Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 10:11 AM JST

PDB ID	:	8XUP
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:

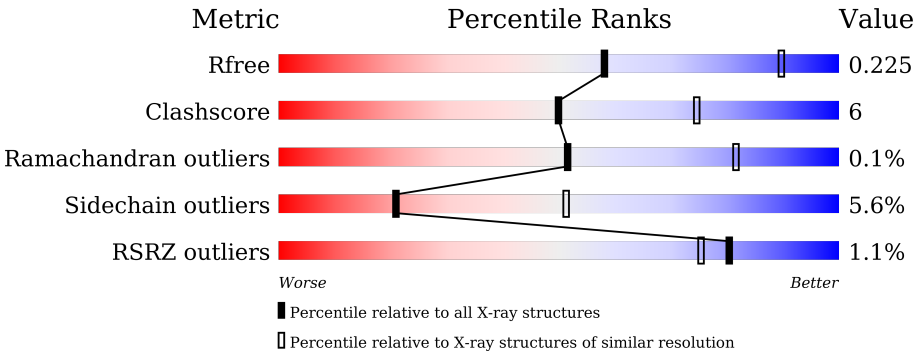
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	79% 8% • 12%
1	B	297	% 74% 12% • 12%
1	C	297	78% 9% • 12%
1	D	297	77% 9% • 13%
2	E	168	% 65% 14% • 19%
2	F	168	2% 60% 17% 5% • 18%

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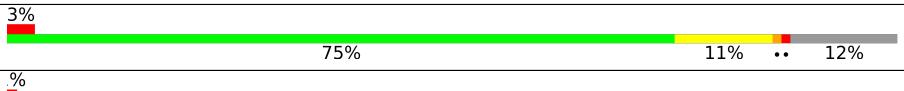
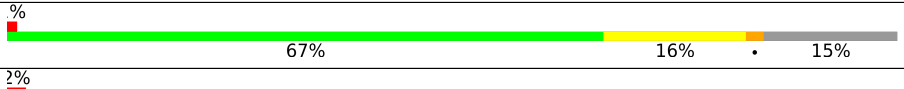
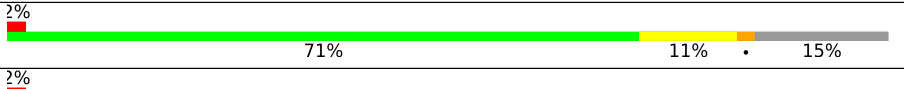
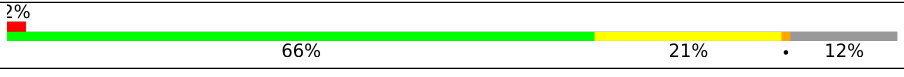
Mol	Chain	Length	Quality of chain
2	G	168	
2	H	168	
2	I	168	
2	J	168	
2	K	168	
2	L	168	

2 Entry composition (i)

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

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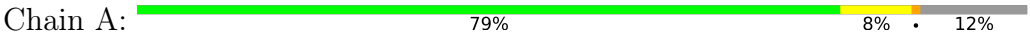
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	17	Total O 17 17	0	0
3	K	22	Total O 22 22	0	0
3	L	7	Total O 7 7	0	0

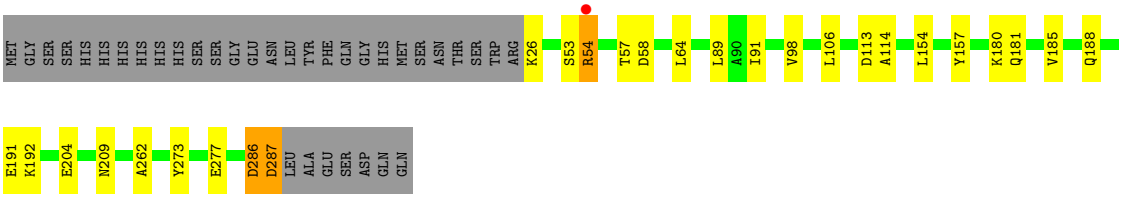
3 Residue-property plots (i)

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

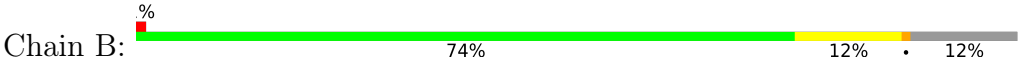
Chain A:

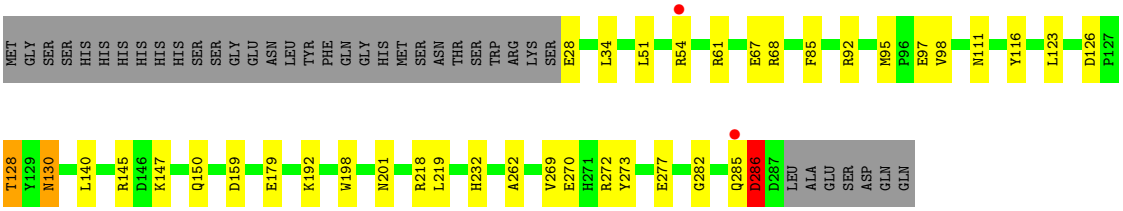




• Molecule 1: Lipoprotein NlpI

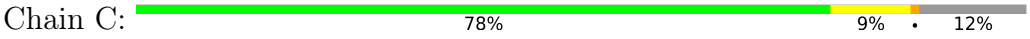
Chain B:

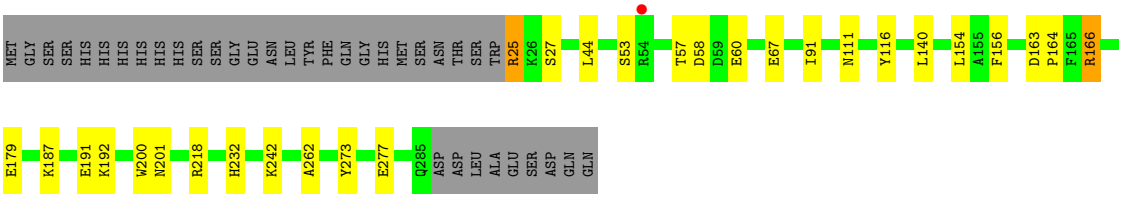




• Molecule 1: Lipoprotein NlpI

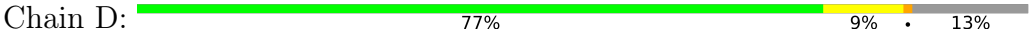
Chain C:

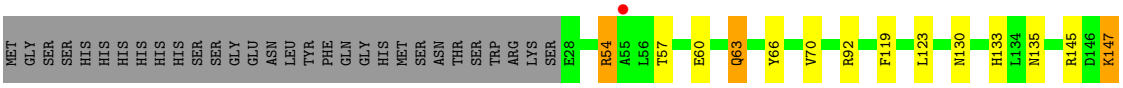


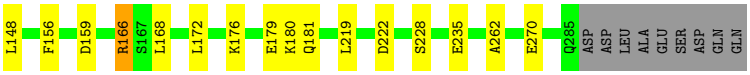


• Molecule 1: Lipoprotein NlpI

Chain D:

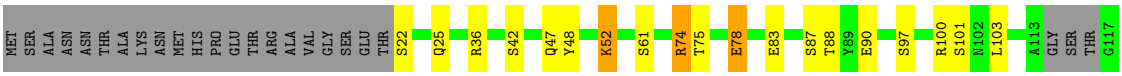






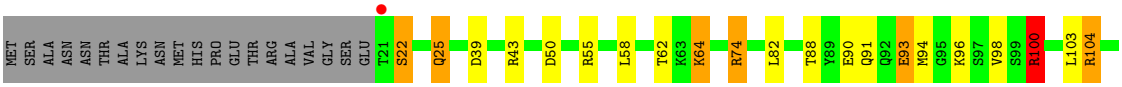
• Molecule 2: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase

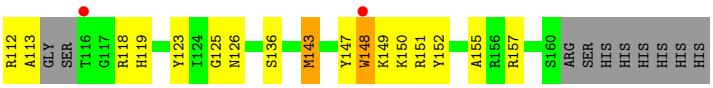
Chain E:



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

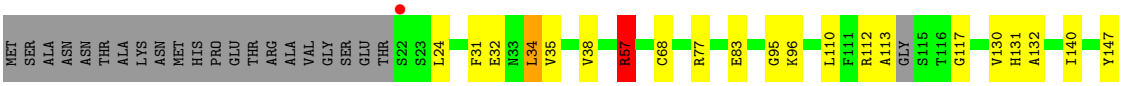
Chain F:





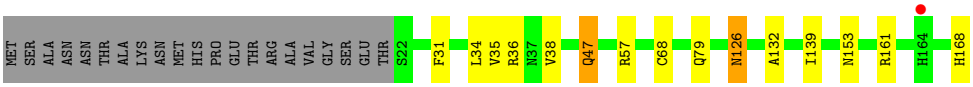
• Molecule 2: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase

Chain G:



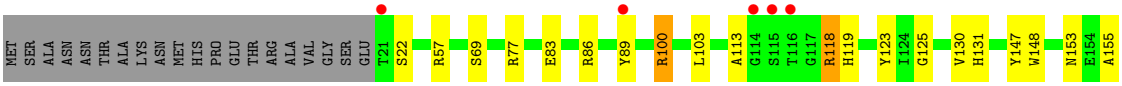
• Molecule 2: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase

Chain H:



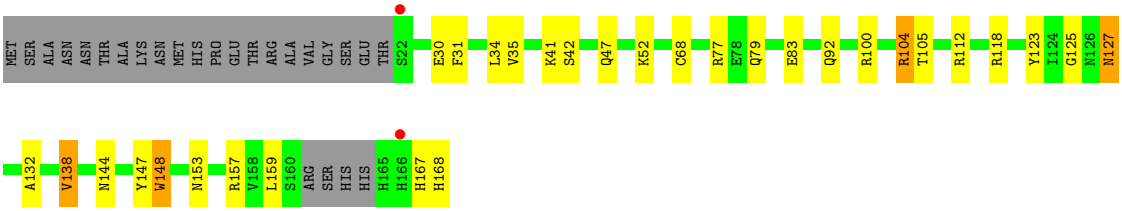
• Molecule 2: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase

Chain I:



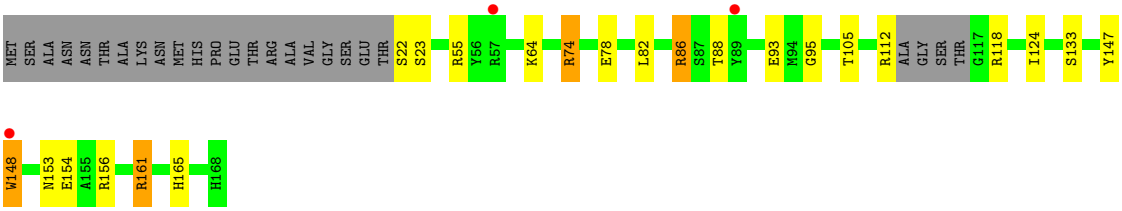
• Molecule 2: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase

Chain J:



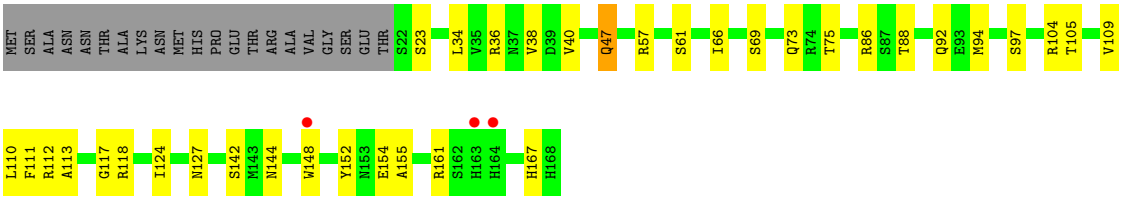
• Molecule 2: Murein DD-endopeptidase MepS/Murein LD-carboxypeptidase

Chain K:



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

Chain L:



4 Data and refinement statistics (i)

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 29.68 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.70-2.80) 99.4 (29.68-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [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 (5.05%)	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 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.39	0/2175	0.71	0/2951
1	B	0.42	0/2151	0.75	2/2920 (0.1%)
1	C	0.41	0/2161	0.72	0/2931
1	D	0.43	1/2135 (0.0%)	0.70	1/2898 (0.0%)
2	E	0.71	5/1114 (0.4%)	0.80	1/1492 (0.1%)
2	F	0.58	2/1128 (0.2%)	0.75	1/1512 (0.1%)
2	G	0.35	0/1210	0.78	0/1622
2	H	0.41	0/1215	0.71	0/1630
2	I	0.37	0/1222	0.70	0/1640
2	J	0.69	5/1175 (0.4%)	0.84	4/1575 (0.3%)
2	K	0.48	1/1192 (0.1%)	0.78	0/1597
2	L	0.65	3/1215 (0.2%)	0.75	1/1630 (0.1%)
All	All	0.48	17/18093 (0.1%)	0.74	10/24398 (0.0%)

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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	148	TRP	CG-CD2	14.22	1.67	1.43
2	L	148	TRP	CD2-CE2	11.59	1.55	1.41
2	J	148	TRP	CG-CD2	11.34	1.62	1.43
2	L	148	TRP	CZ3-CH2	10.04	1.56	1.40
2	F	148	TRP	CD2-CE2	9.57	1.52	1.41
2	F	148	TRP	CZ3-CH2	8.25	1.53	1.40
2	J	148	TRP	CB-CG	8.15	1.65	1.50
2	J	148	TRP	CD1-NE1	7.60	1.50	1.38
2	E	148	TRP	CD2-CE2	6.62	1.49	1.41
2	E	148	TRP	CD1-NE1	6.08	1.48	1.38
2	E	148	TRP	CB-CG	5.83	1.60	1.50
2	K	148	TRP	CZ3-CH2	5.71	1.49	1.40
2	L	148	TRP	CE2-CZ2	5.71	1.49	1.39
2	J	148	TRP	CD2-CE2	5.41	1.47	1.41
2	E	148	TRP	CE3-CZ3	5.27	1.47	1.38
2	J	148	TRP	CG-CD1	5.16	1.44	1.36
1	D	235	GLU	CD-OE2	5.02	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	148	TRP	CD1-CG-CD2	-12.81	96.06	106.30
2	E	148	TRP	CD1-NE1-CE2	7.70	115.93	109.00
2	J	148	TRP	CE2-CD2-CG	7.00	112.90	107.30
2	J	148	TRP	CG-CD2-CE3	-6.04	128.47	133.90
1	B	286	ASP	CB-CA-C	5.73	121.86	110.40
2	L	148	TRP	CH2-CZ2-CE2	-5.39	112.01	117.40
2	F	148	TRP	CH2-CZ2-CE2	-5.34	112.06	117.40
2	J	148	TRP	CG-CD1-NE1	5.22	115.32	110.10
1	B	130	ASN	CB-CA-C	-5.17	100.07	110.40
1	D	145	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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
1	B	68	ARG	Sidechain
1	C	166	ARG	Sidechain
1	C	25	ARG	Sidechain

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Mol	Chain	Res	Type	Group
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 (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	2131	0	2053	13	0
1	B	2107	0	2030	29	0
1	C	2117	0	2053	18	0
1	D	2091	0	2022	20	0
2	E	1096	0	1077	20	0
2	F	1110	0	1091	30	0
2	G	1186	0	1149	13	0
2	H	1190	0	1153	7	0
2	I	1197	0	1160	16	0
2	J	1153	0	1120	20	0
2	K	1168	0	1132	12	0
2	L	1190	0	1153	21	0
3	A	48	0	0	0	0
3	B	37	0	0	1	0
3	C	59	0	0	1	0
3	D	42	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
3	K	22	0	0	1	0
3	L	7	0	0	0	0
All	All	18080	0	17193	201	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 (201) 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
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:CG	2:F:74:ARG:HH11	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: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
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:H:126:ASN:HD22	2:H:126:ASN:N	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:52:LYS:HA	2:J:138:VAL:HG22	1.81	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:E:42:SER:HG	2:J:31:PHE:HD1	1.49	0.59
2:L:112:ARG:HB3	2:L:112:ARG:HH11	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:143:MET:O	2:F:149:LYS:HB3	2.04	0.57
1:B:92:ARG:O	1:B:95:MET:HE2	2.04	0.56
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: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:C:242:LYS:NZ	1:C:277:GLU:OE1	2.32	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
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: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:94:MET:CE	2:F:94:MET:HA	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:160:SER:C	3:E:204:HOH:O	2.48	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: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
2:G:34:LEU:HD12	2:G:34:LEU:C	2.32	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: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
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:D:270:GLU:CD	2:L:167:HIS:HE2	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:156:PHE:CD2	1:D:166:ARG:HG2	2.51	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:HG2	1:B:272:ARG:HH11	1.81	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
1:A:89:LEU:HB2	1:A:98:VAL:HG11	1.98	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:L:110:LEU:HD22	2:L:110:LEU:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:262:ALA:HB1	1:D:262:ALA:HB1	2.02	0.42
2:L:154:GLU:HG2	2:L:155:ALA:N	2.35	0.42
1:A:154:LEU:HD23	1:A:154:LEU:O	2.20	0.42
2:E:87:SER:OG	2:E:90:GLU:HG3	2.19	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: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:B:270:GLU:CD	2:J:167:HIS:HE2	2.24	0.41
1:D:219:LEU:C	1:D:219:LEU:HD23	2.41	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:B:285:GLN:CG	1:B:286:ASP:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

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	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%)	19	49
2	F	134/168 (80%)	128 (96%)	5 (4%)	1 (1%)	22	53
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	51 81

All (2) Ramachandran outliers are listed below:

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

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	224/254 (88%)	213 (95%)	11 (5%)	25 57
1	B	221/254 (87%)	213 (96%)	8 (4%)	35 69
1	C	222/254 (87%)	216 (97%)	6 (3%)	44 78
1	D	219/254 (86%)	210 (96%)	9 (4%)	30 64
2	E	119/146 (82%)	111 (93%)	8 (7%)	16 43
2	F	121/146 (83%)	106 (88%)	15 (12%)	4 14
2	G	129/146 (88%)	119 (92%)	10 (8%)	12 35
2	H	129/146 (88%)	124 (96%)	5 (4%)	32 66
2	I	130/146 (89%)	122 (94%)	8 (6%)	18 47
2	J	125/146 (86%)	118 (94%)	7 (6%)	21 51
2	K	127/146 (87%)	117 (92%)	10 (8%)	12 34
2	L	129/146 (88%)	120 (93%)	9 (7%)	15 40
All	All	1895/2184 (87%)	1789 (94%)	106 (6%)	21 51

All (106) 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	113	ASP
1	A	157	TYR
1	A	180	LYS
1	A	191	GLU
1	A	192	LYS
1	A	287	ASP
1	B	34	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	286	ASP
1	C	25	ARG
1	C	53	SER
1	C	111	ASN
1	C	154	LEU
1	C	179	GLU
1	C	192	LYS
1	D	54	ARG
1	D	63	GLN
1	D	123	LEU
1	D	147	LYS
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	118	ARG
2	E	131	HIS
2	F	22	SER

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Mol	Chain	Res	Type
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	100	ARG
2	F	104	ARG
2	F	126	ASN
2	F	136	SER
2	F	143	MET
2	F	150	LYS
2	G	24	LEU
2	G	32	GLU
2	G	34	LEU
2	G	38	VAL
2	G	57	ARG
2	G	96	LYS
2	G	110	LEU
2	G	131	HIS
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	I	57	ARG
2	I	89	TYR
2	I	100	ARG
2	I	118	ARG
2	I	130	VAL
2	I	131	HIS
2	I	161	ARG
2	I	163	HIS
2	J	30	GLU
2	J	42	SER
2	J	100	ARG
2	J	112	ARG
2	J	127	ASN

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Mol	Chain	Res	Type
2	J	138	VAL
2	J	153	ASN
2	K	22	SER
2	K	23	SER
2	K	55	ARG
2	K	64	LYS
2	K	74	ARG
2	K	86	ARG
2	K	88	THR
2	K	93	GLU
2	K	133	SER
2	K	161	ARG
2	L	23	SER
2	L	38	VAL
2	L	47	GLN
2	L	94	MET
2	L	97	SER
2	L	104	ARG
2	L	109	VAL
2	L	124	ILE
2	L	142	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	GLN
1	A	264	ASN
1	B	135	ASN
1	B	209	ASN
1	B	264	ASN
1	C	111	ASN
1	C	209	ASN
1	C	264	ASN
1	D	87	GLN
1	D	135	ASN
1	D	158	GLN
1	D	209	ASN
1	D	264	ASN
2	F	25	GLN
2	F	102	ASN
2	G	79	GLN
2	G	102	ASN

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Mol	Chain	Res	Type
2	H	25	GLN
2	H	47	GLN
2	H	126	ASN
2	H	144	ASN
2	H	164	HIS
2	H	168	HIS
2	I	128	GLN
2	I	153	ASN
2	I	163	HIS
2	J	25	GLN
2	J	47	GLN
2	K	73	GLN
2	L	25	GLN
2	L	47	GLN
2	L	73	GLN
2	L	92	GLN
2	L	144	ASN
2	L	168	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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^{th} 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%)	-0.45	1 (0%)	92	91	32, 56, 89, 132	0
1	B	260/297 (87%)	-0.36	2 (0%)	86	81	39, 60, 94, 119	0
1	C	261/297 (87%)	-0.53	1 (0%)	92	91	33, 48, 76, 121	0
1	D	258/297 (86%)	-0.43	1 (0%)	92	91	34, 55, 88, 114	0
2	E	136/168 (80%)	-0.39	1 (0%)	87	84	41, 60, 91, 108	0
2	F	138/168 (82%)	-0.31	3 (2%)	62	52	38, 62, 95, 123	0
2	G	146/168 (86%)	-0.37	2 (1%)	75	70	46, 65, 94, 113	0
2	H	147/168 (87%)	-0.43	1 (0%)	87	84	43, 58, 90, 128	0
2	I	148/168 (88%)	-0.26	5 (3%)	45	35	44, 67, 106, 135	0
2	J	143/168 (85%)	-0.31	2 (1%)	75	70	48, 70, 107, 116	0
2	K	143/168 (85%)	-0.39	3 (2%)	63	54	38, 61, 94, 105	0
2	L	147/168 (87%)	-0.18	3 (2%)	65	56	45, 77, 116, 138	0
All	All	2189/2532 (86%)	-0.38	25 (1%)	80	75	32, 60, 98, 138	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	115	SER	5.3
2	I	89	TYR	4.5
2	I	116	THR	4.0
2	J	166	HIS	3.8
2	G	22	SER	3.6
2	L	164	HIS	3.4
2	F	116	THR	3.4
2	E	148	TRP	2.8
2	H	164	HIS	2.8
2	I	21	THR	2.6
1	B	54	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	I	114	GLY	2.5
1	B	285	GLN	2.5
1	A	54	ARG	2.5
2	L	148	TRP	2.4
1	C	54	ARG	2.4
2	F	148	TRP	2.4
2	K	57	ARG	2.3
2	G	164	HIS	2.3
2	J	22	SER	2.2
2	K	148	TRP	2.2
1	D	55	ALA	2.2
2	F	21	THR	2.1
2	L	163	HIS	2.1
2	K	89	TYR	2.1

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.