



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2026 – 04:19 PM JST

PDB ID : 21KU / pdb_000021ku
Title : Structure of Pseudomonas aeruginosa mutant ClpP2-R140A
Authors : Zhao, N.; Bao, R.
Deposited on : 2025-12-17
Resolution : 3.00 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 Phenix2.2
Xtriage (Phenix) : 2.2
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

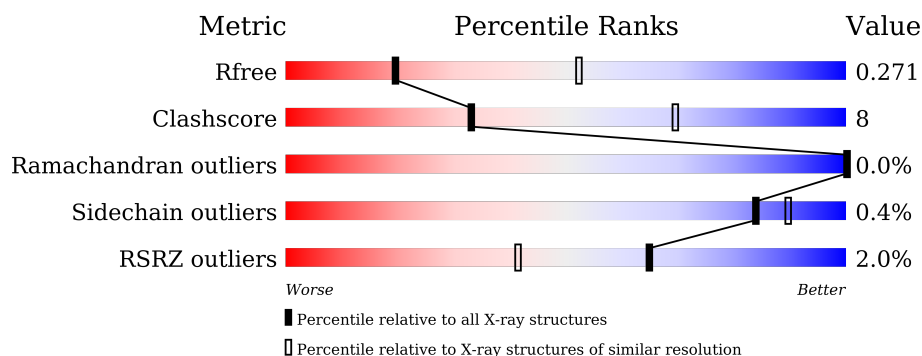
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	207	% 71% 15% 14%
1	B	207	% 70% 17% 13%
1	C	207	3% 62% 22% • 15%
1	D	207	% 69% 19% 12%
1	E	207	% 74% 13% 13%
1	F	207	71% 15% 14%

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Mol	Chain	Length	Quality of chain
1	G	207	
1	H	207	
1	I	207	
1	J	207	
1	K	207	
1	L	207	
1	M	207	
1	N	207	
1	O	207	
1	P	207	
1	Q	207	
1	R	207	
1	S	207	
1	T	207	
1	U	207	
1	V	207	
1	W	207	
1	X	207	
1	Y	207	
1	Z	207	
1	a	207	
1	b	207	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 39105 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 ATP-dependent Clp protease proteolytic subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	179	Total	C	N	O	S	0	0	0
			1391	883	238	264	6			
1	Z	182	Total	C	N	O	S	0	0	0
			1408	894	241	267	6			
1	A	177	Total	C	N	O	S	0	0	0
			1377	874	235	262	6			
1	B	181	Total	C	N	O	S	0	0	0
			1403	891	240	266	6			
1	C	176	Total	C	N	O	S	0	0	0
			1369	868	234	261	6			
1	D	183	Total	C	N	O	S	0	0	0
			1412	896	242	268	6			
1	E	181	Total	C	N	O	S	0	0	0
			1403	891	240	266	6			
1	F	179	Total	C	N	O	S	0	0	0
			1391	883	238	264	6			
1	G	176	Total	C	N	O	S	0	0	0
			1369	868	234	261	6			
1	H	181	Total	C	N	O	S	0	0	0
			1403	891	240	266	6			
1	I	176	Total	C	N	O	S	0	0	0
			1369	868	234	261	6			
1	J	180	Total	C	N	O	S	0	0	0
			1395	885	239	265	6			
1	K	176	Total	C	N	O	S	0	0	0
			1369	868	234	261	6			
1	L	178	Total	C	N	O	S	0	0	0
			1386	880	237	263	6			
1	M	178	Total	C	N	O	S	0	0	0
			1386	880	237	263	6			
1	N	178	Total	C	N	O	S	0	0	0
			1386	880	237	263	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	179	Total	C	N	O	S	0	0	0
			1391	883	238	264	6			
1	P	180	Total	C	N	O	S	0	0	0
			1395	885	239	265	6			
1	Q	178	Total	C	N	O	S	0	0	0
			1386	880	237	263	6			
1	S	178	Total	C	N	O	S	0	0	0
			1386	880	237	263	6			
1	T	181	Total	C	N	O	S	0	0	0
			1403	891	240	266	6			
1	U	178	Total	C	N	O	S	0	0	0
			1386	880	237	263	6			
1	V	176	Total	C	N	O	S	0	0	0
			1369	868	234	261	6			
1	W	183	Total	C	N	O	S	0	0	0
			1412	896	242	268	6			
1	X	179	Total	C	N	O	S	0	0	0
			1391	883	238	264	6			
1	Y	181	Total	C	N	O	S	0	0	0
			1403	891	240	266	6			
1	a	177	Total	C	N	O	S	0	0	0
			1377	874	235	262	6			
1	b	181	Total	C	N	O	S	0	0	0
			1403	891	240	266	6			

There are 196 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-5	HIS	-	expression tag	UNP Q9HYR9
R	-4	HIS	-	expression tag	UNP Q9HYR9
R	-3	HIS	-	expression tag	UNP Q9HYR9
R	-2	HIS	-	expression tag	UNP Q9HYR9
R	-1	HIS	-	expression tag	UNP Q9HYR9
R	0	HIS	-	expression tag	UNP Q9HYR9
R	140	ALA	ARG	engineered mutation	UNP Q9HYR9
Z	-5	HIS	-	expression tag	UNP Q9HYR9
Z	-4	HIS	-	expression tag	UNP Q9HYR9
Z	-3	HIS	-	expression tag	UNP Q9HYR9
Z	-2	HIS	-	expression tag	UNP Q9HYR9
Z	-1	HIS	-	expression tag	UNP Q9HYR9
Z	0	HIS	-	expression tag	UNP Q9HYR9
Z	140	ALA	ARG	engineered mutation	UNP Q9HYR9
A	-5	HIS	-	expression tag	UNP Q9HYR9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	expression tag	UNP Q9HYR9
A	-3	HIS	-	expression tag	UNP Q9HYR9
A	-2	HIS	-	expression tag	UNP Q9HYR9
A	-1	HIS	-	expression tag	UNP Q9HYR9
A	0	HIS	-	expression tag	UNP Q9HYR9
A	140	ALA	ARG	engineered mutation	UNP Q9HYR9
B	-5	HIS	-	expression tag	UNP Q9HYR9
B	-4	HIS	-	expression tag	UNP Q9HYR9
B	-3	HIS	-	expression tag	UNP Q9HYR9
B	-2	HIS	-	expression tag	UNP Q9HYR9
B	-1	HIS	-	expression tag	UNP Q9HYR9
B	0	HIS	-	expression tag	UNP Q9HYR9
B	140	ALA	ARG	engineered mutation	UNP Q9HYR9
C	-5	HIS	-	expression tag	UNP Q9HYR9
C	-4	HIS	-	expression tag	UNP Q9HYR9
C	-3	HIS	-	expression tag	UNP Q9HYR9
C	-2	HIS	-	expression tag	UNP Q9HYR9
C	-1	HIS	-	expression tag	UNP Q9HYR9
C	0	HIS	-	expression tag	UNP Q9HYR9
C	140	ALA	ARG	engineered mutation	UNP Q9HYR9
D	-5	HIS	-	expression tag	UNP Q9HYR9
D	-4	HIS	-	expression tag	UNP Q9HYR9
D	-3	HIS	-	expression tag	UNP Q9HYR9
D	-2	HIS	-	expression tag	UNP Q9HYR9
D	-1	HIS	-	expression tag	UNP Q9HYR9
D	0	HIS	-	expression tag	UNP Q9HYR9
D	140	ALA	ARG	engineered mutation	UNP Q9HYR9
E	-5	HIS	-	expression tag	UNP Q9HYR9
E	-4	HIS	-	expression tag	UNP Q9HYR9
E	-3	HIS	-	expression tag	UNP Q9HYR9
E	-2	HIS	-	expression tag	UNP Q9HYR9
E	-1	HIS	-	expression tag	UNP Q9HYR9
E	0	HIS	-	expression tag	UNP Q9HYR9
E	140	ALA	ARG	engineered mutation	UNP Q9HYR9
F	-5	HIS	-	expression tag	UNP Q9HYR9
F	-4	HIS	-	expression tag	UNP Q9HYR9
F	-3	HIS	-	expression tag	UNP Q9HYR9
F	-2	HIS	-	expression tag	UNP Q9HYR9
F	-1	HIS	-	expression tag	UNP Q9HYR9
F	0	HIS	-	expression tag	UNP Q9HYR9
F	140	ALA	ARG	engineered mutation	UNP Q9HYR9
G	-5	HIS	-	expression tag	UNP Q9HYR9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	HIS	-	expression tag	UNP Q9HYR9
G	-3	HIS	-	expression tag	UNP Q9HYR9
G	-2	HIS	-	expression tag	UNP Q9HYR9
G	-1	HIS	-	expression tag	UNP Q9HYR9
G	0	HIS	-	expression tag	UNP Q9HYR9
G	140	ALA	ARG	engineered mutation	UNP Q9HYR9
H	-5	HIS	-	expression tag	UNP Q9HYR9
H	-4	HIS	-	expression tag	UNP Q9HYR9
H	-3	HIS	-	expression tag	UNP Q9HYR9
H	-2	HIS	-	expression tag	UNP Q9HYR9
H	-1	HIS	-	expression tag	UNP Q9HYR9
H	0	HIS	-	expression tag	UNP Q9HYR9
H	140	ALA	ARG	engineered mutation	UNP Q9HYR9
I	-5	HIS	-	expression tag	UNP Q9HYR9
I	-4	HIS	-	expression tag	UNP Q9HYR9
I	-3	HIS	-	expression tag	UNP Q9HYR9
I	-2	HIS	-	expression tag	UNP Q9HYR9
I	-1	HIS	-	expression tag	UNP Q9HYR9
I	0	HIS	-	expression tag	UNP Q9HYR9
I	140	ALA	ARG	engineered mutation	UNP Q9HYR9
J	-5	HIS	-	expression tag	UNP Q9HYR9
J	-4	HIS	-	expression tag	UNP Q9HYR9
J	-3	HIS	-	expression tag	UNP Q9HYR9
J	-2	HIS	-	expression tag	UNP Q9HYR9
J	-1	HIS	-	expression tag	UNP Q9HYR9
J	0	HIS	-	expression tag	UNP Q9HYR9
J	140	ALA	ARG	engineered mutation	UNP Q9HYR9
K	-5	HIS	-	expression tag	UNP Q9HYR9
K	-4	HIS	-	expression tag	UNP Q9HYR9
K	-3	HIS	-	expression tag	UNP Q9HYR9
K	-2	HIS	-	expression tag	UNP Q9HYR9
K	-1	HIS	-	expression tag	UNP Q9HYR9
K	0	HIS	-	expression tag	UNP Q9HYR9
K	140	ALA	ARG	engineered mutation	UNP Q9HYR9
L	-5	HIS	-	expression tag	UNP Q9HYR9
L	-4	HIS	-	expression tag	UNP Q9HYR9
L	-3	HIS	-	expression tag	UNP Q9HYR9
L	-2	HIS	-	expression tag	UNP Q9HYR9
L	-1	HIS	-	expression tag	UNP Q9HYR9
L	0	HIS	-	expression tag	UNP Q9HYR9
L	140	ALA	ARG	engineered mutation	UNP Q9HYR9
M	-5	HIS	-	expression tag	UNP Q9HYR9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-4	HIS	-	expression tag	UNP Q9HYR9
M	-3	HIS	-	expression tag	UNP Q9HYR9
M	-2	HIS	-	expression tag	UNP Q9HYR9
M	-1	HIS	-	expression tag	UNP Q9HYR9
M	0	HIS	-	expression tag	UNP Q9HYR9
M	140	ALA	ARG	engineered mutation	UNP Q9HYR9
N	-5	HIS	-	expression tag	UNP Q9HYR9
N	-4	HIS	-	expression tag	UNP Q9HYR9
N	-3	HIS	-	expression tag	UNP Q9HYR9
N	-2	HIS	-	expression tag	UNP Q9HYR9
N	-1	HIS	-	expression tag	UNP Q9HYR9
N	0	HIS	-	expression tag	UNP Q9HYR9
N	140	ALA	ARG	engineered mutation	UNP Q9HYR9
O	-5	HIS	-	expression tag	UNP Q9HYR9
O	-4	HIS	-	expression tag	UNP Q9HYR9
O	-3	HIS	-	expression tag	UNP Q9HYR9
O	-2	HIS	-	expression tag	UNP Q9HYR9
O	-1	HIS	-	expression tag	UNP Q9HYR9
O	0	HIS	-	expression tag	UNP Q9HYR9
O	140	ALA	ARG	engineered mutation	UNP Q9HYR9
P	-5	HIS	-	expression tag	UNP Q9HYR9
P	-4	HIS	-	expression tag	UNP Q9HYR9
P	-3	HIS	-	expression tag	UNP Q9HYR9
P	-2	HIS	-	expression tag	UNP Q9HYR9
P	-1	HIS	-	expression tag	UNP Q9HYR9
P	0	HIS	-	expression tag	UNP Q9HYR9
P	140	ALA	ARG	engineered mutation	UNP Q9HYR9
Q	-5	HIS	-	expression tag	UNP Q9HYR9
Q	-4	HIS	-	expression tag	UNP Q9HYR9
Q	-3	HIS	-	expression tag	UNP Q9HYR9
Q	-2	HIS	-	expression tag	UNP Q9HYR9
Q	-1	HIS	-	expression tag	UNP Q9HYR9
Q	0	HIS	-	expression tag	UNP Q9HYR9
Q	140	ALA	ARG	engineered mutation	UNP Q9HYR9
S	-5	HIS	-	expression tag	UNP Q9HYR9
S	-4	HIS	-	expression tag	UNP Q9HYR9
S	-3	HIS	-	expression tag	UNP Q9HYR9
S	-2	HIS	-	expression tag	UNP Q9HYR9
S	-1	HIS	-	expression tag	UNP Q9HYR9
S	0	HIS	-	expression tag	UNP Q9HYR9
S	140	ALA	ARG	engineered mutation	UNP Q9HYR9
T	-5	HIS	-	expression tag	UNP Q9HYR9

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-4	HIS	-	expression tag	UNP Q9HYR9
T	-3	HIS	-	expression tag	UNP Q9HYR9
T	-2	HIS	-	expression tag	UNP Q9HYR9
T	-1	HIS	-	expression tag	UNP Q9HYR9
T	0	HIS	-	expression tag	UNP Q9HYR9
T	140	ALA	ARG	engineered mutation	UNP Q9HYR9
U	-5	HIS	-	expression tag	UNP Q9HYR9
U	-4	HIS	-	expression tag	UNP Q9HYR9
U	-3	HIS	-	expression tag	UNP Q9HYR9
U	-2	HIS	-	expression tag	UNP Q9HYR9
U	-1	HIS	-	expression tag	UNP Q9HYR9
U	0	HIS	-	expression tag	UNP Q9HYR9
U	140	ALA	ARG	engineered mutation	UNP Q9HYR9
V	-5	HIS	-	expression tag	UNP Q9HYR9
V	-4	HIS	-	expression tag	UNP Q9HYR9
V	-3	HIS	-	expression tag	UNP Q9HYR9
V	-2	HIS	-	expression tag	UNP Q9HYR9
V	-1	HIS	-	expression tag	UNP Q9HYR9
V	0	HIS	-	expression tag	UNP Q9HYR9
V	140	ALA	ARG	engineered mutation	UNP Q9HYR9
W	-5	HIS	-	expression tag	UNP Q9HYR9
W	-4	HIS	-	expression tag	UNP Q9HYR9
W	-3	HIS	-	expression tag	UNP Q9HYR9
W	-2	HIS	-	expression tag	UNP Q9HYR9
W	-1	HIS	-	expression tag	UNP Q9HYR9
W	0	HIS	-	expression tag	UNP Q9HYR9
W	140	ALA	ARG	engineered mutation	UNP Q9HYR9
X	-5	HIS	-	expression tag	UNP Q9HYR9
X	-4	HIS	-	expression tag	UNP Q9HYR9
X	-3	HIS	-	expression tag	UNP Q9HYR9
X	-2	HIS	-	expression tag	UNP Q9HYR9
X	-1	HIS	-	expression tag	UNP Q9HYR9
X	0	HIS	-	expression tag	UNP Q9HYR9
X	140	ALA	ARG	engineered mutation	UNP Q9HYR9
Y	-5	HIS	-	expression tag	UNP Q9HYR9
Y	-4	HIS	-	expression tag	UNP Q9HYR9
Y	-3	HIS	-	expression tag	UNP Q9HYR9
Y	-2	HIS	-	expression tag	UNP Q9HYR9
Y	-1	HIS	-	expression tag	UNP Q9HYR9
Y	0	HIS	-	expression tag	UNP Q9HYR9
Y	140	ALA	ARG	engineered mutation	UNP Q9HYR9
a	-5	HIS	-	expression tag	UNP Q9HYR9

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Chain	Residue	Modelled	Actual	Comment	Reference
a	-4	HIS	-	expression tag	UNP Q9HYR9
a	-3	HIS	-	expression tag	UNP Q9HYR9
a	-2	HIS	-	expression tag	UNP Q9HYR9
a	-1	HIS	-	expression tag	UNP Q9HYR9
a	0	HIS	-	expression tag	UNP Q9HYR9
a	140	ALA	ARG	engineered mutation	UNP Q9HYR9
b	-5	HIS	-	expression tag	UNP Q9HYR9
b	-4	HIS	-	expression tag	UNP Q9HYR9
b	-3	HIS	-	expression tag	UNP Q9HYR9
b	-2	HIS	-	expression tag	UNP Q9HYR9
b	-1	HIS	-	expression tag	UNP Q9HYR9
b	0	HIS	-	expression tag	UNP Q9HYR9
b	140	ALA	ARG	engineered mutation	UNP Q9HYR9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	R	6	Total O 6 6	0	0
2	Z	11	Total O 11 11	0	0
2	A	7	Total O 7 7	0	0
2	B	5	Total O 5 5	0	0
2	C	7	Total O 7 7	0	0
2	D	4	Total O 4 4	0	0
2	E	6	Total O 6 6	0	0
2	F	10	Total O 10 10	0	0
2	G	6	Total O 6 6	0	0
2	H	4	Total O 4 4	0	0
2	I	4	Total O 4 4	0	0
2	J	4	Total O 4 4	0	0
2	K	6	Total O 6 6	0	0

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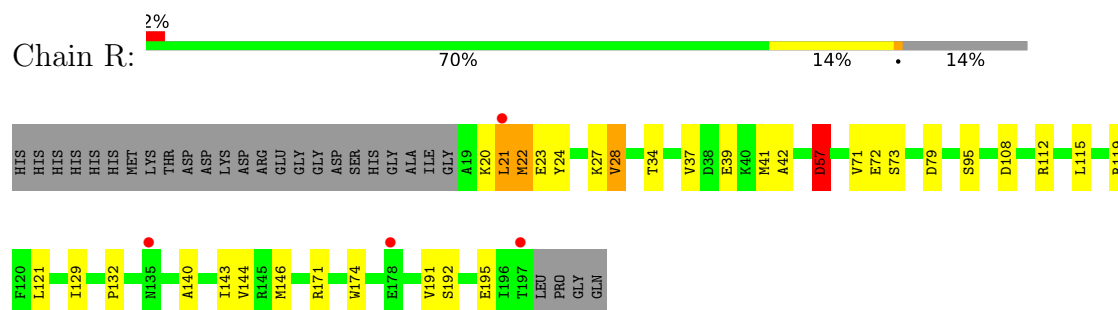
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	7	Total O 7 7	0	0
2	M	9	Total O 9 9	0	0
2	N	5	Total O 5 5	0	0
2	O	7	Total O 7 7	0	0
2	P	6	Total O 6 6	0	0
2	Q	5	Total O 5 5	0	0
2	S	11	Total O 11 11	0	0
2	T	4	Total O 4 4	0	0
2	U	9	Total O 9 9	0	0
2	V	7	Total O 7 7	0	0
2	W	7	Total O 7 7	0	0
2	X	6	Total O 6 6	0	0
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2	a	10	Total O 10 10	0	0
2	b	6	Total O 6 6	0	0

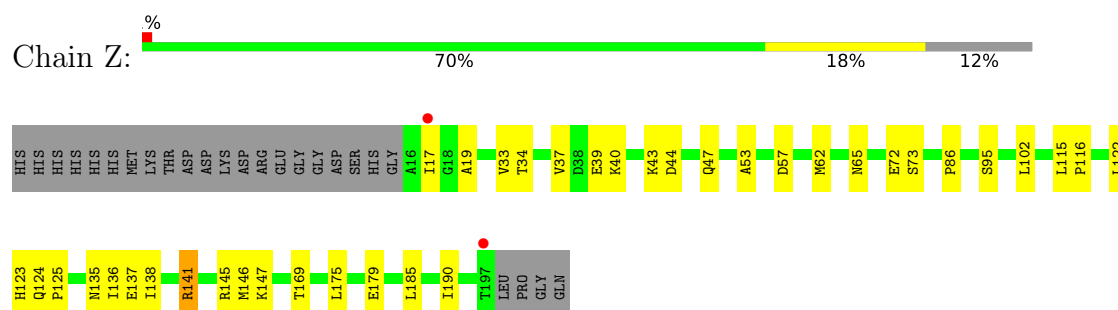
3 Residue-property plots [i](#)

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.

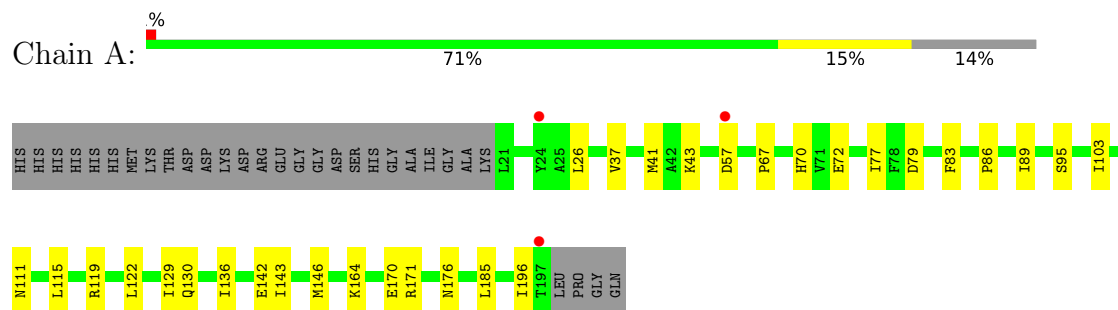
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



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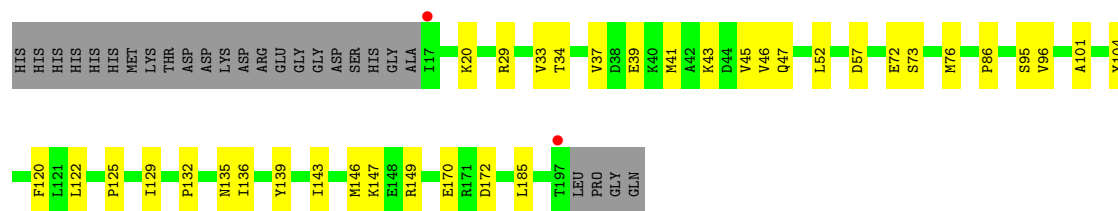


- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

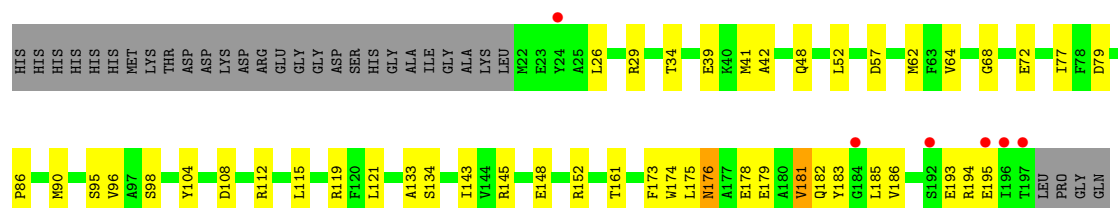


- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

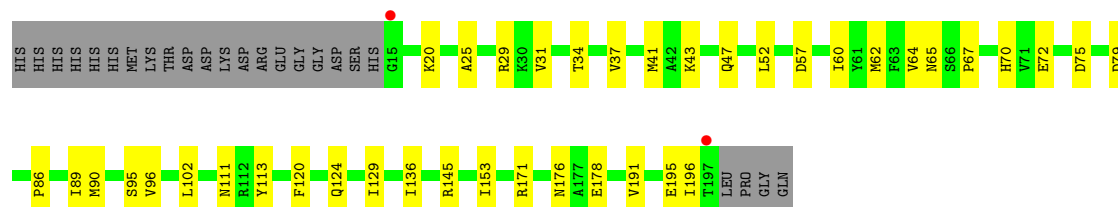




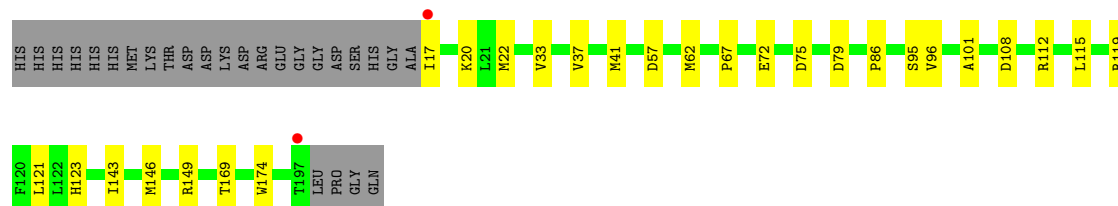
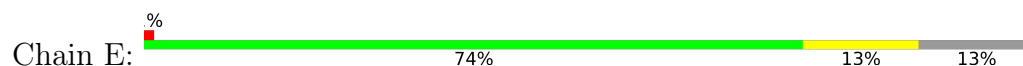
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



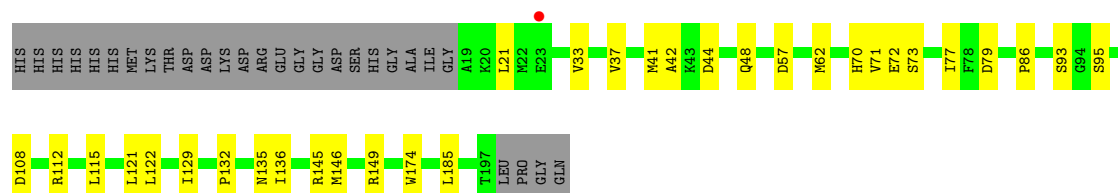
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

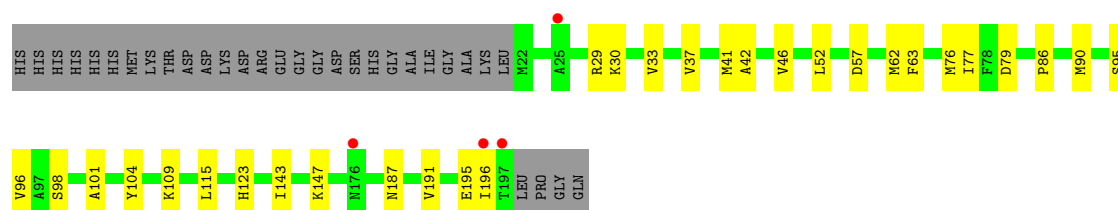


- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



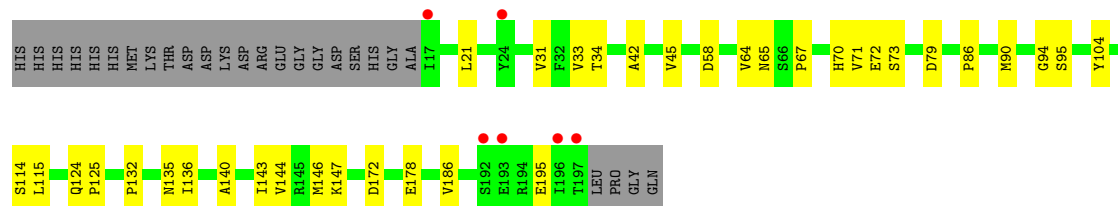
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain G: 



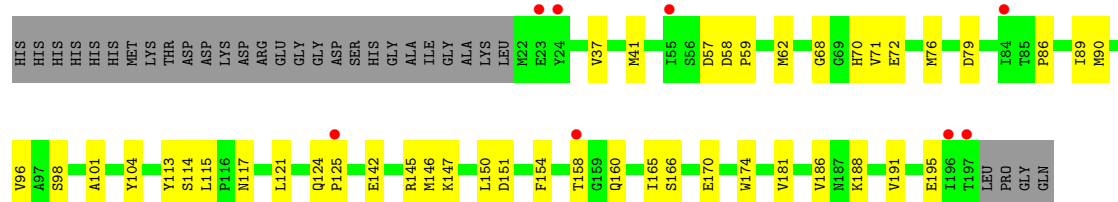
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain H: 



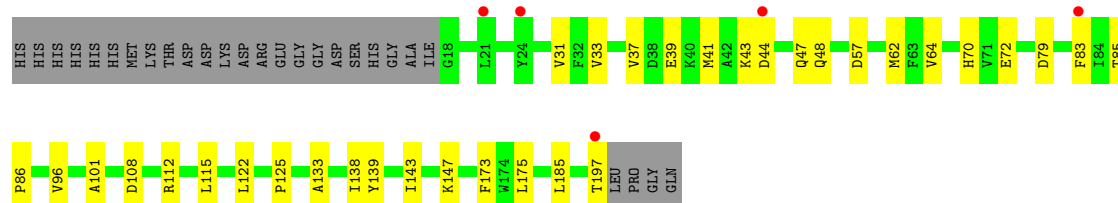
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain I: 



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

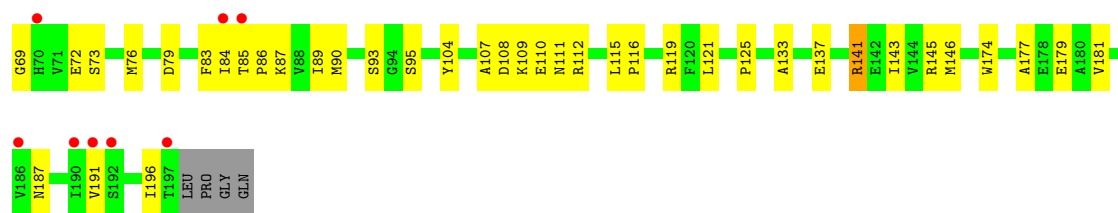
Chain J: 



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

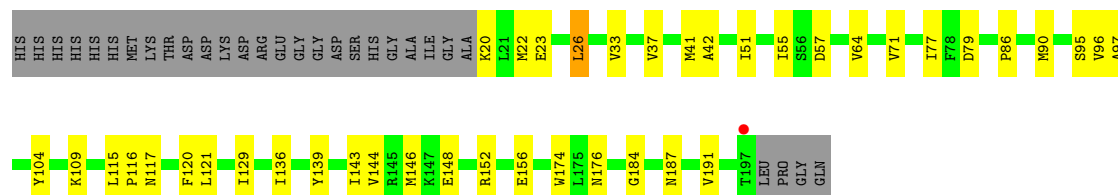
Chain K: 





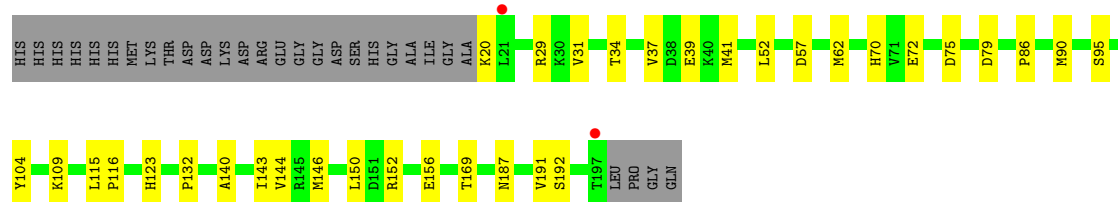
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain L:



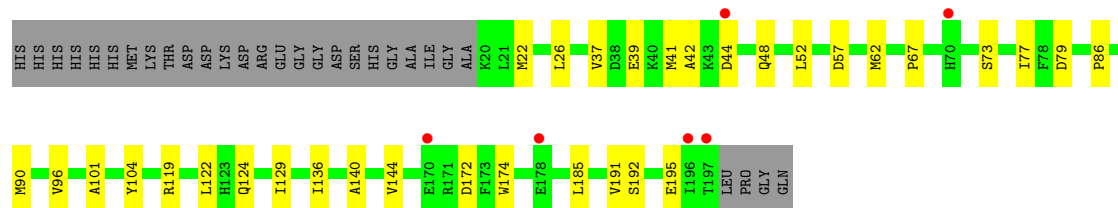
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain M:



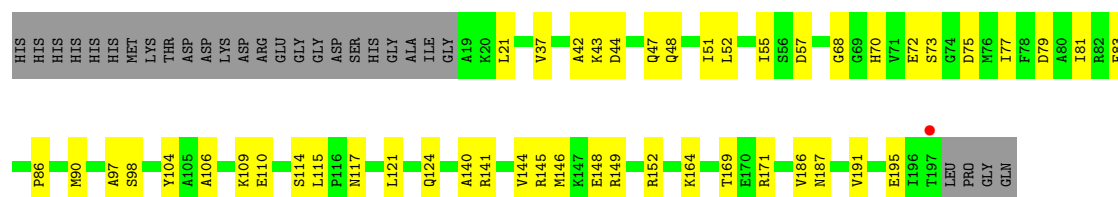
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain N:

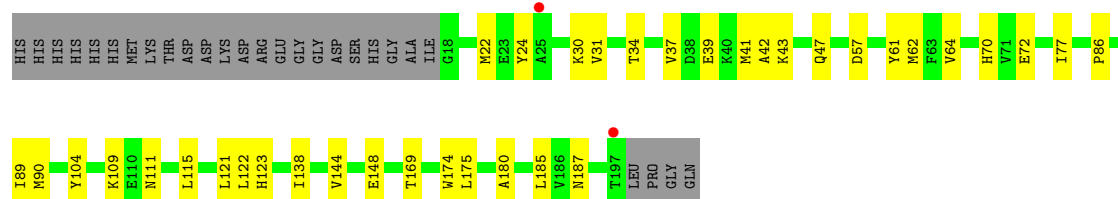


- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

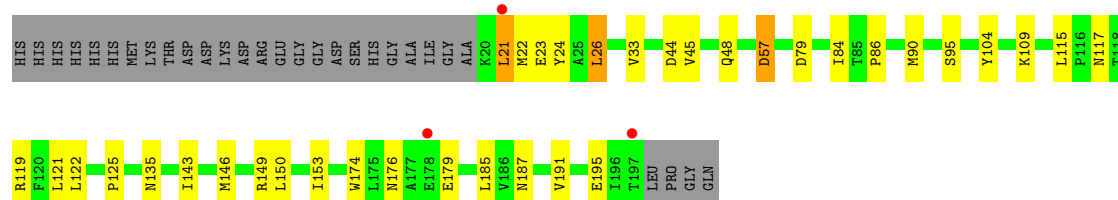
Chain O:



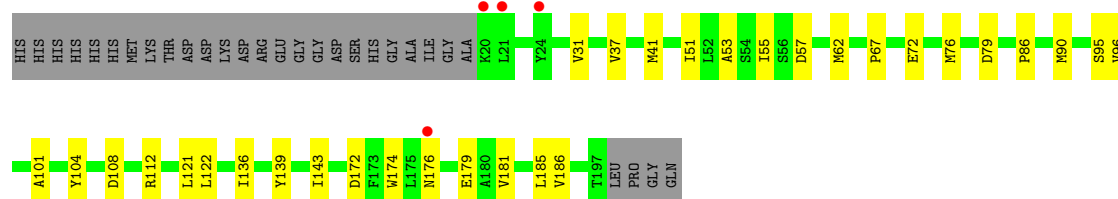
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



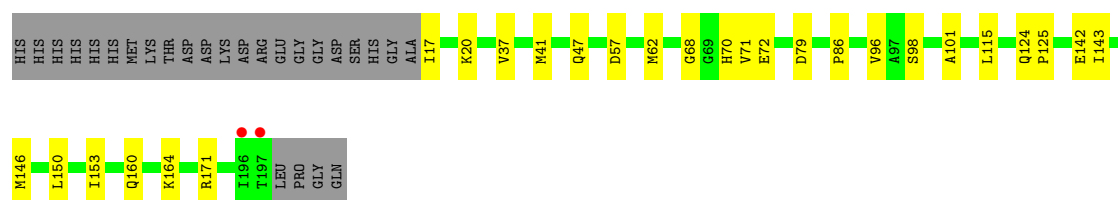
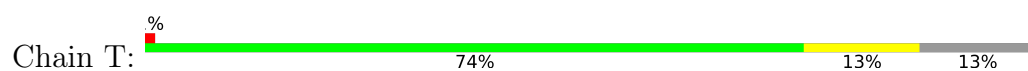
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2





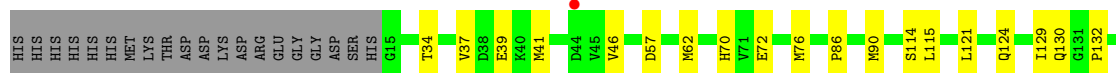
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain V: 72% 13% 15%



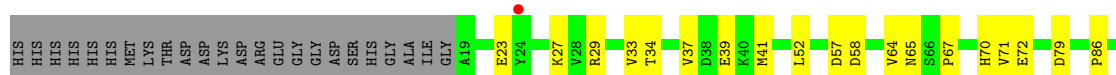
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain W: 73% 15% 12%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain X: 69% 18% 14%



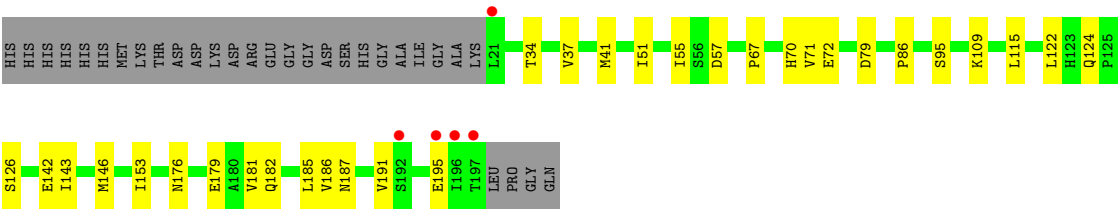
- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain Y: 74% 14% 13%

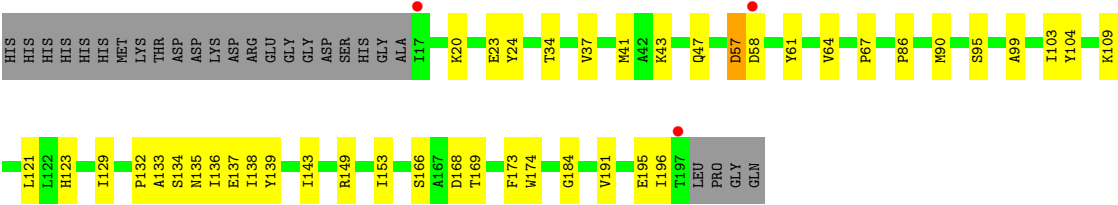


- Molecule 1: ATP-dependent Clp protease proteolytic subunit 2

Chain a: 71% 15% 14%



● Molecule 1: ATP-dependent Clp protease proteolytic subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.66Å 186.90Å 162.07Å 90.00° 91.72° 90.00°	Depositor
Resolution (Å)	37.52 – 3.00 37.52 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.52-3.00) 99.2 (37.52-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.217 , 0.275 0.217 , 0.271	Depositor DCC
R_{free} test set	2002 reflections (1.82%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	39105	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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	0.17	0/1401	0.34	0/1893
1	B	0.24	0/1427	0.40	0/1927
1	C	0.25	0/1393	0.46	1/1882 (0.1%)
1	D	0.33	0/1436	0.52	1/1939 (0.1%)
1	E	0.23	0/1427	0.40	0/1927
1	F	0.22	0/1415	0.39	0/1911
1	G	0.18	0/1393	0.34	0/1882
1	H	0.24	0/1427	0.41	0/1927
1	I	0.27	0/1393	0.44	0/1882
1	J	0.26	0/1419	0.41	0/1916
1	K	0.46	0/1393	0.68	1/1882 (0.1%)
1	L	0.24	0/1410	0.44	1/1904 (0.1%)
1	M	0.19	0/1410	0.35	0/1904
1	N	0.18	0/1410	0.33	0/1904
1	O	0.18	0/1415	0.37	0/1911
1	P	0.27	0/1419	0.48	0/1916
1	Q	0.32	0/1410	0.59	4/1904 (0.2%)
1	R	0.32	0/1415	0.58	2/1911 (0.1%)
1	S	0.31	0/1410	0.50	0/1904
1	T	0.29	0/1427	0.47	1/1927 (0.1%)
1	U	0.26	0/1410	0.53	1/1904 (0.1%)
1	V	0.26	0/1393	0.42	0/1882
1	W	0.29	0/1436	0.45	0/1939
1	X	0.19	0/1415	0.36	0/1911
1	Y	0.31	0/1427	0.58	0/1927
1	Z	0.33	0/1432	0.59	1/1934 (0.1%)
1	a	0.26	0/1401	0.47	0/1893
1	b	0.37	0/1427	0.64	2/1927 (0.1%)
All	All	0.27	0/39591	0.47	15/53470 (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	Y	0	1
1	Z	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	57	ASP	N-CA-C	-7.36	103.39	112.88
1	b	58	ASP	CB-CA-C	6.35	119.50	109.27
1	Z	102	LEU	N-CA-C	-6.28	104.35	111.07
1	R	57	ASP	N-CA-C	-6.20	105.66	112.72
1	Q	57	ASP	N-CA-C	-6.01	105.26	112.59

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Y	152	ARG	Sidechain
1	Z	141	ARG	Sidechain
1	Z	145	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	1377	0	1383	26	0
1	B	1403	0	1415	27	0
1	C	1369	0	1372	37	0
1	D	1412	0	1423	30	0
1	E	1403	0	1415	21	0
1	F	1391	0	1401	22	0
1	G	1369	0	1372	22	0
1	H	1403	0	1415	25	0
1	I	1369	0	1372	31	0
1	J	1395	0	1404	25	0
1	K	1369	0	1372	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1386	0	1396	29	0
1	M	1386	0	1396	25	0
1	N	1386	0	1396	23	0
1	O	1391	0	1401	34	0
1	P	1395	0	1404	25	0
1	Q	1386	0	1396	23	0
1	R	1391	0	1401	31	0
1	S	1386	0	1396	22	0
1	T	1403	0	1415	25	0
1	U	1386	0	1396	29	0
1	V	1369	0	1372	20	0
1	W	1412	0	1423	27	0
1	X	1391	0	1401	25	0
1	Y	1403	0	1415	24	0
1	Z	1408	0	1420	26	0
1	a	1377	0	1383	25	0
1	b	1403	0	1415	28	0
2	A	7	0	0	0	0
2	B	5	0	0	0	0
2	C	7	0	0	0	0
2	D	4	0	0	0	0
2	E	6	0	0	0	0
2	F	10	0	0	0	0
2	G	6	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	0	0
2	K	6	0	0	0	0
2	L	7	0	0	0	0
2	M	9	0	0	1	0
2	N	5	0	0	0	0
2	O	7	0	0	0	0
2	P	6	0	0	0	0
2	Q	5	0	0	0	0
2	R	6	0	0	0	0
2	S	11	0	0	0	0
2	T	4	0	0	0	0
2	U	9	0	0	0	0
2	V	7	0	0	0	0
2	W	7	0	0	0	0
2	X	6	0	0	0	0
2	Y	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	11	0	0	0	0
2	a	10	0	0	1	0
2	b	6	0	0	0	0
All	All	39105	0	39170	610	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 8.

The worst 5 of 610 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:B:72:GLU:HG2	1:D:95:SER:HB3	1.56	0.85
1:A:57:ASP:HA	1:A:86:PRO:HG3	1.62	0.81
1:M:72:GLU:HG2	1:X:95:SER:HB3	1.61	0.80
1:K:110:GLU:HA	1:K:187:ASN:ND2	1.96	0.79
1:O:115:LEU:HD23	1:Q:79:ASP:HB3	1.65	0.79

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	175/207 (84%)	168 (96%)	7 (4%)	0	100	100
1	B	179/207 (86%)	171 (96%)	8 (4%)	0	100	100
1	C	174/207 (84%)	162 (93%)	11 (6%)	1 (1%)	21	56
1	D	181/207 (87%)	173 (96%)	8 (4%)	0	100	100
1	E	179/207 (86%)	171 (96%)	8 (4%)	0	100	100
1	F	177/207 (86%)	170 (96%)	7 (4%)	0	100	100
1	G	174/207 (84%)	165 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	179/207 (86%)	174 (97%)	5 (3%)	0	100	100
1	I	174/207 (84%)	170 (98%)	4 (2%)	0	100	100
1	J	178/207 (86%)	172 (97%)	6 (3%)	0	100	100
1	K	174/207 (84%)	161 (92%)	12 (7%)	1 (1%)	21	56
1	L	176/207 (85%)	173 (98%)	3 (2%)	0	100	100
1	M	176/207 (85%)	164 (93%)	12 (7%)	0	100	100
1	N	176/207 (85%)	169 (96%)	7 (4%)	0	100	100
1	O	177/207 (86%)	169 (96%)	8 (4%)	0	100	100
1	P	178/207 (86%)	173 (97%)	5 (3%)	0	100	100
1	Q	176/207 (85%)	169 (96%)	7 (4%)	0	100	100
1	R	177/207 (86%)	169 (96%)	8 (4%)	0	100	100
1	S	176/207 (85%)	170 (97%)	6 (3%)	0	100	100
1	T	179/207 (86%)	171 (96%)	8 (4%)	0	100	100
1	U	176/207 (85%)	172 (98%)	4 (2%)	0	100	100
1	V	174/207 (84%)	169 (97%)	5 (3%)	0	100	100
1	W	181/207 (87%)	177 (98%)	4 (2%)	0	100	100
1	X	177/207 (86%)	170 (96%)	7 (4%)	0	100	100
1	Y	179/207 (86%)	171 (96%)	8 (4%)	0	100	100
1	Z	180/207 (87%)	173 (96%)	7 (4%)	0	100	100
1	a	175/207 (84%)	168 (96%)	7 (4%)	0	100	100
1	b	179/207 (86%)	172 (96%)	7 (4%)	0	100	100
All	All	4956/5796 (86%)	4756 (96%)	198 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	55	ILE
1	C	194	ARG

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	147/170 (86%)	147 (100%)	0	100	100
1	B	149/170 (88%)	149 (100%)	0	100	100
1	C	146/170 (86%)	145 (99%)	1 (1%)	76	86
1	D	149/170 (88%)	149 (100%)	0	100	100
1	E	149/170 (88%)	149 (100%)	0	100	100
1	F	148/170 (87%)	148 (100%)	0	100	100
1	G	146/170 (86%)	146 (100%)	0	100	100
1	H	149/170 (88%)	148 (99%)	1 (1%)	76	86
1	I	146/170 (86%)	146 (100%)	0	100	100
1	J	148/170 (87%)	147 (99%)	1 (1%)	76	86
1	K	146/170 (86%)	144 (99%)	2 (1%)	59	80
1	L	148/170 (87%)	145 (98%)	3 (2%)	48	76
1	M	148/170 (87%)	148 (100%)	0	100	100
1	N	148/170 (87%)	148 (100%)	0	100	100
1	O	148/170 (87%)	148 (100%)	0	100	100
1	P	148/170 (87%)	148 (100%)	0	100	100
1	Q	148/170 (87%)	146 (99%)	2 (1%)	59	80
1	R	148/170 (87%)	145 (98%)	3 (2%)	48	76
1	S	148/170 (87%)	148 (100%)	0	100	100
1	T	149/170 (88%)	149 (100%)	0	100	100
1	U	148/170 (87%)	148 (100%)	0	100	100
1	V	146/170 (86%)	146 (100%)	0	100	100
1	W	149/170 (88%)	149 (100%)	0	100	100
1	X	148/170 (87%)	148 (100%)	0	100	100
1	Y	149/170 (88%)	149 (100%)	0	100	100
1	Z	149/170 (88%)	148 (99%)	1 (1%)	76	86
1	a	147/170 (86%)	147 (100%)	0	100	100
1	b	149/170 (88%)	148 (99%)	1 (1%)	76	86
All	All	4141/4760 (87%)	4126 (100%)	15 (0%)	84	90

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	52	LEU
1	Q	26	LEU
1	K	141	ARG
1	b	166	SER
1	L	26	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	47	GLN
1	b	187	ASN
1	O	47	GLN
1	Y	111	ASN
1	M	182	GLN

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	177/207 (85%)	0.21	3 (1%) 69 45	35, 48, 71, 95	0
1	B	181/207 (87%)	0.01	2 (1%) 78 57	23, 39, 61, 88	0
1	C	176/207 (85%)	0.43	6 (3%) 48 27	33, 49, 79, 126	0
1	D	183/207 (88%)	0.05	2 (1%) 78 57	27, 39, 62, 100	0
1	E	181/207 (87%)	-0.17	2 (1%) 78 57	17, 32, 55, 79	0
1	F	179/207 (86%)	-0.00	1 (0%) 85 69	24, 37, 64, 80	0
1	G	176/207 (85%)	0.13	4 (2%) 61 38	27, 42, 75, 99	0
1	H	181/207 (87%)	0.10	6 (3%) 49 28	26, 41, 74, 103	0
1	I	176/207 (85%)	0.63	8 (4%) 38 20	39, 56, 84, 98	0
1	J	180/207 (86%)	0.13	5 (2%) 55 32	24, 45, 70, 87	0
1	K	176/207 (85%)	0.72	17 (9%) 13 7	27, 55, 87, 106	0
1	L	178/207 (85%)	-0.12	1 (0%) 85 69	23, 35, 64, 84	0
1	M	178/207 (85%)	0.18	2 (1%) 78 57	30, 46, 78, 103	0
1	N	178/207 (85%)	0.36	6 (3%) 48 27	40, 54, 71, 92	0
1	O	179/207 (86%)	-0.00	1 (0%) 85 69	23, 37, 67, 86	0
1	P	180/207 (86%)	0.12	2 (1%) 78 57	26, 43, 72, 99	0
1	Q	178/207 (85%)	-0.07	3 (1%) 69 45	23, 34, 62, 90	0
1	R	179/207 (86%)	-0.06	4 (2%) 62 39	24, 37, 72, 87	0
1	S	178/207 (85%)	-0.14	4 (2%) 62 39	21, 31, 67, 97	0
1	T	181/207 (87%)	0.00	2 (1%) 78 57	25, 37, 64, 85	0
1	U	178/207 (85%)	-0.02	3 (1%) 69 45	20, 36, 59, 75	0
1	V	176/207 (85%)	-0.07	1 (0%) 85 69	25, 35, 56, 82	0
1	W	183/207 (88%)	0.01	2 (1%) 78 57	25, 38, 60, 81	0
1	X	179/207 (86%)	0.26	3 (1%) 69 45	32, 50, 78, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	181/207 (87%)	0.24	2 (1%) 78 57	30, 44, 67, 79	0
1	Z	182/207 (87%)	-0.14	2 (1%) 78 57	21, 33, 58, 74	0
1	a	177/207 (85%)	0.16	5 (2%) 55 32	28, 40, 78, 121	0
1	b	181/207 (87%)	-0.05	3 (1%) 69 45	25, 35, 54, 82	0
All	All	5012/5796 (86%)	0.10	102 (2%) 65 41	17, 41, 71, 126	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	197	THR	4.8
1	a	196	ILE	4.7
1	H	197	THR	3.9
1	X	197	THR	3.8
1	I	197	THR	3.7

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.