



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 10:13 PM EDT

PDB ID : 6NAY
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 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

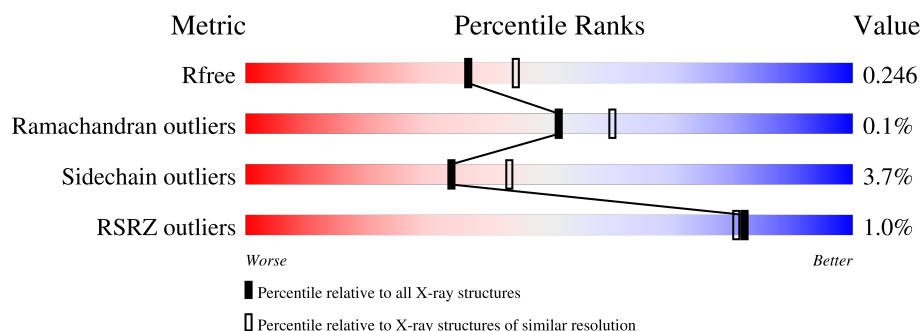
1 Overall quality at a glance

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}	130704	4898 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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	
1	B	217	
1	C	217	
1	D	217	
1	E	217	
1	F	217	

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

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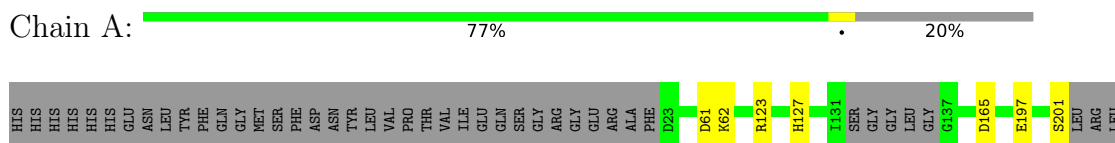
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	b	49	Total	O	0	0
			49	49		

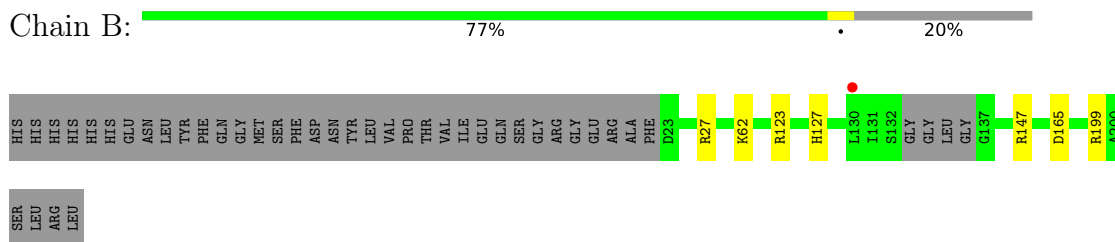
3 Residue-property plots

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.

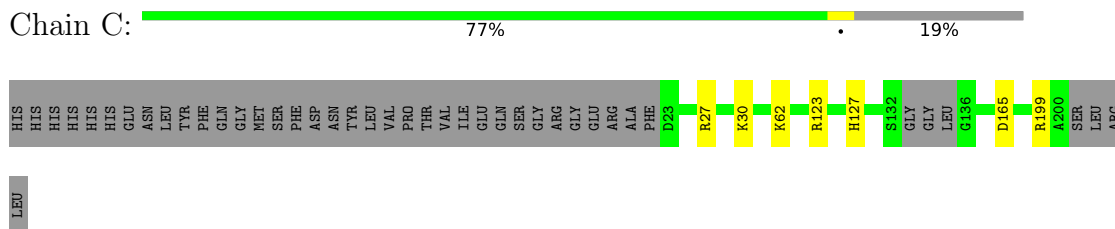
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



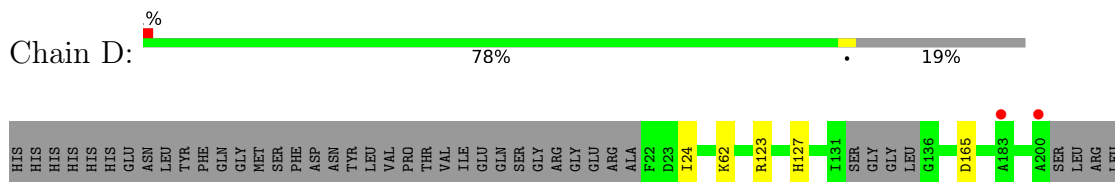
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



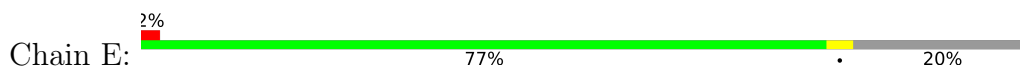
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



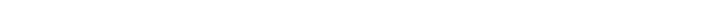
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

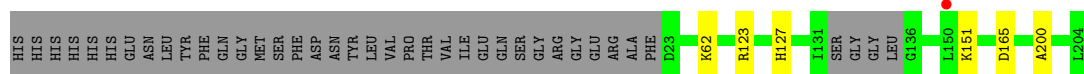


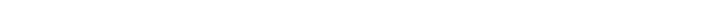
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

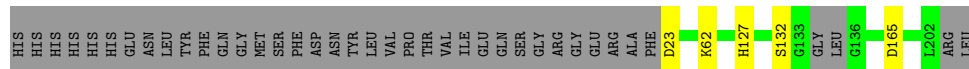


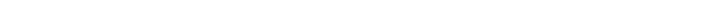


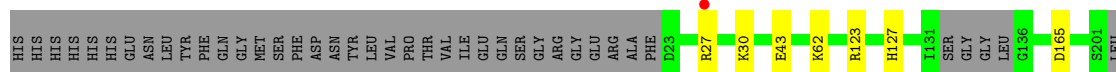
- Chain F:  79% . 18%

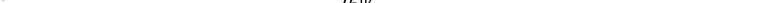


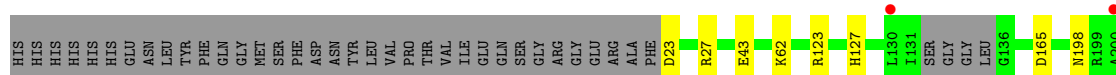
- Chain G:  80% • 18%

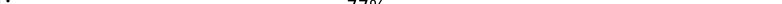


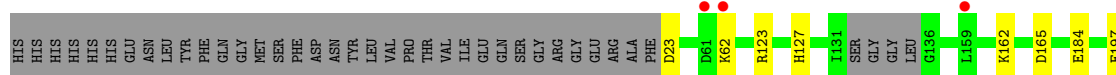
- Chain H:  77% 1% 19%



- Chain I:  76% 20% 4%

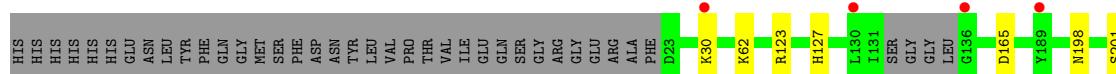
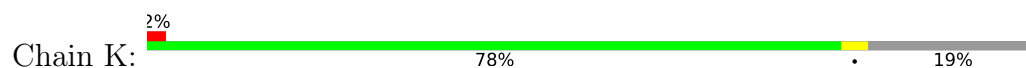


- Chain J: 

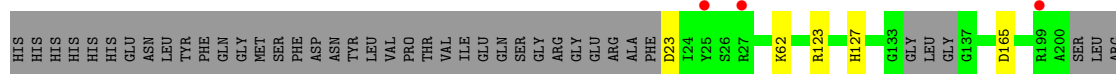
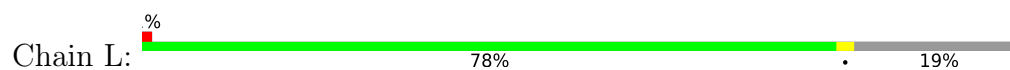




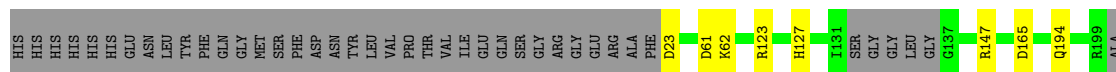
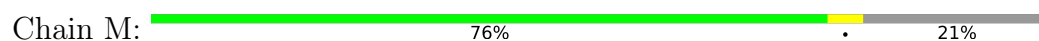
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



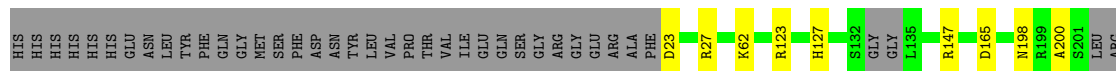
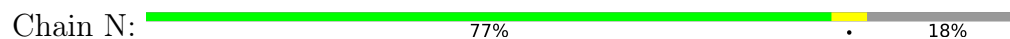
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



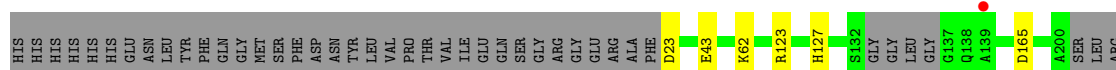
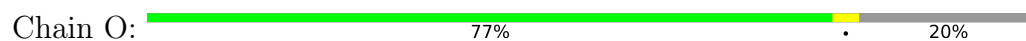
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

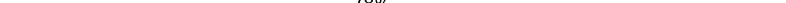


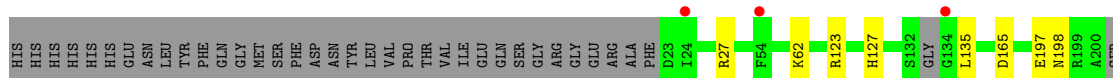
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



LEU

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

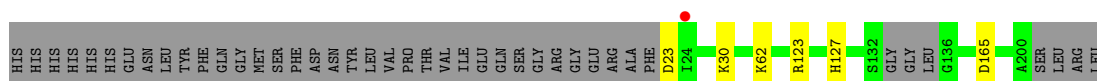
Chain P:  %



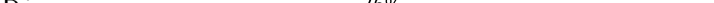
LEU

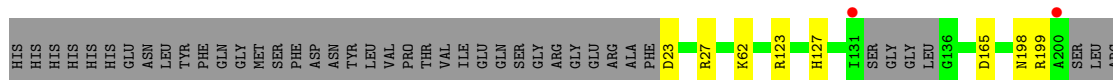
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Q: 78% . 19%



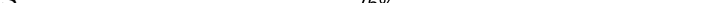
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

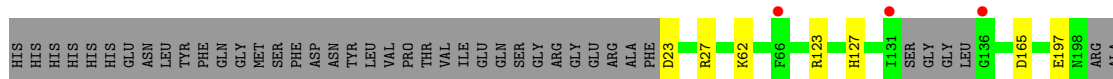
Chain R:  76% 20%



LEU

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

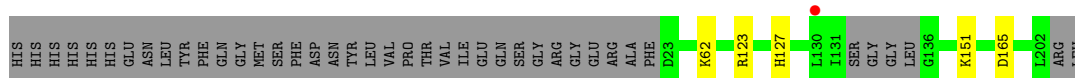
Chain S:  76% 21%



SER

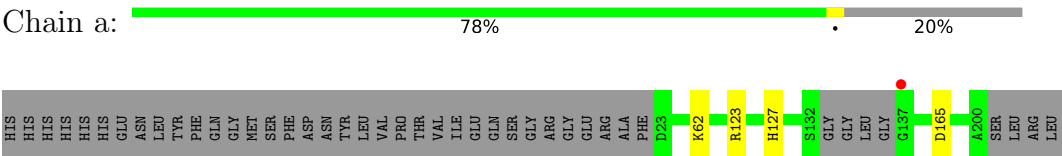
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain T: 79% 19%

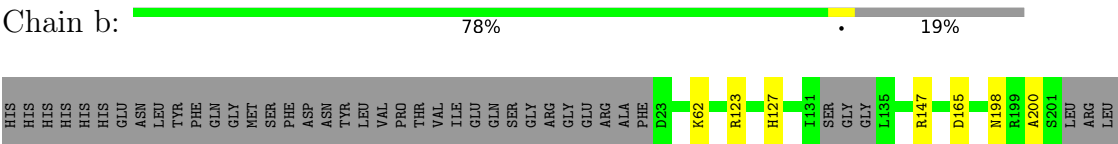


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain U: 78% . 19%



● Molecule 1: ATP-dependent Clp protease proteolytic subunit



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 0.214 , 0.246	Depositor DCC
R_{free} test set	1991 reflections (0.70%)	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)	0.34 , 31.5	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	0.94	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	0.45	0/1374	0.66	0/1849
1	B	0.45	0/1374	0.63	0/1849
1	C	0.45	0/1378	0.62	0/1854
1	D	0.46	0/1384	0.63	0/1862
1	E	0.46	0/1367	0.61	0/1839
1	F	0.46	0/1405	0.64	0/1890
1	G	0.49	0/1396	0.63	0/1878
1	H	1.10	3/1378 (0.2%)	0.68	1/1854 (0.1%)
1	I	0.53	1/1372 (0.1%)	0.69	1/1846 (0.1%)
1	J	0.49	1/1386 (0.1%)	0.65	1/1865 (0.1%)
1	K	0.47	0/1386	0.67	2/1865 (0.1%)
1	L	0.46	0/1378	0.65	0/1854
1	M	0.54	1/1363 (0.1%)	0.67	2/1834 (0.1%)
1	N	0.49	0/1392	0.67	2/1873 (0.1%)
1	O	0.48	1/1374 (0.1%)	0.63	0/1849
1	P	0.46	0/1390	0.65	1/1870 (0.1%)
1	Q	0.43	0/1378	0.60	0/1854
1	R	0.49	0/1372	0.70	4/1846 (0.2%)
1	S	0.50	1/1356 (0.1%)	0.63	0/1825
1	T	0.47	0/1386	0.63	0/1865
1	U	0.43	0/1384	0.62	0/1862
1	V	0.46	0/1378	0.61	0/1854
1	W	0.46	0/1372	0.65	2/1846 (0.1%)
1	X	0.46	0/1386	0.61	0/1865
1	Y	0.49	0/1400	0.73	3/1883 (0.2%)
1	Z	0.47	0/1378	0.64	1/1854 (0.1%)
1	a	0.47	0/1374	0.62	0/1849
1	b	0.55	2/1386 (0.1%)	0.69	2/1865 (0.1%)
All	All	0.51	10/38647 (0.0%)	0.65	22/51999 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	43	GLU	CD-OE1	36.16	1.65	1.25
1	M	194	GLN	CD-OE1	-8.39	1.05	1.24
1	I	43	GLU	CG-CD	-7.73	1.40	1.51
1	H	43	GLU	CG-CD	-6.29	1.42	1.51
1	H	43	GLU	CB-CG	-6.12	1.40	1.52
1	S	197	GLU	CB-CG	-5.99	1.40	1.52
1	O	43	GLU	CB-CG	5.19	1.62	1.52
1	b	147	ARG	CZ-NH2	5.10	1.39	1.33
1	J	197	GLU	CB-CG	-5.01	1.42	1.52
1	b	147	ARG	NE-CZ	5.01	1.39	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	27	ARG	NE-CZ-NH2	-12.59	114.00	120.30
1	Y	27	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	I	198	ASN	C-N-CA	8.32	142.51	121.70
1	N	198	ASN	O-C-N	-8.06	109.81	122.70
1	P	198	ASN	C-N-CA	-7.46	103.06	121.70
1	b	147	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	K	30	LYS	CD-CE-NZ	-6.50	96.75	111.70
1	M	147	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	K	198	ASN	O-C-N	-6.10	112.94	122.70
1	W	43	GLU	CA-CB-CG	5.97	126.55	113.40
1	H	43	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	R	198	ASN	C-N-CA	5.75	136.09	121.70
1	W	198	ASN	C-N-CA	5.69	135.93	121.70
1	M	147	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	R	198	ASN	O-C-N	5.59	131.65	122.70
1	Z	198	ASN	O-C-N	5.59	131.64	122.70
1	R	198	ASN	CA-C-N	-5.53	105.03	117.20
1	Y	27	ARG	CG-CD-NE	-5.36	100.54	111.80
1	J	184	GLU	CA-CB-CG	5.34	125.16	113.40
1	b	198	ASN	O-C-N	-5.23	114.33	122.70
1	R	199	ARG	CA-CB-CG	5.21	124.86	113.40
1	N	198	ASN	CA-C-N	5.17	128.57	117.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	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%)	25	26
1	D	171/217 (79%)	166 (97%)	4 (2%)	1 (1%)	25	26
1	E	169/217 (78%)	164 (97%)	5 (3%)	0	100	100
1	F	174/217 (80%)	168 (97%)	5 (3%)	1 (1%)	25	26
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
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%)	25	26
1	O	170/217 (78%)	165 (97%)	5 (3%)	0	100	100
1	P	173/217 (80%)	166 (96%)	6 (4%)	1 (1%)	25	26
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	25	26
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%)	25	26
All	All	4793/6076 (79%)	4649 (97%)	137 (3%)	7 (0%)	51	60

All (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
1	P	135	LEU
1	Y	133	GLY

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%)	141 (96%)	6 (4%)	30	39
1	B	147/183 (80%)	140 (95%)	7 (5%)	25	32
1	C	147/183 (80%)	141 (96%)	6 (4%)	30	39
1	D	147/183 (80%)	143 (97%)	4 (3%)	44	57
1	E	146/183 (80%)	140 (96%)	6 (4%)	30	39
1	F	150/183 (82%)	145 (97%)	5 (3%)	38	49
1	G	149/183 (81%)	144 (97%)	5 (3%)	37	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	147/183 (80%)	141 (96%)	6 (4%)	30	39
1	I	146/183 (80%)	140 (96%)	6 (4%)	30	39
1	J	148/183 (81%)	142 (96%)	6 (4%)	30	39
1	K	148/183 (81%)	143 (97%)	5 (3%)	37	47
1	L	147/183 (80%)	142 (97%)	5 (3%)	37	47
1	M	146/183 (80%)	141 (97%)	5 (3%)	37	47
1	N	149/183 (81%)	142 (95%)	7 (5%)	26	33
1	O	147/183 (80%)	142 (97%)	5 (3%)	37	47
1	P	148/183 (81%)	142 (96%)	6 (4%)	30	39
1	Q	147/183 (80%)	141 (96%)	6 (4%)	30	39
1	R	146/183 (80%)	140 (96%)	6 (4%)	30	39
1	S	145/183 (79%)	139 (96%)	6 (4%)	30	39
1	T	148/183 (81%)	144 (97%)	4 (3%)	44	57
1	U	148/183 (81%)	142 (96%)	6 (4%)	30	39
1	V	147/183 (80%)	142 (97%)	5 (3%)	37	47
1	W	146/183 (80%)	140 (96%)	6 (4%)	30	39
1	X	148/183 (81%)	142 (96%)	6 (4%)	30	39
1	Y	149/183 (81%)	145 (97%)	4 (3%)	44	57
1	Z	147/183 (80%)	143 (97%)	4 (3%)	44	57
1	a	147/183 (80%)	143 (97%)	4 (3%)	44	57
1	b	148/183 (81%)	144 (97%)	4 (3%)	44	57
All	All	4125/5124 (80%)	3974 (96%)	151 (4%)	34	43

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LYS
1	A	123	ARG
1	A	127	HIS
1	A	165	ASP
1	A	197	GLU
1	A	201	SER
1	B	27	ARG
1	B	62	LYS
1	B	123	ARG

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Mol	Chain	Res	Type
1	B	127	HIS
1	B	147	ARG
1	B	165	ASP
1	B	199	ARG
1	C	27	ARG
1	C	30	LYS
1	C	62	LYS
1	C	123	ARG
1	C	127	HIS
1	C	165	ASP
1	D	62	LYS
1	D	123	ARG
1	D	127	HIS
1	D	165	ASP
1	E	23	ASP
1	E	27	ARG
1	E	62	LYS
1	E	123	ARG
1	E	127	HIS
1	E	165	ASP
1	F	62	LYS
1	F	123	ARG
1	F	127	HIS
1	F	151	LYS
1	F	165	ASP
1	G	23	ASP
1	G	62	LYS
1	G	127	HIS
1	G	132	SER
1	G	165	ASP
1	H	27	ARG
1	H	30	LYS
1	H	62	LYS
1	H	123	ARG
1	H	127	HIS
1	H	165	ASP
1	I	23	ASP
1	I	27	ARG
1	I	62	LYS
1	I	123	ARG
1	I	127	HIS
1	I	165	ASP

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Mol	Chain	Res	Type
1	J	23	ASP
1	J	62	LYS
1	J	123	ARG
1	J	127	HIS
1	J	162	LYS
1	J	165	ASP
1	K	62	LYS
1	K	123	ARG
1	K	127	HIS
1	K	165	ASP
1	K	201	SER
1	L	23	ASP
1	L	62	LYS
1	L	123	ARG
1	L	127	HIS
1	L	165	ASP
1	M	23	ASP
1	M	62	LYS
1	M	123	ARG
1	M	127	HIS
1	M	165	ASP
1	N	23	ASP
1	N	27	ARG
1	N	62	LYS
1	N	123	ARG
1	N	127	HIS
1	N	147	ARG
1	N	165	ASP
1	O	23	ASP
1	O	62	LYS
1	O	123	ARG
1	O	127	HIS
1	O	165	ASP
1	P	27	ARG
1	P	62	LYS
1	P	123	ARG
1	P	127	HIS
1	P	165	ASP
1	P	197	GLU
1	Q	23	ASP
1	Q	30	LYS
1	Q	62	LYS

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Mol	Chain	Res	Type
1	Q	123	ARG
1	Q	127	HIS
1	Q	165	ASP
1	R	23	ASP
1	R	27	ARG
1	R	62	LYS
1	R	123	ARG
1	R	127	HIS
1	R	165	ASP
1	S	23	ASP
1	S	27	ARG
1	S	62	LYS
1	S	123	ARG
1	S	127	HIS
1	S	165	ASP
1	T	62	LYS
1	T	123	ARG
1	T	127	HIS
1	T	165	ASP
1	U	23	ASP
1	U	27	ARG
1	U	62	LYS
1	U	123	ARG
1	U	127	HIS
1	U	165	ASP
1	V	62	LYS
1	V	123	ARG
1	V	127	HIS
1	V	165	ASP
1	V	199	ARG
1	W	23	ASP
1	W	27	ARG
1	W	62	LYS
1	W	123	ARG
1	W	127	HIS
1	W	165	ASP
1	X	23	ASP
1	X	43	GLU
1	X	62	LYS
1	X	123	ARG
1	X	127	HIS
1	X	165	ASP

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Mol	Chain	Res	Type
1	Y	62	LYS
1	Y	123	ARG
1	Y	127	HIS
1	Y	165	ASP
1	Z	23	ASP
1	Z	62	LYS
1	Z	127	HIS
1	Z	165	ASP
1	a	62	LYS
1	a	123	ARG
1	a	127	HIS
1	a	165	ASP
1	b	62	LYS
1	b	123	ARG
1	b	127	HIS
1	b	165	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	194	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 monosaccharides 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	174/217 (80%)	-0.03	0 100 100	27, 34, 65, 102	0
1	B	174/217 (80%)	-0.03	1 (0%) 89 88	26, 33, 57, 74	0
1	C	175/217 (80%)	-0.01	0 100 100	27, 34, 63, 76	0
1	D	175/217 (80%)	0.06	2 (1%) 80 79	30, 37, 69, 82	0
1	E	173/217 (79%)	0.17	5 (2%) 51 49	30, 39, 65, 81	0
1	F	178/217 (82%)	0.11	1 (0%) 89 88	28, 36, 64, 107	0
1	G	178/217 (82%)	0.08	0 100 100	27, 34, 69, 96	0
1	H	175/217 (80%)	0.00	1 (0%) 89 88	28, 34, 62, 83	0
1	I	174/217 (80%)	0.13	2 (1%) 80 79	30, 37, 67, 82	0
1	J	176/217 (81%)	0.17	4 (2%) 60 58	30, 39, 71, 91	0
1	K	176/217 (81%)	0.01	5 (2%) 53 51	28, 35, 63, 84	0
1	L	175/217 (80%)	0.10	3 (1%) 70 68	28, 34, 67, 88	0
1	M	172/217 (79%)	-0.02	0 100 100	28, 34, 60, 80	0
1	N	177/217 (81%)	-0.06	0 100 100	26, 32, 62, 74	0
1	O	174/217 (80%)	0.10	1 (0%) 89 88	27, 34, 60, 79	0
1	P	177/217 (81%)	-0.01	3 (1%) 70 68	26, 33, 62, 108	0
1	Q	175/217 (80%)	-0.02	1 (0%) 89 88	28, 34, 63, 101	0
1	R	174/217 (80%)	0.10	2 (1%) 80 79	29, 37, 65, 82	0
1	S	172/217 (79%)	0.12	3 (1%) 70 68	30, 39, 65, 82	0
1	T	176/217 (81%)	0.01	1 (0%) 89 88	28, 35, 62, 74	0
1	U	176/217 (81%)	0.02	1 (0%) 89 88	28, 33, 64, 87	0
1	V	175/217 (80%)	-0.05	2 (1%) 80 79	28, 34, 64, 79	0
1	W	174/217 (80%)	0.14	2 (1%) 80 79	29, 37, 64, 81	0
1	X	176/217 (81%)	0.18	2 (1%) 80 79	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%)	0.16	5 (2%) 53 51	28, 35, 66, 141	0
1	Z	175/217 (80%)	0.09	1 (0%) 89 88	28, 34, 64, 105	0
1	a	174/217 (80%)	0.05	1 (0%) 89 88	27, 34, 68, 80	0
1	b	176/217 (81%)	-0.01	0 100 100	25, 33, 62, 77	0
All	All	4905/6076 (80%)	0.06	49 (0%) 82 81	25, 35, 66, 141	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	199	ARG	3.6
1	P	54	PHE	3.5
1	Q	24	ILE	2.9
1	S	131	ILE	2.9
1	E	58	ALA	2.8
1	L	27	ARG	2.8
1	B	130	LEU	2.8
1	D	183	ALA	2.7
1	R	200	ALA	2.7
1	Y	132	SER	2.7
1	W	136	GLY	2.7
1	S	136	GLY	2.6
1	J	202	LEU	2.5
1	Z	131	ILE	2.5
1	O	139	ALA	2.5
1	L	25	TYR	2.5
1	W	200	ALA	2.5
1	Y	133	GLY	2.4
1	K	136	GLY	2.4
1	Y	87	PHE	2.4
1	F	150	LEU	2.4
1	E	65	PHE	2.4
1	V	27	ARG	2.4
1	P	24	ILE	2.4
1	E	130	LEU	2.3
1	T	130	LEU	2.3
1	K	130	LEU	2.3
1	J	62	LYS	2.3
1	K	30	LYS	2.3
1	J	61	ASP	2.3
1	I	130	LEU	2.3
1	Y	130	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	27	ARG	2.2
1	P	134	GLY	2.2
1	E	191	LEU	2.2
1	K	202	LEU	2.2
1	X	202	LEU	2.1
1	I	200	ALA	2.1
1	U	132	SER	2.1
1	Y	54	PHE	2.1
1	X	58	ALA	2.1
1	K	189	TYR	2.1
1	a	137	GLY	2.1
1	R	131	ILE	2.1
1	E	159	LEU	2.0
1	V	130	LEU	2.0
1	D	200	ALA	2.0
1	J	159	LEU	2.0
1	S	66	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.