LEU:N	2.37	0.40
1:G:34:MET:HE2	1:G:95:MET:SD	2.62	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	148/156 (95%)	147 (99%)	1 (1%)	0	100	100
1	B	149/156 (96%)	147 (99%)	2 (1%)	0	100	100
1	C	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	D	148/156 (95%)	147 (99%)	1 (1%)	0	100	100
1	E	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
1	F	149/156 (96%)	147 (99%)	2 (1%)	0	100	100
1	G	148/156 (95%)	145 (98%)	2 (1%)	1 (1%)	26	31
1	H	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	I	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	J	149/156 (96%)	145 (97%)	4 (3%)	0	100	100
1	K	149/156 (96%)	146 (98%)	3 (2%)	0	100	100
1	L	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	M	149/156 (96%)	147 (99%)	2 (1%)	0	100	100
1	N	148/156 (95%)	144 (97%)	4 (3%)	0	100	100
1	O	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
1	P	148/156 (95%)	144 (97%)	4 (3%)	0	100	100
1	Q	148/156 (95%)	146 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	S	148/156 (95%)	144 (97%)	4 (3%)	0	100	100
1	T	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	U	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	V	148/156 (95%)	144 (97%)	4 (3%)	0	100	100
1	X	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	Y	148/156 (95%)	142 (96%)	6 (4%)	0	100	100
All	All	3557/3744 (95%)	3493 (98%)	63 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	92	PRO

### 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	132/138 (96%)	119 (90%)	13 (10%)	10	11
1	B	133/138 (96%)	118 (89%)	15 (11%)	7	8
1	C	132/138 (96%)	117 (89%)	15 (11%)	7	7
1	D	132/138 (96%)	117 (89%)	15 (11%)	7	7
1	E	132/138 (96%)	117 (89%)	15 (11%)	7	7
1	F	133/138 (96%)	118 (89%)	15 (11%)	7	8
1	G	132/138 (96%)	116 (88%)	16 (12%)	6	6
1	H	132/138 (96%)	116 (88%)	16 (12%)	6	6
1	I	132/138 (96%)	118 (89%)	14 (11%)	8	9
1	J	133/138 (96%)	120 (90%)	13 (10%)	10	11
1	K	133/138 (96%)	119 (90%)	14 (10%)	8	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	132/138 (96%)	115 (87%)	17 (13%)	5	5
1	M	133/138 (96%)	116 (87%)	17 (13%)	5	5
1	N	132/138 (96%)	116 (88%)	16 (12%)	6	6
1	O	132/138 (96%)	117 (89%)	15 (11%)	7	7
1	P	132/138 (96%)	118 (89%)	14 (11%)	8	9
1	Q	132/138 (96%)	114 (86%)	18 (14%)	5	4
1	R	132/138 (96%)	116 (88%)	16 (12%)	6	6
1	S	132/138 (96%)	116 (88%)	16 (12%)	6	6
1	T	132/138 (96%)	116 (88%)	16 (12%)	6	6
1	U	132/138 (96%)	122 (92%)	10 (8%)	16	20
1	V	132/138 (96%)	120 (91%)	12 (9%)	12	13
1	X	132/138 (96%)	115 (87%)	17 (13%)	5	5
1	Y	131/138 (95%)	115 (88%)	16 (12%)	6	6
All	All	3172/3312 (96%)	2811 (89%)	361 (11%)	7	7

All (361) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	20	LEU
1	A	24	THR
1	A	28	HIS
1	A	42	LEU
1	A	44	GLU
1	A	45	LYS
1	A	65	LEU
1	A	96	ASP
1	A	102	LEU
1	A	114	LYS
1	A	132	LEU
1	A	152	LYS
1	B	13	LEU
1	B	20	LEU
1	B	24	THR
1	B	41	THR
1	B	42	LEU
1	B	44	GLU

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Mol	Chain	Res	Type
1	B	45	LYS
1	B	49	LEU
1	B	65	LEU
1	B	91	LYS
1	B	102	LEU
1	B	114	LYS
1	B	119	LEU
1	B	120	THR
1	B	132	LEU
1	C	13	LEU
1	C	20	LEU
1	C	24	THR
1	C	34	MET
1	C	45	LYS
1	C	55	GLU
1	C	65	LEU
1	C	76	LYS
1	C	96	ASP
1	C	100	GLU
1	C	102	LEU
1	C	120	THR
1	C	132	LEU
1	C	144	TRP
1	C	156	GLU
1	D	13	LEU
1	D	20	LEU
1	D	24	THR
1	D	41	THR
1	D	42	LEU
1	D	45	LYS
1	D	49	LEU
1	D	65	LEU
1	D	85	GLU
1	D	102	LEU
1	D	114	LYS
1	D	122	LYS
1	D	132	LEU
1	D	141	LYS
1	D	156	GLU
1	E	7	VAL
1	E	13	LEU
1	E	20	LEU

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Mol	Chain	Res	Type
1	E	24	THR
1	E	28	HIS
1	E	41	THR
1	E	42	LEU
1	E	45	LYS
1	E	65	LEU
1	E	94	THR
1	E	102	LEU
1	E	120	THR
1	E	122	LYS
1	E	132	LEU
1	E	156	GLU
1	F	7	VAL
1	F	13	LEU
1	F	20	LEU
1	F	24	THR
1	F	28	HIS
1	F	34	MET
1	F	45	LYS
1	F	55	GLU
1	F	58[A]	ASP
1	F	58[B]	ASP
1	F	59	GLU
1	F	65	LEU
1	F	102	LEU
1	F	114	LYS
1	F	132	LEU
1	G	13	LEU
1	G	20	LEU
1	G	24	THR
1	G	28	HIS
1	G	34	MET
1	G	41	THR
1	G	45	LYS
1	G	58	ASP
1	G	65	LEU
1	G	76	LYS
1	G	100	GLU
1	G	102	LEU
1	G	114	LYS
1	G	120	THR
1	G	132	LEU

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Mol	Chain	Res	Type
1	G	156	GLU
1	H	7	VAL
1	H	13	LEU
1	H	20	LEU
1	H	24	THR
1	H	34	MET
1	H	45	LYS
1	H	51	SER
1	H	65	LEU
1	H	93	LYS
1	H	94	THR
1	H	102	LEU
1	H	114	LYS
1	H	120	THR
1	H	132	LEU
1	H	141	LYS
1	H	152	LYS
1	I	13	LEU
1	I	20	LEU
1	I	24	THR
1	I	41	THR
1	I	45	LYS
1	I	49	LEU
1	I	58	ASP
1	I	59	GLU
1	I	65	LEU
1	I	94	THR
1	I	102	LEU
1	I	115	GLN
1	I	122	LYS
1	I	132	LEU
1	J	13	LEU
1	J	20	LEU
1	J	24	THR
1	J	41	THR
1	J	42	LEU
1	J	44	GLU
1	J	45	LYS
1	J	65	LEU
1	J	76	LYS
1	J	94	THR
1	J	102	LEU

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Mol	Chain	Res	Type
1	J	132	LEU
1	J	147	LYS
1	K	13	LEU
1	K	20	LEU
1	K	24	THR
1	K	41	THR
1	K	42	LEU
1	K	45	LYS
1	K	49	LEU
1	K	65	LEU
1	K	94	THR
1	K	100	GLU
1	K	102	LEU
1	K	118	GLU
1	K	119	LEU
1	K	132	LEU
1	L	8	ASP
1	L	13	LEU
1	L	20	LEU
1	L	24	THR
1	L	31	HIS
1	L	41	THR
1	L	42	LEU
1	L	45	LYS
1	L	49	LEU
1	L	65	LEU
1	L	91	LYS
1	L	102	LEU
1	L	114	LYS
1	L	120	THR
1	L	122	LYS
1	L	132	LEU
1	L	152	LYS
1	M	7	VAL
1	M	13	LEU
1	M	20	LEU
1	M	24	THR
1	M	41	THR
1	M	42	LEU
1	M	45	LYS
1	M	59	GLU
1	M	65	LEU

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Mol	Chain	Res	Type
1	M	93	LYS
1	M	100	GLU
1	M	102	LEU
1	M	114	LYS
1	M	118	GLU
1	M	132	LEU
1	M	152	LYS
1	M	156	GLU
1	N	7	VAL
1	N	11	GLU
1	N	13	LEU
1	N	20	LEU
1	N	24	THR
1	N	42	LEU
1	N	55	GLU
1	N	65	LEU
1	N	70	SER
1	N	86	GLU
1	N	102	LEU
1	N	114	LYS
1	N	115	GLN
1	N	126	ASP
1	N	132	LEU
1	N	155	LEU
1	O	7	VAL
1	O	11	GLU
1	O	13	LEU
1	O	20	LEU
1	O	24	THR
1	O	41	THR
1	O	49	LEU
1	O	65	LEU
1	O	85	GLU
1	O	102	LEU
1	O	114	LYS
1	O	119	LEU
1	O	120	THR
1	O	132	LEU
1	O	141	LYS
1	P	7	VAL
1	P	11	GLU
1	P	13	LEU

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Mol	Chain	Res	Type
1	P	20	LEU
1	P	24	THR
1	P	41	THR
1	P	42	LEU
1	P	45	LYS
1	P	65	LEU
1	P	91	LYS
1	P	102	LEU
1	P	115	GLN
1	P	120	THR
1	P	132	LEU
1	Q	13	LEU
1	Q	20	LEU
1	Q	24	THR
1	Q	41	THR
1	Q	42	LEU
1	Q	44	GLU
1	Q	45	LYS
1	Q	49	LEU
1	Q	55	GLU
1	Q	58	ASP
1	Q	65	LEU
1	Q	76	LYS
1	Q	85	GLU
1	Q	91	LYS
1	Q	102	LEU
1	Q	119	LEU
1	Q	120	THR
1	Q	132	LEU
1	R	11	GLU
1	R	13	LEU
1	R	20	LEU
1	R	24	THR
1	R	41	THR
1	R	44	GLU
1	R	45	LYS
1	R	65	LEU
1	R	85	GLU
1	R	91	LYS
1	R	102	LEU
1	R	114	LYS
1	R	122	LYS

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Mol	Chain	Res	Type
1	R	132	LEU
1	R	141	LYS
1	R	156	GLU
1	S	13	LEU
1	S	20	LEU
1	S	24	THR
1	S	41	THR
1	S	45	LYS
1	S	49	LEU
1	S	58	ASP
1	S	65	LEU
1	S	79	LEU
1	S	91	LYS
1	S	100	GLU
1	S	102	LEU
1	S	114	LYS
1	S	122	LYS
1	S	132	LEU
1	S	147	LYS
1	T	13	LEU
1	T	20	LEU
1	T	24	THR
1	T	41	THR
1	T	45	LYS
1	T	49	LEU
1	T	51	SER
1	T	58	ASP
1	T	59	GLU
1	T	65	LEU
1	T	91	LYS
1	T	102	LEU
1	T	119	LEU
1	T	120	THR
1	T	122	LYS
1	T	132	LEU
1	U	8	ASP
1	U	13	LEU
1	U	20	LEU
1	U	24	THR
1	U	41	THR
1	U	45	LYS
1	U	65	LEU

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Mol	Chain	Res	Type
1	U	102	LEU
1	U	114	LYS
1	U	132	LEU
1	V	11	GLU
1	V	20	LEU
1	V	24	THR
1	V	28	HIS
1	V	41	THR
1	V	44	GLU
1	V	45	LYS
1	V	58	ASP
1	V	65	LEU
1	V	102	LEU
1	V	120	THR
1	V	132	LEU
1	X	7	VAL
1	X	13	LEU
1	X	20	LEU
1	X	24	THR
1	X	34	MET
1	X	41	THR
1	X	42	LEU
1	X	45	LYS
1	X	65	LEU
1	X	100	GLU
1	X	102	LEU
1	X	108	LEU
1	X	114	LYS
1	X	119	LEU
1	X	120	THR
1	X	122	LYS
1	X	132	LEU
1	Y	13	LEU
1	Y	20	LEU
1	Y	24	THR
1	Y	28	HIS
1	Y	41	THR
1	Y	42	LEU
1	Y	45	LYS
1	Y	58	ASP
1	Y	65	LEU
1	Y	76	LYS

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Mol	Chain	Res	Type
1	Y	85	GLU
1	Y	94	THR
1	Y	102	LEU
1	Y	114	LYS
1	Y	132	LEU
1	Y	152	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	38	ASN
1	A	115	GLN
1	B	15	HIS
1	B	115	GLN
1	B	129	ASN
1	C	15	HIS
1	C	29	GLN
1	C	129	ASN
1	D	15	HIS
1	D	81	ASN
1	D	115	GLN
1	E	15	HIS
1	E	29	GLN
1	E	129	ASN
1	F	15	HIS
1	G	15	HIS
1	G	29	GLN
1	G	115	GLN
1	G	129	ASN
1	H	15	HIS
1	H	29	GLN
1	H	38	ASN
1	H	81	ASN
1	H	129	ASN
1	I	15	HIS
1	I	29	GLN
1	I	81	ASN
1	I	97	GLN
1	I	129	ASN
1	I	142	HIS
1	J	29	GLN

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Mol	Chain	Res	Type
1	J	81	ASN
1	J	115	GLN
1	K	15	HIS
1	K	29	GLN
1	K	97	GLN
1	K	129	ASN
1	L	29	GLN
1	L	38	ASN
1	L	81	ASN
1	L	129	ASN
1	M	29	GLN
1	M	38	ASN
1	N	81	ASN
1	O	38	ASN
1	O	81	ASN
1	O	129	ASN
1	P	15	HIS
1	P	81	ASN
1	P	129	ASN
1	Q	15	HIS
1	Q	29	GLN
1	Q	81	ASN
1	R	15	HIS
1	R	29	GLN
1	S	15	HIS
1	S	81	ASN
1	T	15	HIS
1	T	29	GLN
1	T	115	GLN
1	T	129	ASN
1	U	15	HIS
1	U	38	ASN
1	U	81	ASN
1	U	97	GLN
1	U	129	ASN
1	V	15	HIS
1	V	81	ASN
1	V	97	GLN
1	V	129	ASN
1	X	15	HIS
1	X	81	ASN
1	Y	15	HIS

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Mol	Chain	Res	Type
1	Y	81	ASN
1	Y	129	ASN

### 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 carbohydrates 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	150/156 (96%)	-0.27	0 100 100	20, 27, 38, 49	0
1	B	150/156 (96%)	-0.32	1 (0%) 89 92	23, 28, 39, 53	0
1	C	150/156 (96%)	-0.35	0 100 100	22, 28, 40, 52	0
1	D	150/156 (96%)	-0.31	0 100 100	22, 28, 40, 50	0
1	E	150/156 (96%)	-0.28	1 (0%) 89 92	22, 28, 39, 49	0
1	F	150/156 (96%)	-0.29	1 (0%) 89 92	22, 28, 40, 52	0
1	G	150/156 (96%)	-0.29	0 100 100	21, 29, 40, 54	0
1	H	150/156 (96%)	-0.23	1 (0%) 89 92	22, 28, 41, 50	0
1	I	150/156 (96%)	-0.24	1 (0%) 89 92	21, 28, 40, 52	0
1	J	150/156 (96%)	-0.31	2 (1%) 79 84	23, 29, 42, 52	0
1	K	150/156 (96%)	-0.28	1 (0%) 89 92	21, 27, 37, 52	0
1	L	150/156 (96%)	-0.19	1 (0%) 89 92	23, 29, 43, 50	0
1	M	150/156 (96%)	-0.21	0 100 100	21, 28, 41, 52	0
1	N	150/156 (96%)	-0.20	1 (0%) 89 92	25, 31, 41, 53	0
1	O	150/156 (96%)	-0.30	0 100 100	23, 29, 42, 53	0
1	P	150/156 (96%)	-0.23	1 (0%) 89 92	24, 31, 42, 52	0
1	Q	150/156 (96%)	-0.29	0 100 100	23, 29, 41, 51	0
1	R	149/156 (95%)	-0.19	1 (0%) 89 92	24, 29, 41, 51	0
1	S	150/156 (96%)	-0.27	0 100 100	25, 31, 42, 50	0
1	T	150/156 (96%)	-0.35	0 100 100	24, 29, 40, 50	0
1	U	150/156 (96%)	-0.28	1 (0%) 89 92	23, 30, 41, 51	0
1	V	150/156 (96%)	-0.35	0 100 100	24, 30, 42, 51	0
1	X	150/156 (96%)	-0.29	2 (1%) 79 84	23, 29, 41, 55	0
1	Y	150/156 (96%)	-0.26	0 100 100	25, 31, 42, 51	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3599/3744 (96%)	-0.28	15 (0%) 93 95	20, 29, 42, 55	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	7	VAL	9.2
1	X	156	GLU	3.9
1	N	156	GLU	3.7
1	H	7	VAL	3.4
1	E	7	VAL	3.4
1	J	7	VAL	3.3
1	P	156	GLU	2.9
1	X	92	PRO	2.8
1	B	156	GLU	2.6
1	J	156	GLU	2.5
1	I	156	GLU	2.3
1	F	156	GLU	2.2
1	U	156	GLU	2.2
1	K	156	GLU	2.1
1	R	156	GLU	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.