



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:37 PM UTC

PDB ID : 8XUP / pdb_00008xup
Title : Crystal structure of lipoprotein NlpI in complex with MepS
Authors : Tzeng, S.R.; Wang, S.; Huang, C.H.
Deposited on : 2024-01-13
Resolution : 2.80 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

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
Xtriage (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

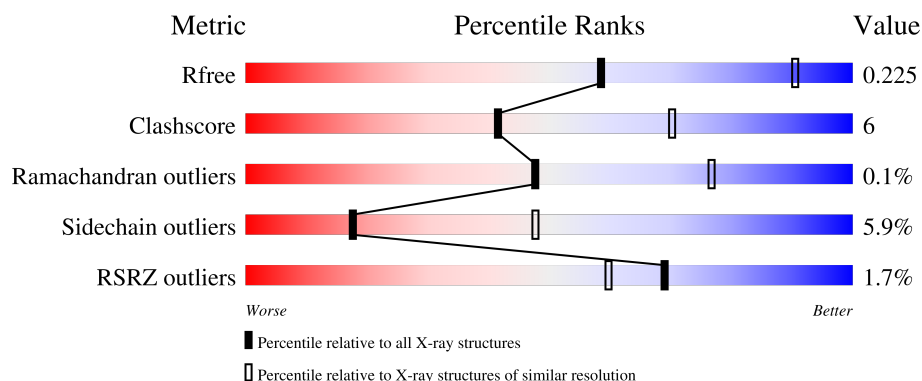
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	297	% 77% 10% • 12%
1	B	297	% 73% 13% • 12%
1	C	297	% 75% 11% • 12%
1	D	297	75% 10% • 13%
2	E	168	% 63% 15% • 19%

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Mol	Chain	Length	Quality of chain
2	F	168	2% 57% 19% 6% 18%
2	G	168	2% 71% 14% •• 13%
2	H	168	3% 77% 9% • 12%
2	I	168	2% 75% 11% • 12%
2	J	168	2% 65% 16% • 15%
2	K	168	2% 70% 12% • 15%
2	L	168	2% 65% 21% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18080 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 Lipoprotein NlpI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	1	0
			2131	1358	352	418	3			
1	B	260	Total	C	N	O	S	0	0	0
			2107	1344	348	412	3			
1	C	261	Total	C	N	O	S	0	0	0
			2117	1351	353	410	3			
1	D	258	Total	C	N	O	S	0	0	0
			2091	1336	346	406	3			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP P0AFB1
A	-1	GLY	-	expression tag	UNP P0AFB1
A	0	SER	-	expression tag	UNP P0AFB1
A	1	SER	-	expression tag	UNP P0AFB1
A	2	HIS	-	expression tag	UNP P0AFB1
A	3	HIS	-	expression tag	UNP P0AFB1
A	4	HIS	-	expression tag	UNP P0AFB1
A	5	HIS	-	expression tag	UNP P0AFB1
A	6	HIS	-	expression tag	UNP P0AFB1
A	7	HIS	-	expression tag	UNP P0AFB1
A	8	SER	-	expression tag	UNP P0AFB1
A	9	SER	-	expression tag	UNP P0AFB1
A	10	GLY	-	expression tag	UNP P0AFB1
A	11	GLU	-	expression tag	UNP P0AFB1
A	12	ASN	-	expression tag	UNP P0AFB1
A	13	LEU	-	expression tag	UNP P0AFB1
A	14	TYR	-	expression tag	UNP P0AFB1
A	15	PHE	-	expression tag	UNP P0AFB1
A	16	GLN	-	expression tag	UNP P0AFB1
A	17	GLY	-	expression tag	UNP P0AFB1
A	18	HIS	-	expression tag	UNP P0AFB1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	UNP P0AFB1
B	-2	MET	-	initiating methionine	UNP P0AFB1
B	-1	GLY	-	expression tag	UNP P0AFB1
B	0	SER	-	expression tag	UNP P0AFB1
B	1	SER	-	expression tag	UNP P0AFB1
B	2	HIS	-	expression tag	UNP P0AFB1
B	3	HIS	-	expression tag	UNP P0AFB1
B	4	HIS	-	expression tag	UNP P0AFB1
B	5	HIS	-	expression tag	UNP P0AFB1
B	6	HIS	-	expression tag	UNP P0AFB1
B	7	HIS	-	expression tag	UNP P0AFB1
B	8	SER	-	expression tag	UNP P0AFB1
B	9	SER	-	expression tag	UNP P0AFB1
B	10	GLY	-	expression tag	UNP P0AFB1
B	11	GLU	-	expression tag	UNP P0AFB1
B	12	ASN	-	expression tag	UNP P0AFB1
B	13	LEU	-	expression tag	UNP P0AFB1
B	14	TYR	-	expression tag	UNP P0AFB1
B	15	PHE	-	expression tag	UNP P0AFB1
B	16	GLN	-	expression tag	UNP P0AFB1
B	17	GLY	-	expression tag	UNP P0AFB1
B	18	HIS	-	expression tag	UNP P0AFB1
B	19	MET	-	expression tag	UNP P0AFB1
C	-2	MET	-	initiating methionine	UNP P0AFB1
C	-1	GLY	-	expression tag	UNP P0AFB1
C	0	SER	-	expression tag	UNP P0AFB1
C	1	SER	-	expression tag	UNP P0AFB1
C	2	HIS	-	expression tag	UNP P0AFB1
C	3	HIS	-	expression tag	UNP P0AFB1
C	4	HIS	-	expression tag	UNP P0AFB1
C	5	HIS	-	expression tag	UNP P0AFB1
C	6	HIS	-	expression tag	UNP P0AFB1
C	7	HIS	-	expression tag	UNP P0AFB1
C	8	SER	-	expression tag	UNP P0AFB1
C	9	SER	-	expression tag	UNP P0AFB1
C	10	GLY	-	expression tag	UNP P0AFB1
C	11	GLU	-	expression tag	UNP P0AFB1
C	12	ASN	-	expression tag	UNP P0AFB1
C	13	LEU	-	expression tag	UNP P0AFB1
C	14	TYR	-	expression tag	UNP P0AFB1
C	15	PHE	-	expression tag	UNP P0AFB1
C	16	GLN	-	expression tag	UNP P0AFB1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	17	GLY	-	expression tag	UNP P0AFB1
C	18	HIS	-	expression tag	UNP P0AFB1
C	19	MET	-	expression tag	UNP P0AFB1
D	-2	MET	-	initiating methionine	UNP P0AFB1
D	-1	GLY	-	expression tag	UNP P0AFB1
D	0	SER	-	expression tag	UNP P0AFB1
D	1	SER	-	expression tag	UNP P0AFB1
D	2	HIS	-	expression tag	UNP P0AFB1
D	3	HIS	-	expression tag	UNP P0AFB1
D	4	HIS	-	expression tag	UNP P0AFB1
D	5	HIS	-	expression tag	UNP P0AFB1
D	6	HIS	-	expression tag	UNP P0AFB1
D	7	HIS	-	expression tag	UNP P0AFB1
D	8	SER	-	expression tag	UNP P0AFB1
D	9	SER	-	expression tag	UNP P0AFB1
D	10	GLY	-	expression tag	UNP P0AFB1
D	11	GLU	-	expression tag	UNP P0AFB1
D	12	ASN	-	expression tag	UNP P0AFB1
D	13	LEU	-	expression tag	UNP P0AFB1
D	14	TYR	-	expression tag	UNP P0AFB1
D	15	PHE	-	expression tag	UNP P0AFB1
D	16	GLN	-	expression tag	UNP P0AFB1
D	17	GLY	-	expression tag	UNP P0AFB1
D	18	HIS	-	expression tag	UNP P0AFB1
D	19	MET	-	expression tag	UNP P0AFB1

- Molecule 2 is a protein called Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	136	Total 1096	C 680	N 206	O 206	S 4	0	0	0
2	F	138	Total 1110	C 688	N 208	O 210	S 4	0	0	0
2	G	146	Total 1186	C 732	N 231	O 219	S 4	0	0	0
2	H	147	Total 1190	C 734	N 232	O 220	S 4	0	0	0
2	I	148	Total 1197	C 738	N 233	O 222	S 4	0	0	0
2	J	143	Total 1153	C 713	N 221	O 215	S 4	0	0	0
2	K	143	Total 1168	C 722	N 228	O 214	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	147	Total	C	N	O	S	0	0	0
			1190	734	232	220	4			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	initiating methionine	UNP P0AFV4
E	163	HIS	-	expression tag	UNP P0AFV4
E	164	HIS	-	expression tag	UNP P0AFV4
E	165	HIS	-	expression tag	UNP P0AFV4
E	166	HIS	-	expression tag	UNP P0AFV4
E	167	HIS	-	expression tag	UNP P0AFV4
E	168	HIS	-	expression tag	UNP P0AFV4
F	1	MET	-	initiating methionine	UNP P0AFV4
F	163	HIS	-	expression tag	UNP P0AFV4
F	164	HIS	-	expression tag	UNP P0AFV4
F	165	HIS	-	expression tag	UNP P0AFV4
F	166	HIS	-	expression tag	UNP P0AFV4
F	167	HIS	-	expression tag	UNP P0AFV4
F	168	HIS	-	expression tag	UNP P0AFV4
G	1	MET	-	initiating methionine	UNP P0AFV4
G	163	HIS	-	expression tag	UNP P0AFV4
G	164	HIS	-	expression tag	UNP P0AFV4
G	165	HIS	-	expression tag	UNP P0AFV4
G	166	HIS	-	expression tag	UNP P0AFV4
G	167	HIS	-	expression tag	UNP P0AFV4
G	168	HIS	-	expression tag	UNP P0AFV4
H	1	MET	-	initiating methionine	UNP P0AFV4
H	163	HIS	-	expression tag	UNP P0AFV4
H	164	HIS	-	expression tag	UNP P0AFV4
H	165	HIS	-	expression tag	UNP P0AFV4
H	166	HIS	-	expression tag	UNP P0AFV4
H	167	HIS	-	expression tag	UNP P0AFV4
H	168	HIS	-	expression tag	UNP P0AFV4
I	1	MET	-	initiating methionine	UNP P0AFV4
I	163	HIS	-	expression tag	UNP P0AFV4
I	164	HIS	-	expression tag	UNP P0AFV4
I	165	HIS	-	expression tag	UNP P0AFV4
I	166	HIS	-	expression tag	UNP P0AFV4
I	167	HIS	-	expression tag	UNP P0AFV4
I	168	HIS	-	expression tag	UNP P0AFV4
J	1	MET	-	initiating methionine	UNP P0AFV4

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Chain	Residue	Modelled	Actual	Comment	Reference
J	163	HIS	-	expression tag	UNP P0AFV4
J	164	HIS	-	expression tag	UNP P0AFV4
J	165	HIS	-	expression tag	UNP P0AFV4
J	166	HIS	-	expression tag	UNP P0AFV4
J	167	HIS	-	expression tag	UNP P0AFV4
J	168	HIS	-	expression tag	UNP P0AFV4
K	1	MET	-	initiating methionine	UNP P0AFV4
K	163	HIS	-	expression tag	UNP P0AFV4
K	164	HIS	-	expression tag	UNP P0AFV4
K	165	HIS	-	expression tag	UNP P0AFV4
K	166	HIS	-	expression tag	UNP P0AFV4
K	167	HIS	-	expression tag	UNP P0AFV4
K	168	HIS	-	expression tag	UNP P0AFV4
L	1	MET	-	initiating methionine	UNP P0AFV4
L	163	HIS	-	expression tag	UNP P0AFV4
L	164	HIS	-	expression tag	UNP P0AFV4
L	165	HIS	-	expression tag	UNP P0AFV4
L	166	HIS	-	expression tag	UNP P0AFV4
L	167	HIS	-	expression tag	UNP P0AFV4
L	168	HIS	-	expression tag	UNP P0AFV4

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	48	Total O 48 48	0	0
3	B	37	Total O 37 37	0	0
3	C	59	Total O 59 59	0	0
3	D	42	Total O 42 42	0	0
3	E	22	Total O 22 22	0	0
3	F	32	Total O 32 32	0	0
3	G	15	Total O 15 15	0	0
3	H	19	Total O 19 19	0	0
3	I	24	Total O 24 24	0	0

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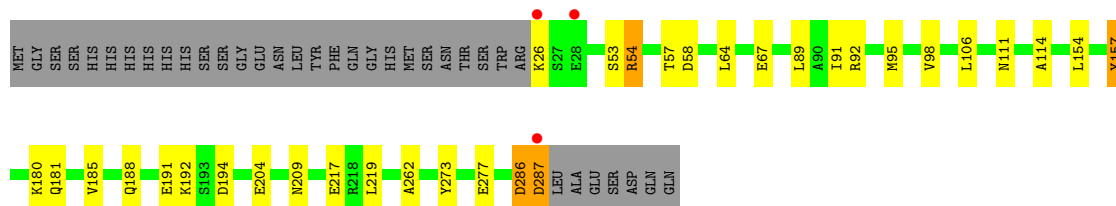
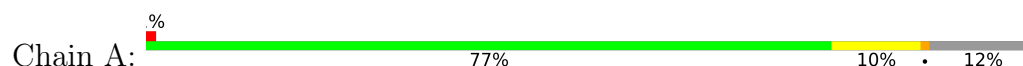
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	17	Total 17	O 17	0	0
3	K	22	Total 22	O 22	0	0
3	L	7	Total 7	O 7	0	0

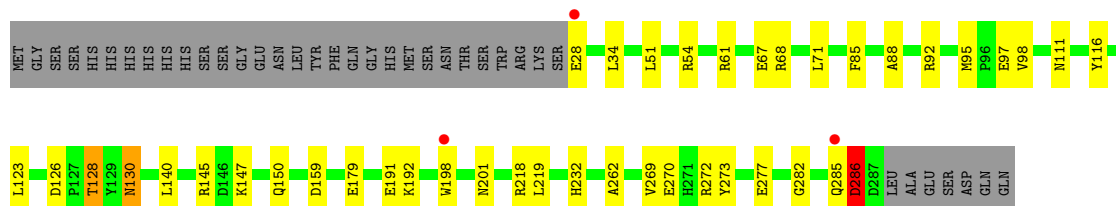
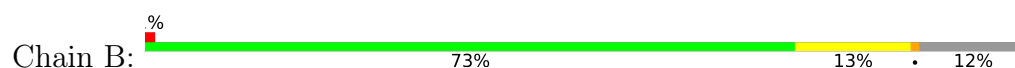
3 Residue-property plots [i](#)

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.

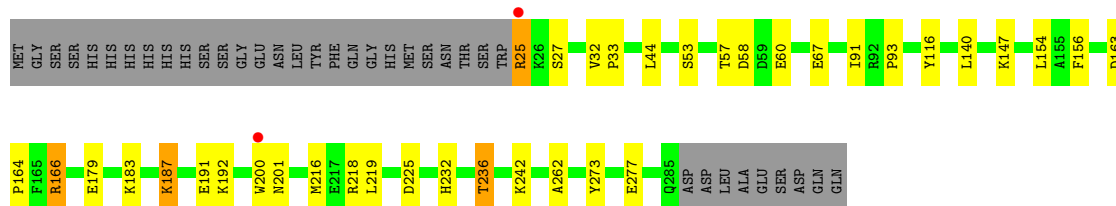
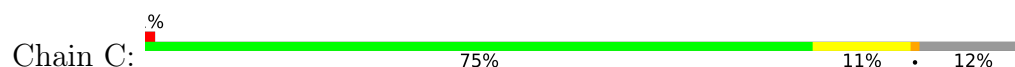
• Molecule 1: Lipoprotein NlpI



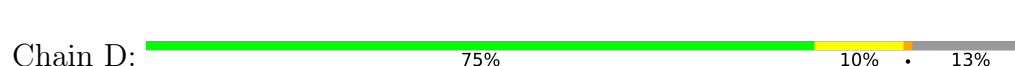
• Molecule 1: Lipoprotein NlpI



• Molecule 1: Lipoprotein NlpI

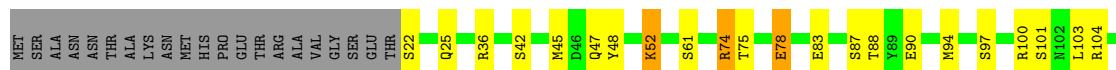


• Molecule 1: Lipoprotein NlpI

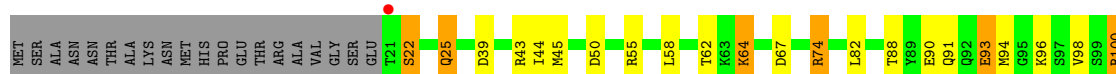




- Molecule 2: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase



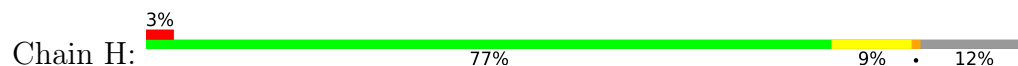
- Molecule 2: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase



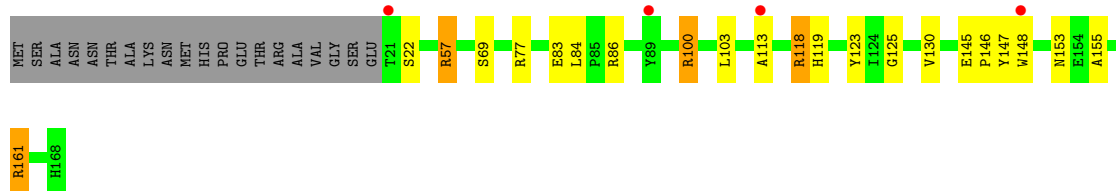
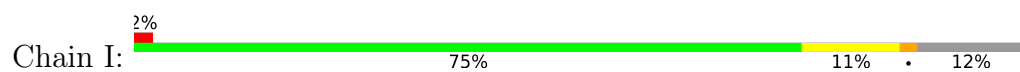
- Molecule 2: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase



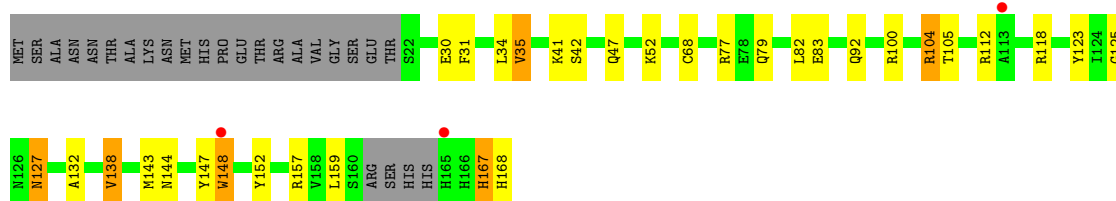
- Molecule 2: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase



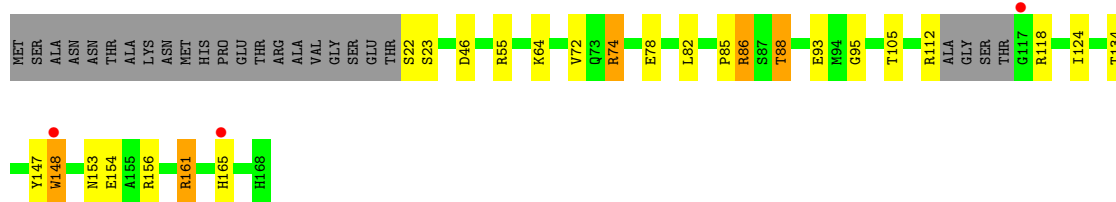
- Molecule 2: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase



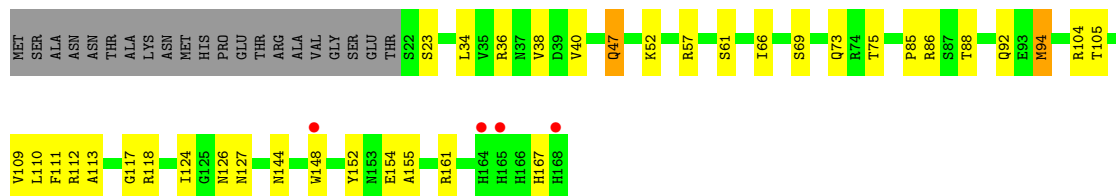
- Molecule 2: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase



- Molecule 2: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase



- Molecule 2: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.19Å 99.44Å 196.24Å 90.00° 104.45° 90.00°	Depositor
Resolution (Å)	29.70 – 2.80 29.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.70-2.80) 99.5 (29.70-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.171 , 0.221 0.177 , 0.225	Depositor DCC
R_{free} test set	4563 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18080	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.20% 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 ⓘ

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	0.54	0/2175	1.06	3/2951 (0.1%)
1	B	0.57	0/2151	1.12	3/2920 (0.1%)
1	C	0.57	0/2161	1.07	3/2931 (0.1%)
1	D	0.56	0/2135	1.06	3/2898 (0.1%)
2	E	0.75	1/1114 (0.1%)	1.07	0/1492
2	F	0.63	2/1128 (0.2%)	1.02	1/1512 (0.1%)
2	G	0.54	0/1210	1.06	2/1622 (0.1%)
2	H	0.56	0/1215	1.00	1/1630 (0.1%)
2	I	0.54	0/1222	1.03	1/1640 (0.1%)
2	J	0.70	2/1175 (0.2%)	1.06	3/1575 (0.2%)
2	K	0.58	0/1192	1.07	3/1597 (0.2%)
2	L	0.66	2/1215 (0.2%)	1.02	0/1630
All	All	0.59	7/18093 (0.0%)	1.06	23/24398 (0.1%)

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	A	0	1
1	B	0	2
1	C	0	2
1	D	0	1
2	E	0	2
2	F	0	3
2	G	0	1
2	H	0	2
2	I	0	2
2	J	0	3
2	K	0	1
2	L	0	2
All	All	0	22

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	148	TRP	CG-CD2	13.38	1.67	1.43
2	J	148	TRP	CG-CD2	10.66	1.62	1.43
2	L	148	TRP	CD2-CE2	8.18	1.55	1.41
2	F	148	TRP	CD2-CE2	6.75	1.52	1.41
2	L	148	TRP	CZ3-CH2	6.27	1.56	1.40
2	J	148	TRP	CD1-NE1	6.20	1.50	1.37
2	F	148	TRP	CZ3-CH2	5.12	1.53	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	148	TRP	CD1-CG-CD2	-6.40	96.06	106.30
2	I	57	ARG	CB-CA-C	6.33	119.88	110.14
1	B	286	ASP	CB-CA-C	6.30	121.86	112.03
2	K	88	THR	CB-CA-C	5.95	122.10	110.67
1	A	111	ASN	CB-CA-C	-5.84	103.36	112.12
2	G	163	HIS	CA-CB-CG	5.82	119.62	113.80
1	C	93	PRO	N-CA-C	5.82	121.51	113.65
1	D	67	GLU	CB-CG-CD	5.80	122.47	112.60
2	J	167	HIS	CA-CB-CG	5.76	119.56	113.80
2	G	134	THR	CA-CB-OG1	-5.58	101.23	109.60
1	A	67	GLU	CB-CG-CD	5.58	122.08	112.60
1	C	236	THR	CA-CB-OG1	-5.53	101.31	109.60
2	F	67	ASP	CA-CB-CG	5.52	118.12	112.60
1	D	107	THR	CA-CB-OG1	5.45	117.78	109.60
2	J	148	TRP	CG-CD2-CE3	-5.43	128.47	133.90
2	H	50	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	286	ASP	CA-CB-CG	5.36	117.96	112.60
1	C	225	ASP	CA-CB-CG	5.33	117.93	112.60
1	D	161	PRO	N-CA-C	5.29	120.55	114.20
2	K	46	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	130	ASN	CB-CA-C	-5.20	100.07	110.42
2	K	148	TRP	CD2-CE2-CZ2	5.13	127.53	122.40
1	A	194	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	ASP	Peptide
1	B	145	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	68	ARG	Sidechain
1	C	166	ARG	Sidechain
1	C	25	ARG	Sidechain
1	D	166	ARG	Sidechain
2	E	157	ARG	Sidechain
2	E	36	ARG	Sidechain
2	F	100	ARG	Sidechain
2	F	112	ARG	Sidechain
2	F	151	ARG	Sidechain
2	G	57	ARG	Sidechain
2	H	161	ARG	Sidechain
2	H	36	ARG	Sidechain
2	I	161	ARG	Sidechain
2	I	22	SER	Peptide
2	J	104	ARG	Sidechain
2	J	157	ARG	Sidechain
2	J	159	LEU	Peptide
2	K	86	ARG	Sidechain
2	L	36	ARG	Sidechain
2	L	57	ARG	Sidechain

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	2131	0	2053	17	0
1	B	2107	0	2030	30	0
1	C	2117	0	2053	21	0
1	D	2091	0	2022	21	0
2	E	1096	0	1077	22	0
2	F	1110	0	1091	35	0
2	G	1186	0	1149	14	0
2	H	1190	0	1153	7	0
2	I	1197	0	1160	19	0
2	J	1153	0	1120	22	0
2	K	1168	0	1132	13	0
2	L	1190	0	1153	22	0
3	A	48	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	37	0	0	1	0
3	C	59	0	0	1	0
3	D	42	0	0	1	0
3	E	22	0	0	2	0
3	F	32	0	0	0	0
3	G	15	0	0	0	0
3	H	19	0	0	1	0
3	I	24	0	0	2	0
3	J	17	0	0	1	0
3	K	22	0	0	1	0
3	L	7	0	0	0	0
All	All	18080	0	17193	222	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.

All (222) 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)
2:I:161:ARG:NH2	3:I:202:HOH:O	2.00	0.94
2:F:94:MET:HE3	2:F:94:MET:HA	1.53	0.91
1:D:54:ARG:HH11	1:D:54:ARG:HB2	1.37	0.89
1:D:54:ARG:HH11	1:D:54:ARG:CB	1.90	0.85
1:B:198:TRP:CZ2	1:B:219:LEU:HA	2.18	0.79
2:E:147:TYR:HE2	2:E:148:TRP:CZ3	2.01	0.79
2:I:83:GLU:OE2	3:I:201:HOH:O	1.99	0.78
2:L:113:ALA:CB	2:L:117:GLY:O	2.34	0.76
2:F:74:ARG:HH11	2:F:74:ARG:CG	1.99	0.75
2:I:118:ARG:HH12	2:I:153:ASN:ND2	1.89	0.71
2:G:77:ARG:NH1	2:G:83:GLU:OE1	2.24	0.70
2:L:92:GLN:NE2	2:L:118:ARG:HH11	1.90	0.69
2:F:25:GLN:HE21	2:F:25:GLN:HA	1.58	0.69
2:E:147:TYR:HD2	2:E:148:TRP:CD2	2.13	0.67
2:L:34:LEU:HD23	2:L:161:ARG:HH21	1.60	0.66
2:F:94:MET:HE1	2:I:84:LEU:C	2.20	0.66
2:L:113:ALA:HB1	2:L:117:GLY:O	1.95	0.66
2:G:57:ARG:NH1	2:G:57:ARG:HG2	2.11	0.65
2:F:74:ARG:HH11	2:F:74:ARG:HG3	1.62	0.65
2:K:74:ARG:NH1	2:K:78:GLU:OE1	2.30	0.65
2:G:57:ARG:HG2	2:G:57:ARG:HH11	1.61	0.64
2:L:69:SER:HB3	2:L:88:THR:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:147:TYR:CD1	2:F:148:TRP:CD2	2.86	0.64
1:D:54:ARG:HB2	1:D:54:ARG:NH1	2.11	0.63
2:F:147:TYR:HE1	2:F:148:TRP:CZ3	2.17	0.63
1:A:54:ARG:NH2	1:B:54:ARG:HH11	1.97	0.63
2:F:94:MET:HE2	2:I:83:GLU:HB3	1.79	0.63
2:H:126:ASN:N	2:H:126:ASN:HD22	1.97	0.63
2:J:47:GLN:NE2	2:J:79:GLN:HE21	1.96	0.63
2:L:92:GLN:NE2	2:L:118:ARG:NH1	2.46	0.63
1:B:28:GLU:OE2	3:B:301:HOH:O	2.16	0.62
1:B:92:ARG:HB3	1:B:95:MET:HE2	1.81	0.61
2:J:52:LYS:HA	2:J:138:VAL:HG22	1.81	0.61
2:L:85:PRO:HD3	2:L:94:MET:HE2	1.82	0.61
2:F:147:TYR:HD1	2:F:148:TRP:CD2	2.19	0.61
2:E:88:THR:HG23	2:E:120:VAL:CG2	2.31	0.61
1:A:54:ARG:HH22	1:B:54:ARG:HH11	1.48	0.60
2:I:118:ARG:HH12	2:I:153:ASN:HD22	1.47	0.60
2:J:104:ARG:HG2	2:J:104:ARG:HH21	1.66	0.60
2:J:47:GLN:HE21	2:J:79:GLN:HE21	1.50	0.60
2:L:112:ARG:HH11	2:L:112:ARG:HB3	1.66	0.59
2:E:147:TYR:CE2	2:E:148:TRP:CE3	2.91	0.59
2:H:47:GLN:NE2	2:H:79:GLN:HE21	2.01	0.59
1:B:198:TRP:CZ2	1:B:219:LEU:CA	2.85	0.58
1:D:63:GLN:HG2	1:D:92:ARG:HH22	1.69	0.58
2:J:68:CYS:HA	2:J:132:ALA:HB3	1.85	0.58
2:F:45:MET:HE1	2:F:130:VAL:HG21	1.86	0.57
1:D:270:GLU:CD	2:L:167:HIS:HE2	2.13	0.57
2:F:143:MET:O	2:F:149:LYS:HB3	2.04	0.57
2:E:147:TYR:CD2	2:E:148:TRP:CD2	2.94	0.56
1:D:270:GLU:OE1	2:L:167:HIS:NE2	2.29	0.56
2:E:160:SER:C	3:E:204:HOH:O	2.48	0.56
2:I:147:TYR:HE2	2:I:148:TRP:CH2	2.24	0.56
2:I:147:TYR:HD2	2:I:148:TRP:CE2	2.24	0.56
2:J:92:GLN:OE1	2:J:118:ARG:NH1	2.38	0.56
2:F:74:ARG:CG	2:F:74:ARG:NH1	2.65	0.55
2:L:113:ALA:HB2	2:L:117:GLY:O	2.07	0.55
1:D:57:THR:HG22	1:D:60:GLU:OE1	2.07	0.55
2:E:147:TYR:CE2	2:E:148:TRP:CZ3	2.91	0.54
2:G:34:LEU:C	2:G:34:LEU:HD12	2.32	0.54
1:A:287:ASP:OD1	1:A:287:ASP:N	2.41	0.54
2:L:73:GLN:HE22	2:L:86:ARG:HB2	1.71	0.54
1:C:242:LYS:NZ	1:C:277:GLU:OE1	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:VAL:O	1:A:188:GLN:HB2	2.08	0.54
1:C:164:PRO:HB3	1:C:200:TRP:CD2	2.42	0.54
2:F:113:ALA:HB3	2:F:119:HIS:HB2	1.90	0.53
2:J:77:ARG:NH2	2:J:83:GLU:OE2	2.42	0.53
2:K:161:ARG:NH2	3:K:201:HOH:O	2.41	0.53
2:K:118:ARG:HH22	2:K:154:GLU:HB3	1.74	0.52
2:E:22:SER:N	3:E:201:HOH:O	2.41	0.52
2:G:95:GLY:HA3	2:G:157:ARG:O	2.10	0.52
1:B:285:GLN:HG3	1:B:286:ASP:N	2.25	0.52
1:A:92:ARG:NH1	1:A:95:MET:HE3	2.25	0.51
2:K:112:ARG:HH11	2:K:153:ASN:HB2	1.75	0.51
1:C:201:ASN:OD1	1:C:218:ARG:NH1	2.42	0.51
2:E:103:LEU:HD21	2:E:155:ALA:CB	2.41	0.51
2:E:45:MET:HE1	2:E:130:VAL:HG21	1.92	0.51
2:J:31:PHE:CE1	2:J:35:VAL:HG21	2.45	0.51
2:E:74:ARG:NH1	2:E:78:GLU:OE1	2.43	0.51
1:C:163:ASP:HB3	1:C:166:ARG:HD2	1.92	0.51
1:B:201:ASN:OD1	1:B:218:ARG:NH1	2.40	0.51
2:G:57:ARG:HH11	2:G:57:ARG:CG	2.24	0.51
2:I:147:TYR:HD2	2:I:148:TRP:CD2	2.29	0.51
1:C:116:TYR:CE1	1:C:140:LEU:HD23	2.47	0.50
2:J:127:ASN:OD1	2:J:144:ASN:ND2	2.39	0.50
1:C:58:ASP:HB3	1:C:91:ILE:CG2	2.42	0.50
2:E:42:SER:HG	2:J:31:PHE:HD1	1.59	0.50
2:I:147:TYR:CD2	2:I:148:TRP:CE2	2.99	0.50
2:J:41:LYS:HB2	2:J:105:THR:HG21	1.94	0.50
1:B:116:TYR:CE2	1:B:140:LEU:HD23	2.47	0.50
2:E:147:TYR:HE2	2:E:148:TRP:CE3	2.28	0.50
1:D:130:ASN:O	1:D:133:HIS:HB2	2.11	0.49
1:B:130:ASN:ND2	1:B:159:ASP:OD2	2.44	0.49
2:I:100:ARG:HG2	2:I:100:ARG:HH11	1.77	0.49
2:J:52:LYS:NZ	3:J:202:HOH:O	2.44	0.49
2:K:118:ARG:NH2	2:K:153:ASN:OD1	2.44	0.49
1:C:164:PRO:HA	1:C:200:TRP:CH2	2.48	0.49
1:D:147:LYS:HD2	1:D:148:LEU:H	1.78	0.49
1:B:126:ASP:OD1	1:B:128:THR:HG22	2.13	0.49
2:G:31:PHE:O	2:G:35:VAL:HG13	2.13	0.49
2:E:88:THR:HG23	2:E:120:VAL:HG22	1.95	0.48
1:B:282:GLY:O	1:B:286:ASP:HB3	2.13	0.48
2:G:112:ARG:HA	2:G:117:GLY:O	2.12	0.48
2:K:95:GLY:O	2:K:156:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:HIS:CE1	2:H:168:HIS:CD2	3.01	0.48
1:D:222:ASP:OD2	3:D:301:HOH:O	2.20	0.48
1:B:88:ALA:HB1	1:B:95:MET:HE1	1.96	0.48
1:D:130:ASN:ND2	1:D:159:ASP:OD2	2.46	0.48
2:E:48:TYR:O	2:E:52:LYS:HB2	2.13	0.48
2:G:147:TYR:HE1	2:G:148:TRP:CH2	2.31	0.48
2:H:153:ASN:ND2	3:H:201:HOH:O	2.47	0.48
2:I:100:ARG:HG2	2:I:100:ARG:NH1	2.27	0.48
1:C:27:SER:HB3	3:C:336:HOH:O	2.13	0.47
1:A:273:TYR:O	1:A:277:GLU:HG2	2.14	0.47
2:F:147:TYR:CE1	2:F:148:TRP:CD2	3.02	0.47
1:B:198:TRP:CE3	1:B:232:HIS:CD2	3.02	0.47
2:I:77:ARG:HD3	2:I:83:GLU:OE1	2.15	0.47
2:F:103:LEU:HD21	2:F:155:ALA:CB	2.45	0.47
2:I:123:TYR:CE2	2:I:125:GLY:HA2	2.50	0.47
2:K:147:TYR:HD2	2:K:148:TRP:CD2	2.32	0.47
1:D:147:LYS:HD3	1:D:148:LEU:HG	1.97	0.47
2:L:34:LEU:HD23	2:L:161:ARG:NH2	2.27	0.47
1:B:51:LEU:O	1:B:61:ARG:NH2	2.49	0.46
1:D:66:TYR:O	1:D:70:VAL:HG23	2.15	0.46
2:F:55:ARG:NH1	2:F:64:LYS:O	2.47	0.46
1:B:192:LYS:O	1:B:192:LYS:HG3	2.15	0.46
2:E:147:TYR:CD2	2:E:148:TRP:CE3	3.04	0.46
2:L:40:VAL:HG12	2:L:105:THR:HG22	1.97	0.46
1:C:57:THR:HB	1:C:60:GLU:H	1.81	0.46
1:B:270:GLU:CD	2:J:167:HIS:HE2	2.24	0.46
1:D:156:PHE:CD2	1:D:166:ARG:HG2	2.51	0.46
1:D:219:LEU:C	1:D:219:LEU:HD23	2.41	0.46
1:A:106:LEU:HD22	1:A:114:ALA:HB3	1.96	0.46
2:K:147:TYR:HD2	2:K:148:TRP:CE2	2.34	0.46
2:E:83:GLU:O	2:K:165:HIS:HE1	1.99	0.45
2:E:22:SER:HB3	2:E:25:GLN:HG2	1.99	0.45
2:L:47:GLN:NE2	2:L:75:THR:OG1	2.50	0.45
1:A:286:ASP:HB2	1:A:287:ASP:OD1	2.16	0.45
1:B:272:ARG:HH11	1:B:272:ARG:HG2	1.81	0.45
1:C:216:MET:HE1	1:C:236:THR:HG21	1.98	0.45
2:F:103:LEU:HD21	2:F:155:ALA:HB2	1.98	0.45
2:F:123:TYR:CE2	2:F:125:GLY:HA2	2.52	0.45
2:F:147:TYR:CE1	2:F:148:TRP:CE3	3.05	0.45
1:A:58:ASP:HB3	1:A:91:ILE:CG2	2.46	0.45
2:I:113:ALA:HB2	2:I:119:HIS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HB2	1:A:98:VAL:HG11	1.98	0.45
2:F:44:ILE:HG22	2:F:45:MET:HE2	1.99	0.45
2:F:91:GLN:HA	2:F:94:MET:HG2	1.99	0.45
2:F:100:ARG:HG3	2:F:152:TYR:CE1	2.51	0.45
2:J:123:TYR:CE2	2:J:125:GLY:HA2	2.51	0.45
2:F:82:LEU:HD23	2:F:82:LEU:HA	1.84	0.45
1:B:128:THR:CG2	2:J:104:ARG:HH11	2.29	0.44
2:K:82:LEU:HD11	2:K:165:HIS:CD2	2.52	0.44
1:A:262:ALA:HB1	1:B:262:ALA:HB1	1.99	0.44
1:A:181:GLN:O	1:A:185:VAL:HG23	2.18	0.44
2:G:130:VAL:HG22	2:G:140:ILE:HG12	2.00	0.44
2:G:143:MET:HE3	2:G:143:MET:HB3	1.91	0.44
2:L:110:LEU:HD22	2:L:110:LEU:N	2.32	0.44
1:D:242:LYS:NZ	1:D:277:GLU:OE2	2.44	0.44
2:F:39:ASP:O	2:F:43:ARG:HG3	2.17	0.44
2:L:127:ASN:ND2	2:L:144:ASN:HD21	2.16	0.44
1:B:67:GLU:HG3	2:J:34:LEU:O	2.18	0.43
1:B:270:GLU:OE1	2:J:167:HIS:NE2	2.47	0.43
1:C:67:GLU:HG3	2:H:34:LEU:O	2.18	0.43
2:F:104:ARG:HH11	2:F:104:ARG:HB3	1.82	0.43
2:G:57:ARG:NH1	2:G:57:ARG:CG	2.81	0.43
2:G:113:ALA:HB2	2:G:151:ARG:HD3	2.00	0.43
2:F:147:TYR:HE1	2:F:148:TRP:CH2	2.36	0.43
2:F:147:TYR:HD1	2:F:148:TRP:CG	2.37	0.43
1:D:119:PHE:CZ	1:D:135:ASN:HB3	2.54	0.43
1:A:219:LEU:C	1:A:219:LEU:HD23	2.44	0.43
2:F:147:TYR:HE1	2:F:148:TRP:CE3	2.36	0.43
2:F:98:VAL:HG11	2:F:157:ARG:NH2	2.34	0.43
2:J:147:TYR:HD2	2:J:148:TRP:CE2	2.37	0.43
1:B:95:MET:HG2	1:B:97:GLU:OE1	2.20	0.42
1:D:54:ARG:HH11	1:D:54:ARG:CG	2.32	0.42
2:K:105:THR:HG23	2:K:124:ILE:HA	2.00	0.42
2:L:69:SER:HB3	2:L:88:THR:CG2	2.48	0.42
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.88	0.42
1:C:116:TYR:CZ	1:C:140:LEU:HD23	2.54	0.42
1:C:219:LEU:C	1:C:219:LEU:HD23	2.44	0.42
1:C:262:ALA:HB1	1:D:262:ALA:HB1	2.02	0.42
2:E:94:MET:HE1	2:K:85:PRO:HD3	1.99	0.42
2:L:154:GLU:HG2	2:L:155:ALA:N	2.35	0.42
1:A:154:LEU:O	1:A:154:LEU:HD23	2.20	0.42
2:E:87:SER:OG	2:E:90:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:145:GLU:O	2:I:146:PRO:C	2.62	0.42
1:B:85:PHE:HB3	1:B:98:VAL:HG13	2.01	0.42
2:E:47:GLN:HG2	2:E:75:THR:OG1	2.20	0.42
1:C:32:VAL:O	1:C:33:PRO:C	2.61	0.42
1:C:164:PRO:HD3	1:C:200:TRP:NE1	2.35	0.42
2:F:88:THR:CG2	2:F:118:ARG:HB3	2.50	0.42
2:H:31:PHE:CE1	2:H:35:VAL:HG11	2.55	0.42
2:L:112:ARG:HH11	2:L:112:ARG:CB	2.33	0.42
2:E:42:SER:OG	2:J:31:PHE:HD1	2.03	0.41
2:F:74:ARG:NH1	2:F:74:ARG:HG2	2.35	0.41
2:L:111:PHE:CD2	2:L:152:TYR:HA	2.55	0.41
1:B:232:HIS:CE1	2:J:168:HIS:CG	3.08	0.41
1:B:269:VAL:HG13	1:B:273:TYR:HE1	1.85	0.41
1:C:156:PHE:CD2	1:C:166:ARG:HG2	2.55	0.41
1:A:92:ARG:HH11	1:A:95:MET:HE3	1.86	0.41
2:F:74:ARG:HH11	2:F:74:ARG:HG2	1.81	0.41
2:F:90:GLU:O	2:F:93:GLU:HG3	2.20	0.41
1:A:204:GLU:HG2	1:A:209:ASN:HD22	1.84	0.41
2:F:82:LEU:HD22	2:I:83:GLU:HG2	2.02	0.41
2:I:103:LEU:HD21	2:I:155:ALA:CB	2.51	0.41
1:A:157:TYR:CD2	1:A:157:TYR:C	2.98	0.41
1:B:285:GLN:CG	1:B:286:ASP:N	2.83	0.41
2:I:69:SER:HB2	2:I:86:ARG:O	2.21	0.41
1:C:273:TYR:O	1:C:277:GLU:HG2	2.21	0.41
1:D:168:LEU:O	1:D:172:LEU:HG	2.20	0.41
2:L:61:SER:HA	2:L:66:ILE:HG13	2.02	0.41
1:B:198:TRP:HZ2	1:B:219:LEU:CA	2.31	0.40
1:B:128:THR:HG23	2:J:104:ARG:HH11	1.86	0.40
1:C:187:LYS:O	1:C:191:GLU:HG2	2.22	0.40
2:H:68:CYS:HA	2:H:132:ALA:HB3	2.02	0.40
1:D:147:LYS:CD	1:D:148:LEU:H	2.34	0.40
2:F:143:MET:HE3	2:F:143:MET:HB3	1.95	0.40
2:G:68:CYS:HA	2:G:132:ALA:HB3	2.02	0.40
2:K:118:ARG:HH21	2:K:153:ASN:HB3	1.86	0.40
1:B:273:TYR:O	1:B:277:GLU:HG2	2.22	0.40
2:J:143:MET:HE1	2:J:152:TYR:CE1	2.57	0.40

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	261/297 (88%)	252 (97%)	9 (3%)	0	100	100
1	B	258/297 (87%)	243 (94%)	15 (6%)	0	100	100
1	C	259/297 (87%)	254 (98%)	5 (2%)	0	100	100
1	D	256/297 (86%)	247 (96%)	9 (4%)	0	100	100
2	E	132/168 (79%)	125 (95%)	6 (4%)	1 (1%)	16	44
2	F	134/168 (80%)	128 (96%)	5 (4%)	1 (1%)	18	47
2	G	142/168 (84%)	136 (96%)	6 (4%)	0	100	100
2	H	145/168 (86%)	140 (97%)	5 (3%)	0	100	100
2	I	146/168 (87%)	140 (96%)	6 (4%)	0	100	100
2	J	139/168 (83%)	133 (96%)	6 (4%)	0	100	100
2	K	139/168 (83%)	135 (97%)	4 (3%)	0	100	100
2	L	145/168 (86%)	130 (90%)	15 (10%)	0	100	100
All	All	2156/2532 (85%)	2063 (96%)	91 (4%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	52	LYS
2	F	22	SER

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	224/254 (88%)	213 (95%)	11 (5%)	22	55
1	B	221/254 (87%)	211 (96%)	10 (4%)	24	58
1	C	222/254 (87%)	214 (96%)	8 (4%)	31	66
1	D	219/254 (86%)	208 (95%)	11 (5%)	22	54
2	E	119/146 (82%)	111 (93%)	8 (7%)	15	42
2	F	121/146 (83%)	106 (88%)	15 (12%)	4	16
2	G	129/146 (88%)	119 (92%)	10 (8%)	11	35
2	H	129/146 (88%)	123 (95%)	6 (5%)	23	57
2	I	130/146 (89%)	126 (97%)	4 (3%)	35	70
2	J	125/146 (86%)	117 (94%)	8 (6%)	16	44
2	K	127/146 (87%)	116 (91%)	11 (9%)	9	30
2	L	129/146 (88%)	120 (93%)	9 (7%)	14	40
All	All	1895/2184 (87%)	1784 (94%)	111 (6%)	18	48

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	53	SER
1	A	54	ARG
1	A	57	THR
1	A	64	LEU
1	A	157	TYR
1	A	180	LYS
1	A	191	GLU
1	A	192	LYS
1	A	217	GLU
1	A	287	ASP
1	B	34	LEU
1	B	71	LEU
1	B	111	ASN
1	B	123	LEU
1	B	128	THR
1	B	147	LYS
1	B	150	GLN
1	B	179	GLU
1	B	191	GLU
1	B	286	ASP
1	C	25	ARG

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Mol	Chain	Res	Type
1	C	53	SER
1	C	147	LYS
1	C	154	LEU
1	C	179	GLU
1	C	183	LYS
1	C	187	LYS
1	C	192	LYS
1	D	54	ARG
1	D	63	GLN
1	D	71	LEU
1	D	123	LEU
1	D	147	LYS
1	D	175	GLN
1	D	176	LYS
1	D	179	GLU
1	D	180	LYS
1	D	181	GLN
1	D	228	SER
2	E	61	SER
2	E	74	ARG
2	E	78	GLU
2	E	97	SER
2	E	100	ARG
2	E	101	SER
2	E	104	ARG
2	E	118	ARG
2	F	22	SER
2	F	25	GLN
2	F	50	ASP
2	F	58	LEU
2	F	62	THR
2	F	64	LYS
2	F	74	ARG
2	F	93	GLU
2	F	96	LYS
2	F	104	ARG
2	F	126	ASN
2	F	130	VAL
2	F	136	SER
2	F	143	MET
2	F	150	LYS
2	G	24	LEU

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Mol	Chain	Res	Type
2	G	32	GLU
2	G	34	LEU
2	G	35	VAL
2	G	38	VAL
2	G	57	ARG
2	G	96	LYS
2	G	110	LEU
2	G	157	ARG
2	G	160	SER
2	H	38	VAL
2	H	47	GLN
2	H	57	ARG
2	H	126	ASN
2	H	139	ILE
2	H	163	HIS
2	I	57	ARG
2	I	100	ARG
2	I	118	ARG
2	I	130	VAL
2	J	30	GLU
2	J	35	VAL
2	J	42	SER
2	J	82	LEU
2	J	100	ARG
2	J	112	ARG
2	J	127	ASN
2	J	138	VAL
2	K	22	SER
2	K	23	SER
2	K	55	ARG
2	K	64	LYS
2	K	72	VAL
2	K	74	ARG
2	K	86	ARG
2	K	88	THR
2	K	93	GLU
2	K	134	THR
2	K	161	ARG
2	L	23	SER
2	L	38	VAL
2	L	47	GLN
2	L	52	LYS

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Mol	Chain	Res	Type
2	L	94	MET
2	L	104	ARG
2	L	109	VAL
2	L	124	ILE
2	L	126	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	108	GLN
1	A	162	ASN
1	A	188	GLN
1	A	197	GLN
1	A	264	ASN
1	A	283	GLN
1	B	135	ASN
1	B	188	GLN
1	B	232	HIS
1	B	264	ASN
1	B	266	HIS
1	C	111	ASN
1	C	209	ASN
1	C	264	ASN
1	D	35	GLN
1	D	87	GLN
1	D	100	ASN
1	D	135	ASN
1	D	158	GLN
1	D	175	GLN
1	D	189	HIS
1	D	209	ASN
1	D	264	ASN
2	E	28	GLN
2	E	73	GLN
2	E	79	GLN
2	E	102	ASN
2	E	126	ASN
2	F	25	GLN
2	F	37	ASN
2	F	73	GLN
2	F	92	GLN

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Mol	Chain	Res	Type
2	F	102	ASN
2	G	79	GLN
2	G	127	ASN
2	G	165	HIS
2	H	25	GLN
2	H	47	GLN
2	H	126	ASN
2	H	127	ASN
2	H	153	ASN
2	H	164	HIS
2	H	168	HIS
2	I	79	GLN
2	I	163	HIS
2	J	25	GLN
2	J	47	GLN
2	J	102	ASN
2	K	102	ASN
2	L	47	GLN
2	L	73	GLN
2	L	92	GLN
2	L	144	ASN
2	L	168	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	262/297 (88%)	-0.51	3 (1%) 78 70	32, 56, 89, 132	1 (0%)
1	B	260/297 (87%)	-0.40	3 (1%) 76 68	39, 60, 94, 119	0
1	C	261/297 (87%)	-0.64	2 (0%) 82 75	33, 48, 76, 121	0
1	D	258/297 (86%)	-0.50	1 (0%) 88 84	34, 55, 88, 114	0
2	E	136/168 (80%)	-0.30	2 (1%) 72 63	41, 60, 91, 108	0
2	F	138/168 (82%)	-0.28	3 (2%) 62 52	38, 62, 95, 123	0
2	G	146/168 (86%)	-0.25	4 (2%) 56 46	46, 65, 94, 113	0
2	H	147/168 (87%)	-0.31	5 (3%) 48 39	43, 58, 90, 128	0
2	I	148/168 (88%)	-0.11	4 (2%) 56 46	44, 67, 106, 135	0
2	J	143/168 (85%)	-0.12	3 (2%) 63 54	48, 70, 107, 116	0
2	K	143/168 (85%)	-0.32	3 (2%) 63 54	38, 61, 94, 105	0
2	L	147/168 (87%)	0.08	4 (2%) 56 46	45, 77, 116, 138	0
All	All	2189/2532 (86%)	-0.35	37 (1%) 69 60	32, 60, 98, 138	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	148	TRP	6.2
2	L	148	TRP	5.6
2	F	148	TRP	5.4
2	J	148	TRP	4.9
2	I	21	THR	4.8
2	K	148	TRP	4.3
2	H	115	SER	4.0
2	I	89	TYR	3.9
2	I	148	TRP	3.5
1	A	287	ASP	3.2
2	F	21	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	198	TRP	2.9
2	E	117	GLY	2.9
2	G	115	SER	2.8
2	H	164	HIS	2.8
2	G	163	HIS	2.7
2	H	116	THR	2.7
2	I	113	ALA	2.6
2	K	165	HIS	2.6
2	L	165	HIS	2.6
1	A	28[A]	GLU	2.5
1	C	25	ARG	2.4
2	L	164	HIS	2.4
1	D	177	LEU	2.4
1	B	28	GLU	2.4
2	J	113	ALA	2.3
2	F	160	SER	2.3
2	H	114	GLY	2.3
2	K	117	GLY	2.2
2	L	168	HIS	2.2
1	C	200	TRP	2.2
2	G	164	HIS	2.1
1	A	26	LYS	2.1
1	B	285	GLN	2.1
2	G	116	THR	2.1
2	J	165	HIS	2.0
2	H	148	TRP	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 oligosaccharides 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.