



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:44 PM UTC

PDB ID : 2IY4 / pdb_00002iy4
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

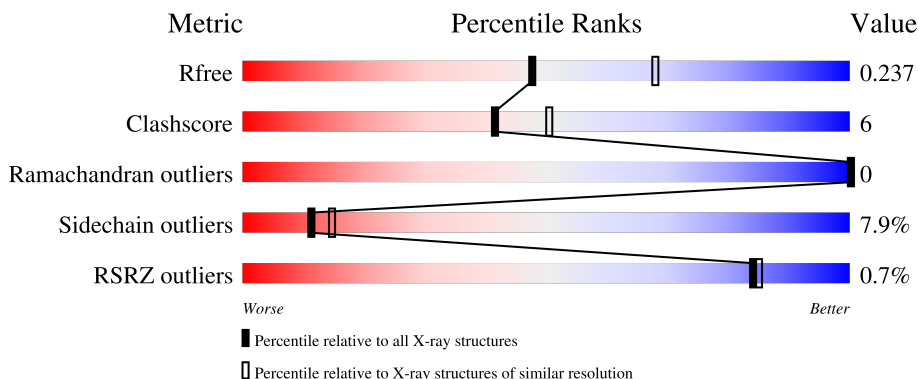
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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.








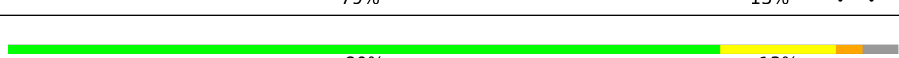


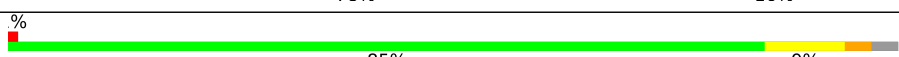

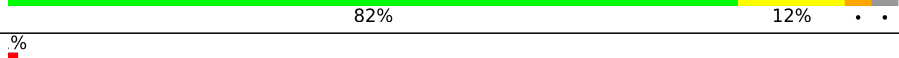
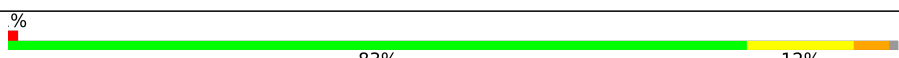







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	156	
1	C	156	
1	D	156	
1	E	156	

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Mol	Chain	Length	Quality of chain
1	F	156	 80% 15% . .
1	G	156	 82% 13% . .
1	H	156	 81% 12% . .
1	I	156	 83% 10% . .
1	J	156	 79% 16% . .
1	K	156	 77% 17% . .
1	L	156	 79% 13% . .
1	M	156	 80% 13% . .
1	N	156	 76% 15% 5% .
1	O	156	 82% 12% . .
1	P	156	 78% 16% . .
1	Q	156	 85% 9% . .
1	R	156	 78% 15% . .
1	S	156	 82% 12% . .
1	T	156	 76% 15% . .
1	U	156	 83% 12% . .
1	V	156	 79% 15% . .
1	X	156	 78% 17% . .
1	Y	156	 80% 15% . .

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	151	1228	786	198	237	7	0	0	0
1	B	150	1222	783	197	235	7	0	0	0
1	C	151	1228	786	198	237	7	0	0	0
1	D	150	1222	783	197	235	7	0	0	0
1	E	150	1222	783	197	235	7	0	0	0
1	F	151	1228	786	198	237	7	0	0	0
1	G	151	1232	788	198	239	7	0	1	0
1	H	150	1222	783	197	235	7	0	0	0
1	I	150	1226	785	197	237	7	0	1	0
1	J	150	1222	783	197	235	7	0	0	0
1	K	150	1222	783	197	235	7	0	0	0
1	L	150	1226	785	197	237	7	0	1	0
1	M	149	1219	780	196	236	7	0	1	0
1	N	150	1226	785	197	237	7	0	1	0
1	O	151	1228	786	198	237	7	0	0	0
1	P	150	1226	785	197	237	7	0	1	0

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

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	2	Total	Fe	0	0
			2	2		
2	F	1	Total	Fe	0	0
			1	1		
2	H	1	Total	Fe	0	0
			1	1		
2	I	1	Total	Fe	0	0
			1	1		
2	J	1	Total	Fe	0	0
			1	1		
2	K	1	Total	Fe	0	0
			1	1		
2	L	1	Total	Fe	0	0
			1	1		
2	M	2	Total	Fe	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	N	2	Total Fe 2 2	0	0
2	P	1	Total Fe 1 1	0	0
2	Q	1	Total Fe 1 1	0	0
2	R	2	Total Fe 2 2	0	0
2	S	1	Total Fe 1 1	0	0
2	U	1	Total Fe 1 1	0	0
2	V	1	Total Fe 1 1	0	0
2	X	1	Total Fe 1 1	0	0
2	Y	1	Total Fe 1 1	0	0

- Molecule 3 is water.

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

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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, 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: 

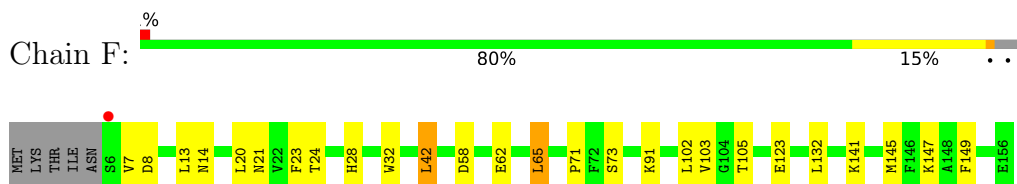


- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

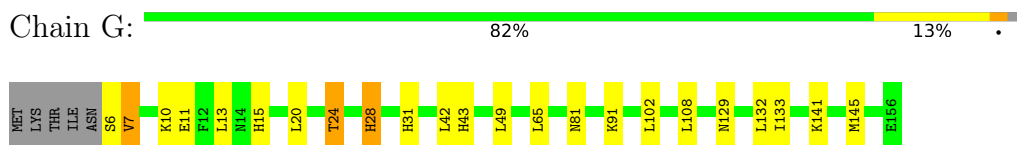
Chain E: 



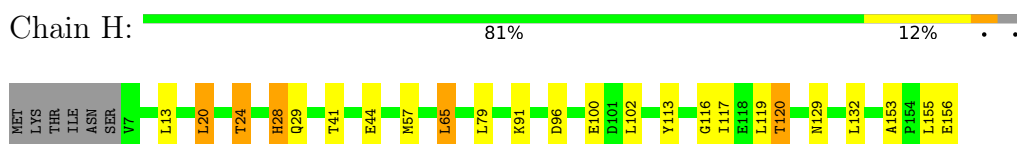
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



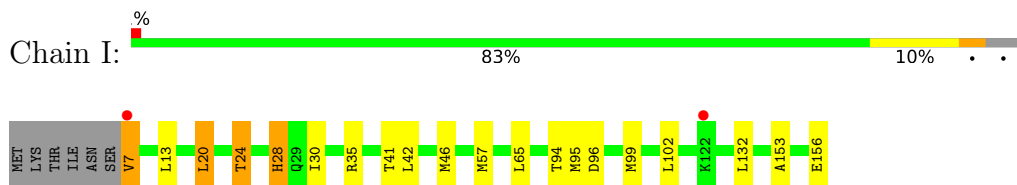
● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



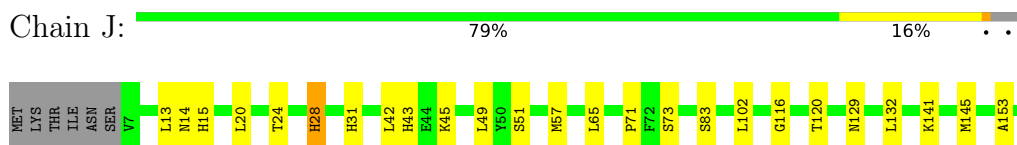
● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



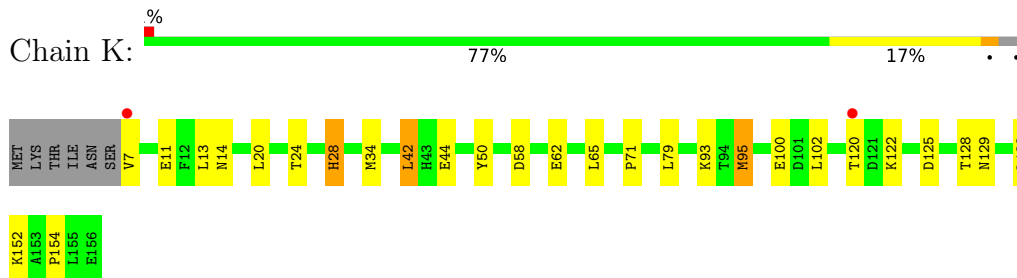
● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



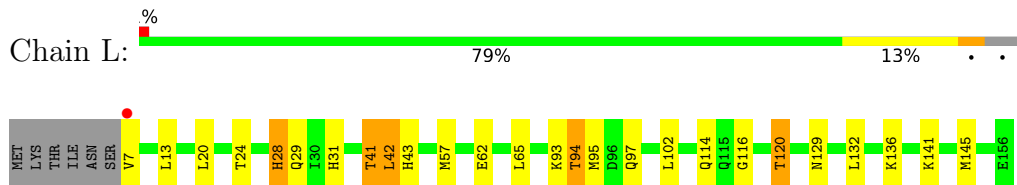
● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN




● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

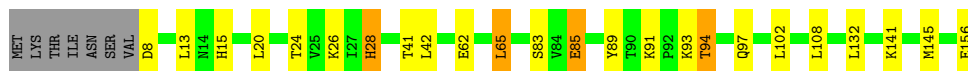


● Molecule 1: NON-HEME IRON-CONTAINING FERRITIN




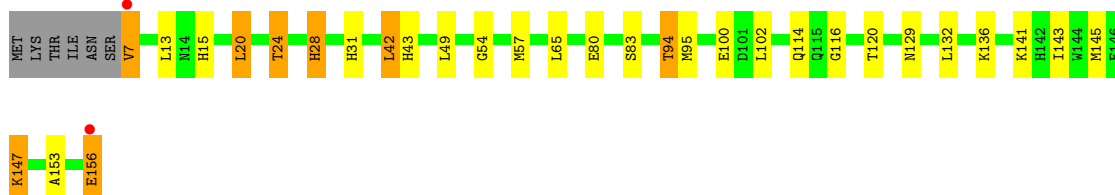
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain M:  80% 13%




- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain N:  76% 15% 5%




- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain O:  82% 12%




- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain P:  78% 16%




- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain Q:  85% 9%




- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain R:  78% 15%

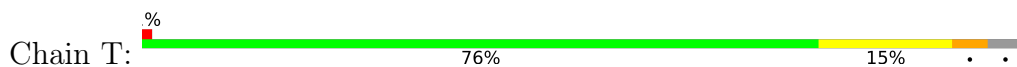


- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

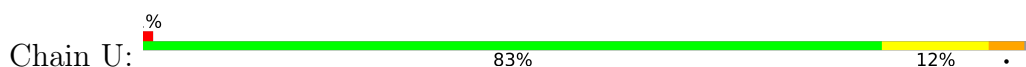
Chain S:  82% 12%



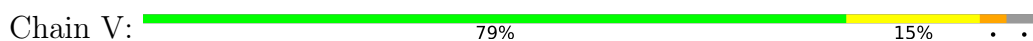
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



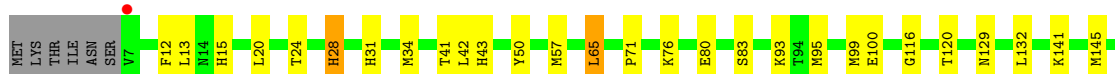
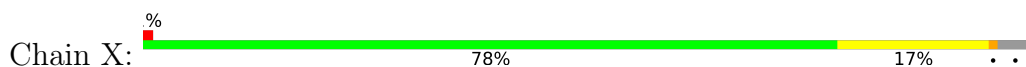
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



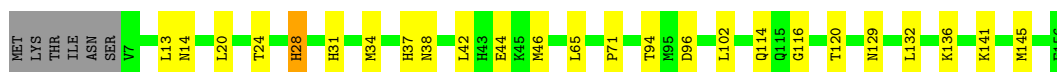
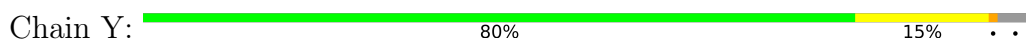
- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



- Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.29Å 172.71Å 135.31Å 90.00° 92.11° 90.00°	Depositor
Resolution (Å)	50.00 – 2.31 50.00 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.31) 99.6 (50.00-2.31)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.31Å)	Xtrriage
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 ²)	26.3	Xtrriage
Anisotropy	0.564	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31295	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

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	0.63	0/1255	0.92	0/1693
1	B	0.66	0/1249	0.95	0/1685
1	C	0.64	0/1255	0.97	2/1693 (0.1%)
1	D	0.63	0/1249	0.93	0/1685
1	E	0.65	0/1249	0.96	0/1685
1	F	0.62	0/1255	0.92	0/1693
1	G	0.64	0/1263	0.93	0/1704
1	H	0.62	0/1249	0.95	0/1685
1	I	0.64	0/1257	0.90	0/1696
1	J	0.64	0/1249	0.93	0/1685
1	K	0.65	0/1249	0.95	0/1685
1	L	0.64	0/1257	0.88	0/1696
1	M	0.66	0/1250	0.93	0/1686
1	N	0.65	0/1257	0.98	0/1696
1	O	0.63	0/1255	0.91	0/1693
1	P	0.68	0/1257	0.95	1/1696 (0.1%)
1	Q	0.66	0/1255	0.93	0/1693
1	R	0.66	0/1255	0.93	0/1693
1	S	0.63	0/1255	0.92	1/1693 (0.1%)
1	T	0.67	0/1257	0.94	0/1696
1	U	0.66	0/1286	0.93	0/1736
1	V	0.63	0/1249	0.95	0/1685
1	X	0.64	0/1249	0.90	0/1685
1	Y	0.60	0/1249	0.93	0/1685
All	All	0.64	0/30110	0.93	4/40622 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	VAL	N-CA-C	6.42	117.17	110.62
1	S	7	VAL	N-CA-C	5.86	118.41	111.09
1	P	19	ASN	N-CA-C	5.26	117.42	111.11
1	C	7	VAL	CB-CA-C	-5.19	105.14	112.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1228	0	1188	14	0
1	B	1222	0	1183	17	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	15	0
1	G	1232	0	1188	11	0
1	H	1222	0	1183	14	0
1	I	1226	0	1183	13	0
1	J	1222	0	1183	14	0
1	K	1222	0	1183	19	0
1	L	1226	0	1183	20	0
1	M	1219	0	1174	14	0
1	N	1226	0	1183	22	0
1	O	1228	0	1188	14	0
1	P	1226	0	1183	21	0
1	Q	1228	0	1188	11	0
1	R	1228	0	1188	22	0
1	S	1228	0	1188	11	0
1	T	1226	0	1183	25	0
1	U	1255	0	1212	18	0
1	V	1222	0	1183	19	0
1	X	1222	0	1183	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	1222	0	1183	16	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	4	0
3	C	72	0	0	5	0
3	D	88	0	0	3	0
3	E	84	0	0	6	0
3	F	82	0	0	3	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	2	0
3	K	65	0	0	1	0
3	L	72	0	0	6	0
3	M	84	0	0	5	0
3	N	78	0	0	8	0
3	O	69	0	0	3	0
3	P	84	0	0	10	0
3	Q	73	0	0	2	0
3	R	82	0	0	10	0
3	S	74	0	0	4	0
3	T	83	0	0	2	0
3	U	88	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	V	68	0	0	4	0
3	X	79	0	0	4	0
3	Y	74	0	0	3	0
All	All	31295	0	28452	372	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 372 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	1.47	0.93
1:E:145:MET:HE3	3:E:2077:HOH:O	1.71	0.90
1:N:141:LYS:HG2	1:N:145:MET:HE2	1.50	0.90

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	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
1	G	150/156 (96%)	148 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [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	134/139 (96%)	124 (92%)	10 (8%)	12	16
1	B	133/139 (96%)	123 (92%)	10 (8%)	12	16
1	C	134/139 (96%)	123 (92%)	11 (8%)	10	14
1	D	133/139 (96%)	122 (92%)	11 (8%)	10	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	133/139 (96%)	121 (91%)	12 (9%)	9	11
1	F	134/139 (96%)	126 (94%)	8 (6%)	17	24
1	G	135/139 (97%)	124 (92%)	11 (8%)	11	14
1	H	133/139 (96%)	120 (90%)	13 (10%)	7	9
1	I	134/139 (96%)	125 (93%)	9 (7%)	15	20
1	J	133/139 (96%)	123 (92%)	10 (8%)	12	16
1	K	133/139 (96%)	121 (91%)	12 (9%)	9	11
1	L	134/139 (96%)	122 (91%)	12 (9%)	9	11
1	M	133/139 (96%)	121 (91%)	12 (9%)	9	11
1	N	134/139 (96%)	120 (90%)	14 (10%)	7	8
1	O	134/139 (96%)	125 (93%)	9 (7%)	15	20
1	P	134/139 (96%)	123 (92%)	11 (8%)	10	14
1	Q	134/139 (96%)	124 (92%)	10 (8%)	12	16
1	R	134/139 (96%)	126 (94%)	8 (6%)	17	24
1	S	134/139 (96%)	124 (92%)	10 (8%)	12	16
1	T	134/139 (96%)	120 (90%)	14 (10%)	7	8
1	U	138/139 (99%)	125 (91%)	13 (9%)	8	10
1	V	133/139 (96%)	124 (93%)	9 (7%)	14	19
1	X	133/139 (96%)	125 (94%)	8 (6%)	17	24
1	Y	133/139 (96%)	126 (95%)	7 (5%)	20	29
All	All	3211/3336 (96%)	2957 (92%)	254 (8%)	11	15

5 of 254 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	132	LEU
1	U	28	HIS
1	N	20	LEU
1	U	20	LEU
1	V	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	31	HIS
1	Q	28	HIS
1	Y	31	HIS
1	N	28	HIS
1	O	43	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 oligosaccharides 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 [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, 95th 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 ²)	Q<0.9
1	A	151/156 (96%)	-0.29	0 100 100	22, 28, 38, 45	0
1	B	150/156 (96%)	-0.31	1 (0%) 84 85	22, 27, 38, 45	0
1	C	151/156 (96%)	-0.29	2 (1%) 75 76	22, 27, 38, 45	0
1	D	150/156 (96%)	-0.37	1 (0%) 84 85	22, 27, 37, 45	0
1	E	150/156 (96%)	-0.33	1 (0%) 84 85	22, 27, 37, 45	0
1	F	151/156 (96%)	-0.38	1 (0%) 84 85	22, 27, 38, 46	0
1	G	151/156 (96%)	-0.34	0 100 100	17, 27, 38, 45	1 (0%)
1	H	150/156 (96%)	-0.37	0 100 100	21, 27, 36, 45	0
1	I	150/156 (96%)	-0.33	2 (1%) 75 76	19, 27, 38, 45	1 (0%)
1	J	150/156 (96%)	-0.31	0 100 100	22, 27, 37, 46	0
1	K	150/156 (96%)	-0.29	2 (1%) 75 76	22, 27, 37, 45	0
1	L	150/156 (96%)	-0.34	1 (0%) 84 85	18, 27, 37, 45	1 (0%)
1	M	149/156 (95%)	-0.37	0 100 100	18, 27, 36, 45	1 (0%)
1	N	150/156 (96%)	-0.37	2 (1%) 75 76	18, 27, 37, 44	1 (0%)
1	O	151/156 (96%)	-0.33	2 (1%) 75 76	22, 27, 38, 52	0
1	P	150/156 (96%)	-0.34	1 (0%) 84 85	18, 27, 37, 45	1 (0%)
1	Q	151/156 (96%)	-0.25	2 (1%) 75 76	23, 27, 38, 49	0
1	R	151/156 (96%)	-0.32	2 (1%) 75 76	22, 27, 37, 51	0
1	S	151/156 (96%)	-0.24	2 (1%) 75 76	23, 27, 38, 49	0
1	T	150/156 (96%)	-0.30	2 (1%) 75 76	19, 27, 37, 45	1 (0%)
1	U	154/156 (98%)	-0.34	1 (0%) 85 86	18, 27, 38, 45	1 (0%)
1	V	150/156 (96%)	-0.32	0 100 100	23, 27, 37, 45	0
1	X	150/156 (96%)	-0.36	1 (0%) 84 85	22, 27, 37, 44	0
1	Y	150/156 (96%)	-0.31	0 100 100	23, 28, 38, 46	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3611/3744 (96%)	-0.33	26 (0%) 84 85	17, 27, 38, 52	8 (0%)

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	6	SER	5.4
1	O	6	SER	4.6
1	S	7	VAL	4.6
1	S	6	SER	4.4
1	X	7	VAL	4.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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, 95th 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 ²)	Q<0.9
2	FE	C	1157	1/1	0.58	0.32	24,24,24,24	1
2	FE	K	1157	1/1	0.63	0.28	27,27,27,27	1
2	FE	M	1158	1/1	0.64	0.35	24,24,24,24	1
2	FE	M	1157	1/1	0.66	0.22	22,22,22,22	1
2	FE	E	1158	1/1	0.68	0.30	23,23,23,23	1
2	FE	I	1157	1/1	0.70	0.30	24,24,24,24	1
2	FE	D	1157	1/1	0.70	0.26	26,26,26,26	1
2	FE	R	1158	1/1	0.74	0.24	17,17,17,17	1
2	FE	J	1157	1/1	0.76	0.23	22,22,22,22	1
2	FE	V	1157	1/1	0.76	0.24	20,20,20,20	1
2	FE	U	1157	1/1	0.79	0.26	16,16,16,16	1
2	FE	N	1158	1/1	0.80	0.20	22,22,22,22	1
2	FE	F	1157	1/1	0.81	0.19	16,16,16,16	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE	R	1157	1/1	0.82	0.18	21,21,21,21	1
2	FE	B	1157	1/1	0.82	0.23	11,11,11,11	1
2	FE	E	1157	1/1	0.82	0.32	17,17,17,17	1
2	FE	P	1157	1/1	0.82	0.34	24,24,24,24	1
2	FE	H	1157	1/1	0.83	0.21	16,16,16,16	1
2	FE	Y	1157	1/1	0.83	0.15	17,17,17,17	1
2	FE	X	1157	1/1	0.84	0.17	16,16,16,16	1
2	FE	L	1157	1/1	0.86	0.18	14,14,14,14	1
2	FE	Q	1157	1/1	0.86	0.17	13,13,13,13	1
2	FE	N	1157	1/1	0.90	0.15	19,19,19,19	1
2	FE	S	1157	1/1	0.90	0.11	10,10,10,10	1

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.