



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 03:47 AM UTC

PDB ID : 6NAY / pdb_00006nay
Title : Crystal structure of Neisseria meningitidis ClpP protease E31A+E58A activated double mutant
Authors : Mabanglo, M.F.; Houry, W.A.
Deposited on : 2018-12-06
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

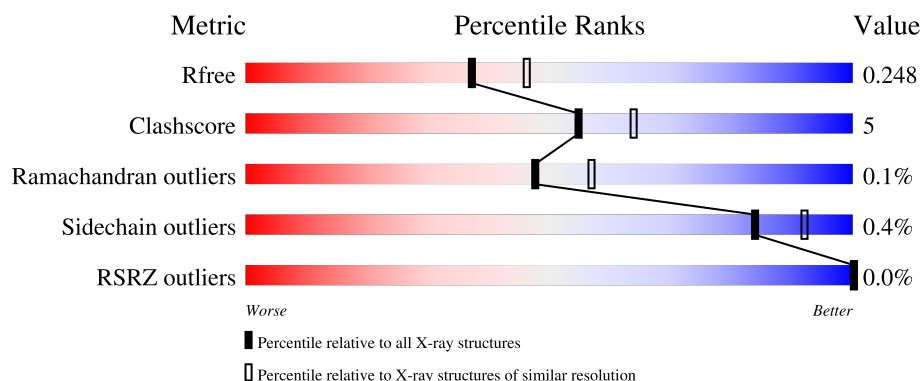
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	217	 68% 12% 20%
1	B	217	 71% 9% 20%
1	C	217	 71% 9% 19%
1	D	217	 71% 10% 19%
1	E	217	 71% 9% 20%

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Mol	Chain	Length	Quality of chain
1	F	217	
1	G	217	
1	H	217	
1	I	217	
1	J	217	
1	K	217	
1	L	217	
1	M	217	
1	N	217	
1	O	217	
1	P	217	
1	Q	217	
1	R	217	
1	S	217	
1	T	217	
1	U	217	
1	V	217	
1	W	217	
1	X	217	
1	Y	217	
1	Z	217	
1	a	217	
1	b	217	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 39500 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1355	855	233	259	8			
1	B	174	Total	C	N	O	S	0	0	0
			1355	855	233	259	8			
1	C	175	Total	C	N	O	S	0	0	0
			1359	857	234	260	8			
1	D	175	Total	C	N	O	S	0	0	0
			1364	863	234	259	8			
1	E	173	Total	C	N	O	S	0	0	0
			1348	851	232	257	8			
1	F	178	Total	C	N	O	S	0	0	0
			1386	875	240	263	8			
1	G	178	Total	C	N	O	S	0	0	0
			1377	868	237	264	8			
1	H	175	Total	C	N	O	S	0	0	0
			1359	857	234	260	8			
1	I	174	Total	C	N	O	S	0	0	0
			1353	854	233	258	8			
1	J	176	Total	C	N	O	S	0	0	0
			1367	863	235	261	8			
1	K	176	Total	C	N	O	S	0	0	0
			1367	863	235	261	8			
1	L	175	Total	C	N	O	S	0	0	0
			1359	857	234	260	8			
1	M	172	Total	C	N	O	S	0	0	0
			1344	849	231	256	8			
1	N	177	Total	C	N	O	S	0	0	0
			1373	866	236	263	8			
1	O	174	Total	C	N	O	S	0	0	0
			1355	855	233	259	8			
1	P	177	Total	C	N	O	S	0	0	0
			1371	865	236	262	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	175	Total	C	N	O	S	0	0	0
			1359	857	234	260	8			
1	R	174	Total	C	N	O	S	0	0	0
			1353	854	233	258	8			
1	S	172	Total	C	N	O	S	0	0	0
			1337	845	228	256	8			
1	T	176	Total	C	N	O	S	0	0	0
			1367	863	235	261	8			
1	U	176	Total	C	N	O	S	0	0	0
			1365	860	235	262	8			
1	V	175	Total	C	N	O	S	0	0	0
			1359	857	234	260	8			
1	W	174	Total	C	N	O	S	0	0	0
			1353	854	233	258	8			
1	X	176	Total	C	N	O	S	0	0	0
			1367	863	235	261	8			
1	Y	179	Total	C	N	O	S	0	0	0
			1381	870	238	265	8			
1	Z	175	Total	C	N	O	S	0	0	0
			1359	857	234	260	8			
1	a	174	Total	C	N	O	S	0	0	0
			1355	855	233	259	8			
1	b	176	Total	C	N	O	S	0	0	0
			1367	863	235	261	8			

There are 420 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
A	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
A	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
A	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
A	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
A	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
A	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
A	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
A	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
A	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
A	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
A	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
A	0	GLY	-	expression tag	UNP A0A0H5Q9L9
A	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
A	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
B	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
B	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
B	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
B	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
B	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
B	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
B	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
B	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
B	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
B	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
B	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
B	0	GLY	-	expression tag	UNP A0A0H5Q9L9
B	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
B	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
C	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
C	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
C	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
C	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
C	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
C	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
C	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
C	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
C	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
C	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
C	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
C	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
C	0	GLY	-	expression tag	UNP A0A0H5Q9L9
C	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
C	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
D	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
D	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
D	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
D	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
D	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
D	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
D	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
D	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
D	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
D	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
D	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
D	-1	GLN	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP A0A0H5Q9L9
D	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
D	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
E	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
E	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
E	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
E	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
E	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
E	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
E	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
E	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
E	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
E	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
E	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
E	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
E	0	GLY	-	expression tag	UNP A0A0H5Q9L9
E	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
E	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
F	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
F	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
F	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
F	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
F	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
F	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
F	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
F	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
F	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
F	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
F	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
F	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
F	0	GLY	-	expression tag	UNP A0A0H5Q9L9
F	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
F	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
G	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
G	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
G	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
G	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
G	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
G	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
G	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
G	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
G	-4	LEU	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
G	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
G	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
G	0	GLY	-	expression tag	UNP A0A0H5Q9L9
G	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
G	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
H	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
H	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
H	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
H	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
H	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
H	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
H	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
H	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
H	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
H	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
H	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
H	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
H	0	GLY	-	expression tag	UNP A0A0H5Q9L9
H	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
H	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
I	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
I	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
I	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
I	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
I	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
I	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
I	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
I	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
I	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
I	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
I	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
I	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
I	0	GLY	-	expression tag	UNP A0A0H5Q9L9
I	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
I	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
J	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
J	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
J	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
J	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
J	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
J	-7	HIS	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
J	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
J	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
J	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
J	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
J	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
J	0	GLY	-	expression tag	UNP A0A0H5Q9L9
J	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
J	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
K	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
K	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
K	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
K	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
K	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
K	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
K	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
K	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
K	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
K	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
K	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
K	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
K	0	GLY	-	expression tag	UNP A0A0H5Q9L9
K	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
K	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
L	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
L	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
L	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
L	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
L	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
L	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
L	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
L	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
L	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
L	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
L	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
L	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
L	0	GLY	-	expression tag	UNP A0A0H5Q9L9
L	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
L	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
M	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
M	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
M	-10	HIS	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
M	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
M	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
M	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
M	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
M	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
M	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
M	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
M	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
M	0	GLY	-	expression tag	UNP A0A0H5Q9L9
M	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
M	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
N	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
N	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
N	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
N	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
N	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
N	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
N	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
N	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
N	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
N	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
N	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
N	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
N	0	GLY	-	expression tag	UNP A0A0H5Q9L9
N	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
N	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
O	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
O	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
O	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
O	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
O	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
O	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
O	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
O	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
O	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
O	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
O	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
O	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
O	0	GLY	-	expression tag	UNP A0A0H5Q9L9
O	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
O	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
P	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
P	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
P	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
P	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
P	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
P	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
P	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
P	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
P	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
P	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
P	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
P	0	GLY	-	expression tag	UNP A0A0H5Q9L9
P	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
P	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
Q	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
Q	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
Q	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
Q	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
Q	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
Q	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
Q	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
Q	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
Q	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
Q	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
Q	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
Q	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
Q	0	GLY	-	expression tag	UNP A0A0H5Q9L9
Q	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
Q	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
R	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
R	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
R	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
R	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
R	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
R	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
R	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
R	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
R	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
R	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
R	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
R	-1	GLN	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
R	0	GLY	-	expression tag	UNP A0A0H5Q9L9
R	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
R	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
S	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
S	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
S	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
S	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
S	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
S	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
S	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
S	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
S	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
S	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
S	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
S	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
S	0	GLY	-	expression tag	UNP A0A0H5Q9L9
S	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
S	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
T	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
T	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
T	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
T	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
T	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
T	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
T	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
T	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
T	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
T	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
T	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
T	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
T	0	GLY	-	expression tag	UNP A0A0H5Q9L9
T	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
T	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
U	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
U	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
U	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
U	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
U	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
U	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
U	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
U	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
U	-4	LEU	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
U	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
U	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
U	0	GLY	-	expression tag	UNP A0A0H5Q9L9
U	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
U	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
V	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
V	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
V	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
V	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
V	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
V	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
V	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
V	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
V	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
V	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
V	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
V	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
V	0	GLY	-	expression tag	UNP A0A0H5Q9L9
V	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
V	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
W	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
W	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
W	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
W	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
W	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
W	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
W	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
W	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
W	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
W	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
W	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
W	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
W	0	GLY	-	expression tag	UNP A0A0H5Q9L9
W	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
W	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
X	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
X	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
X	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
X	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
X	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
X	-7	HIS	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
X	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
X	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
X	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
X	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
X	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
X	0	GLY	-	expression tag	UNP A0A0H5Q9L9
X	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
X	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
Y	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
Y	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
Y	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
Y	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
Y	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
Y	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
Y	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
Y	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
Y	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
Y	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
Y	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
Y	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
Y	0	GLY	-	expression tag	UNP A0A0H5Q9L9
Y	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
Y	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
Z	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
Z	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
Z	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
Z	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
Z	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
Z	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
Z	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
Z	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
Z	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
Z	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
Z	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
Z	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
Z	0	GLY	-	expression tag	UNP A0A0H5Q9L9
Z	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
Z	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
a	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
a	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
a	-10	HIS	-	expression tag	UNP A0A0H5Q9L9

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Chain	Residue	Modelled	Actual	Comment	Reference
a	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
a	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
a	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
a	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
a	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
a	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
a	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
a	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
a	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
a	0	GLY	-	expression tag	UNP A0A0H5Q9L9
a	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
a	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
b	-12	HIS	-	expression tag	UNP A0A0H5Q9L9
b	-11	HIS	-	expression tag	UNP A0A0H5Q9L9
b	-10	HIS	-	expression tag	UNP A0A0H5Q9L9
b	-9	HIS	-	expression tag	UNP A0A0H5Q9L9
b	-8	HIS	-	expression tag	UNP A0A0H5Q9L9
b	-7	HIS	-	expression tag	UNP A0A0H5Q9L9
b	-6	GLU	-	expression tag	UNP A0A0H5Q9L9
b	-5	ASN	-	expression tag	UNP A0A0H5Q9L9
b	-4	LEU	-	expression tag	UNP A0A0H5Q9L9
b	-3	TYR	-	expression tag	UNP A0A0H5Q9L9
b	-2	PHE	-	expression tag	UNP A0A0H5Q9L9
b	-1	GLN	-	expression tag	UNP A0A0H5Q9L9
b	0	GLY	-	expression tag	UNP A0A0H5Q9L9
b	31	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9
b	58	ALA	GLU	engineered mutation	UNP A0A0H5Q9L9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	50	Total O 50 50	0	0
2	B	50	Total O 50 50	0	0
2	C	57	Total O 57 57	0	0
2	D	45	Total O 45 45	0	0
2	E	44	Total O 44 44	0	0
2	F	57	Total O 57 57	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	54	Total 54	O 54	0	0
2	H	56	Total 56	O 56	0	0
2	I	55	Total 55	O 55	0	0
2	J	32	Total 32	O 32	0	0
2	K	44	Total 44	O 44	0	0
2	L	47	Total 47	O 47	0	0
2	M	49	Total 49	O 49	0	0
2	N	53	Total 53	O 53	0	0
2	O	60	Total 60	O 60	0	0
2	P	46	Total 46	O 46	0	0
2	Q	57	Total 57	O 57	0	0
2	R	42	Total 42	O 42	0	0
2	S	32	Total 32	O 32	0	0
2	T	50	Total 50	O 50	0	0
2	U	50	Total 50	O 50	0	0
2	V	64	Total 64	O 64	0	0
2	W	44	Total 44	O 44	0	0
2	X	42	Total 42	O 42	0	0
2	Y	54	Total 54	O 54	0	0
2	Z	51	Total 51	O 51	0	0
2	a	52	Total 52	O 52	0	0

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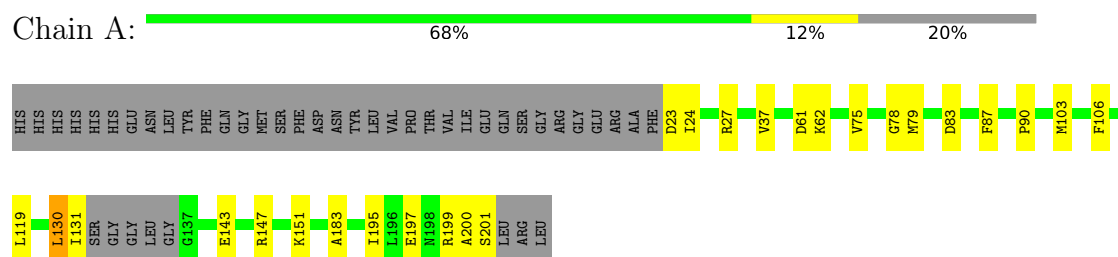
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	b	49	Total	O	0	0
			49	49		

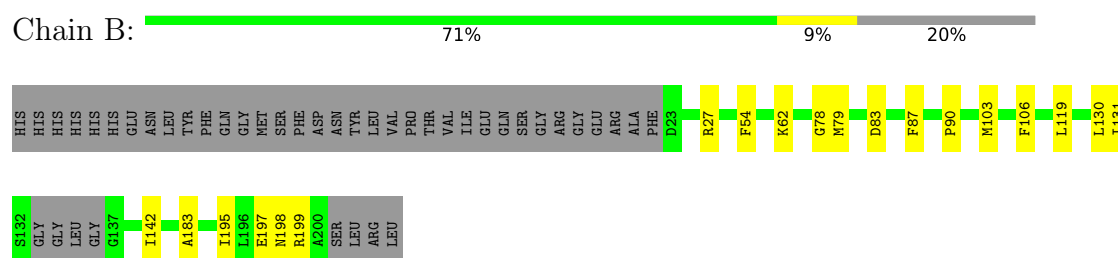
3 Residue-property plots

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.

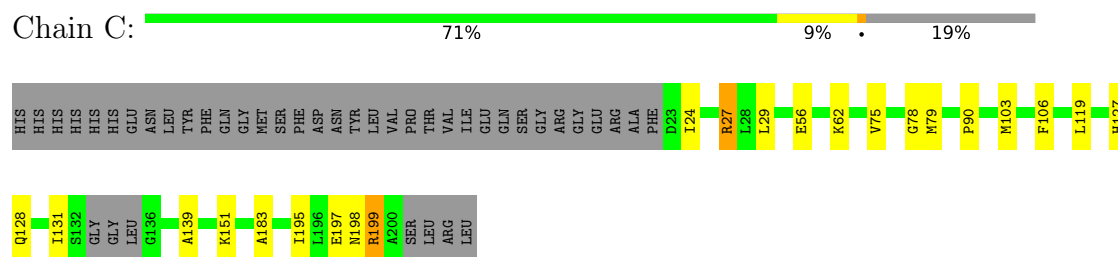
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



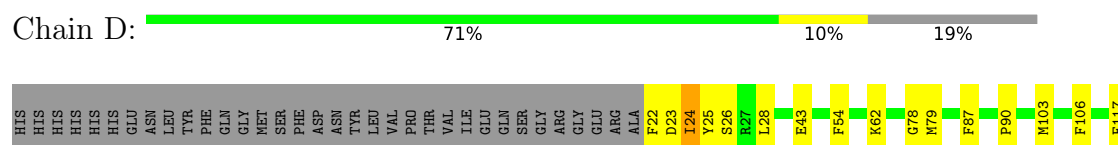
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



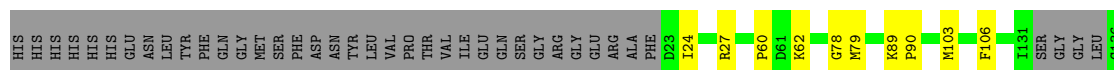
- Molecule 1: ATP-dependent Clp protease proteolytic subunit





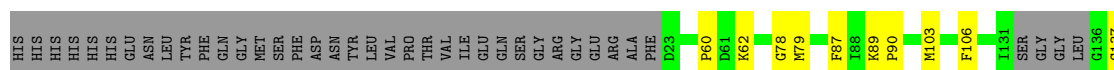
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E: 71% 9% 20%



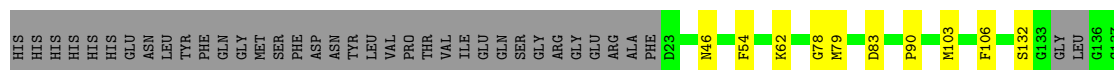
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F: 73% 8% 18%



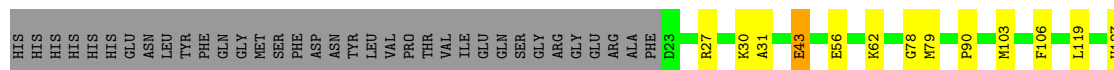
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G: 74% 8% 18%



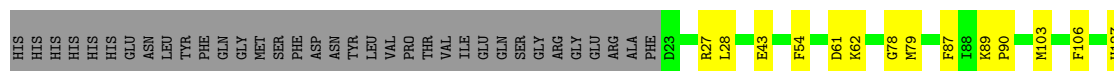
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H: 70% 10% 19%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

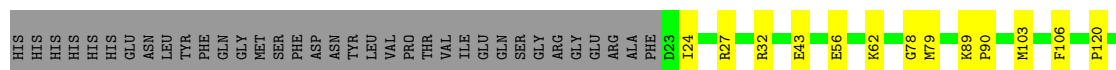
Chain I: 71% 9% 20%





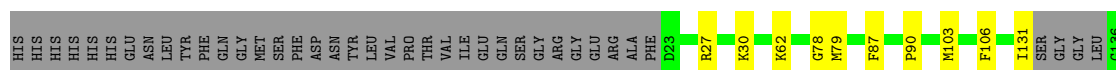
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J: 71% 10% 19%



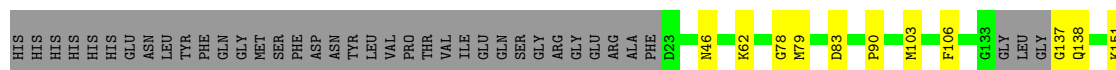
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K: 73% 8% 19%



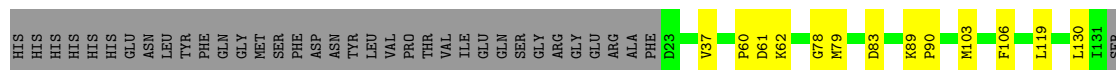
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L: 73% 8% 19%



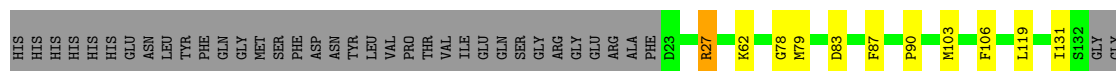
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M: 70% 9% 21%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

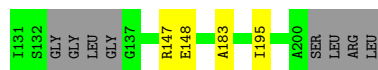
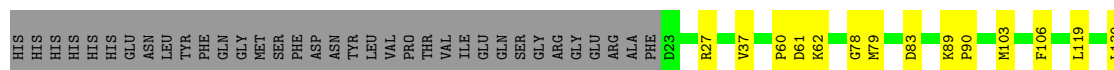
Chain N: 73% 8% 18%





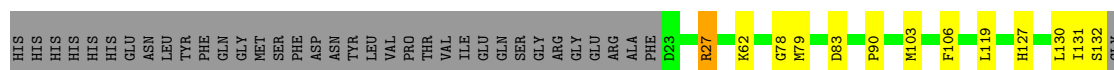
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain O: 72% 8% 20%



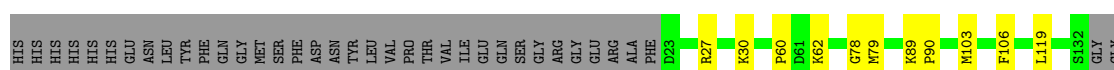
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain P: 72% 9% 18%



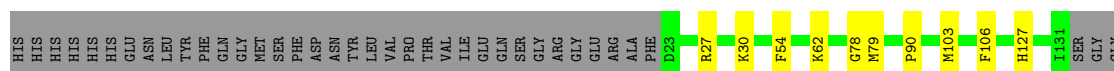
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Q: 74% 6% 19%



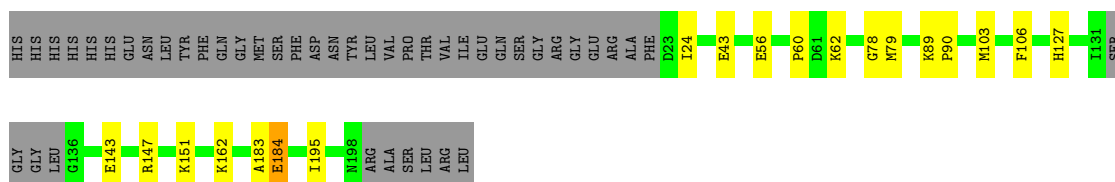
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain R: 71% 9% 20%



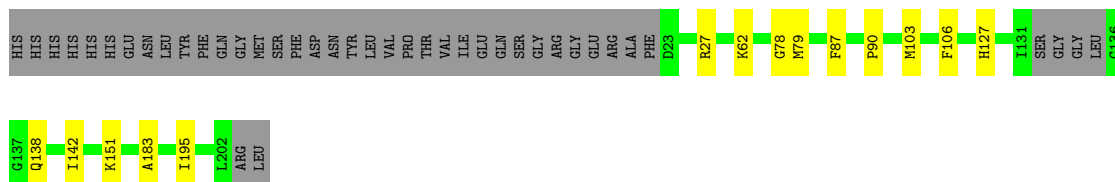
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain S: 71% 8% 21%



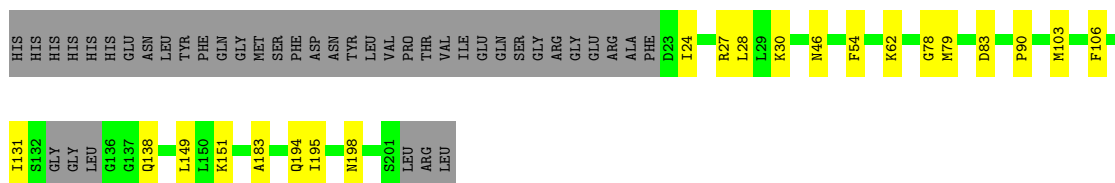
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain T: 75% 6% 19%



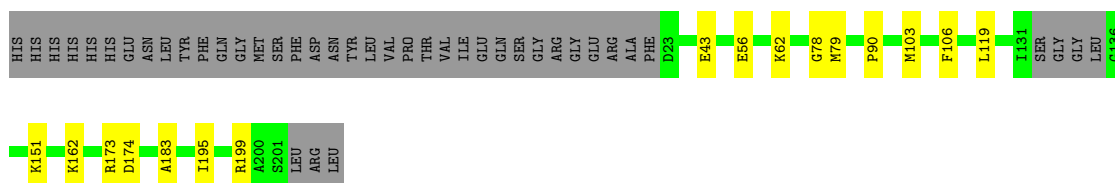
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain U: 71% 10% 19%



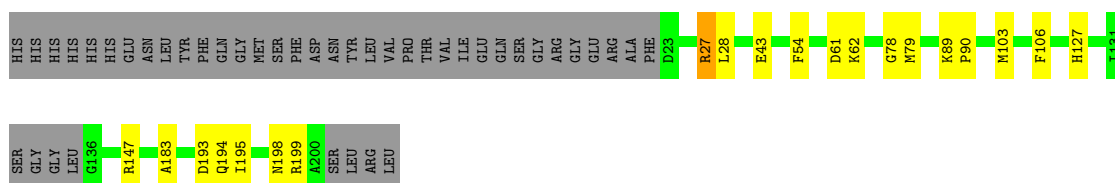
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain V: 73% 7% 19%



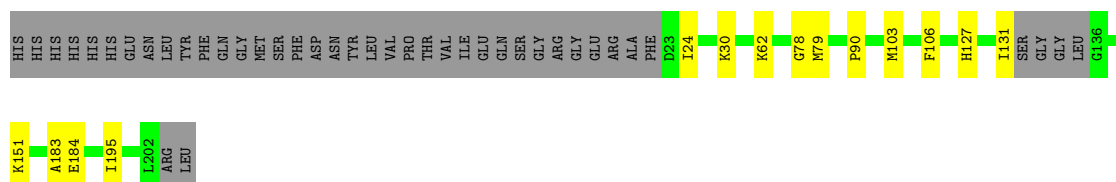
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain W: 71% 9% 20%



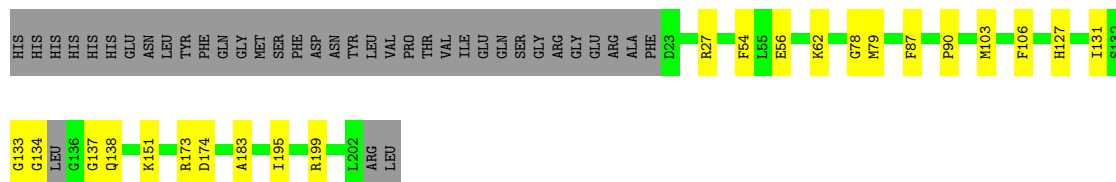
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain X: 75% 6% 19%



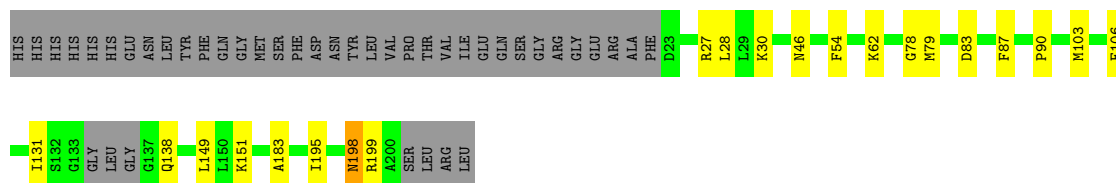
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Y:



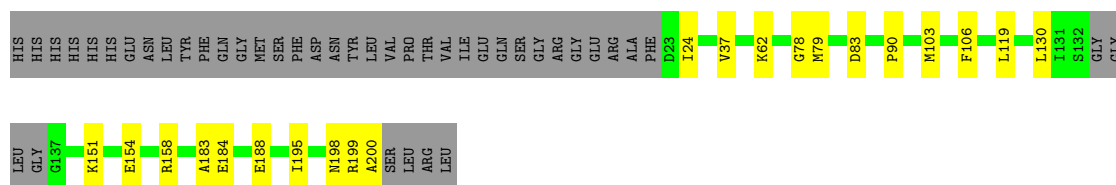
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Z:



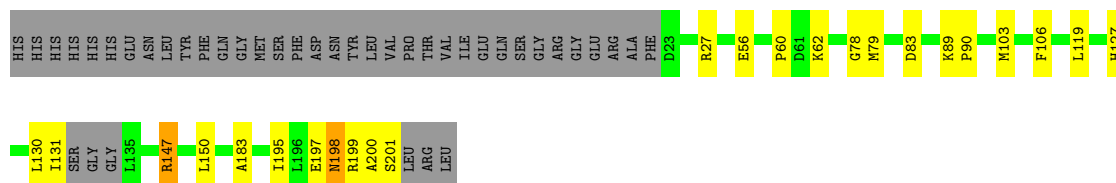
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain a:



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain b:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	98.71Å 119.84Å 127.86Å 90.02° 89.99° 90.02°	Depositor
Resolution (Å)	46.05 – 2.20 46.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (46.05-2.20) 95.1 (46.05-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.214 , 0.245 0.215 , 0.248	Depositor DCC
R_{free} test set	1995 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 24.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.469 for h,-k,-l 0.469 for -h,k,-l 0.470 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	39500	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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	0.44	0/1374	0.70	4/1849 (0.2%)
1	B	0.45	0/1374	0.65	2/1849 (0.1%)
1	C	0.44	0/1378	0.62	2/1854 (0.1%)
1	D	0.43	0/1384	0.68	3/1862 (0.2%)
1	E	0.43	0/1367	0.62	0/1839
1	F	0.46	0/1405	0.66	0/1890
1	G	0.45	0/1396	0.61	0/1878
1	H	0.73	1/1378 (0.1%)	0.69	2/1854 (0.1%)
1	I	0.49	1/1372 (0.1%)	0.75	3/1846 (0.2%)
1	J	0.47	0/1386	0.64	1/1865 (0.1%)
1	K	0.47	0/1386	0.68	1/1865 (0.1%)
1	L	0.46	0/1378	0.67	2/1854 (0.1%)
1	M	0.54	2/1363 (0.1%)	0.63	1/1834 (0.1%)
1	N	0.50	1/1392 (0.1%)	0.66	1/1873 (0.1%)
1	O	0.42	0/1374	0.62	0/1849
1	P	0.48	2/1390 (0.1%)	0.70	2/1870 (0.1%)
1	Q	0.39	0/1378	0.58	0/1854
1	R	0.48	1/1372 (0.1%)	0.77	5/1846 (0.3%)
1	S	0.47	0/1356	0.64	1/1825 (0.1%)
1	T	0.44	0/1386	0.63	0/1865
1	U	0.41	0/1384	0.61	0/1862
1	V	0.41	0/1378	0.58	0/1854
1	W	0.44	1/1372 (0.1%)	0.69	3/1846 (0.2%)
1	X	0.42	0/1386	0.60	0/1865
1	Y	0.47	0/1400	0.66	2/1883 (0.1%)
1	Z	0.45	0/1378	0.69	3/1854 (0.2%)
1	a	0.43	0/1374	0.62	0/1849
1	b	0.55	3/1386 (0.2%)	0.67	1/1865 (0.1%)
All	All	0.47	12/38647 (0.0%)	0.66	39/51999 (0.1%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	43	GLU	CD-OE1	21.09	1.65	1.25
1	M	194	GLN	CD-OE1	-9.50	1.05	1.23
1	b	147	ARG	NE-CZ	5.92	1.39	1.33
1	W	27	ARG	C-O	-5.71	1.17	1.24
1	N	27	ARG	C-O	-5.58	1.17	1.24

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	198	ASN	CA-C-N	11.52	136.09	120.54
1	R	198	ASN	C-N-CA	11.52	136.09	120.54
1	I	198	ASN	CA-C-N	10.98	142.51	121.54
1	I	198	ASN	C-N-CA	10.98	142.51	121.54
1	P	198	ASN	CA-C-N	-9.68	103.06	121.54

There are no chirality outliers.

There are no planarity outliers.

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	1355	0	1366	15	1
1	B	1355	0	1366	19	0
1	C	1359	0	1369	23	0
1	D	1364	0	1373	22	0
1	E	1348	0	1359	18	0
1	F	1386	0	1404	14	0
1	G	1377	0	1388	14	0
1	H	1359	0	1369	23	0
1	I	1353	0	1364	14	0
1	J	1367	0	1380	19	0
1	K	1367	0	1380	17	0
1	L	1359	0	1369	11	0
1	M	1344	0	1356	17	1
1	N	1373	0	1385	10	0
1	O	1355	0	1366	20	0
1	P	1371	0	1383	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	1359	0	1369	9	0
1	R	1353	0	1364	12	0
1	S	1337	0	1346	19	0
1	T	1367	0	1380	9	1
1	U	1365	0	1374	21	0
1	V	1359	0	1369	12	0
1	W	1353	0	1364	15	0
1	X	1367	0	1380	11	0
1	Y	1381	0	1391	15	1
1	Z	1359	0	1369	20	0
1	a	1355	0	1366	18	0
1	b	1367	0	1380	17	0
2	A	50	0	0	2	0
2	B	50	0	0	1	0
2	C	57	0	0	2	0
2	D	45	0	0	0	0
2	E	44	0	0	2	0
2	F	57	0	0	0	0
2	G	54	0	0	2	0
2	H	56	0	0	1	0
2	I	55	0	0	1	0
2	J	32	0	0	1	0
2	K	44	0	0	0	0
2	L	47	0	0	2	0
2	M	49	0	0	0	0
2	N	53	0	0	0	0
2	O	60	0	0	0	0
2	P	46	0	0	0	0
2	Q	57	0	0	0	0
2	R	42	0	0	0	0
2	S	32	0	0	2	0
2	T	50	0	0	0	0
2	U	50	0	0	4	0
2	V	64	0	0	3	0
2	W	44	0	0	0	0
2	X	42	0	0	1	0
2	Y	54	0	0	0	0
2	Z	51	0	0	1	0
2	a	52	0	0	1	0
2	b	49	0	0	0	0
All	All	39500	0	38429	364	2

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 5.

The worst 5 of 364 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:H:43:GLU:OE1	1:H:43:GLU:CD	1.65	1.38
1:D:23:ASP:OD2	1:D:26:SER:OG	1.61	1.15
1:B:142:ILE:HD11	1:K:131:ILE:HG12	1.43	1.00
1:S:184:GLU:HG3	1:S:195:ILE:HD13	1.46	0.96
1:C:199:ARG:H	1:C:199:ARG:HD2	1.37	0.88

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASP:OD2	1:T:151:LYS:NZ[1_545]	2.03	0.17
1:M:61:ASP:OD2	1:Y:151:LYS:NZ[1_554]	2.04	0.16

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	170/217 (78%)	165 (97%)	5 (3%)	0	100	100
1	B	170/217 (78%)	164 (96%)	6 (4%)	0	100	100
1	C	171/217 (79%)	165 (96%)	5 (3%)	1 (1%)	21	23
1	D	171/217 (79%)	166 (97%)	4 (2%)	1 (1%)	21	23
1	E	169/217 (78%)	164 (97%)	5 (3%)	0	100	100
1	F	174/217 (80%)	168 (97%)	5 (3%)	1 (1%)	21	23
1	G	174/217 (80%)	169 (97%)	5 (3%)	0	100	100
1	H	171/217 (79%)	166 (97%)	5 (3%)	0	100	100
1	I	170/217 (78%)	165 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	172/217 (79%)	168 (98%)	4 (2%)	0	100	100
1	K	172/217 (79%)	168 (98%)	4 (2%)	0	100	100
1	L	171/217 (79%)	165 (96%)	6 (4%)	0	100	100
1	M	168/217 (77%)	164 (98%)	4 (2%)	0	100	100
1	N	173/217 (80%)	168 (97%)	4 (2%)	1 (1%)	21	23
1	O	170/217 (78%)	165 (97%)	5 (3%)	0	100	100
1	P	173/217 (80%)	166 (96%)	6 (4%)	1 (1%)	21	23
1	Q	171/217 (79%)	165 (96%)	6 (4%)	0	100	100
1	R	170/217 (78%)	166 (98%)	4 (2%)	0	100	100
1	S	168/217 (77%)	164 (98%)	4 (2%)	0	100	100
1	T	172/217 (79%)	167 (97%)	5 (3%)	0	100	100
1	U	172/217 (79%)	167 (97%)	5 (3%)	0	100	100
1	V	171/217 (79%)	166 (97%)	5 (3%)	0	100	100
1	W	170/217 (78%)	165 (97%)	5 (3%)	0	100	100
1	X	172/217 (79%)	167 (97%)	5 (3%)	0	100	100
1	Y	175/217 (81%)	169 (97%)	5 (3%)	1 (1%)	21	23
1	Z	171/217 (79%)	166 (97%)	5 (3%)	0	100	100
1	a	170/217 (78%)	165 (97%)	5 (3%)	0	100	100
1	b	172/217 (79%)	166 (96%)	5 (3%)	1 (1%)	21	23
All	All	4793/6076 (79%)	4649 (97%)	137 (3%)	7 (0%)	48	57

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	200	ALA
1	N	200	ALA
1	C	199	ARG
1	b	200	ALA
1	D	24	ILE

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	147/183 (80%)	145 (99%)	2 (1%)	59	75
1	B	147/183 (80%)	146 (99%)	1 (1%)	76	87
1	C	147/183 (80%)	146 (99%)	1 (1%)	76	87
1	D	147/183 (80%)	147 (100%)	0	100	100
1	E	146/183 (80%)	146 (100%)	0	100	100
1	F	150/183 (82%)	149 (99%)	1 (1%)	76	87
1	G	149/183 (81%)	148 (99%)	1 (1%)	76	87
1	H	147/183 (80%)	147 (100%)	0	100	100
1	I	146/183 (80%)	145 (99%)	1 (1%)	76	87
1	J	148/183 (81%)	148 (100%)	0	100	100
1	K	148/183 (81%)	147 (99%)	1 (1%)	76	87
1	L	147/183 (80%)	147 (100%)	0	100	100
1	M	146/183 (80%)	146 (100%)	0	100	100
1	N	149/183 (81%)	147 (99%)	2 (1%)	61	76
1	O	147/183 (80%)	147 (100%)	0	100	100
1	P	148/183 (81%)	146 (99%)	2 (1%)	59	75
1	Q	147/183 (80%)	147 (100%)	0	100	100
1	R	146/183 (80%)	146 (100%)	0	100	100
1	S	145/183 (79%)	145 (100%)	0	100	100
1	T	148/183 (81%)	148 (100%)	0	100	100
1	U	148/183 (81%)	146 (99%)	2 (1%)	59	75
1	V	147/183 (80%)	147 (100%)	0	100	100
1	W	146/183 (80%)	145 (99%)	1 (1%)	76	87
1	X	148/183 (81%)	148 (100%)	0	100	100
1	Y	149/183 (81%)	149 (100%)	0	100	100
1	Z	147/183 (80%)	147 (100%)	0	100	100
1	a	147/183 (80%)	147 (100%)	0	100	100
1	b	148/183 (81%)	148 (100%)	0	100	100
All	All	4125/5124 (80%)	4110 (100%)	15 (0%)	84	92

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

Mol	Chain	Res	Type
1	K	201	SER
1	U	27	ARG
1	N	27	ARG
1	W	27	ARG
1	P	197	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	198	ASN
1	Q	194	GLN
1	b	198	ASN
1	Y	194	GLN
1	Y	198	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	174/217 (80%)	-1.02	0	100	100	27, 34, 65, 102	0
1	B	174/217 (80%)	-1.07	0	100	100	26, 33, 57, 74	0
1	C	175/217 (80%)	-1.03	0	100	100	27, 34, 63, 76	0
1	D	175/217 (80%)	-0.99	0	100	100	30, 37, 69, 82	0
1	E	173/217 (79%)	-0.94	0	100	100	30, 39, 65, 81	0
1	F	178/217 (82%)	-1.01	0	100	100	28, 36, 64, 107	0
1	G	178/217 (82%)	-1.03	0	100	100	27, 34, 69, 96	0
1	H	175/217 (80%)	-1.05	0	100	100	28, 34, 62, 83	0
1	I	174/217 (80%)	-0.95	0	100	100	30, 37, 67, 82	0
1	J	176/217 (81%)	-0.95	0	100	100	30, 39, 71, 91	0
1	K	176/217 (81%)	-1.09	0	100	100	28, 35, 63, 84	0
1	L	175/217 (80%)	-0.99	0	100	100	28, 34, 67, 88	0
1	M	172/217 (79%)	-1.04	0	100	100	28, 34, 60, 80	0
1	N	177/217 (81%)	-1.08	0	100	100	26, 32, 62, 74	0
1	O	174/217 (80%)	-1.07	0	100	100	27, 34, 60, 79	0
1	P	177/217 (81%)	-1.09	0	100	100	26, 33, 62, 108	0
1	Q	175/217 (80%)	-1.06	0	100	100	28, 34, 63, 101	0
1	R	174/217 (80%)	-1.01	1 (0%)	85	83	29, 37, 65, 82	0
1	S	172/217 (79%)	-0.93	0	100	100	30, 39, 65, 82	0
1	T	176/217 (81%)	-1.04	0	100	100	28, 35, 62, 74	0
1	U	176/217 (81%)	-1.08	0	100	100	28, 33, 64, 87	0
1	V	175/217 (80%)	-1.07	0	100	100	28, 34, 64, 79	0
1	W	174/217 (80%)	-1.02	0	100	100	29, 37, 64, 81	0
1	X	176/217 (81%)	-0.93	0	100	100	31, 39, 67, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	179/217 (82%)	-1.03	0 100 100	28, 35, 66, 141	0
1	Z	175/217 (80%)	-1.02	0 100 100	28, 34, 64, 105	0
1	a	174/217 (80%)	-0.97	0 100 100	27, 34, 68, 80	0
1	b	176/217 (81%)	-1.08	0 100 100	25, 33, 62, 77	0
All	All	4905/6076 (80%)	-1.02	1 (0%) 100 100	25, 35, 66, 141	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	200	ALA	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.