



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 3, 2023 – 03:53 pm 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 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

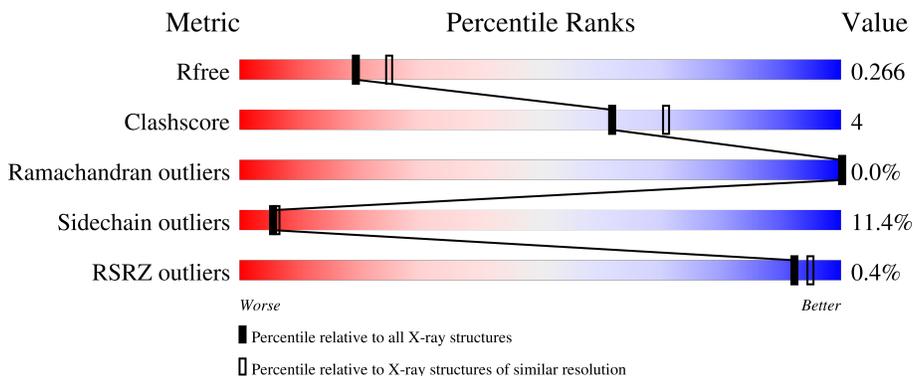
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.



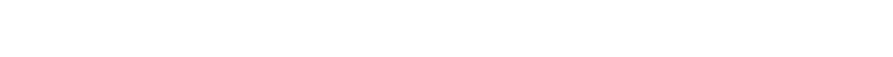
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	156	82% 12% . . .
1	B	156	79% 13% . . .
1	C	156	79% 14% . . .
1	D	156	74% 20% . . .
1	E	156	79% 12% . . .

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Mol	Chain	Length	Quality of chain
1	F	156	 77% 18% ..
1	G	156	 76% 17% . .
1	H	156	 74% 19% . .
1	I	156	 75% 17% . .
1	J	156	 79% 16% . .
1	K	156	 79% 16% . .
1	L	156	 75% 17% . .
1	M	156	 76% 17% . .
1	N	156	 79% 14% . .
1	O	156	 79% 15% . .
1	P	156	 76% 18% ..
1	Q	156	 77% 17% . .
1	R	156	 75% 19% ..
1	S	156	 72% 18% 5% . .
1	T	156	 80% 12% . .
1	U	156	 85% 10% . .
1	V	156	 81% 13% . .
1	X	156	 76% 17% . .
1	Y	156	 80% 15% . .

## 2 Entry composition [i](#)

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

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

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

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain A: 



- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain B: 



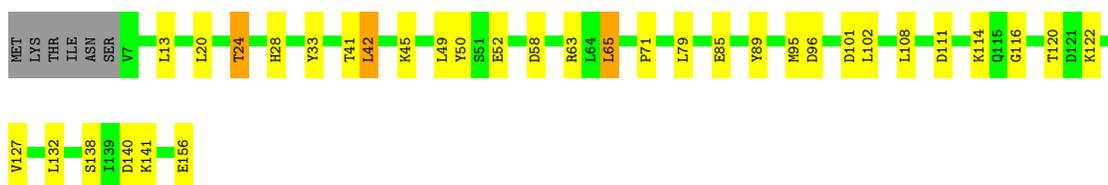
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain C: 



- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain D: 

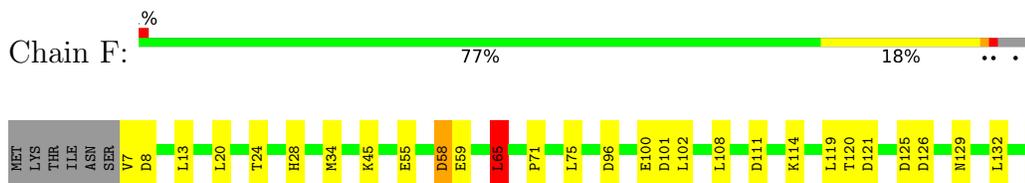


- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

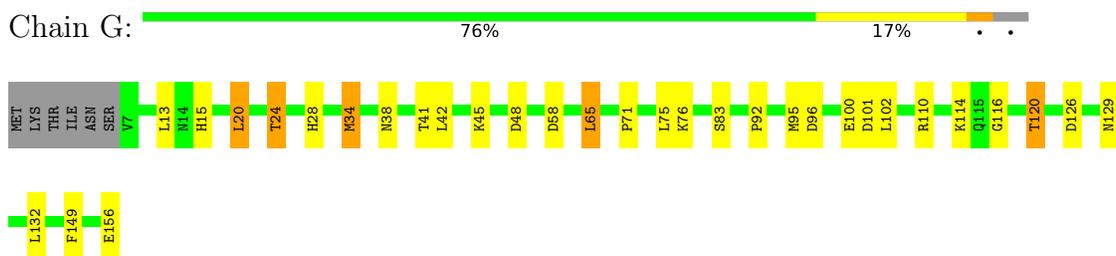
Chain E: 



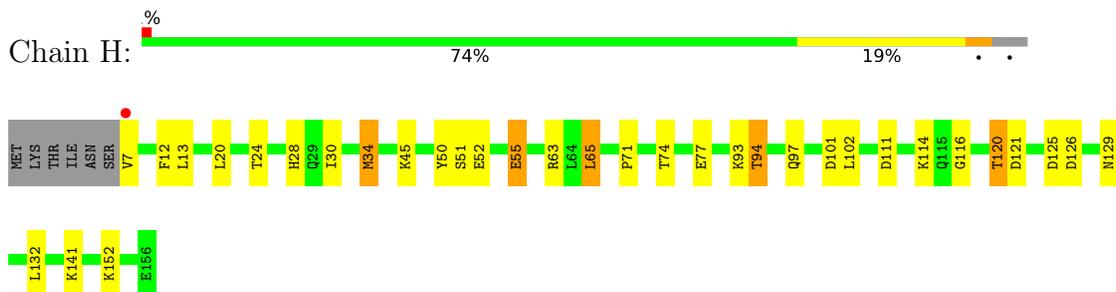
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



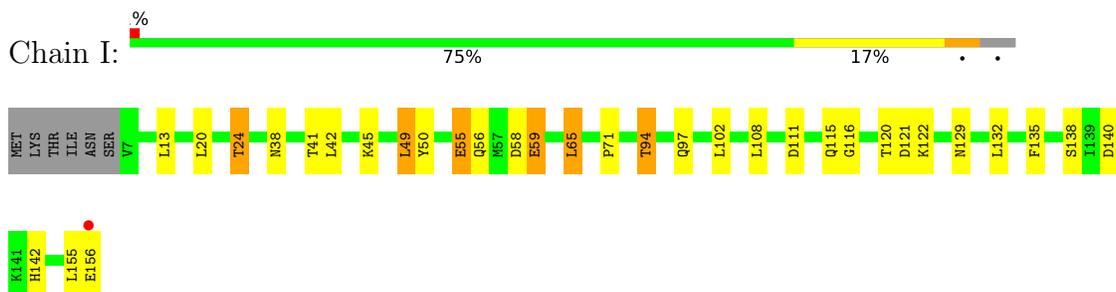
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



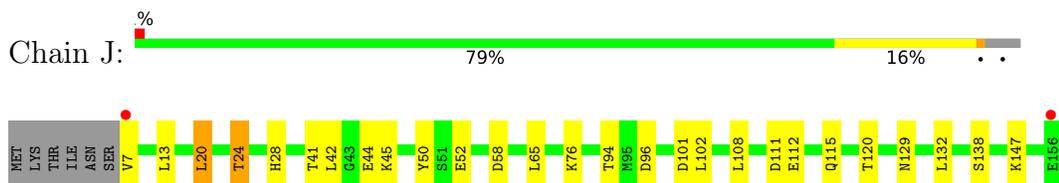
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

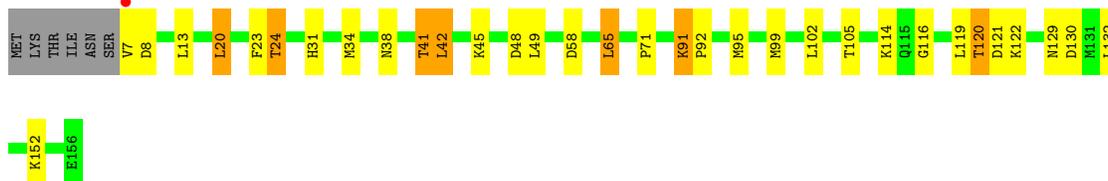
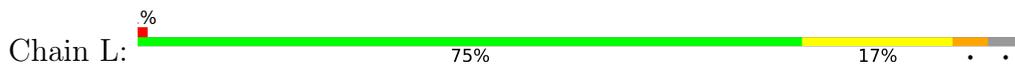


- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

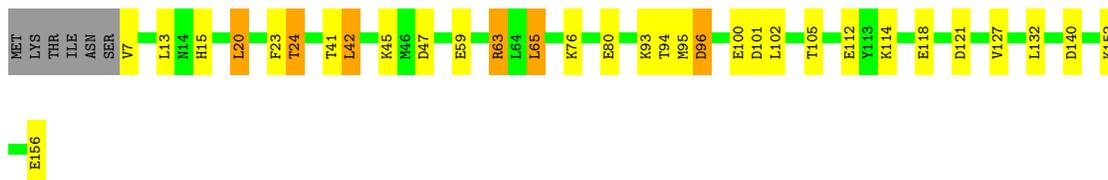




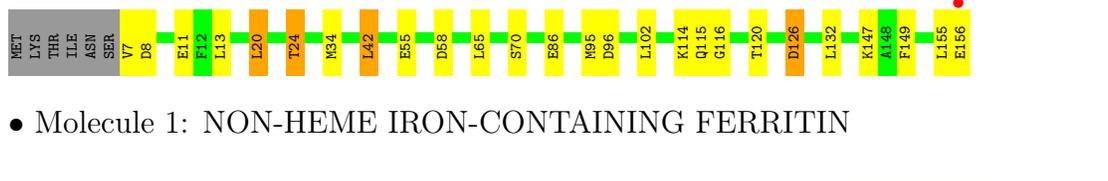
● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



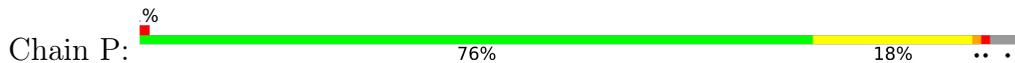
● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



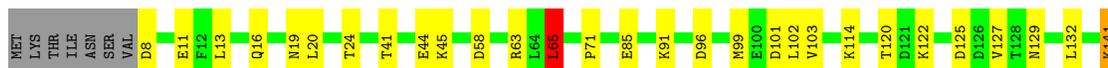
● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain Q:  77% 17%



- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain R:  75% 19%



- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain S:  72% 18% 5%



- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain T:  80% 12%



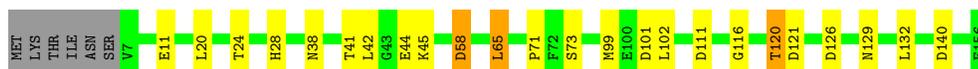
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain U:  85% 10%

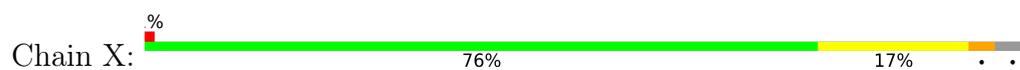


- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain V:  81% 13%



- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.73Å 175.65Å 135.96Å 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 2.29Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.209 , 0.266 0.212 , 0.266	Depositor DCC
$R_{free}$ test set	8694 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtrriage
Anisotropy	0.406	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 26.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	29380	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage'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, 0.333 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	0.81	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

The worst 5 of 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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

The worst 5 of 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

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%)	22	26
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	132/138 (96%)	119 (90%)	13 (10%)	8	9
1	B	133/138 (96%)	118 (89%)	15 (11%)	6	6
1	C	132/138 (96%)	117 (89%)	15 (11%)	5	6
1	D	132/138 (96%)	117 (89%)	15 (11%)	5	6
1	E	132/138 (96%)	117 (89%)	15 (11%)	5	6
1	F	133/138 (96%)	118 (89%)	15 (11%)	6	6
1	G	132/138 (96%)	116 (88%)	16 (12%)	5	5
1	H	132/138 (96%)	116 (88%)	16 (12%)	5	5
1	I	132/138 (96%)	118 (89%)	14 (11%)	6	7
1	J	133/138 (96%)	120 (90%)	13 (10%)	8	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	133/138 (96%)	119 (90%)	14 (10%)	7	8
1	L	132/138 (96%)	115 (87%)	17 (13%)	4	4
1	M	133/138 (96%)	116 (87%)	17 (13%)	4	4
1	N	132/138 (96%)	116 (88%)	16 (12%)	5	5
1	O	132/138 (96%)	117 (89%)	15 (11%)	5	6
1	P	132/138 (96%)	118 (89%)	14 (11%)	6	7
1	Q	132/138 (96%)	114 (86%)	18 (14%)	3	3
1	R	132/138 (96%)	116 (88%)	16 (12%)	5	5
1	S	132/138 (96%)	116 (88%)	16 (12%)	5	5
1	T	132/138 (96%)	116 (88%)	16 (12%)	5	5
1	U	132/138 (96%)	122 (92%)	10 (8%)	13	16
1	V	132/138 (96%)	120 (91%)	12 (9%)	9	11
1	X	132/138 (96%)	115 (87%)	17 (13%)	4	4
1	Y	131/138 (95%)	115 (88%)	16 (12%)	5	5
All	All	3172/3312 (96%)	2811 (89%)	361 (11%)	5	6

5 of 361 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	41	THR
1	S	114	LYS
1	P	120	THR
1	R	20	LEU
1	T	91	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	81	ASN
1	X	15	HIS
1	T	29	GLN
1	U	97	GLN
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 monosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	150/156 (96%)	-0.31	0 100 100	20, 27, 38, 49	0
1	B	150/156 (96%)	-0.37	1 (0%) 87 91	23, 28, 39, 53	0
1	C	150/156 (96%)	-0.40	0 100 100	22, 28, 40, 52	0
1	D	150/156 (96%)	-0.36	0 100 100	22, 28, 40, 50	0
1	E	150/156 (96%)	-0.33	1 (0%) 87 91	22, 28, 39, 49	0
1	F	150/156 (96%)	-0.33	1 (0%) 87 91	22, 28, 40, 52	0
1	G	150/156 (96%)	-0.34	0 100 100	21, 29, 40, 54	0
1	H	150/156 (96%)	-0.28	1 (0%) 87 91	22, 28, 41, 50	0
1	I	150/156 (96%)	-0.29	1 (0%) 87 91	21, 28, 40, 52	0
1	J	150/156 (96%)	-0.35	2 (1%) 77 81	23, 29, 42, 52	0
1	K	150/156 (96%)	-0.33	0 100 100	21, 27, 37, 52	0
1	L	150/156 (96%)	-0.24	1 (0%) 87 91	23, 29, 43, 50	0
1	M	150/156 (96%)	-0.26	0 100 100	21, 28, 41, 52	0
1	N	150/156 (96%)	-0.25	1 (0%) 87 91	25, 31, 41, 53	0
1	O	150/156 (96%)	-0.35	0 100 100	23, 29, 42, 53	0
1	P	150/156 (96%)	-0.28	1 (0%) 87 91	24, 31, 42, 52	0
1	Q	150/156 (96%)	-0.34	0 100 100	23, 29, 41, 51	0
1	R	149/156 (95%)	-0.24	0 100 100	24, 29, 41, 51	0
1	S	150/156 (96%)	-0.32	0 100 100	25, 31, 42, 50	0
1	T	150/156 (96%)	-0.40	0 100 100	24, 29, 40, 50	0
1	U	150/156 (96%)	-0.33	1 (0%) 87 91	23, 30, 41, 51	0
1	V	150/156 (96%)	-0.40	0 100 100	24, 30, 42, 51	0
1	X	150/156 (96%)	-0.34	2 (1%) 77 81	23, 29, 41, 54	0
1	Y	150/156 (96%)	-0.31	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%)	-0.32	13 (0%) 92   95	20, 29, 42, 54	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	7	VAL	8.8
1	X	156	GLU	3.8
1	N	156	GLU	3.7
1	H	7	VAL	3.2
1	E	7	VAL	3.2

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.