



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 10:20 pm BST

PDB ID : 2IY4  
Title : X-ray structure of Dps from *Listeria monocytogenes*  
Authors : Ilari, A.; Bellapadrone, G.; Stefanini, S.; Chiancone, E.  
Deposited on : 2006-07-12  
Resolution : 2.31 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

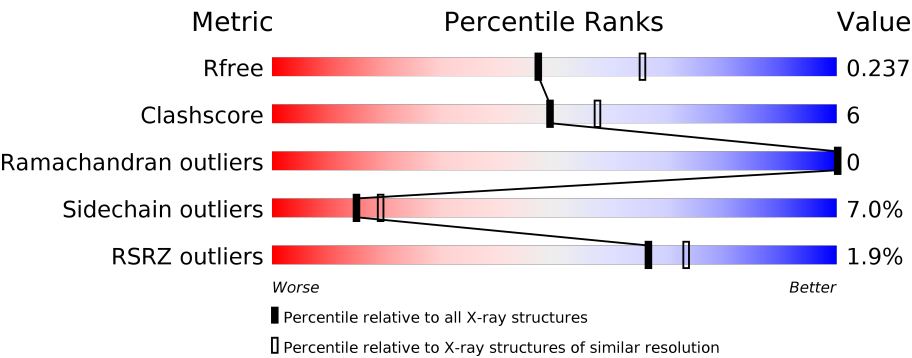
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	156	<div><div>3%</div><div></div><div>84%</div><div>11%</div><div>..</div></div>
1	B	156	<div><div>3%</div><div></div><div>81%</div><div>13%</div><div>..</div></div>
1	C	156	<div><div>3%</div><div></div><div>83%</div><div>12%</div><div>..</div></div>
1	D	156	<div><div>2%</div><div></div><div>85%</div><div>8%</div><div>..</div></div>
1	E	156	<div><div>2%</div><div></div><div>81%</div><div>12%</div><div>..</div></div>
1	F	156	<div><div>%</div><div></div><div>80%</div><div>15%</div><div>..</div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
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 3 unique types of molecules in this entry. The entry contains 31295 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	151	Total	C	N	O	S	0	0	0
			1228	786	198	237	7			
1	B	150	Total	C	N	O	S	0	0	0
			1222	783	197	235	7			
1	C	151	Total	C	N	O	S	0	0	0
			1228	786	198	237	7			
1	D	150	Total	C	N	O	S	0	0	0
			1222	783	197	235	7			
1	E	150	Total	C	N	O	S	0	0	0
			1222	783	197	235	7			
1	F	151	Total	C	N	O	S	0	0	0
			1228	786	198	237	7			
1	G	151	Total	C	N	O	S	0	1	0
			1232	788	198	239	7			
1	H	150	Total	C	N	O	S	0	0	0
			1222	783	197	235	7			
1	I	150	Total	C	N	O	S	0	1	0
			1226	785	197	237	7			
1	J	150	Total	C	N	O	S	0	0	0
			1222	783	197	235	7			
1	K	150	Total	C	N	O	S	0	0	0
			1222	783	197	235	7			
1	L	150	Total	C	N	O	S	0	1	0
			1226	785	197	237	7			
1	M	149	Total	C	N	O	S	0	1	0
			1219	780	196	236	7			
1	N	150	Total	C	N	O	S	0	1	0
			1226	785	197	237	7			
1	O	151	Total	C	N	O	S	0	0	0
			1228	786	198	237	7			
1	P	150	Total	C	N	O	S	0	1	0
			1226	785	197	237	7			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	151	Total 1228	C 786	N 198	O 237	S 7	0	0	0
1	R	151	Total 1228	C 786	N 198	O 237	S 7	0	0	0
1	S	151	Total 1228	C 786	N 198	O 237	S 7	0	0	0
1	T	150	Total 1226	C 785	N 197	O 237	S 7	0	1	0
1	U	154	Total 1255	C 802	N 202	O 244	S 7	0	1	0
1	V	150	Total 1222	C 783	N 197	O 235	S 7	0	0	0
1	X	150	Total 1222	C 783	N 197	O 235	S 7	0	0	0
1	Y	150	Total 1222	C 783	N 197	O 235	S 7	0	0	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total 1	Fe 1	0	0
2	J	1	Total 1	Fe 1	0	0
2	Q	1	Total 1	Fe 1	0	0
2	D	1	Total 1	Fe 1	0	0
2	K	1	Total 1	Fe 1	0	0
2	E	2	Total 2	Fe 2	0	0
2	H	1	Total 1	Fe 1	0	0
2	B	1	Total 1	Fe 1	0	0
2	I	1	Total 1	Fe 1	0	0
2	C	1	Total 1	Fe 1	0	0
2	V	1	Total 1	Fe 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	2	Total 2	Fe 2	0	0
2	U	1	Total 1	Fe 1	0	0
2	X	1	Total 1	Fe 1	0	0
2	R	2	Total 2	Fe 2	0	0
2	Y	1	Total 1	Fe 1	0	0
2	L	1	Total 1	Fe 1	0	0
2	S	1	Total 1	Fe 1	0	0
2	F	1	Total 1	Fe 1	0	0
2	M	2	Total 2	Fe 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total 70	O 70	0	0
3	B	73	Total 73	O 73	0	0
3	C	72	Total 72	O 72	0	0
3	D	88	Total 88	O 88	0	0
3	E	84	Total 84	O 84	0	0
3	F	82	Total 82	O 82	0	0
3	G	76	Total 76	O 76	0	0
3	H	83	Total 83	O 83	0	0
3	I	71	Total 71	O 71	0	0
3	J	69	Total 69	O 69	0	0

*Continued on next page...*

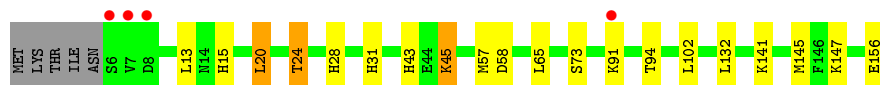
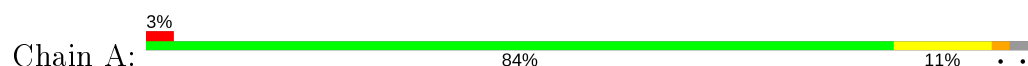
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	65	Total 65	O 65	0	0
3	L	72	Total 72	O 72	0	0
3	M	84	Total 84	O 84	0	0
3	N	78	Total 78	O 78	0	0
3	O	69	Total 69	O 69	0	0
3	P	84	Total 84	O 84	0	0
3	Q	73	Total 73	O 73	0	0
3	R	82	Total 82	O 82	0	0
3	S	74	Total 74	O 74	0	0
3	T	83	Total 83	O 83	0	0
3	U	88	Total 88	O 88	0	0
3	V	68	Total 68	O 68	0	0
3	X	79	Total 79	O 79	0	0
3	Y	74	Total 74	O 74	0	0

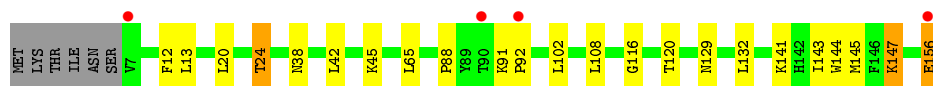
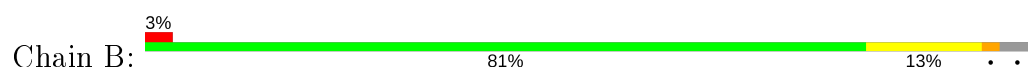
### 3 Residue-property plots [i](#)

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.

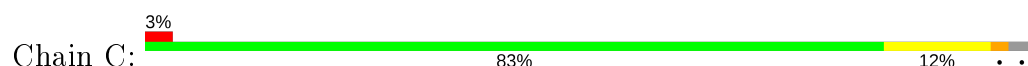
#### • Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



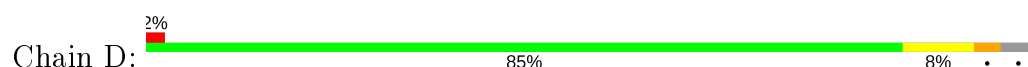
#### • Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



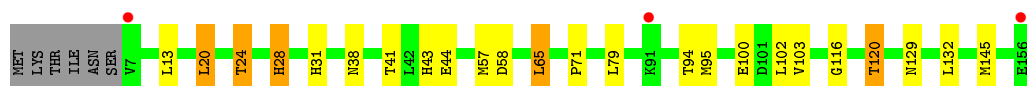
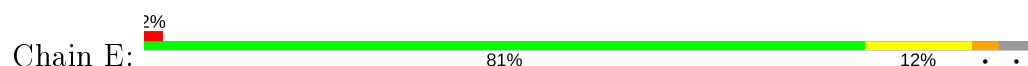
#### • Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



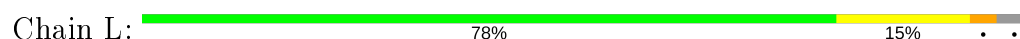
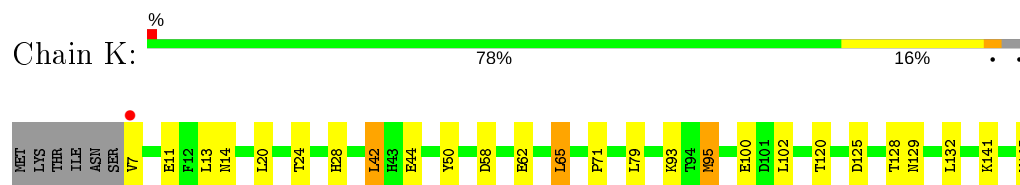
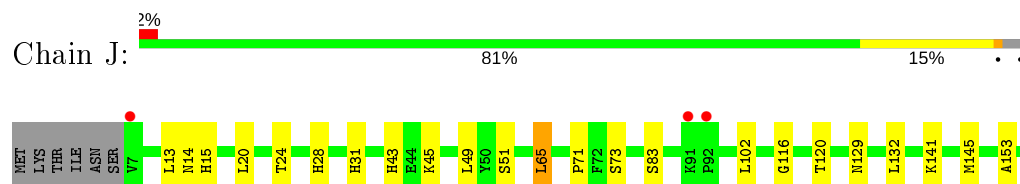
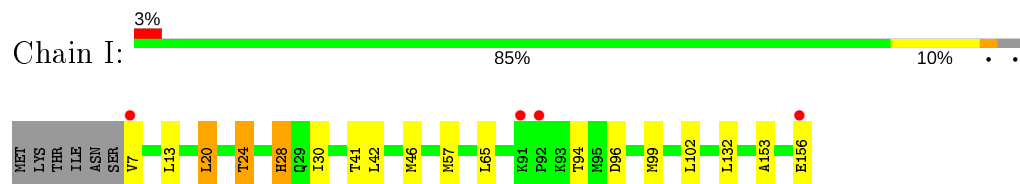
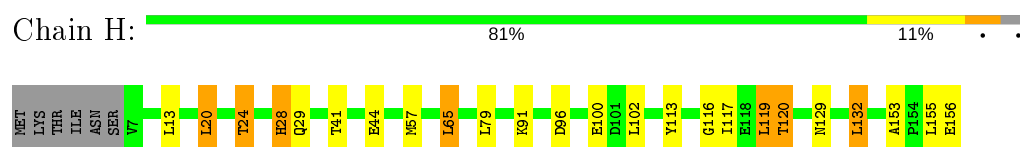
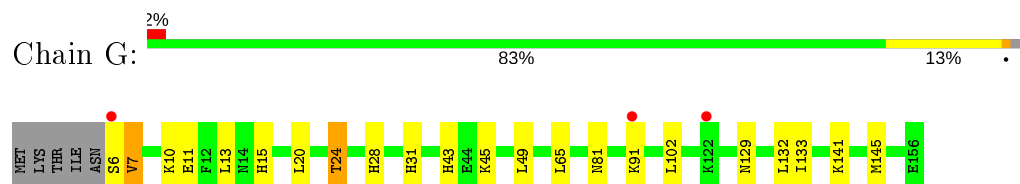
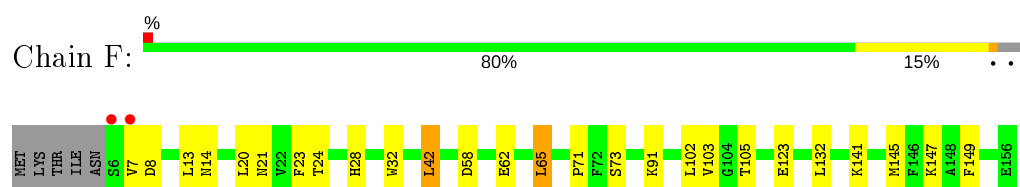
#### • Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

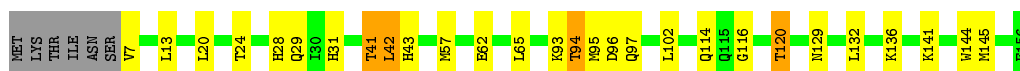


#### • Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

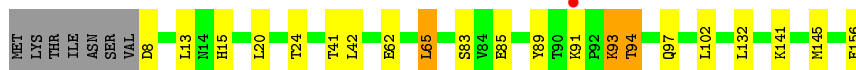
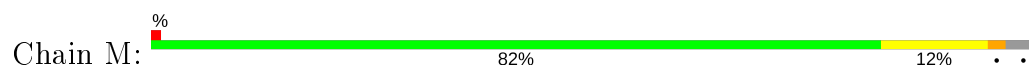


#### • Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

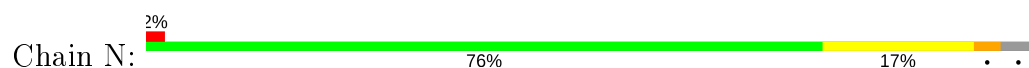




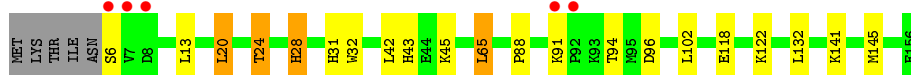
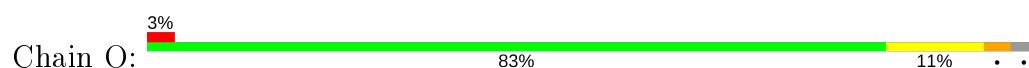
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



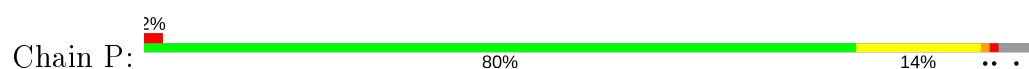
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



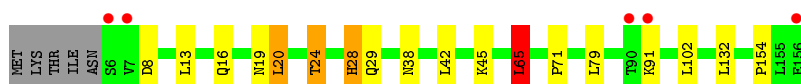
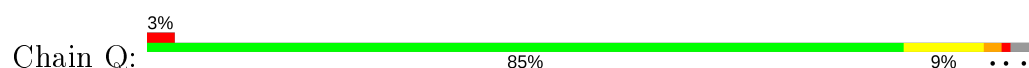
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



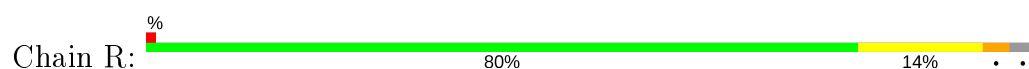
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



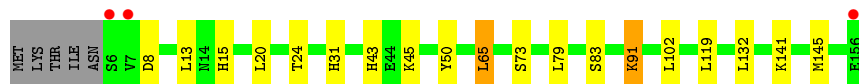
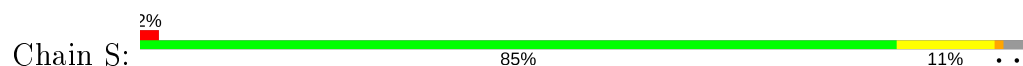
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



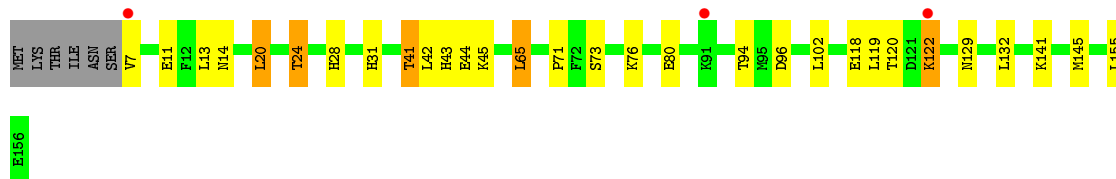
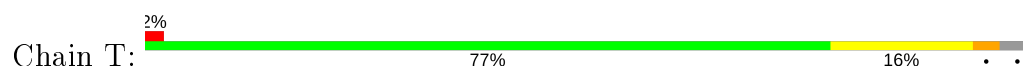
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



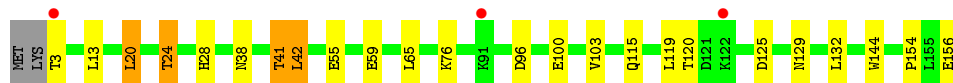
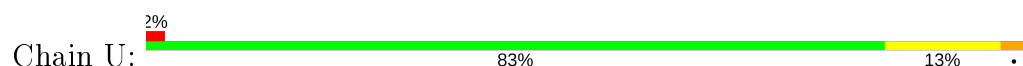
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



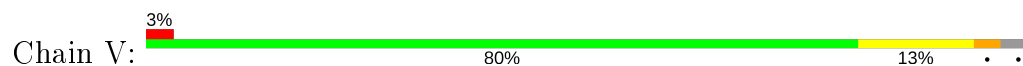
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



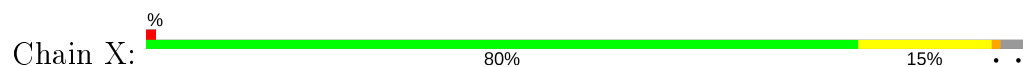
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



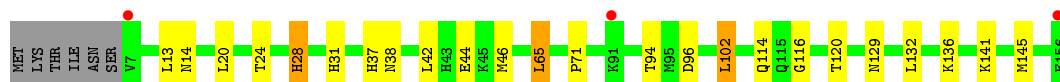
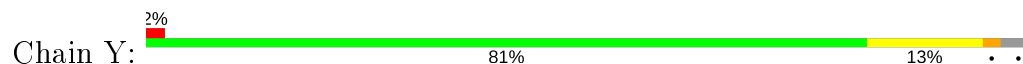
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



- 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, $\alpha$ , $\beta$ , $\gamma$	89.29Å 172.71Å 135.31Å 90.00° 92.11° 90.00°	Depositor
Resolution (Å)	50.00 – 2.31 25.34 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.31) 99.3 (25.34-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.182 , 0.238 0.182 , 0.237	Depositor DCC
$R_{free}$ test set	8944 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	31295	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.54	0/1255	0.62	0/1693
1	B	0.57	0/1249	0.63	0/1685
1	C	0.54	0/1255	0.63	0/1693
1	D	0.54	0/1249	0.62	0/1685
1	E	0.52	0/1249	0.63	0/1685
1	F	0.52	0/1255	0.60	0/1693
1	G	0.53	0/1263	0.63	0/1704
1	H	0.53	0/1249	0.65	2/1685 (0.1%)
1	I	0.54	0/1257	0.62	0/1696
1	J	0.53	0/1249	0.62	1/1685 (0.1%)
1	K	0.53	0/1249	0.64	1/1685 (0.1%)
1	L	0.53	0/1257	0.60	0/1696
1	M	0.53	0/1250	0.60	0/1686
1	N	0.54	0/1257	0.64	0/1696
1	O	0.53	0/1255	0.61	1/1693 (0.1%)
1	P	0.58	0/1257	0.64	1/1696 (0.1%)
1	Q	0.56	0/1255	0.63	1/1693 (0.1%)
1	R	0.55	0/1255	0.62	0/1693
1	S	0.54	0/1255	0.63	1/1693 (0.1%)
1	T	0.56	0/1257	0.63	0/1696
1	U	0.55	0/1286	0.63	0/1736
1	V	0.53	0/1249	0.64	0/1685
1	X	0.54	0/1249	0.60	0/1685
1	Y	0.52	0/1249	0.62	2/1685 (0.1%)
All	All	0.54	0/30110	0.62	10/40622 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	65	LEU	CA-CB-CG	6.04	129.19	115.30
1	J	65	LEU	CA-CB-CG	5.85	128.76	115.30
1	H	119	LEU	CA-CB-CG	5.78	128.60	115.30
1	Q	65	LEU	CA-CB-CG	5.71	128.42	115.30
1	O	65	LEU	CA-CB-CG	5.45	127.82	115.30

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	1228	0	1188	12	0
1	B	1222	0	1183	15	0
1	C	1228	0	1188	16	0
1	D	1222	0	1183	12	0
1	E	1222	0	1183	19	0
1	F	1228	0	1188	14	0
1	G	1232	0	1188	9	0
1	H	1222	0	1183	14	0
1	I	1226	0	1183	11	0
1	J	1222	0	1183	12	0
1	K	1222	0	1183	17	0
1	L	1226	0	1183	20	0
1	M	1219	0	1174	13	0
1	N	1226	0	1183	21	0
1	O	1228	0	1188	10	0
1	P	1226	0	1183	18	0
1	Q	1228	0	1188	11	0
1	R	1228	0	1188	19	0
1	S	1228	0	1188	10	0
1	T	1226	0	1183	23	0
1	U	1255	0	1212	16	0
1	V	1222	0	1183	19	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	1222	0	1183	16	0
1	Y	1222	0	1183	14	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	2	0	0	0	0
2	S	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	X	1	0	0	0	0
2	Y	1	0	0	0	0
3	A	70	0	0	8	0
3	B	73	0	0	3	0
3	C	72	0	0	5	0
3	D	88	0	0	3	0
3	E	84	0	0	7	0
3	F	82	0	0	2	0
3	G	76	0	0	3	0
3	H	83	0	0	4	0
3	I	71	0	0	7	0
3	J	69	0	0	1	0
3	K	65	0	0	1	0
3	L	72	0	0	7	0
3	M	84	0	0	6	0
3	N	78	0	0	6	0
3	O	69	0	0	2	0
3	P	84	0	0	8	0
3	Q	73	0	0	2	0
3	R	82	0	0	9	0
3	S	74	0	0	4	0
3	T	83	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	U	88	0	0	7	0
3	V	68	0	0	5	0
3	X	79	0	0	5	0
3	Y	74	0	0	2	0
All	All	31295	0	28452	344	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 6.

The worst 5 of 344 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:120:THR:HB	3:P:2064:HOH:O	1.64	0.95
1:K:42:LEU:HD23	1:K:95:MET:SD	2.07	0.94
1:R:141:LYS:HG2	1:R:145:MET:HE2	1.51	0.92
1:N:116:GLY:O	1:N:120:THR:HG22	1.75	0.86
1:J:116:GLY:O	1:J:120:THR:HG22	1.75	0.85

There are no symmetry-related clashes.

## 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	149/156 (96%)	148 (99%)	1 (1%)	0	100	100
1	B	148/156 (95%)	147 (99%)	1 (1%)	0	100	100
1	C	149/156 (96%)	148 (99%)	1 (1%)	0	100	100
1	D	148/156 (95%)	145 (98%)	3 (2%)	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	150/156 (96%)	148 (99%)	2 (1%)	0	100	100
1	H	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	I	149/156 (96%)	147 (99%)	2 (1%)	0	100	100
1	J	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	K	148/156 (95%)	147 (99%)	1 (1%)	0	100	100
1	L	149/156 (96%)	147 (99%)	2 (1%)	0	100	100
1	M	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	N	149/156 (96%)	148 (99%)	1 (1%)	0	100	100
1	O	149/156 (96%)	147 (99%)	2 (1%)	0	100	100
1	P	149/156 (96%)	147 (99%)	2 (1%)	0	100	100
1	Q	149/156 (96%)	147 (99%)	2 (1%)	0	100	100
1	R	149/156 (96%)	147 (99%)	2 (1%)	0	100	100
1	S	149/156 (96%)	147 (99%)	2 (1%)	0	100	100
1	T	149/156 (96%)	147 (99%)	2 (1%)	0	100	100
1	U	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
1	V	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	X	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	Y	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
All	All	3571/3744 (95%)	3525 (99%)	46 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	134/139 (96%)	126 (94%)	8 (6%)	19	26
1	B	133/139 (96%)	125 (94%)	8 (6%)	19	26
1	C	134/139 (96%)	126 (94%)	8 (6%)	19	26

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	133/139 (96%)	124 (93%)	9 (7%)	16	20
1	E	133/139 (96%)	122 (92%)	11 (8%)	11	13
1	F	134/139 (96%)	126 (94%)	8 (6%)	19	26
1	G	135/139 (97%)	125 (93%)	10 (7%)	13	17
1	H	133/139 (96%)	120 (90%)	13 (10%)	8	9
1	I	134/139 (96%)	126 (94%)	8 (6%)	19	26
1	J	133/139 (96%)	125 (94%)	8 (6%)	19	26
1	K	133/139 (96%)	123 (92%)	10 (8%)	13	16
1	L	134/139 (96%)	121 (90%)	13 (10%)	8	9
1	M	133/139 (96%)	121 (91%)	12 (9%)	9	11
1	N	134/139 (96%)	123 (92%)	11 (8%)	11	14
1	O	134/139 (96%)	124 (92%)	10 (8%)	13	16
1	P	134/139 (96%)	124 (92%)	10 (8%)	13	16
1	Q	134/139 (96%)	124 (92%)	10 (8%)	13	16
1	R	134/139 (96%)	127 (95%)	7 (5%)	23	32
1	S	134/139 (96%)	128 (96%)	6 (4%)	27	38
1	T	134/139 (96%)	123 (92%)	11 (8%)	11	14
1	U	138/139 (99%)	127 (92%)	11 (8%)	12	15
1	V	133/139 (96%)	125 (94%)	8 (6%)	19	26
1	X	133/139 (96%)	126 (95%)	7 (5%)	22	31
1	Y	133/139 (96%)	126 (95%)	7 (5%)	22	31
All	All	3211/3336 (96%)	2987 (93%)	224 (7%)	15	19

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	VAL
1	M	132	LEU
1	V	65	LEU
1	L	24	THR
1	L	144	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	43	HIS
1	N	114	GLN
1	X	81	ASN
1	L	15	HIS
1	M	15	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	151/156 (96%)	-0.27	4 (2%)	56	63	22, 28, 38, 45	0
1	B	150/156 (96%)	-0.21	4 (2%)	54	62	22, 27, 38, 45	0
1	C	151/156 (96%)	-0.23	5 (3%)	46	53	22, 27, 38, 45	0
1	D	150/156 (96%)	-0.26	3 (2%)	65	72	22, 27, 37, 45	0
1	E	150/156 (96%)	-0.34	3 (2%)	65	72	22, 27, 37, 45	0
1	F	151/156 (96%)	-0.23	2 (1%)	77	81	22, 27, 38, 46	0
1	G	151/156 (96%)	-0.30	3 (1%)	65	72	22, 27, 38, 45	0
1	H	150/156 (96%)	-0.36	0	100	100	21, 27, 36, 45	0
1	I	150/156 (96%)	-0.29	4 (2%)	54	62	22, 27, 38, 45	0
1	J	150/156 (96%)	-0.25	3 (2%)	65	72	22, 27, 37, 46	0
1	K	150/156 (96%)	-0.28	2 (1%)	77	81	22, 27, 37, 45	0
1	L	150/156 (96%)	-0.37	0	100	100	22, 27, 37, 45	0
1	M	149/156 (95%)	-0.32	1 (0%)	87	91	22, 27, 36, 45	0
1	N	150/156 (96%)	-0.38	3 (2%)	65	72	22, 27, 37, 44	0
1	O	151/156 (96%)	-0.22	5 (3%)	46	53	22, 27, 38, 52	0
1	P	150/156 (96%)	-0.25	3 (2%)	65	72	22, 27, 37, 45	0
1	Q	151/156 (96%)	-0.18	5 (3%)	46	53	23, 27, 38, 49	0
1	R	151/156 (96%)	-0.30	2 (1%)	77	81	22, 27, 37, 51	0
1	S	151/156 (96%)	-0.22	3 (1%)	65	72	23, 27, 38, 49	0
1	T	150/156 (96%)	-0.26	3 (2%)	65	72	23, 27, 37, 45	0
1	U	154/156 (98%)	-0.35	3 (1%)	66	73	22, 27, 38, 45	0
1	V	150/156 (96%)	-0.31	4 (2%)	54	62	23, 27, 37, 45	0
1	X	150/156 (96%)	-0.29	1 (0%)	87	91	22, 27, 37, 44	0
1	Y	150/156 (96%)	-0.28	3 (2%)	65	72	23, 28, 38, 46	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3611/3744 (96%)	-0.28	69 (1%) 66 73	21, 27, 38, 52	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	6	SER	9.4
1	Q	6	SER	9.0
1	O	6	SER	8.5
1	X	7	VAL	7.1
1	R	6	SER	6.8

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FE	M	1157	1/1	0.50	0.26	22,22,22,22	1
2	FE	K	1157	1/1	0.65	0.28	27,27,27,27	1
2	FE	R	1158	1/1	0.70	0.26	17,17,17,17	1
2	FE	M	1158	1/1	0.80	0.42	24,24,24,24	1
2	FE	N	1158	1/1	0.80	0.42	22,22,22,22	1
2	FE	V	1157	1/1	0.80	0.23	20,20,20,20	1
2	FE	Q	1157	1/1	0.81	0.18	13,13,13,13	1
2	FE	U	1157	1/1	0.83	0.30	16,16,16,16	1
2	FE	D	1157	1/1	0.83	0.23	26,26,26,26	1
2	FE	J	1157	1/1	0.84	0.18	22,22,22,22	1
2	FE	I	1157	1/1	0.84	0.31	24,24,24,24	1
2	FE	P	1157	1/1	0.84	0.32	24,24,24,24	1
2	FE	N	1157	1/1	0.85	0.17	19,19,19,19	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE	B	1157	1/1	0.86	0.21	11,11,11,11	1
2	FE	E	1158	1/1	0.87	0.35	23,23,23,23	1
2	FE	F	1157	1/1	0.87	0.17	16,16,16,16	1
2	FE	R	1157	1/1	0.88	0.17	21,21,21,21	1
2	FE	X	1157	1/1	0.89	0.19	16,16,16,16	1
2	FE	H	1157	1/1	0.90	0.14	16,16,16,16	1
2	FE	E	1157	1/1	0.90	0.36	17,17,17,17	1
2	FE	L	1157	1/1	0.92	0.20	14,14,14,14	1
2	FE	S	1157	1/1	0.92	0.23	10,10,10,10	1
2	FE	C	1157	1/1	0.93	0.34	24,24,24,24	1
2	FE	Y	1157	1/1	0.94	0.17	17,17,17,17	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.