



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:54 AM UTC

PDB ID : 3V5I / pdb_00003v5i
Title : The crystal structure of the mutant ClpP S98A (Staphylococcus aureus)
Authors : List, A.; Gersch, M.; Groll, M.; Sieber, S.
Deposited on : 2011-12-16
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

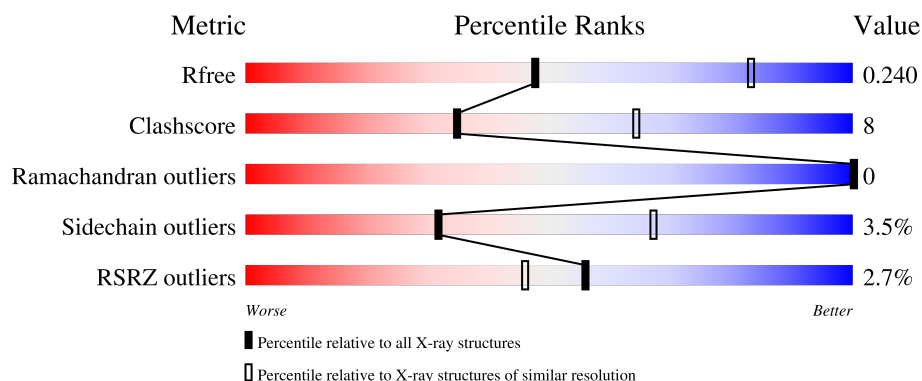
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	203	0% 79% 11% 9%
1	B	203	4% 77% 12% 9%
1	C	203	2% 80% 10% 9%
1	D	203	5% 78% 12% 9%
1	E	203	0% 77% 12% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	203	
1	G	203	
1	H	203	
1	I	203	
1	J	203	
1	K	203	
1	L	203	
1	M	203	
1	N	203	
1	O	203	
1	P	203	
1	Q	203	
1	R	203	
1	S	203	
1	T	203	
1	U	203	
1	V	203	
1	W	203	
1	X	203	
1	Y	203	
1	Z	203	
1	a	203	
1	b	203	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40465 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	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	B	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	C	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	D	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	E	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	F	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	G	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	H	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	I	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	J	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	K	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	L	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	M	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	N	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	O	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	P	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	R	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	S	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	T	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	U	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	V	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	W	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	X	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	Y	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	Z	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	a	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	b	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	ALA	SER	engineered mutation	UNP Q2G036
A	196	TRP	-	expression tag	UNP Q2G036
A	197	SER	-	expression tag	UNP Q2G036
A	198	HIS	-	expression tag	UNP Q2G036
A	199	PRO	-	expression tag	UNP Q2G036
A	200	GLN	-	expression tag	UNP Q2G036
A	201	PHE	-	expression tag	UNP Q2G036
A	202	GLU	-	expression tag	UNP Q2G036
A	203	LYS	-	expression tag	UNP Q2G036
B	98	ALA	SER	engineered mutation	UNP Q2G036
B	196	TRP	-	expression tag	UNP Q2G036
B	197	SER	-	expression tag	UNP Q2G036
B	198	HIS	-	expression tag	UNP Q2G036
B	199	PRO	-	expression tag	UNP Q2G036
B	200	GLN	-	expression tag	UNP Q2G036

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	201	PHE	-	expression tag	UNP Q2G036
B	202	GLU	-	expression tag	UNP Q2G036
B	203	LYS	-	expression tag	UNP Q2G036
C	98	ALA	SER	engineered mutation	UNP Q2G036
C	196	TRP	-	expression tag	UNP Q2G036
C	197	SER	-	expression tag	UNP Q2G036
C	198	HIS	-	expression tag	UNP Q2G036
C	199	PRO	-	expression tag	UNP Q2G036
C	200	GLN	-	expression tag	UNP Q2G036
C	201	PHE	-	expression tag	UNP Q2G036
C	202	GLU	-	expression tag	UNP Q2G036
C	203	LYS	-	expression tag	UNP Q2G036
D	98	ALA	SER	engineered mutation	UNP Q2G036
D	196	TRP	-	expression tag	UNP Q2G036
D	197	SER	-	expression tag	UNP Q2G036
D	198	HIS	-	expression tag	UNP Q2G036
D	199	PRO	-	expression tag	UNP Q2G036
D	200	GLN	-	expression tag	UNP Q2G036
D	201	PHE	-	expression tag	UNP Q2G036
D	202	GLU	-	expression tag	UNP Q2G036
D	203	LYS	-	expression tag	UNP Q2G036
E	98	ALA	SER	engineered mutation	UNP Q2G036
E	196	TRP	-	expression tag	UNP Q2G036
E	197	SER	-	expression tag	UNP Q2G036
E	198	HIS	-	expression tag	UNP Q2G036
E	199	PRO	-	expression tag	UNP Q2G036
E	200	GLN	-	expression tag	UNP Q2G036
E	201	PHE	-	expression tag	UNP Q2G036
E	202	GLU	-	expression tag	UNP Q2G036
E	203	LYS	-	expression tag	UNP Q2G036
F	98	ALA	SER	engineered mutation	UNP Q2G036
F	196	TRP	-	expression tag	UNP Q2G036
F	197	SER	-	expression tag	UNP Q2G036
F	198	HIS	-	expression tag	UNP Q2G036
F	199	PRO	-	expression tag	UNP Q2G036
F	200	GLN	-	expression tag	UNP Q2G036
F	201	PHE	-	expression tag	UNP Q2G036
F	202	GLU	-	expression tag	UNP Q2G036
F	203	LYS	-	expression tag	UNP Q2G036
G	98	ALA	SER	engineered mutation	UNP Q2G036
G	196	TRP	-	expression tag	UNP Q2G036
G	197	SER	-	expression tag	UNP Q2G036

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	198	HIS	-	expression tag	UNP Q2G036
G	199	PRO	-	expression tag	UNP Q2G036
G	200	GLN	-	expression tag	UNP Q2G036
G	201	PHE	-	expression tag	UNP Q2G036
G	202	GLU	-	expression tag	UNP Q2G036
G	203	LYS	-	expression tag	UNP Q2G036
H	98	ALA	SER	engineered mutation	UNP Q2G036
H	196	TRP	-	expression tag	UNP Q2G036
H	197	SER	-	expression tag	UNP Q2G036
H	198	HIS	-	expression tag	UNP Q2G036
H	199	PRO	-	expression tag	UNP Q2G036
H	200	GLN	-	expression tag	UNP Q2G036
H	201	PHE	-	expression tag	UNP Q2G036
H	202	GLU	-	expression tag	UNP Q2G036
H	203	LYS	-	expression tag	UNP Q2G036
I	98	ALA	SER	engineered mutation	UNP Q2G036
I	196	TRP	-	expression tag	UNP Q2G036
I	197	SER	-	expression tag	UNP Q2G036
I	198	HIS	-	expression tag	UNP Q2G036
I	199	PRO	-	expression tag	UNP Q2G036
I	200	GLN	-	expression tag	UNP Q2G036
I	201	PHE	-	expression tag	UNP Q2G036
I	202	GLU	-	expression tag	UNP Q2G036
I	203	LYS	-	expression tag	UNP Q2G036
J	98	ALA	SER	engineered mutation	UNP Q2G036
J	196	TRP	-	expression tag	UNP Q2G036
J	197	SER	-	expression tag	UNP Q2G036
J	198	HIS	-	expression tag	UNP Q2G036
J	199	PRO	-	expression tag	UNP Q2G036
J	200	GLN	-	expression tag	UNP Q2G036
J	201	PHE	-	expression tag	UNP Q2G036
J	202	GLU	-	expression tag	UNP Q2G036
J	203	LYS	-	expression tag	UNP Q2G036
K	98	ALA	SER	engineered mutation	UNP Q2G036
K	196	TRP	-	expression tag	UNP Q2G036
K	197	SER	-	expression tag	UNP Q2G036
K	198	HIS	-	expression tag	UNP Q2G036
K	199	PRO	-	expression tag	UNP Q2G036
K	200	GLN	-	expression tag	UNP Q2G036
K	201	PHE	-	expression tag	UNP Q2G036
K	202	GLU	-	expression tag	UNP Q2G036
K	203	LYS	-	expression tag	UNP Q2G036

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	98	ALA	SER	engineered mutation	UNP Q2G036
L	196	TRP	-	expression tag	UNP Q2G036
L	197	SER	-	expression tag	UNP Q2G036
L	198	HIS	-	expression tag	UNP Q2G036
L	199	PRO	-	expression tag	UNP Q2G036
L	200	GLN	-	expression tag	UNP Q2G036
L	201	PHE	-	expression tag	UNP Q2G036
L	202	GLU	-	expression tag	UNP Q2G036
L	203	LYS	-	expression tag	UNP Q2G036
M	98	ALA	SER	engineered mutation	UNP Q2G036
M	196	TRP	-	expression tag	UNP Q2G036
M	197	SER	-	expression tag	UNP Q2G036
M	198	HIS	-	expression tag	UNP Q2G036
M	199	PRO	-	expression tag	UNP Q2G036
M	200	GLN	-	expression tag	UNP Q2G036
M	201	PHE	-	expression tag	UNP Q2G036
M	202	GLU	-	expression tag	UNP Q2G036
M	203	LYS	-	expression tag	UNP Q2G036
N	98	ALA	SER	engineered mutation	UNP Q2G036
N	196	TRP	-	expression tag	UNP Q2G036
N	197	SER	-	expression tag	UNP Q2G036
N	198	HIS	-	expression tag	UNP Q2G036
N	199	PRO	-	expression tag	UNP Q2G036
N	200	GLN	-	expression tag	UNP Q2G036
N	201	PHE	-	expression tag	UNP Q2G036
N	202	GLU	-	expression tag	UNP Q2G036
N	203	LYS	-	expression tag	UNP Q2G036
O	98	ALA	SER	engineered mutation	UNP Q2G036
O	196	TRP	-	expression tag	UNP Q2G036
O	197	SER	-	expression tag	UNP Q2G036
O	198	HIS	-	expression tag	UNP Q2G036
O	199	PRO	-	expression tag	UNP Q2G036
O	200	GLN	-	expression tag	UNP Q2G036
O	201	PHE	-	expression tag	UNP Q2G036
O	202	GLU	-	expression tag	UNP Q2G036
O	203	LYS	-	expression tag	UNP Q2G036
P	98	ALA	SER	engineered mutation	UNP Q2G036
P	196	TRP	-	expression tag	UNP Q2G036
P	197	SER	-	expression tag	UNP Q2G036
P	198	HIS	-	expression tag	UNP Q2G036
P	199	PRO	-	expression tag	UNP Q2G036
P	200	GLN	-	expression tag	UNP Q2G036

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	201	PHE	-	expression tag	UNP Q2G036
P	202	GLU	-	expression tag	UNP Q2G036
P	203	LYS	-	expression tag	UNP Q2G036
Q	98	ALA	SER	engineered mutation	UNP Q2G036
Q	196	TRP	-	expression tag	UNP Q2G036
Q	197	SER	-	expression tag	UNP Q2G036
Q	198	HIS	-	expression tag	UNP Q2G036
Q	199	PRO	-	expression tag	UNP Q2G036
Q	200	GLN	-	expression tag	UNP Q2G036
Q	201	PHE	-	expression tag	UNP Q2G036
Q	202	GLU	-	expression tag	UNP Q2G036
Q	203	LYS	-	expression tag	UNP Q2G036
R	98	ALA	SER	engineered mutation	UNP Q2G036
R	196	TRP	-	expression tag	UNP Q2G036
R	197	SER	-	expression tag	UNP Q2G036
R	198	HIS	-	expression tag	UNP Q2G036
R	199	PRO	-	expression tag	UNP Q2G036
R	200	GLN	-	expression tag	UNP Q2G036
R	201	PHE	-	expression tag	UNP Q2G036
R	202	GLU	-	expression tag	UNP Q2G036
R	203	LYS	-	expression tag	UNP Q2G036
S	98	ALA	SER	engineered mutation	UNP Q2G036
S	196	TRP	-	expression tag	UNP Q2G036
S	197	SER	-	expression tag	UNP Q2G036
S	198	HIS	-	expression tag	UNP Q2G036
S	199	PRO	-	expression tag	UNP Q2G036
S	200	GLN	-	expression tag	UNP Q2G036
S	201	PHE	-	expression tag	UNP Q2G036
S	202	GLU	-	expression tag	UNP Q2G036
S	203	LYS	-	expression tag	UNP Q2G036
T	98	ALA	SER	engineered mutation	UNP Q2G036
T	196	TRP	-	expression tag	UNP Q2G036
T	197	SER	-	expression tag	UNP Q2G036
T	198	HIS	-	expression tag	UNP Q2G036
T	199	PRO	-	expression tag	UNP Q2G036
T	200	GLN	-	expression tag	UNP Q2G036
T	201	PHE	-	expression tag	UNP Q2G036
T	202	GLU	-	expression tag	UNP Q2G036
T	203	LYS	-	expression tag	UNP Q2G036
U	98	ALA	SER	engineered mutation	UNP Q2G036
U	196	TRP	-	expression tag	UNP Q2G036
U	197	SER	-	expression tag	UNP Q2G036

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
U	198	HIS	-	expression tag	UNP Q2G036
U	199	PRO	-	expression tag	UNP Q2G036
U	200	GLN	-	expression tag	UNP Q2G036
U	201	PHE	-	expression tag	UNP Q2G036
U	202	GLU	-	expression tag	UNP Q2G036
U	203	LYS	-	expression tag	UNP Q2G036
V	98	ALA	SER	engineered mutation	UNP Q2G036
V	196	TRP	-	expression tag	UNP Q2G036
V	197	SER	-	expression tag	UNP Q2G036
V	198	HIS	-	expression tag	UNP Q2G036
V	199	PRO	-	expression tag	UNP Q2G036
V	200	GLN	-	expression tag	UNP Q2G036
V	201	PHE	-	expression tag	UNP Q2G036
V	202	GLU	-	expression tag	UNP Q2G036
V	203	LYS	-	expression tag	UNP Q2G036
W	98	ALA	SER	engineered mutation	UNP Q2G036
W	196	TRP	-	expression tag	UNP Q2G036
W	197	SER	-	expression tag	UNP Q2G036
W	198	HIS	-	expression tag	UNP Q2G036
W	199	PRO	-	expression tag	UNP Q2G036
W	200	GLN	-	expression tag	UNP Q2G036
W	201	PHE	-	expression tag	UNP Q2G036
W	202	GLU	-	expression tag	UNP Q2G036
W	203	LYS	-	expression tag	UNP Q2G036
X	98	ALA	SER	engineered mutation	UNP Q2G036
X	196	TRP	-	expression tag	UNP Q2G036
X	197	SER	-	expression tag	UNP Q2G036
X	198	HIS	-	expression tag	UNP Q2G036
X	199	PRO	-	expression tag	UNP Q2G036
X	200	GLN	-	expression tag	UNP Q2G036
X	201	PHE	-	expression tag	UNP Q2G036
X	202	GLU	-	expression tag	UNP Q2G036
X	203	LYS	-	expression tag	UNP Q2G036
Y	98	ALA	SER	engineered mutation	UNP Q2G036
Y	196	TRP	-	expression tag	UNP Q2G036
Y	197	SER	-	expression tag	UNP Q2G036
Y	198	HIS	-	expression tag	UNP Q2G036
Y	199	PRO	-	expression tag	UNP Q2G036
Y	200	GLN	-	expression tag	UNP Q2G036
Y	201	PHE	-	expression tag	UNP Q2G036
Y	202	GLU	-	expression tag	UNP Q2G036
Y	203	LYS	-	expression tag	UNP Q2G036

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Z	98	ALA	SER	engineered mutation	UNP Q2G036
Z	196	TRP	-	expression tag	UNP Q2G036
Z	197	SER	-	expression tag	UNP Q2G036
Z	198	HIS	-	expression tag	UNP Q2G036
Z	199	PRO	-	expression tag	UNP Q2G036
Z	200	GLN	-	expression tag	UNP Q2G036
Z	201	PHE	-	expression tag	UNP Q2G036
Z	202	GLU	-	expression tag	UNP Q2G036
Z	203	LYS	-	expression tag	UNP Q2G036
a	98	ALA	SER	engineered mutation	UNP Q2G036
a	196	TRP	-	expression tag	UNP Q2G036
a	197	SER	-	expression tag	UNP Q2G036
a	198	HIS	-	expression tag	UNP Q2G036
a	199	PRO	-	expression tag	UNP Q2G036
a	200	GLN	-	expression tag	UNP Q2G036
a	201	PHE	-	expression tag	UNP Q2G036
a	202	GLU	-	expression tag	UNP Q2G036
a	203	LYS	-	expression tag	UNP Q2G036
b	98	ALA	SER	engineered mutation	UNP Q2G036
b	196	TRP	-	expression tag	UNP Q2G036
b	197	SER	-	expression tag	UNP Q2G036
b	198	HIS	-	expression tag	UNP Q2G036
b	199	PRO	-	expression tag	UNP Q2G036
b	200	GLN	-	expression tag	UNP Q2G036
b	201	PHE	-	expression tag	UNP Q2G036
b	202	GLU	-	expression tag	UNP Q2G036
b	203	LYS	-	expression tag	UNP Q2G036

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	22	Total O 22 22	0	0
2	C	16	Total O 16 16	0	0
2	D	22	Total O 22 22	0	0
2	E	31	Total O 31 31	0	0
2	F	44	Total O 44 44	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	33	Total O 33 33	0	0
2	H	38	Total O 38 38	0	0
2	I	31	Total O 31 31	0	0
2	J	20	Total O 20 20	0	0
2	K	41	Total O 41 41	0	0
2	L	31	Total O 31 31	0	0
2	M	31	Total O 31 31	0	0
2	N	28	Total O 28 28	0	0
2	O	19	Total O 19 19	0	0
2	P	18	Total O 18 18	0	0
2	Q	18	Total O 18 18	0	0
2	R	21	Total O 21 21	0	0
2	S	14	Total O 14 14	0	0
2	T	19	Total O 19 19	0	0
2	U	14	Total O 14 14	0	0
2	V	20	Total O 20 20	0	0
2	W	16	Total O 16 16	0	0
2	X	20	Total O 20 20	0	0
2	Y	20	Total O 20 20	0	0
2	Z	16	Total O 16 16	0	0
2	a	20	Total O 20 20	0	0

Continued on next page...

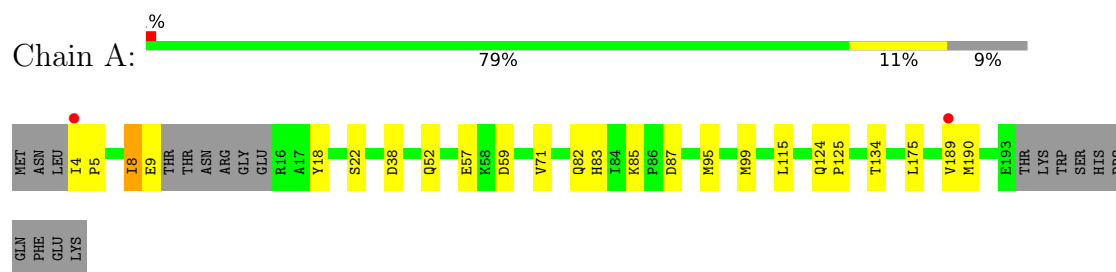
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	b	25	Total	O	0	0
			25	25		

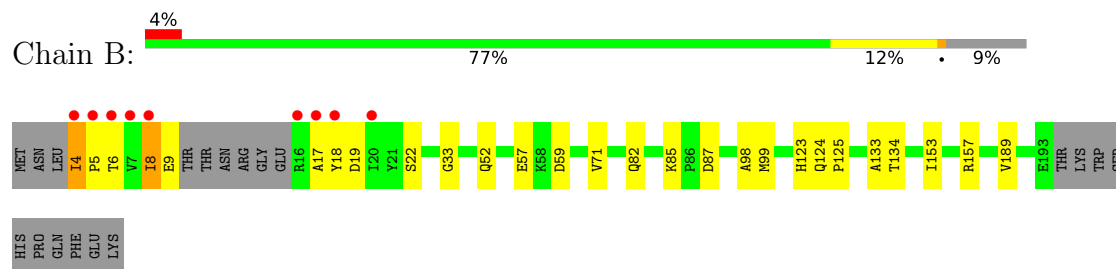
3 Residue-property plots

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.

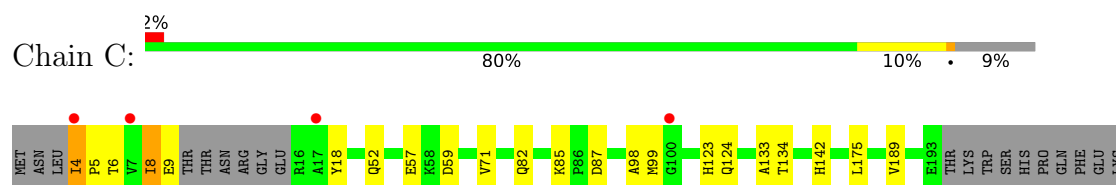
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



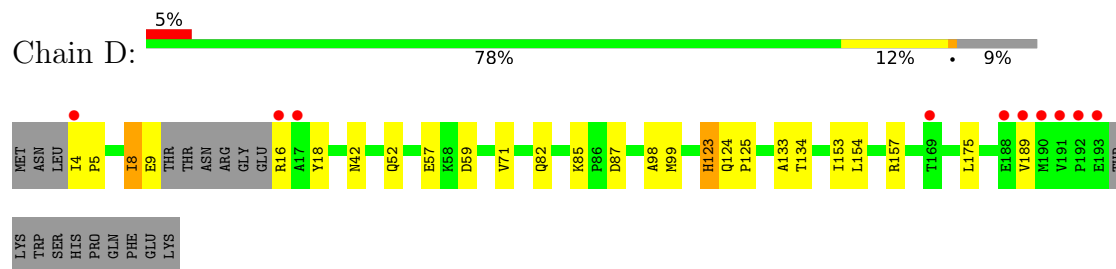
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



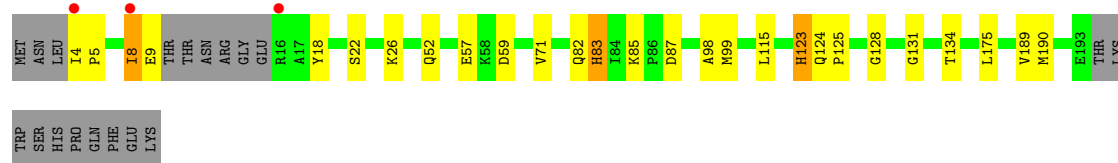
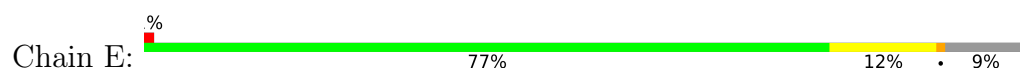
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



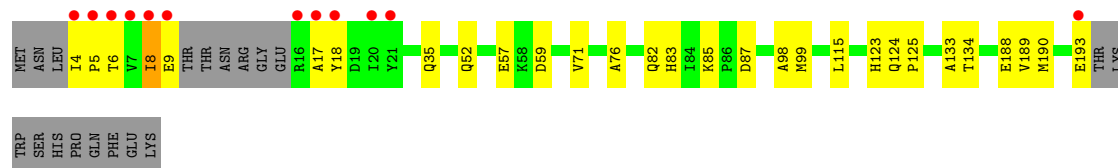
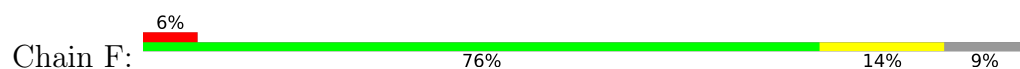
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



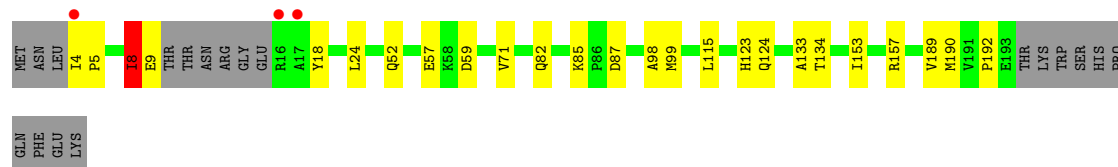
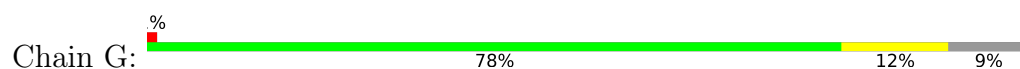
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



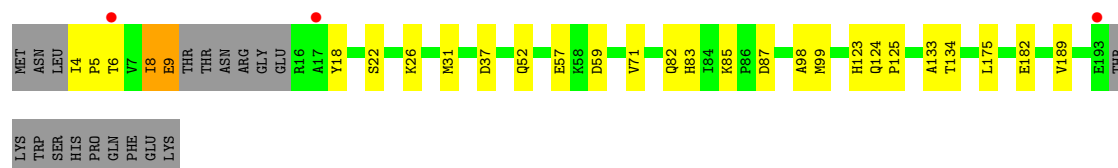
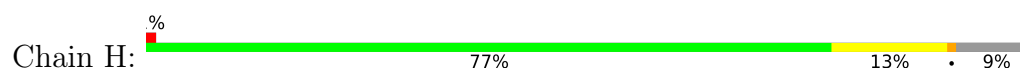
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



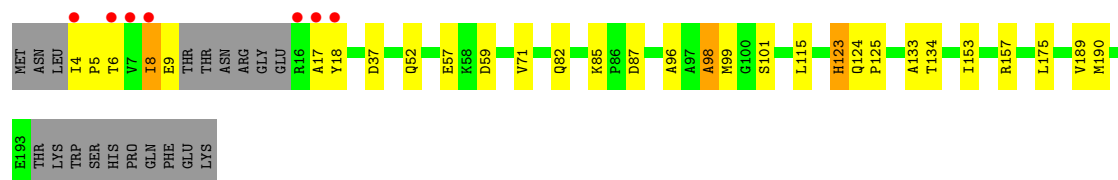
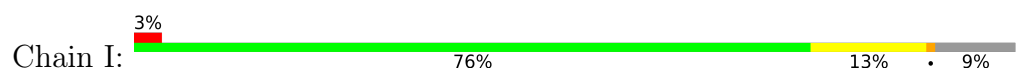
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



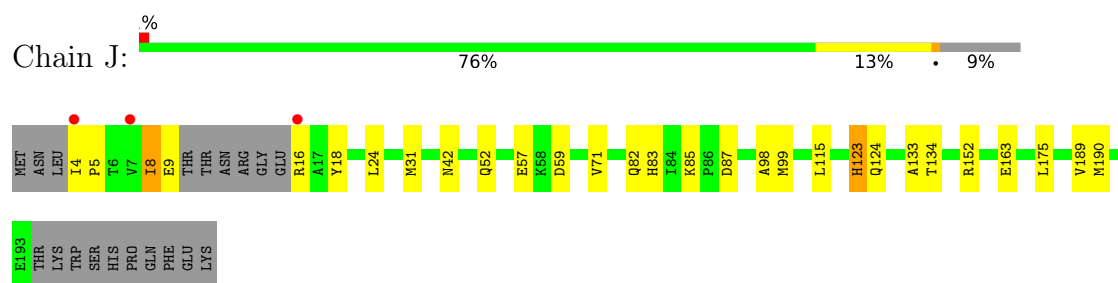
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



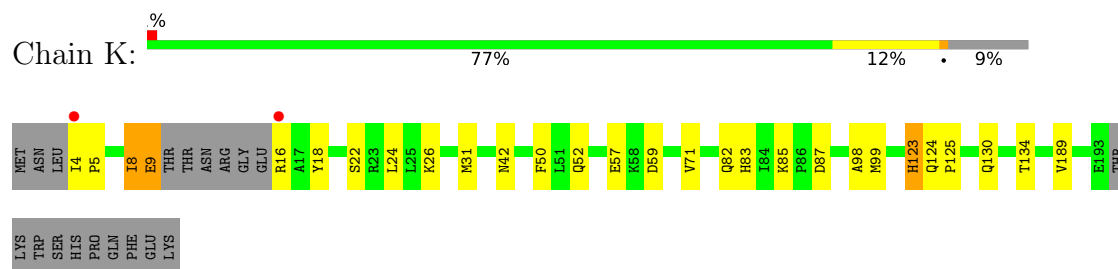
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



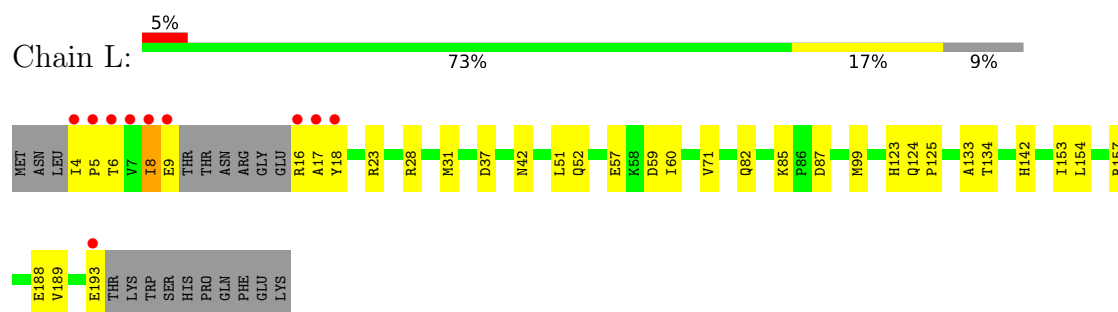
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



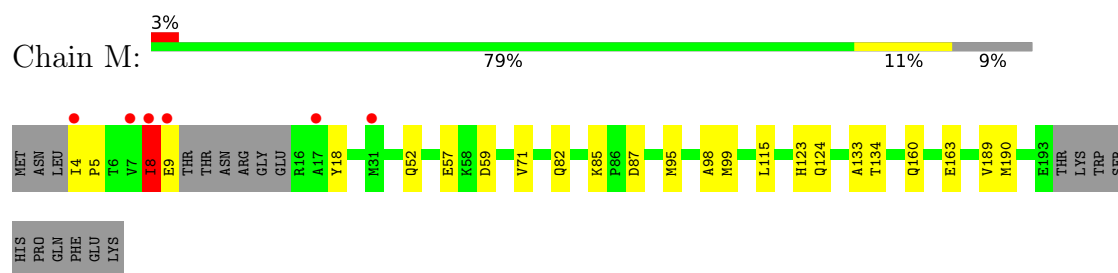
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



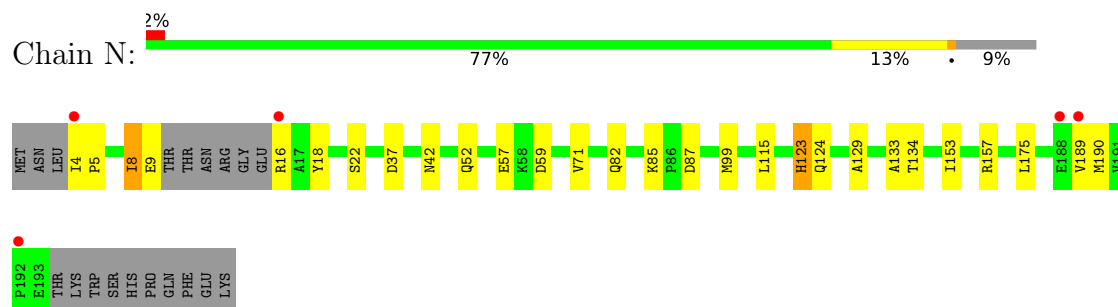
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



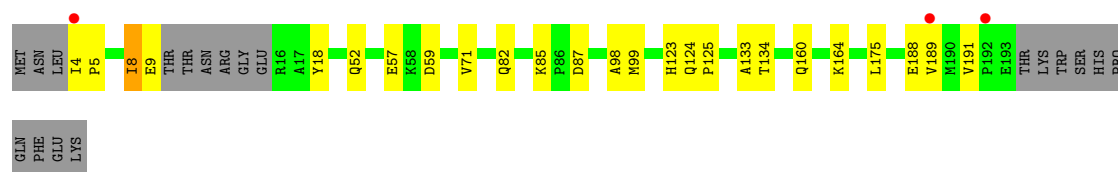
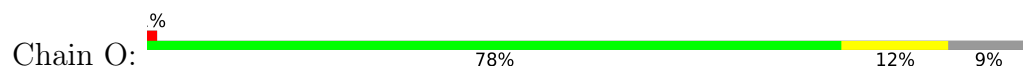
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



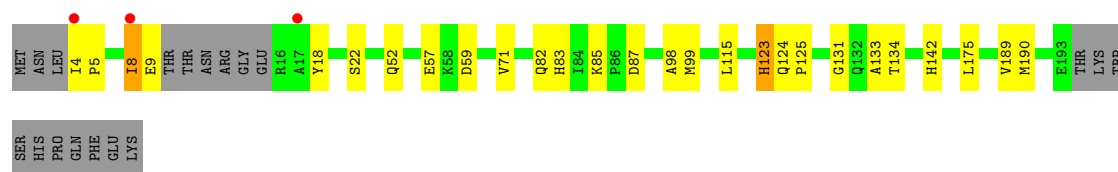
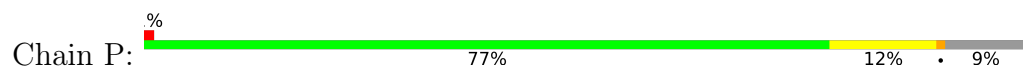
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



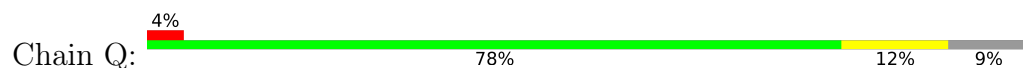
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



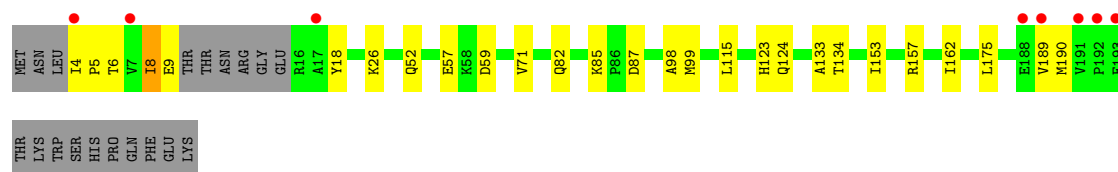
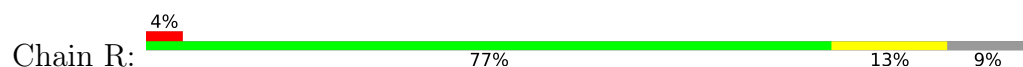
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



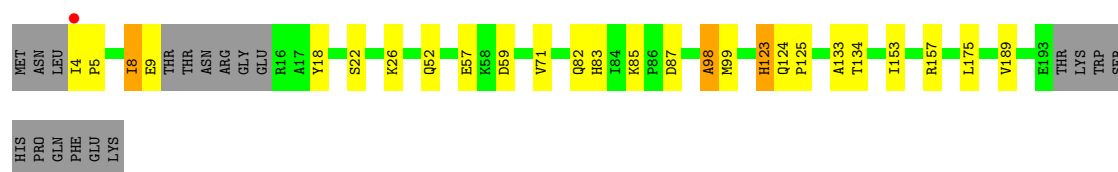
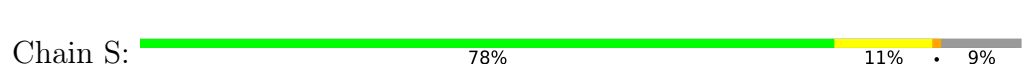
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



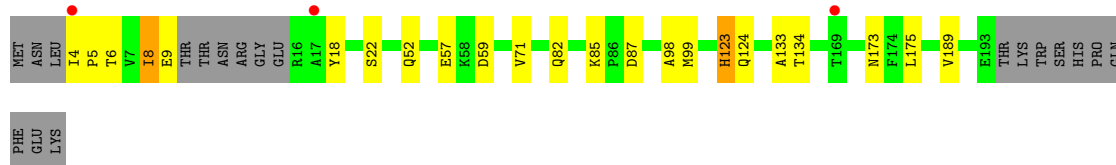
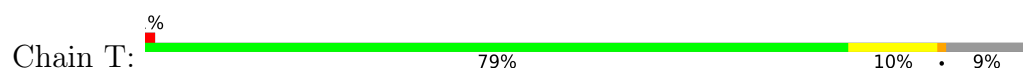
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



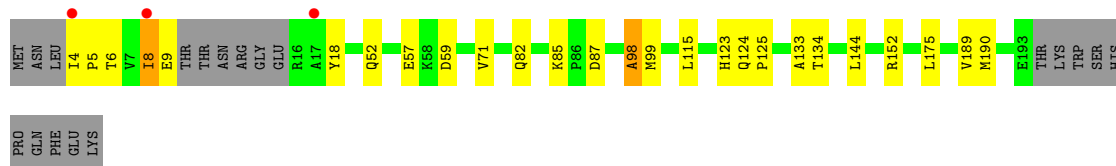
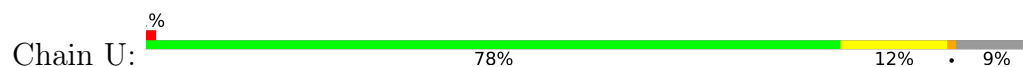
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



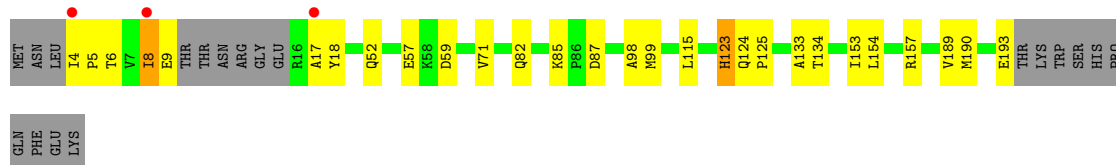
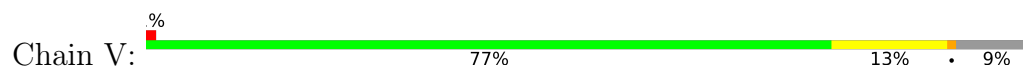
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



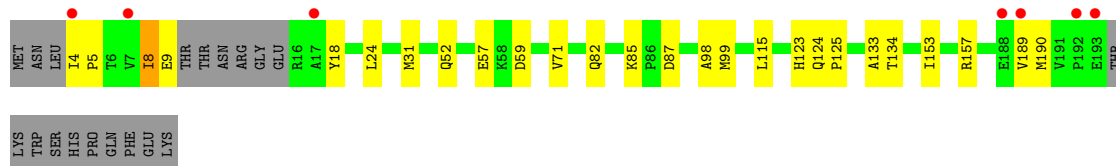
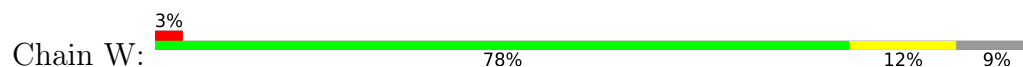
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



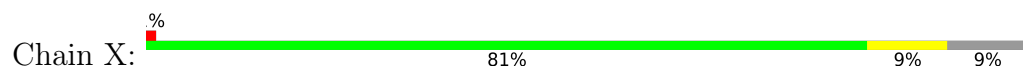
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



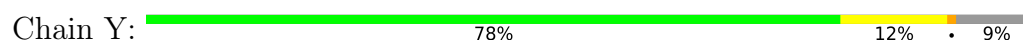
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

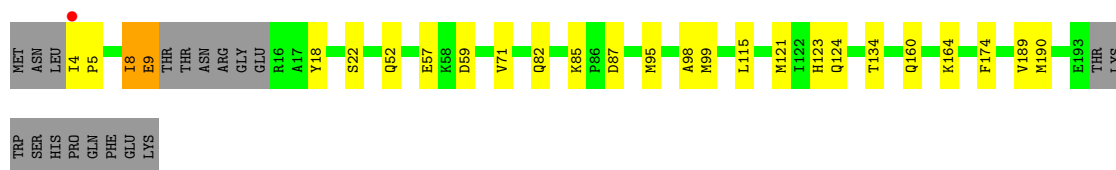


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

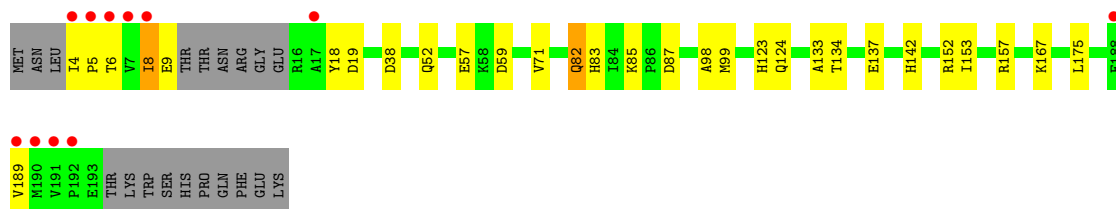
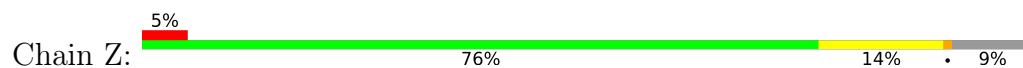


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

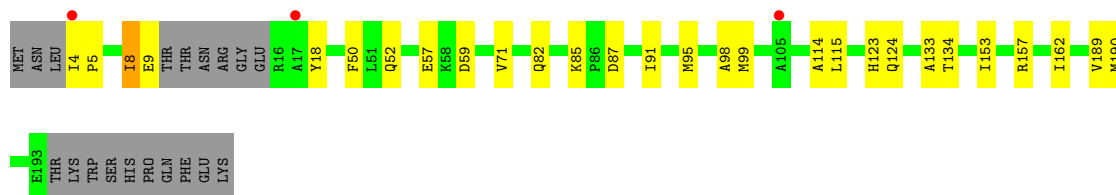
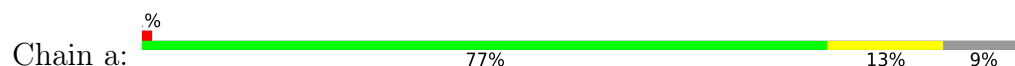




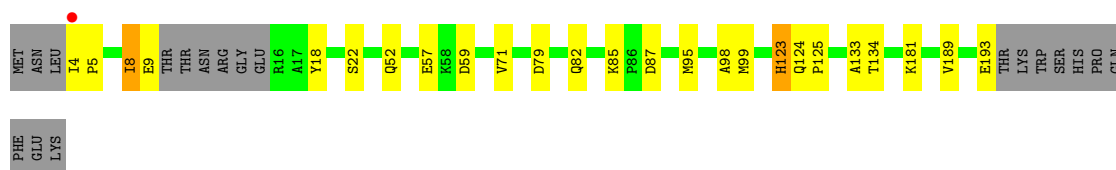
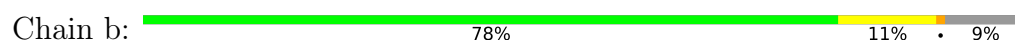
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- 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	97.55Å 109.73Å 171.41Å 73.10° 78.68° 71.46°	Depositor
Resolution (Å)	24.80 – 2.80 24.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (24.80-2.80) 95.6 (24.80-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.216 , 0.242 0.216 , 0.240	Depositor DCC
R_{free} test set	7542 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	40465	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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	0.84	1/1439 (0.1%)	0.93	0/1942
1	B	0.75	0/1439	0.92	2/1942 (0.1%)
1	C	0.81	1/1439 (0.1%)	0.91	2/1942 (0.1%)
1	D	0.84	0/1439	0.92	0/1942
1	E	1.00	2/1439 (0.1%)	1.00	1/1942 (0.1%)
1	F	1.00	0/1439	1.00	1/1942 (0.1%)
1	G	0.91	0/1439	0.99	2/1942 (0.1%)
1	H	1.01	1/1439 (0.1%)	0.99	0/1942
1	I	0.91	0/1439	0.95	1/1942 (0.1%)
1	J	0.82	2/1439 (0.1%)	0.90	0/1942
1	K	0.90	2/1439 (0.1%)	0.95	0/1942
1	L	0.93	1/1439 (0.1%)	0.94	0/1942
1	M	0.96	0/1439	0.98	2/1942 (0.1%)
1	N	1.01	1/1439 (0.1%)	1.00	0/1942
1	O	0.84	0/1439	0.90	0/1942
1	P	0.88	3/1439 (0.2%)	0.91	1/1942 (0.1%)
1	Q	0.87	1/1439 (0.1%)	0.92	0/1942
1	R	0.81	0/1439	0.93	0/1942
1	S	0.87	1/1439 (0.1%)	0.92	1/1942 (0.1%)
1	T	0.84	0/1439	0.89	0/1942
1	U	0.77	0/1439	0.90	1/1942 (0.1%)
1	V	0.83	0/1439	0.94	0/1942
1	W	0.81	0/1439	0.91	0/1942
1	X	0.82	0/1439	0.92	0/1942
1	Y	0.80	0/1439	0.89	0/1942
1	Z	0.73	0/1439	0.91	0/1942
1	a	0.76	0/1439	0.92	0/1942
1	b	0.85	0/1439	0.94	0/1942
All	All	0.87	16/40292 (0.0%)	0.94	14/54376 (0.0%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	83	HIS	CE1-NE2	6.25	1.38	1.32
1	K	83	HIS	CG-CD2	5.90	1.42	1.35
1	P	83	HIS	CG-CD2	5.67	1.42	1.35
1	K	83	HIS	CE1-NE2	5.65	1.38	1.32
1	Q	142	HIS	CG-CD2	5.63	1.42	1.35
1	E	83	HIS	CG-CD2	5.44	1.41	1.35
1	S	83	HIS	CG-CD2	5.36	1.41	1.35
1	J	83	HIS	CG-CD2	5.34	1.41	1.35
1	H	83	HIS	CG-CD2	5.33	1.41	1.35
1	P	142	HIS	CG-CD2	5.25	1.41	1.35
1	L	142	HIS	CG-CD2	5.23	1.41	1.35
1	N	123	HIS	CG-CD2	5.20	1.41	1.35
1	A	83	HIS	CG-CD2	5.20	1.41	1.35
1	J	83	HIS	CE1-NE2	5.13	1.37	1.32
1	P	83	HIS	CE1-NE2	5.12	1.37	1.32
1	C	142	HIS	CG-CD2	5.07	1.41	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	8	ILE	CB-CA-C	-6.12	102.81	111.38
1	M	8	ILE	N-CA-C	6.04	118.47	109.17
1	F	76	ALA	N-CA-C	-6.01	104.81	111.36
1	P	131	GLY	N-CA-C	5.45	117.07	111.56
1	C	4	ILE	CA-C-N	-5.40	115.02	120.31
1	C	4	ILE	C-N-CA	-5.40	115.02	120.31
1	B	4	ILE	CA-C-N	-5.33	115.09	120.31
1	B	4	ILE	C-N-CA	-5.33	115.09	120.31
1	E	131	GLY	N-CA-C	5.26	116.88	111.56
1	G	98	ALA	CB-CA-C	-5.21	110.54	116.54
1	U	98	ALA	CB-CA-C	-5.18	110.59	116.54
1	M	8	ILE	CB-CA-C	-5.17	104.14	111.38
1	S	98	ALA	CB-CA-C	-5.11	110.66	116.54
1	I	98	ALA	CB-CA-C	-5.01	110.78	116.54

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	1421	0	1437	20	0
1	B	1421	0	1437	33	0
1	C	1421	0	1437	23	0
1	D	1421	0	1437	25	0
1	E	1421	0	1437	39	0
1	F	1421	0	1437	39	0
1	G	1421	0	1437	19	0
1	H	1421	0	1437	30	0
1	I	1421	0	1437	34	0
1	J	1421	0	1437	27	0
1	K	1421	0	1437	38	0
1	L	1421	0	1437	42	0
1	M	1421	0	1437	20	0
1	N	1421	0	1437	22	0
1	O	1421	0	1437	28	0
1	P	1421	0	1437	22	0
1	Q	1421	0	1437	26	0
1	R	1421	0	1437	28	0
1	S	1421	0	1437	24	0
1	T	1421	0	1437	25	0
1	U	1421	0	1437	25	0
1	V	1421	0	1437	27	0
1	W	1421	0	1437	22	0
1	X	1421	0	1437	18	0
1	Y	1421	0	1437	25	0
1	Z	1421	0	1437	35	0
1	a	1421	0	1437	31	0
1	b	1421	0	1437	22	0
2	A	29	0	0	3	0
2	B	22	0	0	6	0
2	C	16	0	0	1	0
2	D	22	0	0	2	0
2	E	31	0	0	8	0
2	F	44	0	0	5	0
2	G	33	0	0	3	0
2	H	38	0	0	8	0
2	I	31	0	0	8	0
2	J	20	0	0	3	0
2	K	41	0	0	11	0
2	L	31	0	0	7	0
2	M	31	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	28	0	0	3	0
2	O	19	0	0	8	0
2	P	18	0	0	0	0
2	Q	18	0	0	1	0
2	R	21	0	0	3	0
2	S	14	0	0	2	0
2	T	19	0	0	2	0
2	U	14	0	0	1	0
2	V	20	0	0	3	0
2	W	16	0	0	0	0
2	X	20	0	0	1	0
2	Y	20	0	0	5	0
2	Z	16	0	0	8	0
2	a	20	0	0	11	0
2	b	25	0	0	5	0
All	All	40465	0	40236	603	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (603) 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:K:18:TYR:OH	1:L:8:ILE:HG12	1.26	1.32
1:E:18:TYR:OH	1:F:8:ILE:HG12	1.16	1.24
1:S:18:TYR:OH	1:T:8:ILE:HG12	1.46	1.14
2:Y:308:HOH:O	1:Z:4:ILE:HG22	1.44	1.14
1:H:18:TYR:OH	1:I:8:ILE:HG12	1.47	1.13
2:K:314:HOH:O	1:L:17:ALA:HB1	1.47	1.12
1:F:8:ILE:HG22	2:F:305:HOH:O	1.47	1.11
1:Y:164:LYS:HB3	2:Y:317:HOH:O	1.50	1.10
1:K:8:ILE:CG2	2:K:318:HOH:O	2.00	1.09
1:V:17:ALA:HB1	2:b:307:HOH:O	1.54	1.08
1:Q:18:TYR:OH	1:R:8:ILE:HG12	1.53	1.06
1:B:8:ILE:HG22	2:B:307:HOH:O	1.53	1.05
1:A:18:TYR:OH	1:B:8:ILE:HG12	1.54	1.05
1:B:18:TYR:OH	1:C:8:ILE:HG12	1.55	1.05
2:E:321:HOH:O	1:F:17:ALA:HB1	1.55	1.05
1:I:6:THR:HG21	2:I:302:HOH:O	1.58	1.03
1:S:4:ILE:HG13	2:S:311:HOH:O	1.60	1.02
1:Y:18:TYR:OH	1:Z:8:ILE:HG12	1.58	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:TYR:OH	1:F:8:ILE:CG1	2.08	1.01
1:K:22:SER:HB3	1:L:6:THR:O	1.60	0.99
2:H:336:HOH:O	1:I:5:PRO:HB3	1.59	0.98
1:P:18:TYR:OH	1:Q:8:ILE:HG12	1.63	0.98
1:V:8:ILE:HG12	1:b:18:TYR:OH	1.64	0.98
1:D:18:TYR:OH	1:E:8:ILE:HG12	1.63	0.97
1:H:8:ILE:HG12	1:N:18:TYR:OH	1.64	0.96
1:H:8:ILE:HG22	2:H:313:HOH:O	1.64	0.96
1:E:18:TYR:CZ	1:F:8:ILE:HG12	2.01	0.95
1:T:18:TYR:OH	1:U:8:ILE:HG12	1.64	0.95
1:F:188:GLU:HG2	2:F:320:HOH:O	1.66	0.94
1:Z:83:HIS:HD2	2:a:309:HOH:O	1.50	0.92
1:X:18:TYR:OH	1:Y:8:ILE:HG12	1.71	0.90
1:A:95:MET:HG2	2:A:306:HOH:O	1.72	0.90
1:K:18:TYR:OH	1:L:8:ILE:CG1	2.17	0.88
1:Z:18:TYR:OH	1:a:8:ILE:HG12	1.71	0.88
1:R:18:TYR:OH	1:S:8:ILE:HG12	1.73	0.88
1:E:18:TYR:HH	1:F:8:ILE:HG12	1.11	0.87
1:V:18:TYR:OH	1:W:8:ILE:HG12	1.73	0.87
1:E:22:SER:HB3	1:F:6:THR:O	1.75	0.86
1:O:8:ILE:HG12	1:U:18:TYR:OH	1.75	0.85
1:K:18:TYR:CZ	1:L:8:ILE:HG12	2.11	0.85
1:O:18:TYR:OH	1:P:8:ILE:HG12	1.76	0.85
1:E:8:ILE:CG2	2:E:311:HOH:O	2.26	0.84
1:Y:9:GLU:O	2:Y:305:HOH:O	1.97	0.82
1:I:8:ILE:HG22	2:I:314:HOH:O	1.76	0.82
1:K:8:ILE:HG22	2:K:318:HOH:O	1.73	0.81
1:F:4:ILE:HA	2:F:302:HOH:O	1.80	0.80
1:J:18:TYR:OH	1:K:8:ILE:HG12	1.82	0.79
1:L:8:ILE:HG22	2:L:303:HOH:O	1.83	0.79
1:Y:160:GLN:HB3	2:Y:317:HOH:O	1.82	0.79
1:a:18:TYR:OH	1:b:8:ILE:HG12	1.83	0.78
1:D:16:ARG:NH1	2:D:319:HOH:O	2.16	0.78
1:G:4:ILE:HG23	1:G:5:PRO:HD3	1.65	0.78
1:a:8:ILE:HG22	2:a:320:HOH:O	1.84	0.78
1:K:8:ILE:HG23	2:K:318:HOH:O	1.68	0.77
1:C:4:ILE:HG22	2:C:308:HOH:O	1.85	0.76
1:I:17:ALA:HB1	2:I:302:HOH:O	1.84	0.76
1:L:4:ILE:N	2:L:316:HOH:O	2.18	0.75
1:V:17:ALA:CB	2:b:307:HOH:O	2.20	0.75
1:F:18:TYR:OH	1:G:8:ILE:HG12	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:8:ILE:HA	2:K:318:HOH:O	1.87	0.73
1:W:18:TYR:OH	1:X:8:ILE:HG12	1.88	0.73
1:B:6:THR:HG22	2:B:320:HOH:O	1.89	0.73
1:D:4:ILE:HG23	1:D:5:PRO:HD3	1.70	0.73
1:M:95:MET:HG2	2:M:327:HOH:O	1.89	0.73
1:K:9:GLU:O	2:K:326:HOH:O	2.06	0.72
1:K:26:LYS:HE2	1:L:8:ILE:HD11	1.71	0.72
1:O:188:GLU:HG3	2:O:305:HOH:O	1.89	0.72
1:M:18:TYR:OH	1:N:8:ILE:HG12	1.90	0.72
1:T:134:THR:H	1:a:124:GLN:HE22	1.38	0.71
1:Q:4:ILE:HA	2:Q:305:HOH:O	1.89	0.70
1:H:18:TYR:CZ	1:I:8:ILE:HG12	2.26	0.70
1:D:134:THR:H	1:H:124:GLN:HE22	1.40	0.70
2:X:313:HOH:O	1:Y:95:MET:HG2	1.90	0.70
1:X:4:ILE:HG23	1:X:5:PRO:HD3	1.72	0.70
2:K:314:HOH:O	1:L:17:ALA:CB	2.19	0.70
1:E:18:TYR:HH	1:F:8:ILE:CG1	1.95	0.69
1:a:8:ILE:CG2	2:a:320:HOH:O	2.38	0.69
1:I:4:ILE:HD13	2:N:323:HOH:O	1.93	0.69
1:J:16:ARG:HB2	2:J:305:HOH:O	1.91	0.69
1:I:4:ILE:HA	2:I:303:HOH:O	1.94	0.68
1:H:4:ILE:HG23	1:H:5:PRO:HD3	1.77	0.67
2:H:320:HOH:O	1:I:6:THR:HB	1.94	0.67
1:R:4:ILE:HG23	1:R:5:PRO:HD3	1.76	0.67
1:T:18:TYR:HA	2:T:319:HOH:O	1.94	0.67
1:A:8:ILE:HG12	1:G:18:TYR:OH	1.94	0.67
1:E:134:THR:H	1:N:124:GLN:HE22	1.41	0.67
1:E:8:ILE:HG23	2:E:311:HOH:O	1.93	0.67
1:L:28:ARG:NH2	2:L:331:HOH:O	2.28	0.66
1:M:160:GLN:OE1	1:Q:159:GLY:HA2	1.95	0.66
1:S:59:ASP:HB2	1:S:87:ASP:O	1.96	0.66
1:U:134:THR:H	1:Z:124:GLN:HE22	1.42	0.66
1:K:82:GLN:HA	1:K:82:GLN:NE2	2.11	0.66
1:F:4:ILE:HG22	2:F:317:HOH:O	1.96	0.66
1:Z:82:GLN:HA	1:Z:82:GLN:NE2	2.11	0.66
1:N:4:ILE:HG23	1:N:5:PRO:HD3	1.77	0.65
1:L:18:TYR:OH	1:M:8:ILE:HG12	1.96	0.65
1:A:4:ILE:HG23	1:A:5:PRO:HD3	1.78	0.65
1:R:82:GLN:HA	1:R:82:GLN:NE2	2.13	0.64
1:T:52:GLN:NE2	1:T:85:LYS:H	1.96	0.64
1:F:124:GLN:HE21	1:M:133:ALA:HB3	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:134:THR:H	1:Y:124:GLN:HE22	1.45	0.64
1:W:82:GLN:NE2	1:W:82:GLN:HA	2.13	0.64
1:F:115:LEU:HD21	1:F:190:MET:HE2	1.78	0.64
1:L:60:ILE:HD11	2:L:331:HOH:O	1.96	0.64
1:R:52:GLN:HE21	1:R:85:LYS:H	1.45	0.64
1:J:4:ILE:HG23	1:J:5:PRO:HD3	1.78	0.64
1:A:52:GLN:HE21	1:A:85:LYS:H	1.46	0.64
1:S:4:ILE:HG23	1:S:5:PRO:HD3	1.80	0.64
1:a:95:MET:HG2	2:a:318:HOH:O	1.98	0.63
1:a:85:LYS:HG2	2:b:316:HOH:O	1.97	0.63
2:E:321:HOH:O	1:F:6:THR:HG21	1.98	0.63
1:O:124:GLN:HE22	1:Y:134:THR:H	1.47	0.63
1:S:71:VAL:HG22	1:S:99:MET:HE3	1.79	0.63
1:B:18:TYR:HH	1:C:8:ILE:HG12	1.61	0.63
1:O:191:VAL:HA	2:O:307:HOH:O	1.97	0.63
1:P:52:GLN:NE2	1:P:85:LYS:H	1.96	0.63
1:U:71:VAL:HG22	1:U:99:MET:HE3	1.79	0.63
1:E:26:LYS:HE2	1:F:8:ILE:HD11	1.79	0.63
1:I:18:TYR:OH	1:J:8:ILE:HG12	1.99	0.63
1:O:4:ILE:HG23	1:O:5:PRO:HD3	1.81	0.63
1:S:134:THR:H	1:b:124:GLN:HE22	1.47	0.63
1:O:8:ILE:HG23	2:O:317:HOH:O	1.97	0.62
1:C:18:TYR:OH	1:D:8:ILE:HG12	1.99	0.62
1:M:4:ILE:HG23	1:M:5:PRO:HD3	1.81	0.62
1:a:4:ILE:HG23	1:a:5:PRO:HD3	1.82	0.62
1:H:18:TYR:HA	2:H:320:HOH:O	1.99	0.62
1:F:59:ASP:HB2	1:F:87:ASP:O	2.00	0.62
1:U:124:GLN:HE22	1:Z:134:THR:H	1.47	0.62
1:Z:82:GLN:HA	1:Z:82:GLN:HE21	1.64	0.61
1:A:71:VAL:HG22	1:A:99:MET:HE3	1.83	0.61
1:C:82:GLN:HA	1:C:82:GLN:NE2	2.15	0.61
1:X:82:GLN:NE2	1:X:82:GLN:HA	2.14	0.61
1:P:71:VAL:HG22	1:P:99:MET:HE3	1.83	0.61
1:Z:142:HIS:HD2	2:Z:310:HOH:O	1.81	0.61
2:a:313:HOH:O	1:b:95:MET:HG2	2.00	0.61
1:E:8:ILE:HG22	2:E:311:HOH:O	1.91	0.61
1:a:50:PHE:HA	2:a:302:HOH:O	1.99	0.61
1:I:17:ALA:HB3	2:I:311:HOH:O	2.00	0.61
1:Y:52:GLN:HE21	1:Y:85:LYS:H	1.48	0.61
1:H:9:GLU:O	2:H:306:HOH:O	2.17	0.61
1:Y:52:GLN:NE2	1:Y:85:LYS:H	1.99	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:8:ILE:CG2	2:H:313:HOH:O	2.35	0.60
1:a:71:VAL:HG22	1:a:99:MET:HE3	1.83	0.60
1:b:59:ASP:HB2	1:b:87:ASP:O	2.01	0.60
1:A:52:GLN:NE2	1:A:85:LYS:H	1.99	0.60
1:U:4:ILE:HG23	1:U:5:PRO:HD3	1.84	0.60
1:E:82:GLN:HA	1:E:82:GLN:NE2	2.16	0.60
1:G:133:ALA:HB3	1:L:124:GLN:HE21	1.66	0.60
1:J:71:VAL:HG22	1:J:99:MET:HE3	1.83	0.60
1:P:52:GLN:HE21	1:P:85:LYS:H	1.50	0.59
1:a:52:GLN:HE21	1:a:85:LYS:H	1.48	0.59
2:E:321:HOH:O	1:F:17:ALA:CB	2.29	0.59
1:W:52:GLN:HE21	1:W:85:LYS:H	1.50	0.59
1:a:52:GLN:NE2	1:a:85:LYS:H	2.00	0.59
1:B:134:THR:H	1:J:124:GLN:HE22	1.50	0.59
1:b:193:GLU:HG3	2:b:302:HOH:O	2.01	0.59
1:Q:4:ILE:HG23	1:Q:5:PRO:HD3	1.83	0.59
1:J:163:GLU:HA	2:J:308:HOH:O	2.02	0.59
1:L:71:VAL:HG22	1:L:99:MET:HE3	1.85	0.59
1:Q:71:VAL:HG22	1:Q:99:MET:HE3	1.83	0.59
1:S:133:ALA:HB3	1:b:124:GLN:HE21	1.68	0.59
1:S:52:GLN:HE21	1:S:85:LYS:H	1.51	0.59
1:D:82:GLN:HA	1:D:82:GLN:NE2	2.18	0.58
1:J:82:GLN:HA	1:J:82:GLN:NE2	2.17	0.58
1:H:98:ALA:HB1	2:H:307:HOH:O	2.03	0.58
1:B:124:GLN:HE22	1:J:134:THR:H	1.51	0.58
1:I:59:ASP:HB2	1:I:87:ASP:O	2.03	0.58
1:b:71:VAL:HG22	1:b:99:MET:HE3	1.84	0.58
1:C:59:ASP:HB2	1:C:87:ASP:O	2.03	0.58
1:C:71:VAL:HG22	1:C:99:MET:HE3	1.84	0.58
2:K:308:HOH:O	1:L:193:GLU:C	2.46	0.58
2:Z:311:HOH:O	1:a:5:PRO:CG	2.51	0.58
1:O:82:GLN:NE2	1:O:82:GLN:HA	2.18	0.58
1:T:52:GLN:HE21	1:T:85:LYS:H	1.49	0.58
1:C:52:GLN:NE2	1:C:85:LYS:H	2.02	0.58
1:E:18:TYR:CE1	1:F:8:ILE:HG12	2.39	0.58
1:Q:124:GLN:HE21	1:W:133:ALA:HB3	1.68	0.58
1:R:26:LYS:HB2	2:R:315:HOH:O	2.03	0.58
1:S:124:GLN:HE21	1:b:133:ALA:HB3	1.68	0.58
1:L:52:GLN:HE21	1:L:85:LYS:H	1.52	0.58
1:L:188:GLU:HG2	2:L:318:HOH:O	2.04	0.57
1:W:4:ILE:HG23	1:W:5:PRO:HD3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:4:ILE:HG23	1:Y:5:PRO:HD3	1.84	0.57
1:Z:4:ILE:HG23	1:Z:5:PRO:HD3	1.86	0.57
1:D:124:GLN:HE22	1:H:134:THR:H	1.52	0.57
1:F:83:HIS:HD2	2:G:333:HOH:O	1.85	0.57
1:Q:18:TYR:CZ	1:R:8:ILE:HG12	2.39	0.57
1:L:82:GLN:HA	1:L:82:GLN:NE2	2.18	0.57
1:T:4:ILE:HG23	1:T:5:PRO:HD3	1.85	0.57
1:a:91:ILE:HG23	2:a:317:HOH:O	2.03	0.57
1:W:71:VAL:HG22	1:W:99:MET:HE3	1.87	0.57
1:C:52:GLN:HE21	1:C:85:LYS:H	1.52	0.57
1:K:130:GLN:HG3	2:K:320:HOH:O	2.04	0.57
1:S:133:ALA:HB3	1:b:124:GLN:NE2	2.20	0.57
1:b:4:ILE:HG23	1:b:5:PRO:HD3	1.87	0.57
1:N:59:ASP:HB2	1:N:87:ASP:O	2.04	0.57
1:T:124:GLN:HE21	1:a:133:ALA:HB3	1.69	0.57
1:O:52:GLN:HE21	1:O:85:LYS:H	1.53	0.56
1:W:52:GLN:NE2	1:W:85:LYS:H	2.03	0.56
1:E:52:GLN:HE21	1:E:85:LYS:H	1.51	0.56
1:L:52:GLN:NE2	1:L:85:LYS:H	2.02	0.56
1:B:98:ALA:HB2	1:B:123:HIS:HE1	1.70	0.56
1:K:82:GLN:HA	1:K:82:GLN:HE21	1.70	0.56
1:O:160:GLN:HB3	2:O:318:HOH:O	2.04	0.56
1:Q:52:GLN:NE2	1:Q:85:LYS:H	2.03	0.56
1:R:52:GLN:NE2	1:R:85:LYS:H	2.03	0.56
1:B:124:GLN:HE21	1:J:133:ALA:HB3	1.71	0.56
1:C:82:GLN:HA	1:C:82:GLN:HE21	1.71	0.56
1:K:8:ILE:CA	2:K:318:HOH:O	2.50	0.56
1:X:52:GLN:HE21	1:X:85:LYS:H	1.54	0.56
1:Q:134:THR:H	1:W:124:GLN:HE22	1.52	0.56
1:H:59:ASP:HB2	1:H:87:ASP:O	2.06	0.56
1:E:4:ILE:HG23	1:E:5:PRO:HD3	1.88	0.56
1:I:6:THR:CG2	2:I:302:HOH:O	2.34	0.56
1:F:124:GLN:NE2	1:M:133:ALA:HB3	2.20	0.56
1:G:124:GLN:HE22	1:L:134:THR:H	1.52	0.56
1:G:133:ALA:HB3	1:L:124:GLN:NE2	2.19	0.56
1:S:52:GLN:NE2	1:S:85:LYS:H	2.03	0.56
1:P:4:ILE:HG23	1:P:5:PRO:HD3	1.88	0.55
1:Q:59:ASP:HB2	1:Q:87:ASP:O	2.06	0.55
1:C:98:ALA:HB2	1:C:123:HIS:HE1	1.72	0.55
1:G:124:GLN:HE21	1:L:133:ALA:HB3	1.72	0.55
1:Z:59:ASP:HB2	1:Z:87:ASP:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:98:ALA:HB2	1:Z:123:HIS:HE1	1.71	0.55
1:E:8:ILE:HA	2:E:311:HOH:O	2.05	0.55
1:G:82:GLN:NE2	1:G:82:GLN:HA	2.22	0.55
1:Q:82:GLN:HA	1:Q:82:GLN:NE2	2.21	0.55
1:b:52:GLN:NE2	1:b:85:LYS:H	2.05	0.55
1:C:4:ILE:HG23	1:C:5:PRO:HD3	1.88	0.55
1:P:82:GLN:HA	1:P:82:GLN:NE2	2.22	0.55
1:R:71:VAL:HG22	1:R:99:MET:HE3	1.89	0.55
1:D:59:ASP:HB2	1:D:87:ASP:O	2.07	0.55
1:L:59:ASP:HB2	1:L:87:ASP:O	2.07	0.55
1:O:52:GLN:NE2	1:O:85:LYS:H	2.05	0.55
1:R:82:GLN:HA	1:R:82:GLN:HE21	1.72	0.55
1:D:4:ILE:CG2	1:D:5:PRO:HD3	2.37	0.54
1:K:59:ASP:HB2	1:K:87:ASP:O	2.08	0.54
1:B:71:VAL:HG22	1:B:99:MET:HE3	1.89	0.54
1:I:71:VAL:HG22	1:I:99:MET:HE3	1.90	0.54
1:Y:18:TYR:CZ	1:Z:8:ILE:HG12	2.40	0.54
1:A:82:GLN:HA	1:A:82:GLN:NE2	2.22	0.54
1:D:52:GLN:NE2	1:D:85:LYS:H	2.05	0.54
1:K:52:GLN:NE2	1:K:85:LYS:H	2.04	0.54
1:S:18:TYR:CZ	1:T:8:ILE:HG12	2.39	0.54
1:U:82:GLN:HA	1:U:82:GLN:NE2	2.22	0.54
1:V:71:VAL:HG22	1:V:99:MET:HE3	1.90	0.54
1:C:124:GLN:HE21	1:I:133:ALA:HB3	1.72	0.54
1:F:134:THR:H	1:M:124:GLN:HE22	1.54	0.54
1:M:52:GLN:NE2	1:M:85:LYS:H	2.06	0.54
1:O:133:ALA:HB3	1:Y:124:GLN:HE21	1.73	0.54
1:b:52:GLN:HE21	1:b:85:LYS:H	1.55	0.54
1:T:59:ASP:HB2	1:T:87:ASP:O	2.08	0.54
1:V:82:GLN:HA	1:V:82:GLN:NE2	2.23	0.54
1:K:71:VAL:HG22	1:K:99:MET:HE3	1.90	0.54
1:T:134:THR:H	1:a:124:GLN:NE2	2.05	0.54
1:E:124:GLN:HE22	1:N:134:THR:H	1.53	0.54
1:F:193:GLU:HG3	2:F:327:HOH:O	2.07	0.54
1:G:52:GLN:HE21	1:G:85:LYS:H	1.56	0.54
1:V:4:ILE:HG23	1:V:5:PRO:HD3	1.89	0.54
1:C:134:THR:H	1:I:124:GLN:HE22	1.57	0.53
1:Z:52:GLN:HE21	1:Z:85:LYS:H	1.55	0.53
1:a:59:ASP:HB2	1:a:87:ASP:O	2.08	0.53
1:B:98:ALA:HB2	1:B:123:HIS:CE1	2.43	0.53
1:F:82:GLN:NE2	1:F:82:GLN:HA	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:17:ALA:CB	2:I:311:HOH:O	2.56	0.53
1:G:134:THR:H	1:L:124:GLN:HE22	1.56	0.53
1:V:52:GLN:NE2	1:V:85:LYS:H	2.06	0.53
1:Q:52:GLN:HE21	1:Q:85:LYS:H	1.54	0.53
1:T:124:GLN:NE2	1:a:133:ALA:HB3	2.24	0.53
1:E:52:GLN:NE2	1:E:85:LYS:H	2.06	0.53
1:R:98:ALA:HB2	1:R:123:HIS:HE1	1.74	0.53
1:M:98:ALA:HB2	1:M:123:HIS:HE1	1.74	0.53
1:E:71:VAL:HG22	1:E:99:MET:HE3	1.89	0.53
1:H:71:VAL:HG22	1:H:99:MET:HE3	1.89	0.53
1:Q:98:ALA:HB2	1:Q:123:HIS:HE1	1.73	0.53
2:Z:311:HOH:O	1:a:5:PRO:CB	2.57	0.53
1:D:52:GLN:HE21	1:D:85:LYS:H	1.55	0.53
1:G:71:VAL:HG22	1:G:99:MET:HE3	1.91	0.53
1:N:52:GLN:NE2	1:N:85:LYS:H	2.06	0.53
1:B:22:SER:HB3	1:C:6:THR:O	2.09	0.53
1:D:71:VAL:HG22	1:D:99:MET:HE3	1.91	0.53
1:G:59:ASP:HB2	1:G:87:ASP:O	2.09	0.53
1:N:71:VAL:HG22	1:N:99:MET:HE3	1.91	0.53
1:L:51:LEU:C	2:L:331:HOH:O	2.52	0.52
1:P:124:GLN:HE22	1:X:134:THR:H	1.56	0.52
1:S:82:GLN:HA	1:S:82:GLN:NE2	2.24	0.52
1:V:52:GLN:HE21	1:V:85:LYS:H	1.56	0.52
1:E:59:ASP:HB2	1:E:87:ASP:O	2.09	0.52
1:Q:124:GLN:NE2	1:W:133:ALA:HB3	2.24	0.52
1:Z:52:GLN:NE2	1:Z:85:LYS:H	2.06	0.52
1:E:115:LEU:HD21	1:E:190:MET:HE2	1.92	0.52
1:J:59:ASP:HB2	1:J:87:ASP:O	2.09	0.52
1:b:98:ALA:HB2	1:b:123:HIS:CE1	2.45	0.52
1:A:18:TYR:CZ	1:B:8:ILE:HG12	2.44	0.52
1:U:52:GLN:NE2	1:U:85:LYS:H	2.08	0.52
1:F:124:GLN:HE22	1:M:134:THR:H	1.57	0.52
1:X:4:ILE:CG2	1:X:5:PRO:HD3	2.39	0.52
1:Y:71:VAL:HG22	1:Y:99:MET:HE3	1.91	0.52
1:C:133:ALA:HB3	1:I:124:GLN:HE21	1.74	0.52
1:J:52:GLN:NE2	1:J:85:LYS:H	2.07	0.52
1:N:52:GLN:HE21	1:N:85:LYS:H	1.58	0.52
1:O:71:VAL:HG22	1:O:99:MET:HE3	1.92	0.52
1:U:59:ASP:HB2	1:U:87:ASP:O	2.10	0.52
1:G:52:GLN:NE2	1:G:85:LYS:H	2.08	0.52
1:H:22:SER:HB3	1:I:6:THR:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:52:GLN:HE21	1:K:85:LYS:H	1.57	0.51
1:L:4:ILE:HG23	1:L:5:PRO:HD3	1.92	0.51
1:Q:124:GLN:HE22	1:W:134:THR:H	1.57	0.51
1:a:91:ILE:CG2	2:a:317:HOH:O	2.56	0.51
1:B:4:ILE:HG23	1:B:5:PRO:HD3	1.91	0.51
1:D:82:GLN:HA	1:D:82:GLN:HE21	1.76	0.51
1:N:82:GLN:NE2	1:N:82:GLN:HA	2.25	0.51
1:U:134:THR:H	1:Z:124:GLN:NE2	2.08	0.51
1:X:52:GLN:NE2	1:X:85:LYS:H	2.08	0.51
1:Z:98:ALA:HB2	1:Z:123:HIS:CE1	2.45	0.51
1:A:59:ASP:HB2	1:A:87:ASP:O	2.11	0.51
1:a:82:GLN:HA	1:a:82:GLN:NE2	2.25	0.51
1:A:124:GLN:HE22	1:K:134:THR:H	1.58	0.51
1:B:124:GLN:NE2	1:J:133:ALA:HB3	2.25	0.51
1:a:98:ALA:HB2	1:a:123:HIS:HE1	1.76	0.51
1:B:52:GLN:NE2	1:B:85:LYS:H	2.09	0.51
1:I:82:GLN:HA	1:I:82:GLN:NE2	2.26	0.51
1:K:18:TYR:CE1	1:L:8:ILE:HG23	2.46	0.51
1:R:124:GLN:HE21	1:V:133:ALA:HB3	1.76	0.51
1:T:98:ALA:HB2	1:T:123:HIS:CE1	2.45	0.51
1:Y:59:ASP:HB2	1:Y:87:ASP:O	2.10	0.51
1:C:133:ALA:HB3	1:I:124:GLN:NE2	2.26	0.51
1:D:134:THR:H	1:H:124:GLN:NE2	2.07	0.51
2:I:331:HOH:O	1:J:31:MET:HE3	2.10	0.51
1:T:98:ALA:HB2	1:T:123:HIS:HE1	1.74	0.51
1:J:52:GLN:HE21	1:J:85:LYS:H	1.58	0.51
1:A:95:MET:CG	2:A:306:HOH:O	2.45	0.50
1:E:18:TYR:CE1	1:F:8:ILE:HG23	2.46	0.50
1:M:71:VAL:HG22	1:M:99:MET:HE3	1.93	0.50
1:U:52:GLN:HE21	1:U:85:LYS:H	1.59	0.50
1:U:98:ALA:HB2	1:U:123:HIS:HE1	1.77	0.50
1:G:124:GLN:NE2	1:L:133:ALA:HB3	2.26	0.50
1:Z:167:LYS:HB2	2:Z:312:HOH:O	2.10	0.50
1:E:123:HIS:CD2	2:N:304:HOH:O	2.64	0.50
1:O:134:THR:H	1:Y:124:GLN:NE2	2.10	0.50
1:S:124:GLN:NE2	1:b:133:ALA:HB3	2.26	0.50
1:S:124:GLN:HE22	1:b:134:THR:H	1.59	0.50
1:T:18:TYR:CZ	1:U:8:ILE:HG12	2.47	0.50
1:Y:22:SER:HB3	1:Z:6:THR:O	2.11	0.50
1:E:82:GLN:HA	1:E:82:GLN:HE21	1.75	0.50
2:E:327:HOH:O	1:F:17:ALA:HB3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:82:GLN:NE2	1:K:82:GLN:CA	2.75	0.50
1:T:133:ALA:HB3	1:a:124:GLN:HE21	1.77	0.50
1:B:82:GLN:HA	1:B:82:GLN:NE2	2.26	0.50
1:C:124:GLN:NE2	1:I:133:ALA:HB3	2.27	0.50
1:G:4:ILE:CG2	1:G:5:PRO:HD3	2.39	0.50
1:M:98:ALA:HB2	1:M:123:HIS:CE1	2.47	0.50
1:T:82:GLN:HA	1:T:82:GLN:NE2	2.27	0.50
1:X:82:GLN:HA	1:X:82:GLN:HE21	1.77	0.49
1:B:59:ASP:HB2	1:B:87:ASP:O	2.12	0.49
1:D:133:ALA:HB3	1:H:124:GLN:HE21	1.78	0.49
1:W:59:ASP:HB2	1:W:87:ASP:O	2.11	0.49
1:b:181:LYS:HE2	2:b:319:HOH:O	2.12	0.49
1:R:133:ALA:HB3	1:V:124:GLN:HE21	1.78	0.49
1:a:114:ALA:HA	2:a:317:HOH:O	2.11	0.49
1:B:52:GLN:HE21	1:B:85:LYS:H	1.59	0.49
1:T:124:GLN:HE22	1:a:134:THR:H	1.61	0.49
1:Z:152:ARG:HD3	2:Z:308:HOH:O	2.11	0.49
1:H:52:GLN:NE2	1:H:85:LYS:H	2.10	0.49
1:O:98:ALA:HB2	1:O:123:HIS:HE1	1.78	0.49
1:V:98:ALA:HB2	1:V:123:HIS:HE1	1.78	0.49
1:B:18:TYR:CZ	1:C:8:ILE:HG12	2.43	0.49
1:b:98:ALA:HB2	1:b:123:HIS:HE1	1.76	0.49
1:K:26:LYS:HE2	1:L:8:ILE:CD1	2.40	0.49
1:P:134:THR:H	1:X:124:GLN:HE22	1.61	0.49
1:G:192:PRO:HA	2:G:333:HOH:O	2.13	0.49
1:a:115:LEU:HD21	1:a:190:MET:HE2	1.95	0.49
1:E:18:TYR:CZ	1:F:8:ILE:CG2	2.96	0.48
1:I:52:GLN:NE2	1:I:85:LYS:H	2.11	0.48
1:K:124:GLN:HB2	1:K:125:PRO:HD2	1.94	0.48
1:K:18:TYR:CE1	1:L:8:ILE:HG12	2.46	0.48
1:N:16:ARG:NH1	2:N:319:HOH:O	2.46	0.48
1:R:59:ASP:HB2	1:R:87:ASP:O	2.12	0.48
1:Z:4:ILE:HA	2:Z:307:HOH:O	2.13	0.48
1:F:4:ILE:HG23	1:F:5:PRO:HD3	1.95	0.48
1:U:124:GLN:NE2	1:Z:134:THR:H	2.10	0.48
1:U:133:ALA:HB3	1:Z:124:GLN:HE21	1.79	0.48
1:P:59:ASP:HB2	1:P:87:ASP:O	2.13	0.48
1:T:71:VAL:HG22	1:T:99:MET:HE3	1.94	0.48
1:O:59:ASP:HB2	1:O:87:ASP:O	2.13	0.48
1:F:52:GLN:NE2	1:F:85:LYS:H	2.11	0.48
1:H:82:GLN:HA	1:H:82:GLN:NE2	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:82:GLN:HA	1:J:82:GLN:HE21	1.78	0.48
1:B:59:ASP:HB3	2:B:312:HOH:O	2.14	0.48
1:M:59:ASP:HB2	1:M:87:ASP:O	2.13	0.48
1:Q:98:ALA:HB2	1:Q:123:HIS:CE1	2.48	0.48
1:R:98:ALA:HB2	1:R:123:HIS:CE1	2.48	0.48
1:T:22:SER:HB3	1:U:6:THR:O	2.13	0.48
1:V:193:GLU:CG	2:V:304:HOH:O	2.62	0.48
1:F:83:HIS:CD2	2:G:333:HOH:O	2.65	0.47
1:X:59:ASP:HB2	1:X:87:ASP:O	2.13	0.47
1:Z:71:VAL:HG22	1:Z:99:MET:HE3	1.96	0.47
1:K:18:TYR:CZ	1:L:8:ILE:CG2	2.96	0.47
1:R:4:ILE:CG2	1:R:5:PRO:HD3	2.43	0.47
1:V:115:LEU:HD21	1:V:190:MET:HE2	1.97	0.47
1:B:6:THR:CG2	2:B:320:HOH:O	2.55	0.47
1:C:98:ALA:HB2	1:C:123:HIS:CE1	2.48	0.47
1:E:134:THR:H	1:N:124:GLN:NE2	2.09	0.47
1:F:52:GLN:HE21	1:F:85:LYS:H	1.63	0.47
1:H:8:ILE:HG12	1:N:18:TYR:CZ	2.48	0.47
1:O:98:ALA:HB2	1:O:123:HIS:CE1	2.50	0.47
1:O:164:LYS:HB3	2:O:318:HOH:O	2.15	0.47
1:U:124:GLN:HE21	1:Z:133:ALA:HB3	1.79	0.47
1:K:98:ALA:HB1	2:K:303:HOH:O	2.14	0.47
1:O:133:ALA:HB3	1:Y:124:GLN:NE2	2.30	0.47
1:S:26:LYS:HE2	1:T:8:ILE:HD11	1.96	0.47
1:Y:98:ALA:HB2	1:Y:123:HIS:HE1	1.80	0.47
1:C:124:GLN:HE22	1:I:134:THR:H	1.63	0.47
1:K:98:ALA:HB2	1:K:123:HIS:CE1	2.49	0.47
1:M:52:GLN:HE21	1:M:85:LYS:H	1.62	0.47
1:R:82:GLN:NE2	1:R:82:GLN:CA	2.77	0.47
1:V:6:THR:O	1:b:22:SER:HB3	2.14	0.47
1:F:71:VAL:HG22	1:F:99:MET:HE3	1.97	0.47
1:D:98:ALA:HB2	1:D:123:HIS:HE1	1.79	0.46
1:I:115:LEU:HD21	1:I:190:MET:HE2	1.97	0.46
1:K:98:ALA:HB2	1:K:123:HIS:HE1	1.80	0.46
1:V:193:GLU:HG3	2:V:304:HOH:O	2.15	0.46
1:B:133:ALA:HB3	1:J:124:GLN:HE21	1.80	0.46
1:K:4:ILE:HG23	1:K:5:PRO:HD3	1.97	0.46
1:P:133:ALA:HB3	1:X:124:GLN:HE21	1.80	0.46
1:a:98:ALA:HB2	1:a:123:HIS:CE1	2.49	0.46
1:R:115:LEU:HD21	1:R:190:MET:HE2	1.97	0.46
1:Q:82:GLN:HA	1:Q:82:GLN:HE21	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:52:GLN:HE21	1:H:85:LYS:H	1.63	0.46
1:O:124:GLN:NE2	1:Y:134:THR:H	2.13	0.46
1:R:124:GLN:NE2	1:V:133:ALA:HB3	2.30	0.46
1:S:22:SER:HB3	1:T:6:THR:O	2.16	0.46
1:A:8:ILE:H	1:A:8:ILE:HG13	1.55	0.46
1:E:98:ALA:HB2	1:E:123:HIS:HE1	1.81	0.46
1:J:152:ARG:HD3	2:J:304:HOH:O	2.16	0.46
1:E:82:GLN:NE2	1:E:82:GLN:CA	2.79	0.46
1:N:4:ILE:CG2	1:N:5:PRO:HD3	2.46	0.46
1:V:98:ALA:HB2	1:V:123:HIS:CE1	2.50	0.46
1:D:124:GLN:HE21	1:H:133:ALA:HB3	1.81	0.45
1:P:18:TYR:CZ	1:Q:8:ILE:HG12	2.50	0.45
1:R:134:THR:H	1:V:124:GLN:HE22	1.62	0.45
1:V:153:ILE:O	1:V:157:ARG:HG3	2.16	0.45
1:Y:8:ILE:HG23	2:Y:312:HOH:O	2.15	0.45
1:B:124:GLN:HB2	1:B:125:PRO:HD2	1.98	0.45
1:K:18:TYR:CZ	1:L:8:ILE:HG21	2.51	0.45
1:M:82:GLN:HA	1:M:82:GLN:NE2	2.30	0.45
1:P:98:ALA:HB2	1:P:123:HIS:HE1	1.81	0.45
1:X:8:ILE:H	1:X:8:ILE:HG13	1.58	0.45
1:N:37:ASP:OD2	1:N:37:ASP:C	2.59	0.45
1:U:144:LEU:HD11	1:Z:137:GLU:HG3	1.98	0.45
1:E:98:ALA:HB2	1:E:123:HIS:CE1	2.52	0.45
1:F:124:GLN:HB2	1:F:125:PRO:HD2	1.98	0.45
1:J:98:ALA:HB2	1:J:123:HIS:HE1	1.82	0.45
1:Y:82:GLN:HA	1:Y:82:GLN:NE2	2.32	0.45
2:A:304:HOH:O	1:K:123:HIS:CD2	2.68	0.45
1:a:153:ILE:O	1:a:157:ARG:HG3	2.16	0.45
1:X:71:VAL:HG22	1:X:99:MET:HE3	1.98	0.45
1:E:18:TYR:CZ	1:F:8:ILE:HG21	2.52	0.45
1:H:182:GLU:HG2	2:H:338:HOH:O	2.17	0.45
1:G:153:ILE:O	1:G:157:ARG:HG3	2.17	0.45
1:H:4:ILE:CG2	1:H:5:PRO:HD3	2.46	0.45
1:R:124:GLN:HE22	1:V:134:THR:H	1.64	0.45
1:M:115:LEU:HD21	1:M:190:MET:HE2	1.98	0.44
1:V:124:GLN:HB2	1:V:125:PRO:HD2	1.99	0.44
1:O:82:GLN:HA	1:O:82:GLN:HE21	1.79	0.44
1:S:98:ALA:HB1	2:S:301:HOH:O	2.17	0.44
1:S:98:ALA:HB2	1:S:123:HIS:HE1	1.81	0.44
1:B:17:ALA:CB	2:B:308:HOH:O	2.65	0.44
1:E:8:ILE:H	1:E:8:ILE:HG13	1.63	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:42:ASN:HD21	1:K:31:MET:HB3	1.83	0.44
1:U:115:LEU:HD21	1:U:190:MET:HE2	1.99	0.44
1:A:4:ILE:CG2	1:A:5:PRO:HD3	2.46	0.44
1:W:82:GLN:HA	1:W:82:GLN:HE21	1.79	0.44
1:A:22:SER:HB3	1:B:6:THR:O	2.17	0.44
1:O:188:GLU:CG	2:O:305:HOH:O	2.58	0.44
1:I:52:GLN:HE21	1:I:85:LYS:H	1.65	0.44
1:J:98:ALA:HB2	1:J:123:HIS:CE1	2.52	0.44
1:K:42:ASN:HD21	1:L:31:MET:HB3	1.83	0.44
1:O:188:GLU:HG2	2:O:315:HOH:O	2.16	0.44
1:Q:22:SER:HB3	1:R:6:THR:O	2.18	0.44
2:V:303:HOH:O	1:W:31:MET:HE3	2.18	0.44
1:E:124:GLN:HE21	1:N:133:ALA:HB3	1.83	0.44
1:I:4:ILE:HG23	1:I:5:PRO:HD3	2.00	0.44
1:Q:134:THR:H	1:W:124:GLN:NE2	2.15	0.44
1:Y:115:LEU:HD21	1:Y:190:MET:HE2	2.00	0.44
1:O:8:ILE:H	1:O:8:ILE:HG13	1.57	0.44
1:S:4:ILE:CG2	1:S:5:PRO:HD3	2.47	0.44
1:b:82:GLN:HA	1:b:82:GLN:NE2	2.33	0.44
1:L:153:ILE:O	1:L:157:ARG:HG3	2.18	0.44
1:O:8:ILE:HG12	1:U:18:TYR:CZ	2.52	0.44
1:U:8:ILE:H	1:U:8:ILE:HG13	1.59	0.44
1:A:124:GLN:HB2	1:A:125:PRO:HD2	2.00	0.43
1:H:124:GLN:HB2	1:H:125:PRO:HD2	1.99	0.43
1:P:22:SER:HB3	1:Q:6:THR:O	2.18	0.43
1:H:26:LYS:HE2	1:I:8:ILE:HD11	2.00	0.43
1:P:124:GLN:NE2	1:X:134:THR:H	2.14	0.43
1:W:8:ILE:H	1:W:8:ILE:HG13	1.58	0.43
1:J:4:ILE:CG2	1:J:5:PRO:HD3	2.46	0.43
1:L:124:GLN:HB2	1:L:125:PRO:HD2	2.01	0.43
1:P:115:LEU:HD21	1:P:190:MET:HE2	2.00	0.43
1:Q:133:ALA:HB3	1:W:124:GLN:HE21	1.83	0.43
1:R:162:ILE:HG23	2:R:318:HOH:O	2.17	0.43
1:Z:82:GLN:NE2	1:Z:82:GLN:CA	2.77	0.43
1:D:124:GLN:HB2	1:D:125:PRO:HD2	2.00	0.43
1:I:153:ILE:O	1:I:157:ARG:HG3	2.19	0.43
1:W:115:LEU:HD21	1:W:190:MET:HE2	2.01	0.43
1:W:153:ILE:O	1:W:157:ARG:HG3	2.18	0.43
1:Z:19:ASP:N	2:Z:314:HOH:O	2.51	0.43
1:R:133:ALA:HB3	1:V:124:GLN:NE2	2.34	0.43
1:T:133:ALA:HB3	1:a:124:GLN:NE2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:59:ASP:HB2	1:V:87:ASP:O	2.18	0.43
1:V:154:LEU:HD12	1:V:154:LEU:HA	1.89	0.43
1:a:162:ILE:HG23	2:a:311:HOH:O	2.19	0.43
1:D:98:ALA:HB2	1:D:123:HIS:CE1	2.53	0.43
1:O:82:GLN:NE2	1:O:82:GLN:CA	2.81	0.43
1:V:8:ILE:H	1:V:8:ILE:HG13	1.66	0.43
1:Y:98:ALA:HB2	1:Y:123:HIS:CE1	2.54	0.43
1:B:153:ILE:O	1:B:157:ARG:HG3	2.18	0.43
1:Q:4:ILE:CG2	1:Q:5:PRO:HD3	2.48	0.43
1:Q:124:GLN:HB2	1:Q:125:PRO:HD2	2.01	0.43
1:Z:142:HIS:CD2	2:Z:310:HOH:O	2.65	0.43
1:E:124:GLN:HB2	1:E:125:PRO:HD2	2.01	0.43
1:J:115:LEU:HD21	1:J:190:MET:HE2	2.01	0.43
1:K:8:ILE:H	1:K:8:ILE:HG13	1.57	0.43
1:I:115:LEU:HD21	1:I:190:MET:CE	2.49	0.42
1:P:124:GLN:HE21	1:X:133:ALA:HB3	1.84	0.42
1:R:153:ILE:O	1:R:157:ARG:HG3	2.19	0.42
1:C:8:ILE:H	1:C:8:ILE:HG13	1.58	0.42
1:R:8:ILE:H	1:R:8:ILE:HG13	1.62	0.42
1:B:8:ILE:H	1:B:8:ILE:HG13	1.63	0.42
1:E:83:HIS:NE2	1:F:190:MET:HE3	2.33	0.42
1:S:98:ALA:HB2	1:S:123:HIS:CE1	2.54	0.42
1:B:134:THR:H	1:J:124:GLN:NE2	2.17	0.42
1:K:50:PHE:CE1	1:L:23:ARG:HG2	2.54	0.42
1:R:162:ILE:CG2	2:R:318:HOH:O	2.67	0.42
1:B:19:ASP:N	2:B:310:HOH:O	2.52	0.42
1:M:95:MET:CG	2:M:327:HOH:O	2.57	0.42
1:P:124:GLN:HB2	1:P:125:PRO:HD2	2.02	0.42
1:U:124:GLN:HB2	1:U:125:PRO:HD2	2.00	0.42
1:L:37:ASP:OD2	1:L:37:ASP:C	2.62	0.42
1:P:4:ILE:CG2	1:P:5:PRO:HD3	2.50	0.42
1:U:152:ARG:NH2	2:U:312:HOH:O	2.48	0.42
1:F:133:ALA:HB3	1:M:124:GLN:HE21	1.84	0.42
1:G:115:LEU:HD21	1:G:190:MET:HE2	2.01	0.42
1:P:133:ALA:HB3	1:X:124:GLN:NE2	2.35	0.42
1:Z:99:MET:HE2	1:Z:99:MET:HA	2.00	0.42
1:D:133:ALA:HB3	1:H:124:GLN:NE2	2.35	0.42
1:E:115:LEU:HD21	1:E:190:MET:CE	2.50	0.42
1:L:42:ASN:HB2	2:L:302:HOH:O	2.19	0.42
1:O:124:GLN:HB2	1:O:125:PRO:HD2	2.01	0.42
1:Z:8:ILE:H	1:Z:8:ILE:HG13	1.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASP:HB3	1:B:33:GLY:O	2.19	0.41
1:E:99:MET:HE2	1:E:99:MET:HA	2.01	0.41
1:S:124:GLN:HB2	1:S:125:PRO:HD2	2.02	0.41
1:B:133:ALA:HB3	1:J:124:GLN:NE2	2.35	0.41
1:E:128:GLY:HA2	1:N:129:ALA:O	2.19	0.41
1:F:8:ILE:H	1:F:8:ILE:HG13	1.62	0.41
1:I:37:ASP:OD2	1:I:37:ASP:C	2.63	0.41
1:M:163:GLU:HB2	2:M:301:HOH:O	2.20	0.41
1:Z:4:ILE:CG2	1:Z:5:PRO:HD3	2.50	0.41
1:A:115:LEU:HD21	1:A:190:MET:HE2	2.01	0.41
1:T:173:ASN:HA	2:T:315:HOH:O	2.19	0.41
1:V:115:LEU:CD1	1:b:79:ASP:HB3	2.51	0.41
1:W:98:ALA:HB2	1:W:123:HIS:HE1	1.86	0.41
1:D:124:GLN:NE2	1:H:133:ALA:HB3	2.36	0.41
1:H:31:MET:HB3	1:N:42:ASN:HD21	1.86	0.41
1:J:82:GLN:NE2	1:J:82:GLN:CA	2.84	0.41
1:N:115:LEU:HD21	1:N:190:MET:HE2	2.02	0.41
1:a:8:ILE:H	1:a:8:ILE:HG13	1.61	0.41
1:b:124:GLN:HB2	1:b:125:PRO:HD2	2.02	0.41
1:C:82:GLN:NE2	1:C:82:GLN:CA	2.81	0.41
1:K:16:ARG:NH2	1:L:16:ARG:HA	2.36	0.41
1:R:115:LEU:HD21	1:R:190:MET:CE	2.50	0.41
1:L:82:GLN:HA	1:L:82:GLN:HE21	1.82	0.41
1:S:153:ILE:O	1:S:157:ARG:HG3	2.20	0.41
1:Q:124:GLN:NE2	1:W:134:THR:H	2.17	0.41
1:B:124:GLN:NE2	1:J:134:THR:H	2.17	0.41
1:D:42:ASN:ND2	2:D:321:HOH:O	2.54	0.41
1:D:154:LEU:HD12	1:D:154:LEU:HA	1.97	0.41
1:E:124:GLN:NE2	1:N:134:THR:H	2.18	0.41
1:F:98:ALA:HB2	1:F:123:HIS:HE1	1.86	0.41
1:I:96:ALA:O	1:I:101:SER:HB3	2.20	0.41
1:L:154:LEU:HD12	1:L:154:LEU:HA	1.92	0.41
2:O:319:HOH:O	1:P:8:ILE:HG13	2.20	0.41
1:W:124:GLN:HB2	1:W:125:PRO:HD2	2.03	0.41
1:X:99:MET:HE2	1:X:99:MET:HA	2.03	0.41
1:Y:121:MET:HG3	1:Y:174:PHE:CE1	2.56	0.41
1:Z:38:ASP:HB2	2:a:306:HOH:O	2.19	0.41
1:Z:153:ILE:O	1:Z:157:ARG:HG3	2.20	0.41
1:D:99:MET:HE2	1:D:99:MET:HA	2.03	0.41
1:I:98:ALA:HB2	1:I:123:HIS:HE1	1.84	0.41
1:G:134:THR:H	1:L:124:GLN:NE2	2.18	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:98:ALA:HB2	1:P:123:HIS:CE1	2.56	0.40
1:T:4:ILE:CG2	1:T:5:PRO:HD3	2.49	0.40
1:A:134:THR:H	1:K:124:GLN:HE22	1.70	0.40
1:I:124:GLN:HB2	1:I:125:PRO:HD2	2.02	0.40
1:U:133:ALA:HB3	1:Z:124:GLN:NE2	2.36	0.40
1:D:153:ILE:O	1:D:157:ARG:HG3	2.21	0.40
1:H:37:ASP:OD2	1:H:37:ASP:C	2.64	0.40
1:A:82:GLN:HA	1:A:82:GLN:HE21	1.85	0.40
1:H:6:THR:O	1:N:22:SER:HB3	2.21	0.40
1:N:153:ILE:O	1:N:157:ARG:HG3	2.22	0.40
1:U:98:ALA:HB2	1:U:123:HIS:CE1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	B	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	C	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	D	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	E	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	F	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	G	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	H	180/203 (89%)	174 (97%)	6 (3%)	0	100	100
1	I	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	J	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	K	180/203 (89%)	176 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	M	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	N	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	O	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	P	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	Q	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	R	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	S	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	T	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	U	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	V	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	W	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	X	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	Y	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	Z	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	a	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	b	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
All	All	5040/5684 (89%)	4942 (98%)	98 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	152/170 (89%)	147 (97%)	5 (3%)	33	69
1	B	152/170 (89%)	148 (97%)	4 (3%)	40	75
1	C	152/170 (89%)	147 (97%)	5 (3%)	33	69
1	D	152/170 (89%)	146 (96%)	6 (4%)	28	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	152/170 (89%)	146 (96%)	6 (4%)	28	64
1	F	152/170 (89%)	147 (97%)	5 (3%)	33	69
1	G	152/170 (89%)	146 (96%)	6 (4%)	28	64
1	H	152/170 (89%)	146 (96%)	6 (4%)	28	64
1	I	152/170 (89%)	146 (96%)	6 (4%)	28	64
1	J	152/170 (89%)	145 (95%)	7 (5%)	24	58
1	K	152/170 (89%)	146 (96%)	6 (4%)	28	64
1	L	152/170 (89%)	147 (97%)	5 (3%)	33	69
1	M	152/170 (89%)	148 (97%)	4 (3%)	40	75
1	N	152/170 (89%)	146 (96%)	6 (4%)	28	64
1	O	152/170 (89%)	147 (97%)	5 (3%)	33	69
1	P	152/170 (89%)	146 (96%)	6 (4%)	28	64
1	Q	152/170 (89%)	147 (97%)	5 (3%)	33	69
1	R	152/170 (89%)	147 (97%)	5 (3%)	33	69
1	S	152/170 (89%)	146 (96%)	6 (4%)	28	64
1	T	152/170 (89%)	146 (96%)	6 (4%)	28	64
1	U	152/170 (89%)	147 (97%)	5 (3%)	33	69
1	V	152/170 (89%)	147 (97%)	5 (3%)	33	69
1	W	152/170 (89%)	147 (97%)	5 (3%)	33	69
1	X	152/170 (89%)	146 (96%)	6 (4%)	28	64
1	Y	152/170 (89%)	148 (97%)	4 (3%)	40	75
1	Z	152/170 (89%)	146 (96%)	6 (4%)	28	64
1	a	152/170 (89%)	148 (97%)	4 (3%)	40	75
1	b	152/170 (89%)	147 (97%)	5 (3%)	33	69
All	All	4256/4760 (89%)	4106 (96%)	150 (4%)	32	67

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	9	GLU
1	A	57	GLU
1	A	175	LEU
1	A	189	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	8	ILE
1	B	9	GLU
1	B	57	GLU
1	B	189	VAL
1	C	8	ILE
1	C	9	GLU
1	C	57	GLU
1	C	175	LEU
1	C	189	VAL
1	D	8	ILE
1	D	9	GLU
1	D	57	GLU
1	D	123	HIS
1	D	175	LEU
1	D	189	VAL
1	E	8	ILE
1	E	9	GLU
1	E	57	GLU
1	E	123	HIS
1	E	175	LEU
1	E	189	VAL
1	F	8	ILE
1	F	9	GLU
1	F	35	GLN
1	F	57	GLU
1	F	189	VAL
1	G	8	ILE
1	G	9	GLU
1	G	24	LEU
1	G	57	GLU
1	G	123	HIS
1	G	189	VAL
1	H	8	ILE
1	H	9	GLU
1	H	57	GLU
1	H	123	HIS
1	H	175	LEU
1	H	189	VAL
1	I	8	ILE
1	I	9	GLU
1	I	57	GLU
1	I	123	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	175	LEU
1	I	189	VAL
1	J	8	ILE
1	J	9	GLU
1	J	24	LEU
1	J	57	GLU
1	J	123	HIS
1	J	175	LEU
1	J	189	VAL
1	K	8	ILE
1	K	9	GLU
1	K	24	LEU
1	K	57	GLU
1	K	123	HIS
1	K	189	VAL
1	L	8	ILE
1	L	9	GLU
1	L	57	GLU
1	L	123	HIS
1	L	189	VAL
1	M	8	ILE
1	M	9	GLU
1	M	57	GLU
1	M	189	VAL
1	N	8	ILE
1	N	9	GLU
1	N	57	GLU
1	N	123	HIS
1	N	175	LEU
1	N	189	VAL
1	O	8	ILE
1	O	9	GLU
1	O	57	GLU
1	O	175	LEU
1	O	189	VAL
1	P	8	ILE
1	P	9	GLU
1	P	57	GLU
1	P	123	HIS
1	P	175	LEU
1	P	189	VAL
1	Q	8	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	9	GLU
1	Q	57	GLU
1	Q	175	LEU
1	Q	189	VAL
1	R	8	ILE
1	R	9	GLU
1	R	57	GLU
1	R	175	LEU
1	R	189	VAL
1	S	8	ILE
1	S	9	GLU
1	S	57	GLU
1	S	123	HIS
1	S	175	LEU
1	S	189	VAL
1	T	8	ILE
1	T	9	GLU
1	T	57	GLU
1	T	123	HIS
1	T	175	LEU
1	T	189	VAL
1	U	8	ILE
1	U	9	GLU
1	U	57	GLU
1	U	175	LEU
1	U	189	VAL
1	V	8	ILE
1	V	9	GLU
1	V	57	GLU
1	V	123	HIS
1	V	189	VAL
1	W	8	ILE
1	W	9	GLU
1	W	24	LEU
1	W	57	GLU
1	W	189	VAL
1	X	8	ILE
1	X	9	GLU
1	X	57	GLU
1	X	123	HIS
1	X	175	LEU
1	X	189	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Y	8	ILE
1	Y	9	GLU
1	Y	57	GLU
1	Y	189	VAL
1	Z	8	ILE
1	Z	9	GLU
1	Z	57	GLU
1	Z	82	GLN
1	Z	175	LEU
1	Z	189	VAL
1	a	8	ILE
1	a	9	GLU
1	a	57	GLU
1	a	189	VAL
1	b	8	ILE
1	b	9	GLU
1	b	57	GLU
1	b	123	HIS
1	b	189	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	52	GLN
1	A	82	GLN
1	A	124	GLN
1	A	130	GLN
1	B	42	ASN
1	B	47	GLN
1	B	52	GLN
1	B	82	GLN
1	B	123	HIS
1	B	124	GLN
1	C	42	ASN
1	C	47	GLN
1	C	52	GLN
1	C	82	GLN
1	C	123	HIS
1	C	124	GLN
1	D	42	ASN
1	D	52	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	82	GLN
1	D	123	HIS
1	D	124	GLN
1	E	42	ASN
1	E	52	GLN
1	E	82	GLN
1	E	123	HIS
1	E	124	GLN
1	E	130	GLN
1	F	42	ASN
1	F	52	GLN
1	F	82	GLN
1	F	123	HIS
1	F	124	GLN
1	F	151	ASN
1	F	166	GLN
1	G	52	GLN
1	G	82	GLN
1	G	123	HIS
1	G	124	GLN
1	H	42	ASN
1	H	52	GLN
1	H	82	GLN
1	H	123	HIS
1	H	124	GLN
1	I	47	GLN
1	I	82	GLN
1	I	123	HIS
1	I	124	GLN
1	J	42	ASN
1	J	52	GLN
1	J	82	GLN
1	J	117	ASN
1	J	123	HIS
1	J	124	GLN
1	K	42	ASN
1	K	52	GLN
1	K	82	GLN
1	K	117	ASN
1	K	123	HIS
1	K	124	GLN
1	K	130	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	47	GLN
1	L	52	GLN
1	L	82	GLN
1	L	123	HIS
1	L	124	GLN
1	M	47	GLN
1	M	52	GLN
1	M	82	GLN
1	M	123	HIS
1	M	124	GLN
1	N	42	ASN
1	N	52	GLN
1	N	82	GLN
1	N	123	HIS
1	N	124	GLN
1	O	42	ASN
1	O	52	GLN
1	O	82	GLN
1	O	123	HIS
1	O	124	GLN
1	P	42	ASN
1	P	47	GLN
1	P	52	GLN
1	P	82	GLN
1	P	123	HIS
1	P	124	GLN
1	Q	42	ASN
1	Q	52	GLN
1	Q	82	GLN
1	Q	123	HIS
1	Q	124	GLN
1	R	42	ASN
1	R	52	GLN
1	R	82	GLN
1	R	123	HIS
1	R	124	GLN
1	S	42	ASN
1	S	52	GLN
1	S	82	GLN
1	S	123	HIS
1	S	124	GLN
1	T	42	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	52	GLN
1	T	82	GLN
1	T	123	HIS
1	T	124	GLN
1	U	42	ASN
1	U	52	GLN
1	U	82	GLN
1	U	117	ASN
1	U	123	HIS
1	U	124	GLN
1	V	52	GLN
1	V	82	GLN
1	V	117	ASN
1	V	123	HIS
1	V	124	GLN
1	W	42	ASN
1	W	52	GLN
1	W	82	GLN
1	W	123	HIS
1	W	124	GLN
1	X	42	ASN
1	X	52	GLN
1	X	82	GLN
1	X	123	HIS
1	X	124	GLN
1	Y	42	ASN
1	Y	47	GLN
1	Y	52	GLN
1	Y	82	GLN
1	Y	117	ASN
1	Y	123	HIS
1	Y	124	GLN
1	Y	130	GLN
1	Z	42	ASN
1	Z	52	GLN
1	Z	82	GLN
1	Z	123	HIS
1	Z	124	GLN
1	Z	130	GLN
1	a	52	GLN
1	a	82	GLN
1	a	123	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	124	GLN
1	a	130	GLN
1	b	42	ASN
1	b	52	GLN
1	b	82	GLN
1	b	123	HIS
1	b	124	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	184/203 (90%)	-0.06	2 (1%) 78 70	73, 82, 110, 172	0
1	B	184/203 (90%)	0.16	9 (4%) 35 27	80, 89, 155, 224	0
1	C	184/203 (90%)	0.03	4 (2%) 62 52	78, 91, 111, 150	0
1	D	184/203 (90%)	0.07	10 (5%) 31 24	65, 82, 112, 392	0
1	E	184/203 (90%)	-0.16	3 (1%) 70 61	59, 69, 94, 122	0
1	F	184/203 (90%)	-0.03	12 (6%) 25 18	60, 68, 108, 206	0
1	G	184/203 (90%)	-0.21	3 (1%) 70 61	65, 74, 94, 137	0
1	H	184/203 (90%)	-0.23	3 (1%) 70 61	58, 69, 97, 127	0
1	I	184/203 (90%)	-0.11	7 (3%) 44 35	64, 77, 101, 197	0
1	J	184/203 (90%)	-0.10	3 (1%) 70 61	71, 85, 104, 146	0
1	K	184/203 (90%)	-0.12	2 (1%) 78 70	67, 80, 96, 126	0
1	L	184/203 (90%)	0.04	10 (5%) 31 24	64, 76, 118, 281	0
1	M	184/203 (90%)	-0.13	6 (3%) 49 39	64, 73, 91, 124	0
1	N	184/203 (90%)	-0.17	5 (2%) 56 46	60, 70, 98, 244	0
1	O	184/203 (90%)	0.00	3 (1%) 70 61	71, 86, 111, 190	0
1	P	184/203 (90%)	-0.13	3 (1%) 70 61	67, 80, 115, 175	0
1	Q	184/203 (90%)	0.01	8 (4%) 40 31	67, 79, 120, 161	0
1	R	184/203 (90%)	-0.11	8 (4%) 40 31	74, 87, 134, 227	0
1	S	184/203 (90%)	-0.21	1 (0%) 87 82	70, 81, 102, 128	0
1	T	184/203 (90%)	-0.11	3 (1%) 70 61	70, 83, 105, 149	0
1	U	184/203 (90%)	-0.04	3 (1%) 70 61	74, 91, 111, 149	0
1	V	184/203 (90%)	-0.08	3 (1%) 70 61	72, 84, 102, 172	0
1	W	184/203 (90%)	-0.01	7 (3%) 44 35	73, 85, 122, 240	0
1	X	184/203 (90%)	-0.18	3 (1%) 70 61	69, 81, 115, 167	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	184/203 (90%)	-0.04	1 (0%) 87 82	74, 88, 132, 161	0
1	Z	184/203 (90%)	0.33	11 (5%) 27 21	89, 100, 168, 303	0
1	a	184/203 (90%)	0.17	3 (1%) 70 61	79, 99, 124, 154	0
1	b	184/203 (90%)	-0.11	1 (0%) 87 82	69, 80, 122, 159	0
All	All	5152/5684 (90%)	-0.05	137 (2%) 56 46	58, 82, 116, 392	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	ILE	9.8
1	D	189	VAL	8.4
1	F	17	ALA	7.4
1	F	7	VAL	7.3
1	L	4	ILE	7.2
1	L	5	PRO	6.7
1	D	190	MET	6.4
1	L	7	VAL	6.3
1	D	192	PRO	6.2
1	A	4	ILE	5.7
1	Z	17	ALA	5.4
1	W	189	VAL	5.3
1	F	5	PRO	5.2
1	D	191	VAL	5.2
1	Q	17	ALA	5.1
1	I	7	VAL	5.0
1	F	8	ILE	5.0
1	O	189	VAL	4.9
1	F	4	ILE	4.9
1	F	6	THR	4.8
1	F	16	ARG	4.6
1	I	4	ILE	4.4
1	L	17	ALA	4.3
1	I	17	ALA	4.3
1	R	4	ILE	4.2
1	L	18	TYR	4.2
1	Y	4	ILE	4.2
1	N	189	VAL	4.1
1	M	4	ILE	4.0
1	a	4	ILE	4.0
1	L	16	ARG	3.9
1	L	6	THR	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	b	4	ILE	3.9
1	B	5	PRO	3.8
1	W	17	ALA	3.8
1	Z	7	VAL	3.7
1	J	4	ILE	3.5
1	L	8	ILE	3.5
1	Z	189	VAL	3.5
1	O	4	ILE	3.5
1	B	16	ARG	3.4
1	R	189	VAL	3.3
1	T	4	ILE	3.3
1	U	8	ILE	3.1
1	B	17	ALA	3.1
1	B	7	VAL	3.1
1	Z	192	PRO	3.1
1	F	21	TYR	3.0
1	M	17	ALA	3.0
1	W	192	PRO	3.0
1	Z	6	THR	3.0
1	D	4	ILE	3.0
1	I	16	ARG	3.0
1	V	4	ILE	2.9
1	V	8	ILE	2.9
1	F	18	TYR	2.9
1	C	17	ALA	2.9
1	F	9	GLU	2.9
1	H	17	ALA	2.9
1	M	9	GLU	2.9
1	A	189	VAL	2.9
1	Z	5	PRO	2.9
1	D	188	GLU	2.9
1	L	9	GLU	2.9
1	Z	188	GLU	2.9
1	E	4	ILE	2.9
1	D	17	ALA	2.8
1	X	4	ILE	2.8
1	D	193	GLU	2.7
1	F	193	GLU	2.7
1	Z	191	VAL	2.7
1	K	4	ILE	2.7
1	R	7	VAL	2.7
1	C	100	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	R	191	VAL	2.7
1	Q	8	ILE	2.7
1	S	4	ILE	2.7
1	I	18	TYR	2.7
1	G	16	ARG	2.7
1	I	8	ILE	2.6
1	P	4	ILE	2.6
1	Z	4	ILE	2.6
1	N	192	PRO	2.6
1	O	192	PRO	2.5
1	B	8	ILE	2.5
1	X	5	PRO	2.5
1	R	192	PRO	2.5
1	L	193	GLU	2.5
1	H	6	THR	2.5
1	R	17	ALA	2.5
1	C	4	ILE	2.4
1	N	188	GLU	2.4
1	Z	190	MET	2.4
1	E	8	ILE	2.4
1	N	4	ILE	2.4
1	W	4	ILE	2.4
1	M	8	ILE	2.4
1	W	7	VAL	2.4
1	K	16	ARG	2.4
1	V	17	ALA	2.4
1	G	17	ALA	2.3
1	G	4	ILE	2.3
1	E	16	ARG	2.3
1	R	188	GLU	2.3
1	B	6	THR	2.3
1	D	16	ARG	2.3
1	R	193	GLU	2.2
1	a	105	ALA	2.2
1	I	6	THR	2.2
1	M	31	MET	2.2
1	H	193	GLU	2.2
1	U	17	ALA	2.2
1	Q	6	THR	2.2
1	W	188	GLU	2.2
1	W	193	GLU	2.2
1	B	20	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	16	ARG	2.2
1	D	169	THR	2.2
1	X	17	ALA	2.2
1	T	17	ALA	2.1
1	Q	185	LEU	2.1
1	P	8	ILE	2.1
1	Z	8	ILE	2.1
1	C	7	VAL	2.1
1	Q	7	VAL	2.1
1	T	169	THR	2.1
1	P	17	ALA	2.1
1	Q	4	ILE	2.1
1	J	7	VAL	2.1
1	F	20	ILE	2.1
1	J	16	ARG	2.0
1	U	4	ILE	2.0
1	Q	188	GLU	2.0
1	B	18	TYR	2.0
1	a	17	ALA	2.0
1	Q	18	TYR	2.0
1	M	7	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.