Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2022 – 04:38 pm BST

PDB ID	:	7P81
Title	:	Crystal structure of ClpP from Bacillus subtilis in complex with ADEP2 (compact state)
Authors	:	Lee, B.-G.; Kim, L.; Kim, M.K.; Kwon, D.H.; Song, H.K.
Deposited on	:	2021-07-21
Resolution	:	2.79 Å(reported)

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

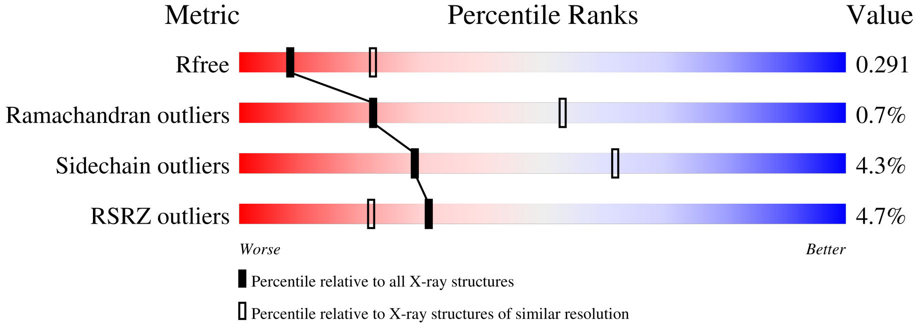
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

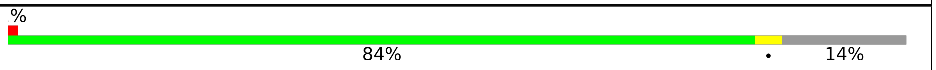
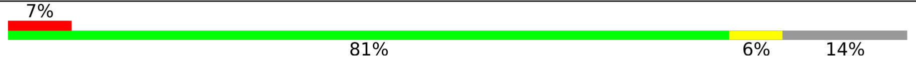
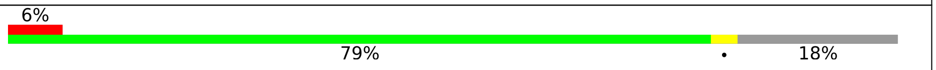
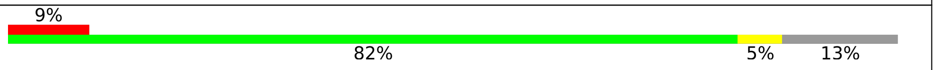
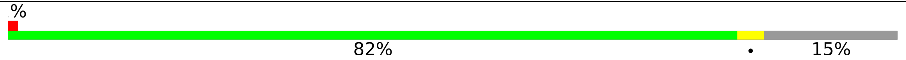
The reported resolution of this entry is 2.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	199	
1	B	199	
1	C	199	
1	D	199	
1	E	199	
1	F	199	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	199	% 83% 6% 11%
1	H	199	7% 82% 5% 14%
1	I	199	9% 84% • • 11%
1	J	199	4% 82% 5% 13%
1	K	199	% 82% • 14%
1	L	199	7% 80% 6% 14%
1	M	199	6% 81% • 16%
1	N	199	12% 80% • 16%
1	O	199	3% 84% • 13%
1	P	199	% 85% • 11%
1	Q	199	4% 81% 5% 14%
1	R	199	% 81% • • 16%
1	S	199	6% 85% • 13%
1	T	199	2% 81% • 16%
1	U	199	4% 81% • 15%
1	V	199	2% 84% • 12%
1	W	199	3% 87% • 12%
1	X	199	4% 82% • • 15%
1	Y	199	7% 79% • 17%
1	Z	199	8% 80% • • 15%
1	a	199	% 82% • 16%
1	b	199	2% 83% • • 12%
2	c	7	29% 71%
2	d	7	29% 71%
2	e	7	29% 29% 71%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	f	7	🟥 14% 🟩 29% 🟨 71%
2	g	7	🟩 29% 🟨 71%
2	h	7	🟩 29% 🟨 71%
2	i	7	🟩 29% 🟨 71%
2	j	7	🟩 29% 🟨 71%
2	k	7	🟩 29% 🟨 71%
2	l	7	🟥 14% 🟩 29% 🟨 71%
2	m	7	🟩 29% 🟨 71%
2	n	7	🟩 29% 🟨 71%
2	o	7	🟩 29% 🟨 71%
2	p	7	🟩 14% 🟨 86%
2	q	7	🟩 29% 🟨 71%
2	r	7	🟩 29% 🟨 71%
2	t	7	🟩 29% 🟨 71%
2	u	7	🟩 29% 🟨 71%
2	v	7	🟩 29% 🟨 71%
2	w	7	🟩 29% 🟨 71%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38248 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	172	Total C N O S 1319 841 219 252 7	0	0	0
1	B	176	Total C N O S 1354 861 229 257 7	0	0	0
1	C	172	Total C N O S 1315 839 219 250 7	0	0	0
1	D	164	Total C N O S 1260 801 211 241 7	0	0	0
1	E	174	Total C N O S 1323 843 221 252 7	0	0	0
1	F	169	Total C N O S 1292 822 216 247 7	0	0	0
1	G	177	Total C N O S 1358 863 228 260 7	0	0	0
1	H	172	Total C N O S 1317 839 219 252 7	0	0	0
1	I	177	Total C N O S 1351 859 227 258 7	0	0	0
1	J	173	Total C N O S 1318 840 220 251 7	0	0	0
1	K	171	Total C N O S 1311 837 218 249 7	0	0	0
1	L	171	Total C N O S 1311 837 218 249 7	0	0	0
1	M	168	Total C N O S 1284 816 215 246 7	0	0	0
1	N	168	Total C N O S 1294 824 215 248 7	0	0	0
1	O	174	Total C N O S 1333 851 221 254 7	0	0	0
1	P	177	Total C N O S 1362 867 230 258 7	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	Q	172	Total C N O S 1317 839 219 252 7	0	0	0
1	R	168	Total C N O S 1293 825 215 246 7	0	0	0
1	S	174	Total C N O S 1327 845 221 254 7	0	0	0
1	T	168	Total C N O S 1290 822 215 246 7	0	0	0
1	U	170	Total C N O S 1307 832 219 249 7	0	0	0
1	V	175	Total C N O S 1343 854 223 259 7	0	0	0
1	W	176	Total C N O S 1348 857 229 255 7	0	0	0
1	X	169	Total C N O S 1294 824 216 247 7	0	0	0
1	Y	165	Total C N O S 1262 801 212 242 7	0	0	0
1	Z	169	Total C N O S 1292 822 216 247 7	0	0	0
1	a	168	Total C N O S 1290 822 215 246 7	0	0	0
1	b	175	Total C N O S 1344 855 226 256 7	0	0	0

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	LEU	-	expression tag	UNP P80244
A	193	GLU	-	expression tag	UNP P80244
A	194	HIS	-	expression tag	UNP P80244
A	195	HIS	-	expression tag	UNP P80244
A	196	HIS	-	expression tag	UNP P80244
A	197	HIS	-	expression tag	UNP P80244
A	198	HIS	-	expression tag	UNP P80244
A	199	HIS	-	expression tag	UNP P80244
B	192	LEU	-	expression tag	UNP P80244
B	193	GLU	-	expression tag	UNP P80244
B	194	HIS	-	expression tag	UNP P80244
B	195	HIS	-	expression tag	UNP P80244
B	196	HIS	-	expression tag	UNP P80244
B	197	HIS	-	expression tag	UNP P80244
B	198	HIS	-	expression tag	UNP P80244

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	199	HIS	-	expression tag	UNP P80244
C	192	LEU	-	expression tag	UNP P80244
C	193	GLU	-	expression tag	UNP P80244
C	194	HIS	-	expression tag	UNP P80244
C	195	HIS	-	expression tag	UNP P80244
C	196	HIS	-	expression tag	UNP P80244
C	197	HIS	-	expression tag	UNP P80244
C	198	HIS	-	expression tag	UNP P80244
C	199	HIS	-	expression tag	UNP P80244
D	192	LEU	-	expression tag	UNP P80244
D	193	GLU	-	expression tag	UNP P80244
D	194	HIS	-	expression tag	UNP P80244
D	195	HIS	-	expression tag	UNP P80244
D	196	HIS	-	expression tag	UNP P80244
D	197	HIS	-	expression tag	UNP P80244
D	198	HIS	-	expression tag	UNP P80244
D	199	HIS	-	expression tag	UNP P80244
E	192	LEU	-	expression tag	UNP P80244
E	193	GLU	-	expression tag	UNP P80244
E	194	HIS	-	expression tag	UNP P80244
E	195	HIS	-	expression tag	UNP P80244
E	196	HIS	-	expression tag	UNP P80244
E	197	HIS	-	expression tag	UNP P80244
E	198	HIS	-	expression tag	UNP P80244
E	199	HIS	-	expression tag	UNP P80244
F	192	LEU	-	expression tag	UNP P80244
F	193	GLU	-	expression tag	UNP P80244
F	194	HIS	-	expression tag	UNP P80244
F	195	HIS	-	expression tag	UNP P80244
F	196	HIS	-	expression tag	UNP P80244
F	197	HIS	-	expression tag	UNP P80244
F	198	HIS	-	expression tag	UNP P80244
F	199	HIS	-	expression tag	UNP P80244
G	192	LEU	-	expression tag	UNP P80244
G	193	GLU	-	expression tag	UNP P80244
G	194	HIS	-	expression tag	UNP P80244
G	195	HIS	-	expression tag	UNP P80244
G	196	HIS	-	expression tag	UNP P80244
G	197	HIS	-	expression tag	UNP P80244
G	198	HIS	-	expression tag	UNP P80244
G	199	HIS	-	expression tag	UNP P80244
H	192	LEU	-	expression tag	UNP P80244

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	193	GLU	-	expression tag	UNP P80244
H	194	HIS	-	expression tag	UNP P80244
H	195	HIS	-	expression tag	UNP P80244
H	196	HIS	-	expression tag	UNP P80244
H	197	HIS	-	expression tag	UNP P80244
H	198	HIS	-	expression tag	UNP P80244
H	199	HIS	-	expression tag	UNP P80244
I	192	LEU	-	expression tag	UNP P80244
I	193	GLU	-	expression tag	UNP P80244
I	194	HIS	-	expression tag	UNP P80244
I	195	HIS	-	expression tag	UNP P80244
I	196	HIS	-	expression tag	UNP P80244
I	197	HIS	-	expression tag	UNP P80244
I	198	HIS	-	expression tag	UNP P80244
I	199	HIS	-	expression tag	UNP P80244
J	192	LEU	-	expression tag	UNP P80244
J	193	GLU	-	expression tag	UNP P80244
J	194	HIS	-	expression tag	UNP P80244
J	195	HIS	-	expression tag	UNP P80244
J	196	HIS	-	expression tag	UNP P80244
J	197	HIS	-	expression tag	UNP P80244
J	198	HIS	-	expression tag	UNP P80244
J	199	HIS	-	expression tag	UNP P80244
K	192	LEU	-	expression tag	UNP P80244
K	193	GLU	-	expression tag	UNP P80244
K	194	HIS	-	expression tag	UNP P80244
K	195	HIS	-	expression tag	UNP P80244
K	196	HIS	-	expression tag	UNP P80244
K	197	HIS	-	expression tag	UNP P80244
K	198	HIS	-	expression tag	UNP P80244
K	199	HIS	-	expression tag	UNP P80244
L	192	LEU	-	expression tag	UNP P80244
L	193	GLU	-	expression tag	UNP P80244
L	194	HIS	-	expression tag	UNP P80244
L	195	HIS	-	expression tag	UNP P80244
L	196	HIS	-	expression tag	UNP P80244
L	197	HIS	-	expression tag	UNP P80244
L	198	HIS	-	expression tag	UNP P80244
L	199	HIS	-	expression tag	UNP P80244
M	192	LEU	-	expression tag	UNP P80244
M	193	GLU	-	expression tag	UNP P80244
M	194	HIS	-	expression tag	UNP P80244

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	195	HIS	-	expression tag	UNP P80244
M	196	HIS	-	expression tag	UNP P80244
M	197	HIS	-	expression tag	UNP P80244
M	198	HIS	-	expression tag	UNP P80244
M	199	HIS	-	expression tag	UNP P80244
N	192	LEU	-	expression tag	UNP P80244
N	193	GLU	-	expression tag	UNP P80244
N	194	HIS	-	expression tag	UNP P80244
N	195	HIS	-	expression tag	UNP P80244
N	196	HIS	-	expression tag	UNP P80244
N	197	HIS	-	expression tag	UNP P80244
N	198	HIS	-	expression tag	UNP P80244
N	199	HIS	-	expression tag	UNP P80244
O	192	LEU	-	expression tag	UNP P80244
O	193	GLU	-	expression tag	UNP P80244
O	194	HIS	-	expression tag	UNP P80244
O	195	HIS	-	expression tag	UNP P80244
O	196	HIS	-	expression tag	UNP P80244
O	197	HIS	-	expression tag	UNP P80244
O	198	HIS	-	expression tag	UNP P80244
O	199	HIS	-	expression tag	UNP P80244
P	192	LEU	-	expression tag	UNP P80244
P	193	GLU	-	expression tag	UNP P80244
P	194	HIS	-	expression tag	UNP P80244
P	195	HIS	-	expression tag	UNP P80244
P	196	HIS	-	expression tag	UNP P80244
P	197	HIS	-	expression tag	UNP P80244
P	198	HIS	-	expression tag	UNP P80244
P	199	HIS	-	expression tag	UNP P80244
Q	192	LEU	-	expression tag	UNP P80244
Q	193	GLU	-	expression tag	UNP P80244
Q	194	HIS	-	expression tag	UNP P80244
Q	195	HIS	-	expression tag	UNP P80244
Q	196	HIS	-	expression tag	UNP P80244
Q	197	HIS	-	expression tag	UNP P80244
Q	198	HIS	-	expression tag	UNP P80244
Q	199	HIS	-	expression tag	UNP P80244
R	192	LEU	-	expression tag	UNP P80244
R	193	GLU	-	expression tag	UNP P80244
R	194	HIS	-	expression tag	UNP P80244
R	195	HIS	-	expression tag	UNP P80244
R	196	HIS	-	expression tag	UNP P80244

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	197	HIS	-	expression tag	UNP P80244
R	198	HIS	-	expression tag	UNP P80244
R	199	HIS	-	expression tag	UNP P80244
S	192	LEU	-	expression tag	UNP P80244
S	193	GLU	-	expression tag	UNP P80244
S	194	HIS	-	expression tag	UNP P80244
S	195	HIS	-	expression tag	UNP P80244
S	196	HIS	-	expression tag	UNP P80244
S	197	HIS	-	expression tag	UNP P80244
S	198	HIS	-	expression tag	UNP P80244
S	199	HIS	-	expression tag	UNP P80244
T	192	LEU	-	expression tag	UNP P80244
T	193	GLU	-	expression tag	UNP P80244
T	194	HIS	-	expression tag	UNP P80244
T	195	HIS	-	expression tag	UNP P80244
T	196	HIS	-	expression tag	UNP P80244
T	197	HIS	-	expression tag	UNP P80244
T	198	HIS	-	expression tag	UNP P80244
T	199	HIS	-	expression tag	UNP P80244
U	192	LEU	-	expression tag	UNP P80244
U	193	GLU	-	expression tag	UNP P80244
U	194	HIS	-	expression tag	UNP P80244
U	195	HIS	-	expression tag	UNP P80244
U	196	HIS	-	expression tag	UNP P80244
U	197	HIS	-	expression tag	UNP P80244
U	198	HIS	-	expression tag	UNP P80244
U	199	HIS	-	expression tag	UNP P80244
V	192	LEU	-	expression tag	UNP P80244
V	193	GLU	-	expression tag	UNP P80244
V	194	HIS	-	expression tag	UNP P80244
V	195	HIS	-	expression tag	UNP P80244
V	196	HIS	-	expression tag	UNP P80244
V	197	HIS	-	expression tag	UNP P80244
V	198	HIS	-	expression tag	UNP P80244
V	199	HIS	-	expression tag	UNP P80244
W	192	LEU	-	expression tag	UNP P80244
W	193	GLU	-	expression tag	UNP P80244
W	194	HIS	-	expression tag	UNP P80244
W	195	HIS	-	expression tag	UNP P80244
W	196	HIS	-	expression tag	UNP P80244
W	197	HIS	-	expression tag	UNP P80244
W	198	HIS	-	expression tag	UNP P80244

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
W	199	HIS	-	expression tag	UNP P80244
X	192	LEU	-	expression tag	UNP P80244
X	193	GLU	-	expression tag	UNP P80244
X	194	HIS	-	expression tag	UNP P80244
X	195	HIS	-	expression tag	UNP P80244
X	196	HIS	-	expression tag	UNP P80244
X	197	HIS	-	expression tag	UNP P80244
X	198	HIS	-	expression tag	UNP P80244
X	199	HIS	-	expression tag	UNP P80244
Y	192	LEU	-	expression tag	UNP P80244
Y	193	GLU	-	expression tag	UNP P80244
Y	194	HIS	-	expression tag	UNP P80244
Y	195	HIS	-	expression tag	UNP P80244
Y	196	HIS	-	expression tag	UNP P80244
Y	197	HIS	-	expression tag	UNP P80244
Y	198	HIS	-	expression tag	UNP P80244
Y	199	HIS	-	expression tag	UNP P80244
Z	192	LEU	-	expression tag	UNP P80244
Z	193	GLU	-	expression tag	UNP P80244
Z	194	HIS	-	expression tag	UNP P80244
Z	195	HIS	-	expression tag	UNP P80244
Z	196	HIS	-	expression tag	UNP P80244
Z	197	HIS	-	expression tag	UNP P80244
Z	198	HIS	-	expression tag	UNP P80244
Z	199	HIS	-	expression tag	UNP P80244
a	192	LEU	-	expression tag	UNP P80244
a	193	GLU	-	expression tag	UNP P80244
a	194	HIS	-	expression tag	UNP P80244
a	195	HIS	-	expression tag	UNP P80244
a	196	HIS	-	expression tag	UNP P80244
a	197	HIS	-	expression tag	UNP P80244
a	198	HIS	-	expression tag	UNP P80244
a	199	HIS	-	expression tag	UNP P80244
b	192	LEU	-	expression tag	UNP P80244
b	193	GLU	-	expression tag	UNP P80244
b	194	HIS	-	expression tag	UNP P80244
b	195	HIS	-	expression tag	UNP P80244
b	196	HIS	-	expression tag	UNP P80244
b	197	HIS	-	expression tag	UNP P80244
b	198	HIS	-	expression tag	UNP P80244
b	199	HIS	-	expression tag	UNP P80244

- Molecule 2 is a protein called ADEP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	c	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	d	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	e	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	f	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	g	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	h	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	i	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	j	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	k	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	l	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	m	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	n	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	o	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	p	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	q	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	r	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	t	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	u	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	v	7	Total 57	C 41	F 2	N 6	O 8	0	0	0
2	w	7	Total 57	C 41	F 2	N 6	O 8	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total O 6 6	0	0
3	B	17	Total O 17 17	0	0
3	C	11	Total O 11 11	0	0
3	D	13	Total O 13 13	0	0
3	E	16	Total O 16 16	0	0
3	F	10	Total O 10 10	0	0
3	G	17	Total O 17 17	0	0
3	H	6	Total O 6 6	0	0
3	I	3	Total O 3 3	0	0
3	J	9	Total O 9 9	0	0
3	K	19	Total O 19 19	0	0
3	L	13	Total O 13 13	0	0
3	M	11	Total O 11 11	0	0
3	N	5	Total O 5 5	0	0
3	O	7	Total O 7 7	0	0
3	P	6	Total O 6 6	0	0
3	Q	15	Total O 15 15	0	0
3	R	10	Total O 10 10	0	0
3	S	12	Total O 12 12	0	0
3	T	14	Total O 14 14	0	0
3	U	12	Total O 12 12	0	0
3	V	5	Total O 5 5	0	0

Continued on next page...

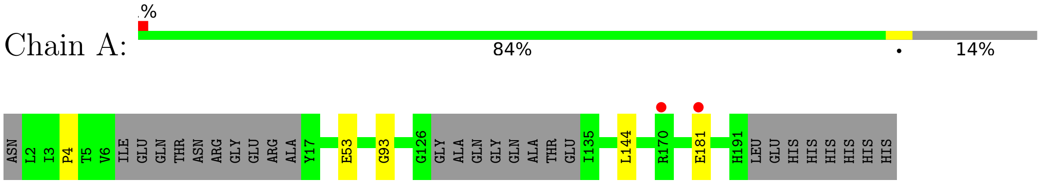
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	W	9	Total O 9 9	0	0
3	X	8	Total O 8 8	0	0
3	Y	5	Total O 5 5	0	0
3	Z	9	Total O 9 9	0	0
3	a	10	Total O 10 10	0	0
3	b	12	Total O 12 12	0	0
3	f	1	Total O 1 1	0	0
3	g	2	Total O 2 2	0	0
3	h	1	Total O 1 1	0	0
3	j	1	Total O 1 1	0	0
3	m	2	Total O 2 2	0	0
3	o	1	Total O 1 1	0	0
3	v	1	Total O 1 1	0	0

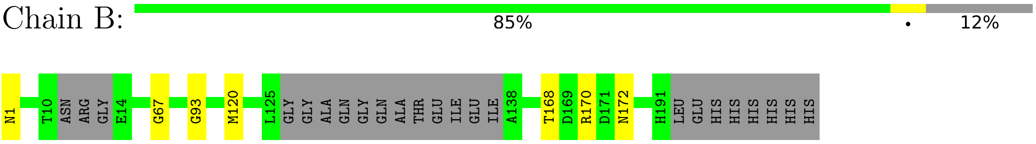
3 Residue-property plots ⓘ

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.

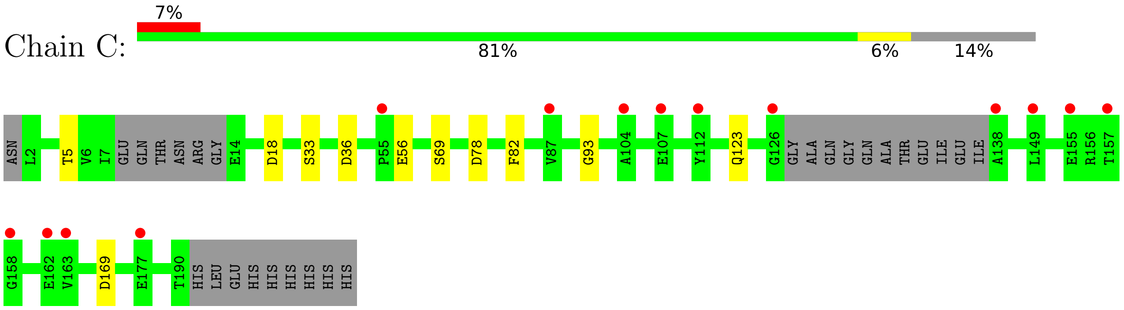
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



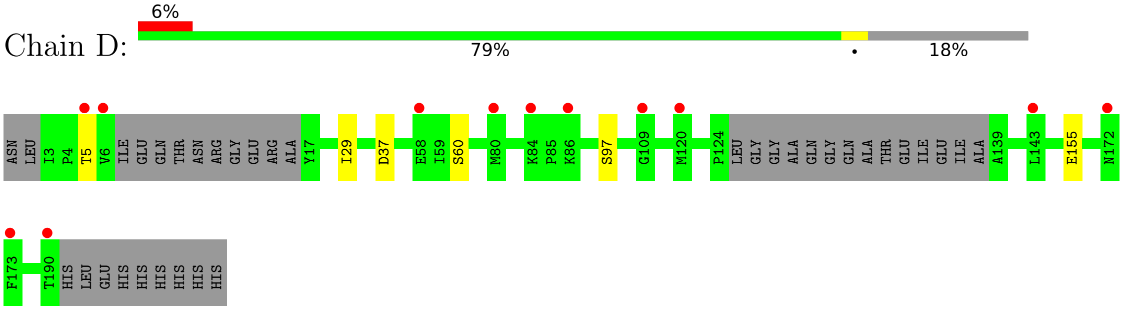
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



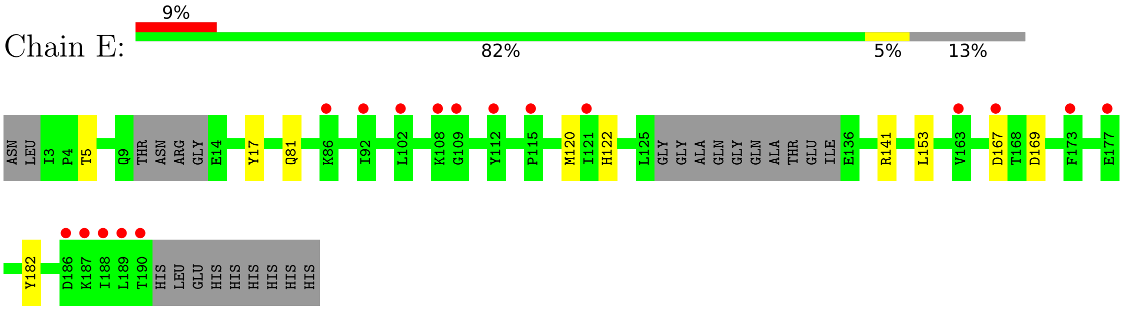
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



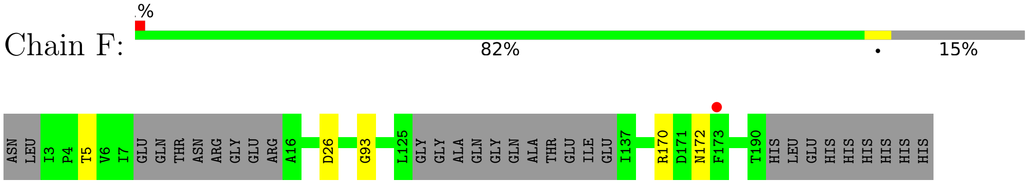
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



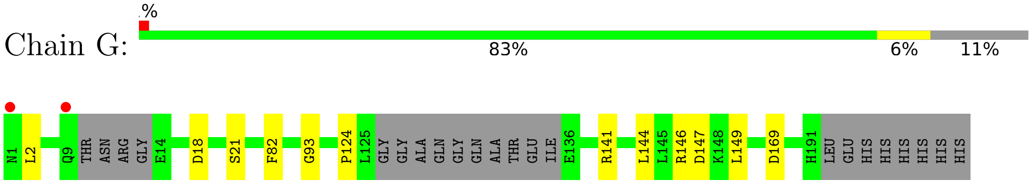
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



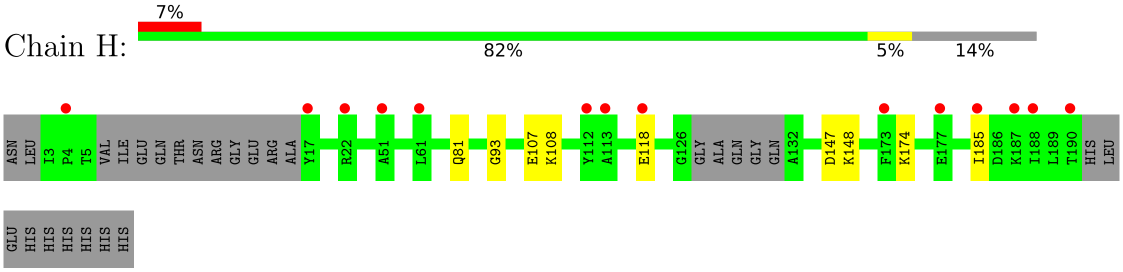
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



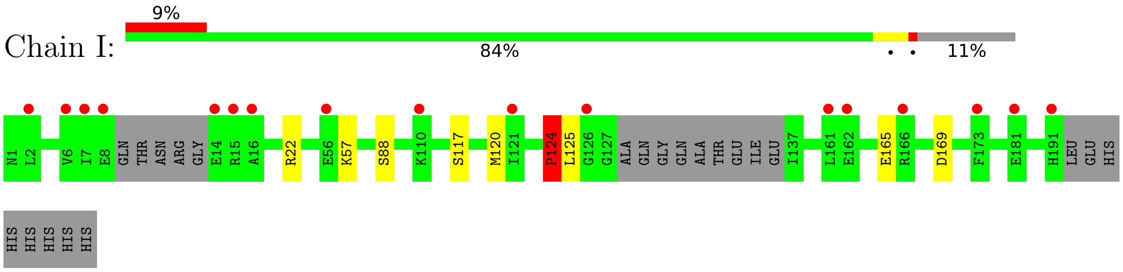
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



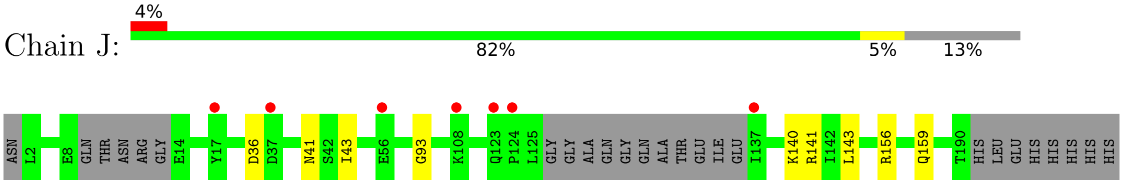
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

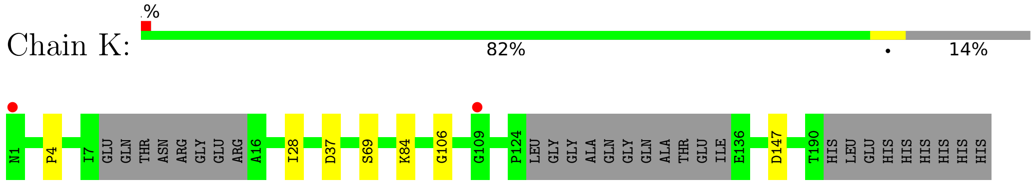


• Molecule 1: ATP-dependent Clp protease proteolytic subunit



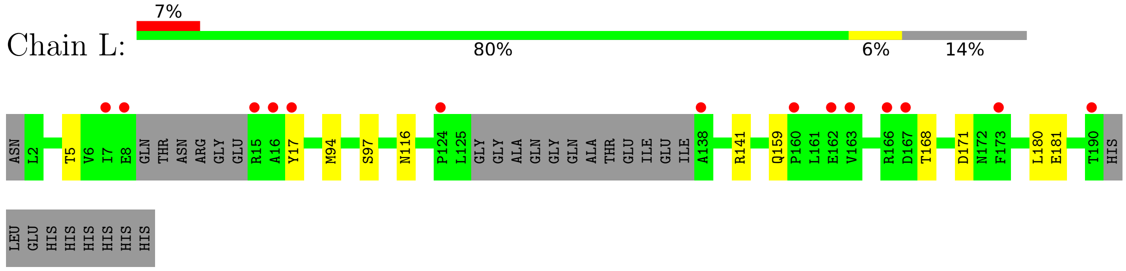
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



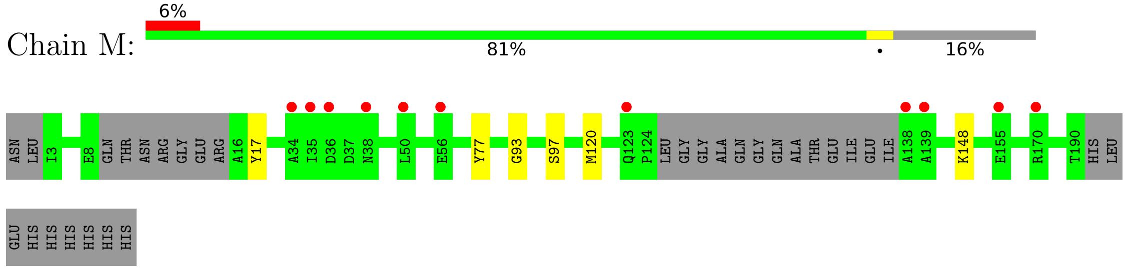
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



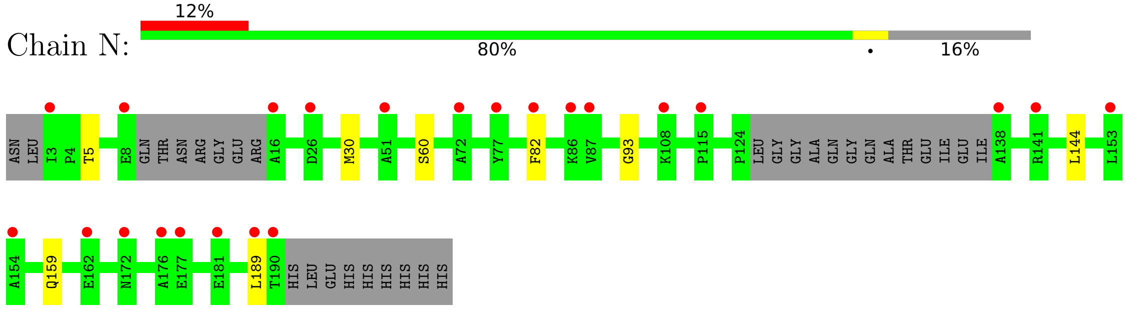
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



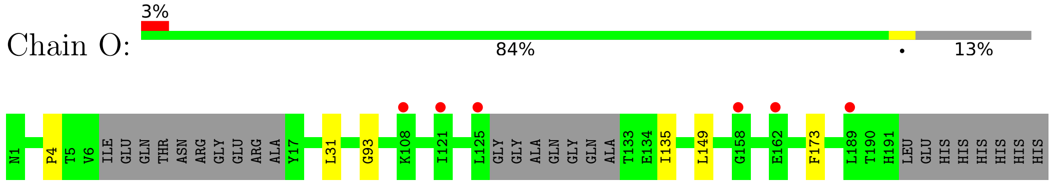
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:



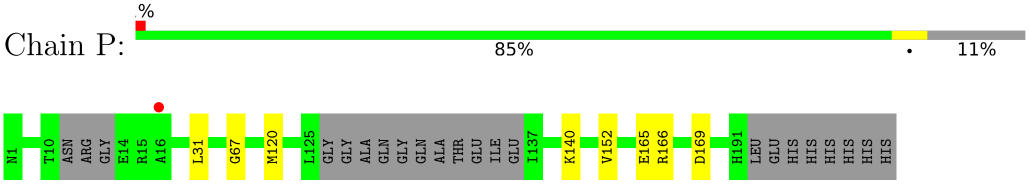
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain O:



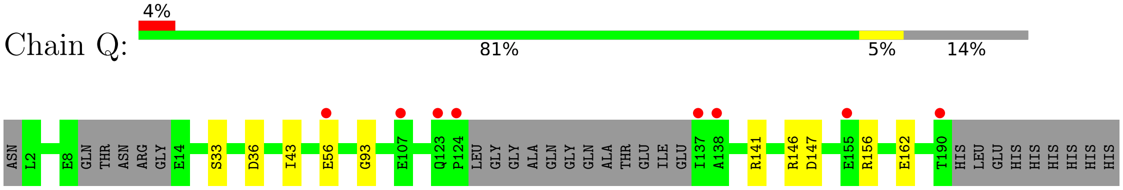
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain P:



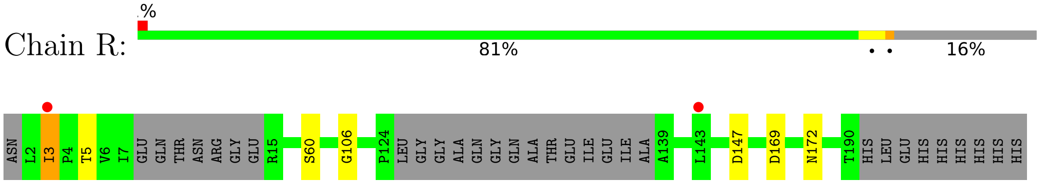
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Q:



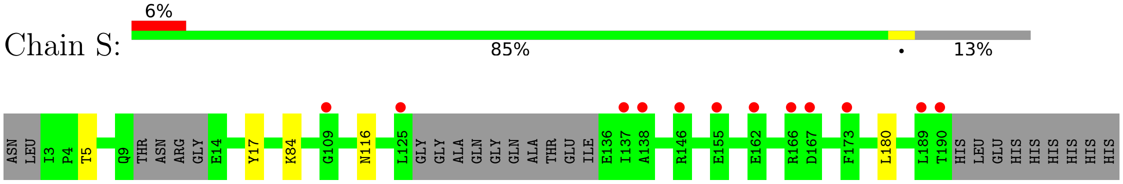
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain R:



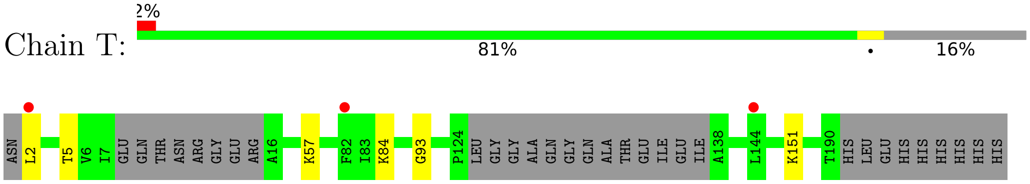
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain S:



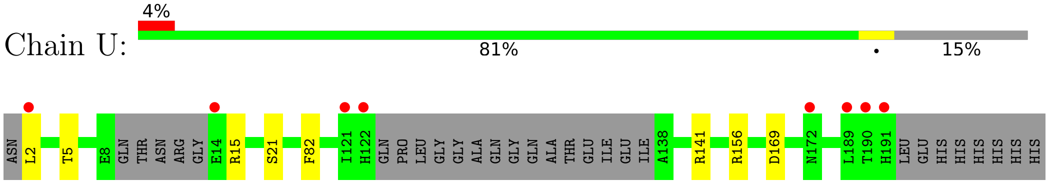
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain T:



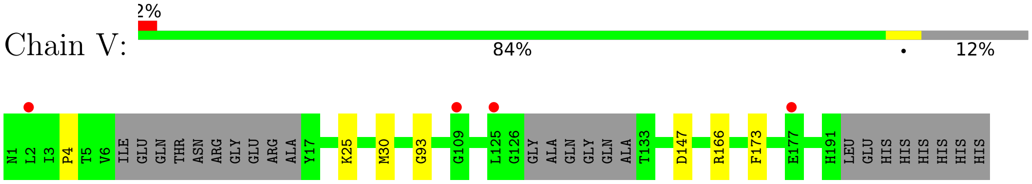
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain U:



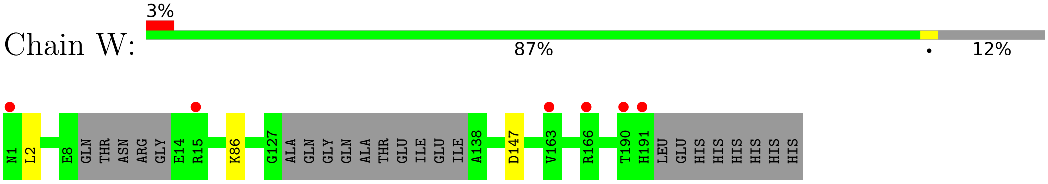
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain V:



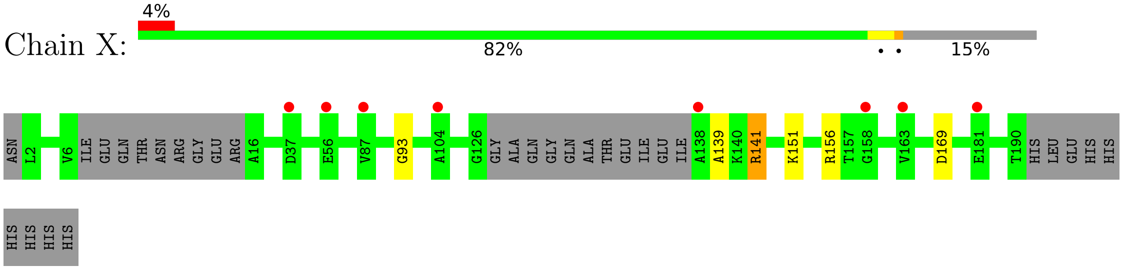
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain W:



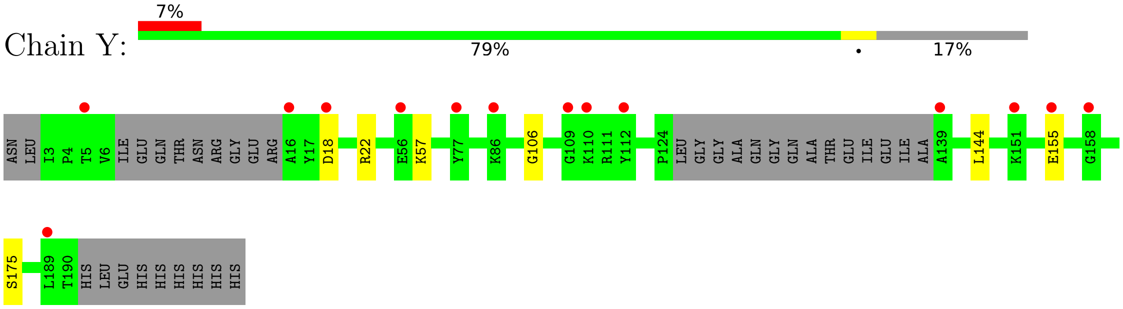
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain X:



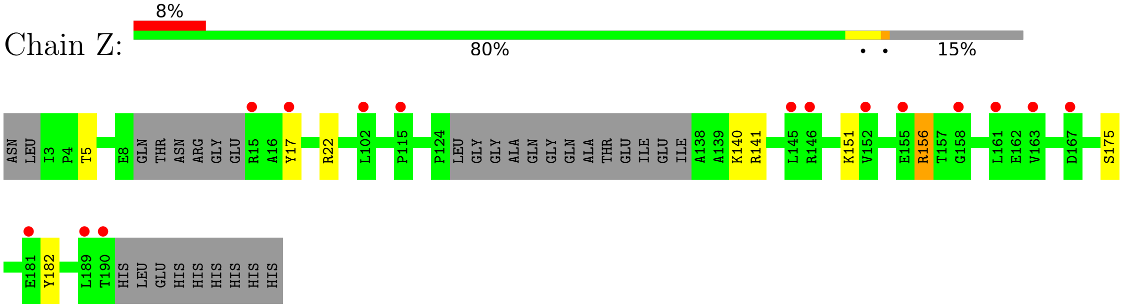
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Y:



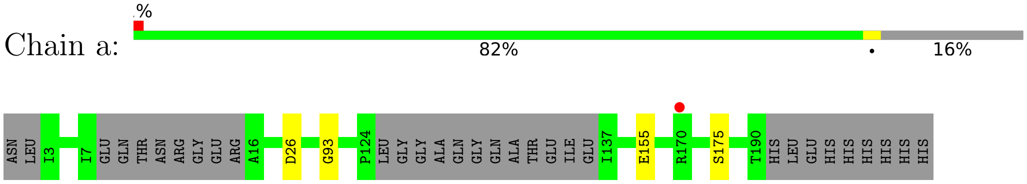
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Z:



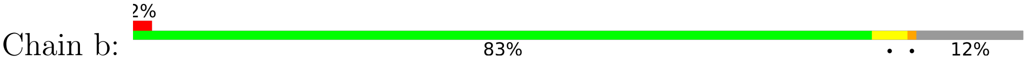
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

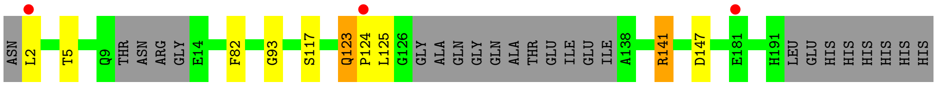
Chain a:



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

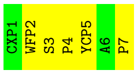
Chain b:





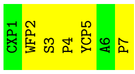
- Molecule 2: ADEP2

Chain c:



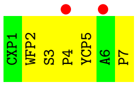
- Molecule 2: ADEP2

Chain d:



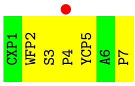
- Molecule 2: ADEP2

Chain e:



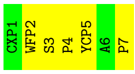
- Molecule 2: ADEP2

Chain f:



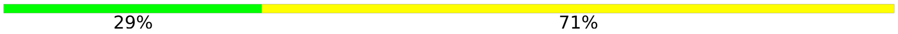
- Molecule 2: ADEP2

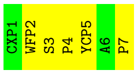
Chain g:



- Molecule 2: ADEP2

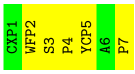
Chain h:





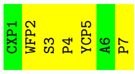
- Molecule 2: ADEP2

Chain i:



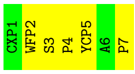
- Molecule 2: ADEP2

Chain j:



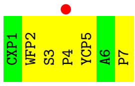
- Molecule 2: ADEP2

Chain k:



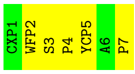
- Molecule 2: ADEP2

Chain l:



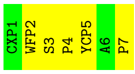
- Molecule 2: ADEP2

Chain m:



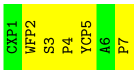
- Molecule 2: ADEP2

Chain n:



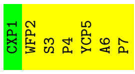
- Molecule 2: ADEP2

Chain o:



- Molecule 2: ADEP2

Chain p:

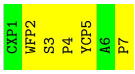


- Molecule 2: ADEP2

Chain q:

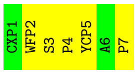
- Molecule 2: ADEP2

Chain r:



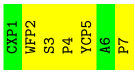
- Molecule 2: ADEP2

Chain t:



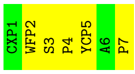
- Molecule 2: ADEP2

Chain u:



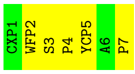
- Molecule 2: ADEP2

Chain v:



- Molecule 2: ADEP2

Chain w:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	112.98Å 173.07Å 160.00Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	45.51 – 2.79 45.51 – 2.79	Depositor EDS
% Data completeness (in resolution range)	95.8 (45.51-2.79) 91.1 (45.51-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	0.65 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.235 , 0.290 0.235 , 0.291	Depositor DCC
R_{free} test set	2019 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	38248	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8373e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MP8, CXP, WFP, YCP

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	0.29	0/1334	0.53	0/1798
1	B	0.32	0/1370	0.55	0/1847
1	C	0.30	0/1330	0.53	0/1793
1	D	0.29	0/1274	0.56	0/1716
1	E	0.29	0/1338	0.58	0/1805
1	F	0.27	0/1307	0.51	0/1762
1	G	0.33	0/1373	0.54	0/1851
1	H	0.30	0/1332	0.55	0/1795
1	I	0.32	0/1367	0.60	3/1843 (0.2%)
1	J	0.30	0/1333	0.56	0/1798
1	K	0.31	0/1326	0.54	0/1788
1	L	0.28	0/1326	0.56	0/1788
1	M	0.33	0/1299	0.56	0/1751
1	N	0.27	0/1309	0.52	0/1764
1	O	0.29	0/1348	0.51	0/1818
1	P	0.31	0/1378	0.54	0/1858
1	Q	0.32	0/1332	0.57	0/1796
1	R	0.32	0/1308	0.60	0/1763
1	S	0.31	0/1342	0.58	0/1810
1	T	0.28	0/1305	0.51	0/1759
1	U	0.30	0/1321	0.54	0/1779
1	V	0.30	0/1358	0.54	0/1831
1	W	0.27	0/1364	0.52	0/1838
1	X	0.33	0/1309	0.57	0/1764
1	Y	0.32	0/1276	0.57	0/1719
1	Z	0.33	0/1307	0.55	0/1762
1	a	0.26	0/1305	0.51	0/1759
1	b	0.37	1/1359 (0.1%)	0.59	2/1831 (0.1%)
2	c	4.20	3/17 (17.6%)	1.41	0/21
2	d	4.22	3/17 (17.6%)	1.23	0/21
2	e	4.41	5/17 (29.4%)	1.40	0/21
2	f	4.31	4/17 (23.5%)	1.16	0/21

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	g	4.24	4/17 (23.5%)	1.55	0/21
2	h	4.43	5/17 (29.4%)	1.59	0/21
2	i	4.35	4/17 (23.5%)	1.10	0/21
2	j	4.34	4/17 (23.5%)	1.27	0/21
2	k	4.41	4/17 (23.5%)	1.09	0/21
2	l	4.51	5/17 (29.4%)	1.26	0/21
2	m	4.41	3/17 (17.6%)	1.43	0/21
2	n	4.42	3/17 (17.6%)	1.26	0/21
2	o	4.40	3/17 (17.6%)	1.24	0/21
2	p	4.26	4/17 (23.5%)	1.70	1/21 (4.8%)
2	q	4.42	4/17 (23.5%)	1.26	0/21
2	r	4.39	4/17 (23.5%)	1.34	0/21
2	t	4.25	4/17 (23.5%)	1.27	0/21
2	u	4.31	4/17 (23.5%)	1.15	0/21
2	v	4.21	3/17 (17.6%)	1.46	0/21
2	w	4.40	4/17 (23.5%)	1.30	0/21
All	All	0.51	78/37570 (0.2%)	0.56	6/50606 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	G	0	1
1	J	0	1
1	Q	0	1
1	U	0	2
1	X	0	2
1	Y	0	1
1	Z	0	1
1	b	0	1
All	All	0	11

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	f	4	PRO	N-CD	12.28	1.65	1.47
2	h	4	PRO	N-CD	12.11	1.64	1.47
2	l	4	PRO	N-CD	11.99	1.64	1.47
2	r	4	PRO	N-CD	11.82	1.64	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	k	4	PRO	N-CD	11.72	1.64	1.47
2	w	4	PRO	N-CD	11.69	1.64	1.47
2	j	4	PRO	N-CD	11.65	1.64	1.47
2	e	4	PRO	N-CD	11.54	1.64	1.47
2	i	4	PRO	N-CD	11.54	1.64	1.47
2	p	4	PRO	N-CD	11.52	1.64	1.47
2	q	4	PRO	N-CD	11.46	1.63	1.47
2	c	4	PRO	N-CD	11.41	1.63	1.47
2	u	4	PRO	N-CD	11.40	1.63	1.47
2	d	4	PRO	N-CD	11.35	1.63	1.47
2	t	4	PRO	N-CD	11.31	1.63	1.47
2	v	4	PRO	N-CD	11.22	1.63	1.47
2	o	4	PRO	N-CD	11.20	1.63	1.47
2	m	4	PRO	N-CD	11.17	1.63	1.47
2	n	4	PRO	N-CD	11.11	1.63	1.47
2	g	4	PRO	N-CD	10.92	1.63	1.47
2	n	4	PRO	N-CA	-8.77	1.32	1.47
2	o	4	PRO	N-CA	-8.70	1.32	1.47
2	w	4	PRO	N-CA	-8.27	1.33	1.47
2	r	4	PRO	N-CA	-8.23	1.33	1.47
2	g	4	PRO	N-CA	-8.21	1.33	1.47
2	l	4	PRO	N-CA	-8.20	1.33	1.47
2	k	4	PRO	N-CA	-8.17	1.33	1.47
2	q	4	PRO	N-CA	-8.14	1.33	1.47
2	t	4	PRO	N-CA	-7.96	1.33	1.47
2	j	4	PRO	N-CA	-7.91	1.33	1.47
2	i	4	PRO	N-CA	-7.85	1.33	1.47
2	h	4	PRO	N-CA	-7.83	1.33	1.47
2	p	4	PRO	N-CA	-7.77	1.34	1.47
2	u	4	PRO	N-CA	-7.75	1.34	1.47
2	c	4	PRO	N-CA	-7.73	1.34	1.47
1	b	124	PRO	N-CD	7.72	1.58	1.47
2	m	4	PRO	N-CA	-7.66	1.34	1.47
2	d	4	PRO	N-CA	-7.49	1.34	1.47
2	v	4	PRO	N-CA	-7.36	1.34	1.47
2	f	4	PRO	N-CA	-7.18	1.35	1.47
2	e	4	PRO	N-CA	-7.09	1.35	1.47
2	m	3	SER	CB-OG	6.49	1.50	1.42
2	e	3	SER	C-N	6.46	1.46	1.34
2	q	3	SER	CB-OG	6.45	1.50	1.42
2	n	3	SER	CB-OG	6.26	1.50	1.42
2	l	3	SER	CB-OG	6.07	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	u	3	SER	CB-OG	5.92	1.50	1.42
2	d	3	SER	C-N	5.91	1.45	1.34
2	h	3	SER	C-N	5.79	1.45	1.34
2	k	3	SER	CB-OG	5.76	1.49	1.42
2	g	3	SER	CB-OG	5.76	1.49	1.42
2	c	3	SER	C-N	5.71	1.45	1.34
2	o	3	SER	CB-OG	5.66	1.49	1.42
2	l	3	SER	C-N	5.62	1.45	1.34
2	i	3	SER	CB-OG	5.59	1.49	1.42
2	r	3	SER	CB-OG	5.55	1.49	1.42
2	e	3	SER	CB-OG	5.54	1.49	1.42
2	j	3	SER	CB-OG	5.47	1.49	1.42
2	t	3	SER	CB-OG	5.40	1.49	1.42
2	t	3	SER	C-N	5.39	1.44	1.34
2	q	3	SER	C-N	5.36	1.44	1.34
2	i	3	SER	C-N	5.34	1.44	1.34
2	f	3	SER	C-N	5.33	1.44	1.34
2	w	3	SER	CB-OG	5.33	1.49	1.42
2	p	3	SER	C-N	5.32	1.44	1.34
2	p	4	PRO	CA-CB	5.28	1.64	1.53
2	h	3	SER	CB-OG	5.24	1.49	1.42
2	j	3	SER	C-N	5.22	1.44	1.34
2	k	4	PRO	CA-CB	5.20	1.64	1.53
2	e	4	PRO	CA-CB	5.15	1.63	1.53
2	l	4	PRO	CA-CB	5.14	1.63	1.53
2	h	4	PRO	CA-CB	5.14	1.63	1.53
2	u	4	PRO	CA-CB	5.14	1.63	1.53
2	r	3	SER	C-N	5.13	1.44	1.34
2	f	4	PRO	CA-CB	5.13	1.63	1.53
2	w	4	PRO	CA-CB	5.12	1.63	1.53
2	v	3	SER	CB-OG	5.03	1.48	1.42
2	g	3	SER	C-N	5.01	1.43	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	125	LEU	N-CA-CB	-8.64	93.12	110.40
1	I	124	PRO	N-CA-CB	-7.40	94.42	103.30
1	I	124	PRO	CB-CA-C	-5.74	97.65	112.00
2	p	6	ALA	N-CA-CB	-5.73	102.08	110.10
1	I	124	PRO	N-CA-C	5.60	126.66	112.10
1	b	124	PRO	N-CA-C	-5.54	97.69	112.10

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	170	ARG	Sidechain
1	G	146	ARG	Sidechain
1	J	141	ARG	Sidechain
1	Q	141	ARG	Sidechain
1	U	141	ARG	Sidechain
1	U	156	ARG	Sidechain
1	X	141	ARG	Sidechain
1	X	156	ARG	Sidechain
1	Y	22	ARG	Sidechain
1	Z	156	ARG	Sidechain
1	b	141	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	166/199 (83%)	157 (95%)	7 (4%)	2 (1%)	13	39
1	B	170/199 (85%)	162 (95%)	6 (4%)	2 (1%)	13	39
1	C	166/199 (83%)	155 (93%)	10 (6%)	1 (1%)	25	56
1	D	158/199 (79%)	145 (92%)	13 (8%)	0	100	100
1	E	168/199 (84%)	151 (90%)	17 (10%)	0	100	100
1	F	163/199 (82%)	154 (94%)	8 (5%)	1 (1%)	25	56
1	G	171/199 (86%)	162 (95%)	7 (4%)	2 (1%)	13	39
1	H	166/199 (83%)	157 (95%)	8 (5%)	1 (1%)	25	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	171/199 (86%)	159 (93%)	11 (6%)	1 (1%)	25	56
1	J	167/199 (84%)	156 (93%)	10 (6%)	1 (1%)	25	56
1	K	165/199 (83%)	155 (94%)	8 (5%)	2 (1%)	13	39
1	L	165/199 (83%)	153 (93%)	12 (7%)	0	100	100
1	M	162/199 (81%)	152 (94%)	9 (6%)	1 (1%)	25	56
1	N	162/199 (81%)	155 (96%)	5 (3%)	2 (1%)	13	39
1	O	168/199 (84%)	159 (95%)	6 (4%)	3 (2%)	8	28
1	P	171/199 (86%)	160 (94%)	10 (6%)	1 (1%)	25	56
1	Q	166/199 (83%)	152 (92%)	13 (8%)	1 (1%)	25	56
1	R	162/199 (81%)	153 (94%)	7 (4%)	2 (1%)	13	39
1	S	168/199 (84%)	157 (94%)	11 (6%)	0	100	100
1	T	162/199 (81%)	153 (94%)	8 (5%)	1 (1%)	25	56
1	U	164/199 (82%)	156 (95%)	8 (5%)	0	100	100
1	V	169/199 (85%)	163 (96%)	4 (2%)	2 (1%)	13	39
1	W	170/199 (85%)	158 (93%)	12 (7%)	0	100	100
1	X	163/199 (82%)	155 (95%)	6 (4%)	2 (1%)	13	39
1	Y	159/199 (80%)	150 (94%)	8 (5%)	1 (1%)	25	56
1	Z	163/199 (82%)	150 (92%)	13 (8%)	0	100	100
1	a	162/199 (81%)	153 (94%)	8 (5%)	1 (1%)	25	56
1	b	169/199 (85%)	162 (96%)	5 (3%)	2 (1%)	13	39
2	c	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	d	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	e	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	f	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	g	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	h	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	i	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	j	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	k	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	l	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	m	3/7 (43%)	2 (67%)	1 (33%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	n	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	o	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	p	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	q	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	r	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	t	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	u	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	v	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	w	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
All	All	4696/5712 (82%)	4394 (94%)	270 (6%)	32 (1%)	22	53

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	124	PRO
1	K	4	PRO
1	O	4	PRO
1	O	135	ILE
1	A	93	GLY
1	G	124	PRO
1	H	93	GLY
1	J	93	GLY
1	V	93	GLY
1	X	139	ALA
1	F	93	GLY
1	N	189	LEU
1	Q	93	GLY
1	R	106	GLY
1	X	93	GLY
1	A	4	PRO
1	B	67	GLY
1	C	93	GLY
1	P	67	GLY
1	V	4	PRO
1	K	106	GLY
1	O	93	GLY
1	R	3	ILE
1	T	93	GLY
1	Y	106	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	b	93	GLY
1	b	123	GLN
1	G	93	GLY
1	M	93	GLY
1	N	93	GLY
1	a	93	GLY
1	B	93	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	142/165 (86%)	139 (98%)	3 (2%)	53	84
1	B	145/165 (88%)	141 (97%)	4 (3%)	43	77
1	C	141/165 (86%)	131 (93%)	10 (7%)	14	39
1	D	137/165 (83%)	131 (96%)	6 (4%)	28	61
1	E	140/165 (85%)	130 (93%)	10 (7%)	14	39
1	F	138/165 (84%)	134 (97%)	4 (3%)	42	76
1	G	145/165 (88%)	136 (94%)	9 (6%)	18	47
1	H	141/165 (86%)	133 (94%)	8 (6%)	20	50
1	I	144/165 (87%)	135 (94%)	9 (6%)	18	46
1	J	140/165 (85%)	133 (95%)	7 (5%)	24	56
1	K	141/165 (86%)	136 (96%)	5 (4%)	36	70
1	L	141/165 (86%)	130 (92%)	11 (8%)	12	35
1	M	137/165 (83%)	132 (96%)	5 (4%)	35	69
1	N	140/165 (85%)	134 (96%)	6 (4%)	29	62
1	O	143/165 (87%)	140 (98%)	3 (2%)	53	84
1	P	146/165 (88%)	139 (95%)	7 (5%)	25	58
1	Q	141/165 (86%)	133 (94%)	8 (6%)	20	50
1	R	140/165 (85%)	134 (96%)	6 (4%)	29	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	141/165 (86%)	136 (96%)	5 (4%)	36	70
1	T	139/165 (84%)	134 (96%)	5 (4%)	35	69
1	U	140/165 (85%)	134 (96%)	6 (4%)	29	62
1	V	145/165 (88%)	140 (97%)	5 (3%)	37	71
1	W	144/165 (87%)	141 (98%)	3 (2%)	53	84
1	X	139/165 (84%)	136 (98%)	3 (2%)	52	83
1	Y	136/165 (82%)	131 (96%)	5 (4%)	34	68
1	Z	138/165 (84%)	129 (94%)	9 (6%)	17	44
1	a	139/165 (84%)	136 (98%)	3 (2%)	52	83
1	b	144/165 (87%)	137 (95%)	7 (5%)	25	57
2	c	2/2 (100%)	2 (100%)	0	100	100
2	d	2/2 (100%)	2 (100%)	0	100	100
2	e	2/2 (100%)	2 (100%)	0	100	100
2	f	2/2 (100%)	2 (100%)	0	100	100
2	g	2/2 (100%)	2 (100%)	0	100	100
2	h	2/2 (100%)	2 (100%)	0	100	100
2	i	2/2 (100%)	2 (100%)	0	100	100
2	j	2/2 (100%)	2 (100%)	0	100	100
2	k	2/2 (100%)	2 (100%)	0	100	100
2	l	2/2 (100%)	2 (100%)	0	100	100
2	m	2/2 (100%)	2 (100%)	0	100	100
2	n	2/2 (100%)	2 (100%)	0	100	100
2	o	2/2 (100%)	2 (100%)	0	100	100
2	p	2/2 (100%)	2 (100%)	0	100	100
2	q	2/2 (100%)	2 (100%)	0	100	100
2	r	2/2 (100%)	2 (100%)	0	100	100
2	t	2/2 (100%)	2 (100%)	0	100	100
2	u	2/2 (100%)	2 (100%)	0	100	100
2	v	2/2 (100%)	2 (100%)	0	100	100
2	w	2/2 (100%)	2 (100%)	0	100	100
All	All	3987/4660 (86%)	3815 (96%)	172 (4%)	29	62

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	144	LEU
1	A	181	GLU
1	B	1	ASN
1	B	120	MET
1	B	168	THR
1	B	172	ASN
1	C	5	THR
1	C	18	ASP
1	C	33	SER
1	C	36	ASP
1	C	56	GLU
1	C	69	SER
1	C	78	ASP
1	C	82	PHE
1	C	123	GLN
1	C	169	ASP
1	D	5	THR
1	D	29	ILE
1	D	37	ASP
1	D	60	SER
1	D	97	SER
1	D	155	GLU
1	E	5	THR
1	E	17	TYR
1	E	81	GLN
1	E	120	MET
1	E	122	HIS
1	E	141	ARG
1	E	153	LEU
1	E	167	ASP
1	E	169	ASP
1	E	182	TYR
1	F	5	THR
1	F	26	ASP
1	F	170	ARG
1	F	172	ASN
1	G	2	LEU
1	G	18	ASP
1	G	21	SER
1	G	82	PHE
1	G	141	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	144	LEU
1	G	147	ASP
1	G	149	LEU
1	G	169	ASP
1	H	81	GLN
1	H	107	GLU
1	H	108	LYS
1	H	118	GLU
1	H	147	ASP
1	H	148	LYS
1	H	174	LYS
1	H	185	ILE
1	I	22	ARG
1	I	57	LYS
1	I	88	SER
1	I	117	SER
1	I	120	MET
1	I	124	PRO
1	I	125	LEU
1	I	165	GLU
1	I	169	ASP
1	J	36	ASP
1	J	41	ASN
1	J	43	ILE
1	J	140	LYS
1	J	143	LEU
1	J	156	ARG
1	J	159	GLN
1	K	28	ILE
1	K	37	ASP
1	K	69	SER
1	K	84	LYS
1	K	147	ASP
1	L	5	THR
1	L	17	TYR
1	L	94	MET
1	L	97	SER
1	L	116	ASN
1	L	141	ARG
1	L	159	GLN
1	L	168	THR
1	L	171	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	180	LEU
1	L	181	GLU
1	M	17	TYR
1	M	77	TYR
1	M	97	SER
1	M	120	MET
1	M	148	LYS
1	N	5	THR
1	N	30	MET
1	N	60	SER
1	N	82	PHE
1	N	144	LEU
1	N	159	GLN
1	O	31	LEU
1	O	149	LEU
1	O	173	PHE
1	P	31	LEU
1	P	120	MET
1	P	140	LYS
1	P	152	VAL
1	P	165	GLU
1	P	166	ARG
1	P	169	ASP
1	Q	33	SER
1	Q	36	ASP
1	Q	43	ILE
1	Q	56	GLU
1	Q	146	ARG
1	Q	147	ASP
1	Q	156	ARG
1	Q	162	GLU
1	R	3	ILE
1	R	5	THR
1	R	60	SER
1	R	147	ASP
1	R	169	ASP
1	R	172	ASN
1	S	5	THR
1	S	17	TYR
1	S	84	LYS
1	S	116	ASN
1	S	180	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	2	LEU
1	T	5	THR
1	T	57	LYS
1	T	84	LYS
1	T	151	LYS
1	U	2	LEU
1	U	5	THR
1	U	15	ARG
1	U	21	SER
1	U	82	PHE
1	U	169	ASP
1	V	25	LYS
1	V	30	MET
1	V	147	ASP
1	V	166	ARG
1	V	173	PHE
1	W	2	LEU
1	W	86	LYS
1	W	147	ASP
1	X	141	ARG
1	X	151	LYS
1	X	169	ASP
1	Y	18	ASP
1	Y	57	LYS
1	Y	144	LEU
1	Y	155	GLU
1	Y	175	SER
1	Z	5	THR
1	Z	17	TYR
1	Z	22	ARG
1	Z	140	LYS
1	Z	141	ARG
1	Z	151	LYS
1	Z	156	ARG
1	Z	175	SER
1	Z	182	TYR
1	a	26	ASP
1	a	155	GLU
1	a	175	SER
1	b	2	LEU
1	b	5	THR
1	b	82	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	b	117	SER
1	b	123	GLN
1	b	141	ARG
1	b	147	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

60 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	WFP	u	2	2	12,13,14	0.98	0	14,17,19	2.24	6 (42%)
2	WFP	i	2	2	12,13,14	0.99	0	14,17,19	1.87	5 (35%)
2	WFP	t	2	2	12,13,14	0.94	0	14,17,19	1.61	4 (28%)
2	YCP	d	5	2	6,8,9	1.59	1 (16%)	5,9,11	3.02	3 (60%)
2	WFP	r	2	2	12,13,14	0.88	0	14,17,19	2.27	6 (42%)
2	WFP	v	2	2	12,13,14	1.01	0	14,17,19	1.72	4 (28%)
2	WFP	f	2	2	12,13,14	0.92	0	14,17,19	2.21	6 (42%)
2	WFP	j	2	2	12,13,14	1.05	1 (8%)	14,17,19	2.18	6 (42%)
2	WFP	q	2	2	12,13,14	0.81	0	14,17,19	1.95	6 (42%)
2	YCP	i	5	2	6,8,9	1.52	1 (16%)	5,9,11	3.02	3 (60%)
2	MP8	e	7	2	5,8,9	5.79	3 (60%)	3,10,12	1.59	1 (33%)
2	MP8	l	7	2	5,8,9	5.83	3 (60%)	3,10,12	1.77	1 (33%)
2	MP8	r	7	2	5,8,9	5.68	3 (60%)	3,10,12	1.43	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	MP8	g	7	2	5,8,9	5.69	3 (60%)	3,10,12	1.95	1 (33%)
2	MP8	m	7	2	5,8,9	5.71	3 (60%)	3,10,12	0.84	0
2	MP8	c	7	2	5,8,9	5.77	3 (60%)	3,10,12	1.32	0
2	WFP	d	2	2	12,13,14	1.10	0	14,17,19	1.64	4 (28%)
2	WFP	p	2	2	12,13,14	1.03	0	14,17,19	1.62	2 (14%)
2	WFP	w	2	2	12,13,14	1.00	0	14,17,19	1.55	3 (21%)
2	MP8	h	7	2	5,8,9	5.91	3 (60%)	3,10,12	1.02	0
2	MP8	n	7	2	5,8,9	5.70	3 (60%)	3,10,12	1.44	1 (33%)
2	MP8	t	7	2	5,8,9	5.82	3 (60%)	3,10,12	1.56	1 (33%)
2	YCP	r	5	2	6,8,9	1.48	1 (16%)	5,9,11	3.08	3 (60%)
2	MP8	j	7	2	5,8,9	5.83	3 (60%)	3,10,12	2.05	2 (66%)
2	MP8	v	7	2	5,8,9	5.75	3 (60%)	3,10,12	0.67	0
2	YCP	j	5	2	6,8,9	1.77	1 (16%)	5,9,11	1.50	2 (40%)
2	YCP	h	5	2	6,8,9	1.56	1 (16%)	5,9,11	2.48	3 (60%)
2	YCP	t	5	2	6,8,9	1.56	1 (16%)	5,9,11	2.63	2 (40%)
2	WFP	o	2	2	12,13,14	0.82	0	14,17,19	2.23	6 (42%)
2	WFP	e	2	2	12,13,14	1.19	1 (8%)	14,17,19	2.07	5 (35%)
2	YCP	u	5	2	6,8,9	1.76	2 (33%)	5,9,11	1.55	1 (20%)
2	WFP	h	2	2	12,13,14	1.10	0	14,17,19	1.74	6 (42%)
2	YCP	w	5	2	6,8,9	1.56	1 (16%)	5,9,11	2.09	2 (40%)
2	YCP	n	5	2	6,8,9	1.63	1 (16%)	5,9,11	1.74	2 (40%)
2	MP8	i	7	2	5,8,9	5.76	3 (60%)	3,10,12	1.51	1 (33%)
2	MP8	d	7	2	5,8,9	5.82	3 (60%)	3,10,12	1.37	1 (33%)
2	YCP	v	5	2	6,8,9	1.79	2 (33%)	5,9,11	0.92	0
2	YCP	q	5	2	6,8,9	1.52	1 (16%)	5,9,11	3.04	3 (60%)
2	WFP	l	2	2	12,13,14	1.15	1 (8%)	14,17,19	2.83	9 (64%)
2	YCP	p	5	2	6,8,9	1.76	2 (33%)	5,9,11	1.86	1 (20%)
2	YCP	k	5	2	6,8,9	1.66	1 (16%)	5,9,11	1.77	2 (40%)
2	WFP	n	2	2	12,13,14	0.89	0	14,17,19	1.78	7 (50%)
2	YCP	m	5	2	6,8,9	1.61	1 (16%)	5,9,11	2.26	2 (40%)
2	YCP	c	5	2	6,8,9	1.68	1 (16%)	5,9,11	2.02	3 (60%)
2	YCP	e	5	2	6,8,9	1.66	2 (33%)	5,9,11	1.54	1 (20%)
2	WFP	c	2	2	12,13,14	0.91	1 (8%)	14,17,19	2.82	8 (57%)
2	MP8	w	7	2	5,8,9	5.85	3 (60%)	3,10,12	1.98	2 (66%)
2	YCP	o	5	2	6,8,9	1.72	1 (16%)	5,9,11	1.92	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
2	MP8	u	7	2	5,8,9	5.90	3 (60%)	3,10,12	2.16	2 (66%)
2	YCP	g	5	2	6,8,9	1.55	1 (16%)	5,9,11	2.80	2 (40%)
2	YCP	l	5	2	6,8,9	1.58	1 (16%)	5,9,11	2.43	3 (60%)
2	WFP	k	2	2	12,13,14	0.87	0	14,17,19	1.80	4 (28%)
2	WFP	m	2	2	12,13,14	0.83	1 (8%)	14,17,19	1.93	5 (35%)
2	MP8	f	7	2	5,8,9	5.93	3 (60%)	3,10,12	1.31	1 (33%)
2	MP8	k	7	2	5,8,9	5.73	3 (60%)	3,10,12	1.58	1 (33%)
2	MP8	q	7	2	5,8,9	5.81	3 (60%)	3,10,12	1.62	0
2	YCP	f	5	2	6,8,9	1.68	1 (16%)	5,9,11	1.44	1 (20%)
2	WFP	g	2	2	12,13,14	0.81	0	14,17,19	1.51	2 (14%)
2	MP8	p	7	2	5,8,9	5.52	3 (60%)	3,10,12	0.60	0
2	MP8	o	7	2	5,8,9	5.89	3 (60%)	3,10,12	2.06	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WFP	u	2	2	-	0/5/6/8	0/1/1/1
2	WFP	i	2	2	-	2/5/6/8	0/1/1/1
2	WFP	t	2	2	-	1/5/6/8	0/1/1/1
2	YCP	d	5	2	-	0/1/10/12	0/1/1/1
2	WFP	r	2	2	-	2/5/6/8	0/1/1/1
2	WFP	v	2	2	-	2/5/6/8	0/1/1/1
2	WFP	f	2	2	-	1/5/6/8	0/1/1/1
2	WFP	j	2	2	-	2/5/6/8	0/1/1/1
2	WFP	q	2	2	-	1/5/6/8	0/1/1/1
2	YCP	i	5	2	-	0/1/10/12	0/1/1/1
2	MP8	e	7	2	-	0/0/11/13	0/1/1/1
2	MP8	l	7	2	-	0/0/11/13	0/1/1/1
2	MP8	r	7	2	-	0/0/11/13	0/1/1/1
2	MP8	g	7	2	-	0/0/11/13	0/1/1/1
2	MP8	m	7	2	-	0/0/11/13	0/1/1/1
2	MP8	c	7	2	-	0/0/11/13	0/1/1/1
2	WFP	d	2	2	-	2/5/6/8	0/1/1/1
2	WFP	p	2	2	-	2/5/6/8	0/1/1/1
2	WFP	w	2	2	-	1/5/6/8	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MP8	h	7	2	-	0/0/11/13	0/1/1/1
2	MP8	n	7	2	-	0/0/11/13	0/1/1/1
2	MP8	t	7	2	-	0/0/11/13	0/1/1/1
2	YCP	r	5	2	-	0/1/10/12	0/1/1/1
2	MP8	j	7	2	-	0/0/11/13	0/1/1/1
2	MP8	v	7	2	-	0/0/11/13	0/1/1/1
2	YCP	j	5	2	-	0/1/10/12	1/1/1/1
2	YCP	h	5	2	-	0/1/10/12	0/1/1/1
2	YCP	t	5	2	-	0/1/10/12	0/1/1/1
2	WFP	o	2	2	-	2/5/6/8	0/1/1/1
2	WFP	e	2	2	-	1/5/6/8	0/1/1/1
2	YCP	u	5	2	-	0/1/10/12	1/1/1/1
2	WFP	h	2	2	-	2/5/6/8	0/1/1/1
2	YCP	w	5	2	-	0/1/10/12	0/1/1/1
2	YCP	n	5	2	-	0/1/10/12	0/1/1/1
2	MP8	i	7	2	-	0/0/11/13	0/1/1/1
2	MP8	d	7	2	-	0/0/11/13	0/1/1/1
2	YCP	v	5	2	-	1/1/10/12	1/1/1/1
2	YCP	q	5	2	-	0/1/10/12	0/1/1/1
2	WFP	l	2	2	-	2/5/6/8	0/1/1/1
2	YCP	p	5	2	-	0/1/10/12	1/1/1/1
2	YCP	k	5	2	-	0/1/10/12	1/1/1/1
2	WFP	n	2	2	-	0/5/6/8	0/1/1/1
2	YCP	m	5	2	-	0/1/10/12	0/1/1/1
2	YCP	c	5	2	-	1/1/10/12	0/1/1/1
2	YCP	e	5	2	-	0/1/10/12	1/1/1/1
2	WFP	c	2	2	-	2/5/6/8	0/1/1/1
2	MP8	w	7	2	-	0/0/11/13	0/1/1/1
2	YCP	o	5	2	-	0/1/10/12	1/1/1/1
2	MP8	u	7	2	-	0/0/11/13	0/1/1/1
2	YCP	g	5	2	-	0/1/10/12	0/1/1/1
2	YCP	l	5	2	-	0/1/10/12	0/1/1/1
2	WFP	k	2	2	-	0/5/6/8	0/1/1/1
2	WFP	m	2	2	-	2/5/6/8	0/1/1/1
2	MP8	f	7	2	-	0/0/11/13	0/1/1/1
2	MP8	k	7	2	-	0/0/11/13	0/1/1/1
2	MP8	q	7	2	-	0/0/11/13	0/1/1/1
2	YCP	f	5	2	-	0/1/10/12	1/1/1/1
2	WFP	g	2	2	-	1/5/6/8	0/1/1/1
2	MP8	p	7	2	-	0/0/11/13	0/1/1/1
2	MP8	o	7	2	-	0/0/11/13	0/1/1/1

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	h	7	MP8	CB-CA	-10.82	1.30	1.54
2	o	7	MP8	CB-CA	-10.81	1.30	1.54
2	j	7	MP8	CB-CA	-10.79	1.30	1.54
2	f	7	MP8	CB-CA	-10.78	1.30	1.54
2	w	7	MP8	CB-CA	-10.77	1.30	1.54
2	u	7	MP8	CB-CA	-10.76	1.30	1.54
2	t	7	MP8	CB-CA	-10.63	1.31	1.54
2	q	7	MP8	CB-CA	-10.58	1.31	1.54
2	c	7	MP8	CB-CA	-10.53	1.31	1.54
2	i	7	MP8	CB-CA	-10.53	1.31	1.54
2	e	7	MP8	CB-CA	-10.52	1.31	1.54
2	l	7	MP8	CB-CA	-10.49	1.31	1.54
2	d	7	MP8	CB-CA	-10.46	1.31	1.54
2	v	7	MP8	CB-CA	-10.36	1.31	1.54
2	n	7	MP8	CB-CA	-10.27	1.31	1.54
2	g	7	MP8	CB-CA	-10.25	1.31	1.54
2	m	7	MP8	CB-CA	-10.21	1.32	1.54
2	k	7	MP8	CB-CA	-10.15	1.32	1.54
2	p	7	MP8	CB-CA	-10.08	1.32	1.54
2	r	7	MP8	CB-CA	-10.07	1.32	1.54
2	f	7	MP8	O-C	6.11	1.44	1.19
2	l	7	MP8	O-C	6.11	1.44	1.19
2	d	7	MP8	O-C	6.08	1.44	1.19
2	t	7	MP8	O-C	6.04	1.44	1.19
2	k	7	MP8	O-C	6.03	1.44	1.19
2	h	7	MP8	O-C	6.00	1.43	1.19
2	e	7	MP8	O-C	5.99	1.43	1.19
2	r	7	MP8	O-C	5.99	1.43	1.19
2	m	7	MP8	O-C	5.98	1.43	1.19
2	u	7	MP8	O-C	5.87	1.43	1.19
2	v	7	MP8	O-C	5.86	1.43	1.19
2	q	7	MP8	O-C	5.86	1.43	1.19
2	i	7	MP8	O-C	5.84	1.43	1.19
2	o	7	MP8	O-C	5.83	1.43	1.19
2	c	7	MP8	O-C	5.78	1.43	1.19
2	g	7	MP8	O-C	5.68	1.42	1.19
2	j	7	MP8	O-C	5.68	1.42	1.19
2	n	7	MP8	O-C	5.63	1.42	1.19
2	w	7	MP8	O-C	5.58	1.42	1.19
2	p	7	MP8	O-C	5.50	1.41	1.19
2	r	7	MP8	CD-N	-4.72	1.30	1.47
2	n	7	MP8	CD-N	-4.70	1.30	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	g	7	MP8	CD-N	-4.69	1.30	1.47
2	k	7	MP8	CD-N	-4.66	1.30	1.47
2	u	7	MP8	CD-N	-4.65	1.30	1.47
2	w	7	MP8	CD-N	-4.64	1.30	1.47
2	v	7	MP8	CD-N	-4.58	1.31	1.47
2	o	7	MP8	CD-N	-4.56	1.31	1.47
2	q	7	MP8	CD-N	-4.54	1.31	1.47
2	d	7	MP8	CD-N	-4.52	1.31	1.47
2	l	7	MP8	CD-N	-4.43	1.31	1.47
2	j	7	MP8	CD-N	-4.43	1.31	1.47
2	m	7	MP8	CD-N	-4.39	1.31	1.47
2	h	7	MP8	CD-N	-4.38	1.31	1.47
2	c	7	MP8	CD-N	-4.37	1.31	1.47
2	f	7	MP8	CD-N	-4.36	1.31	1.47
2	e	7	MP8	CD-N	-4.34	1.31	1.47
2	i	7	MP8	CD-N	-4.32	1.32	1.47
2	t	7	MP8	CD-N	-4.24	1.32	1.47
2	p	7	MP8	CD-N	-4.20	1.32	1.47
2	j	5	YCP	CG-CB	-3.49	1.44	1.53
2	o	5	YCP	CG-CB	-3.36	1.44	1.53
2	p	5	YCP	CG-CB	-3.34	1.44	1.53
2	v	5	YCP	CG-CB	-3.33	1.44	1.53
2	u	5	YCP	CG-CB	-3.32	1.44	1.53
2	m	5	YCP	CG-CB	-3.28	1.44	1.53
2	f	5	YCP	CG-CB	-3.26	1.44	1.53
2	c	5	YCP	CG-CB	-3.25	1.44	1.53
2	n	5	YCP	CG-CB	-3.25	1.44	1.53
2	k	5	YCP	CG-CB	-3.18	1.44	1.53
2	e	5	YCP	CG-CB	-3.17	1.44	1.53
2	i	5	YCP	CG-CB	-3.12	1.45	1.53
2	w	5	YCP	CG-CB	-3.08	1.45	1.53
2	g	5	YCP	CG-CB	-3.07	1.45	1.53
2	t	5	YCP	CG-CB	-3.05	1.45	1.53
2	l	5	YCP	CG-CB	-3.05	1.45	1.53
2	r	5	YCP	CG-CB	-3.02	1.45	1.53
2	d	5	YCP	CG-CB	-2.99	1.45	1.53
2	h	5	YCP	CG-CB	-2.96	1.45	1.53
2	q	5	YCP	CG-CB	-2.88	1.45	1.53
2	c	2	WFP	CZ-CE1	2.28	1.41	1.37
2	e	2	WFP	CZ-CE1	2.19	1.41	1.37
2	v	5	YCP	CE-N	2.17	1.53	1.47
2	u	5	YCP	CE-N	2.16	1.53	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	2	WFP	CZ-CE1	2.05	1.41	1.37
2	m	2	WFP	CD2-CE2	2.04	1.41	1.37
2	p	5	YCP	CE-N	2.03	1.52	1.47
2	l	2	WFP	CZ-CE1	2.00	1.41	1.37
2	e	5	YCP	CE-N	2.00	1.52	1.47

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	c	2	WFP	CG-CB-CA	-6.58	100.77	114.10
2	f	2	WFP	CB-CA-C	-6.03	100.16	111.47
2	j	2	WFP	CG-CB-CA	-5.29	103.40	114.10
2	q	5	YCP	CG-CB-CA	5.05	118.47	110.98
2	u	2	WFP	CG-CB-CA	-4.97	104.04	114.10
2	r	5	YCP	CD-CG-CB	4.89	121.39	111.42
2	i	5	YCP	CD-CG-CB	4.70	121.01	111.42
2	d	5	YCP	CD-CG-CB	4.54	120.68	111.42
2	r	2	WFP	CG-CB-CA	-4.51	104.96	114.10
2	o	2	WFP	CB-CA-C	-4.47	103.09	111.47
2	o	2	WFP	CG-CB-CA	-4.46	105.06	114.10
2	l	2	WFP	CD1-CE1-CZ	-4.35	118.03	123.52
2	r	5	YCP	CG-CB-CA	4.16	117.16	110.98
2	m	5	YCP	CD-CG-CB	4.13	119.83	111.42
2	g	5	YCP	CG-CB-CA	4.11	117.09	110.98
2	l	2	WFP	F2-CE2-CD2	4.09	124.10	118.25
2	g	5	YCP	CD-CG-CB	4.07	119.72	111.42
2	t	5	YCP	CD-CG-CB	4.00	119.57	111.42
2	l	2	WFP	CB-CG-CD1	-3.97	113.63	120.44
2	r	2	WFP	CB-CA-C	-3.96	104.04	111.47
2	i	5	YCP	CG-CB-CA	3.96	116.86	110.98
2	m	2	WFP	CG-CB-CA	-3.92	106.16	114.10
2	q	5	YCP	CD-CG-CB	3.89	119.34	111.42
2	v	2	WFP	CB-CA-C	-3.83	104.29	111.47
2	d	5	YCP	CG-CB-CA	3.83	116.66	110.98
2	k	2	WFP	CG-CB-CA	-3.77	106.47	114.10
2	l	2	WFP	CE2-CZ-CE1	3.77	121.99	116.13
2	i	2	WFP	CG-CB-CA	-3.76	106.48	114.10
2	l	2	WFP	CB-CA-C	-3.75	104.45	111.47
2	l	5	YCP	CD-CG-CB	3.66	118.88	111.42
2	p	2	WFP	CB-CA-C	-3.65	104.63	111.47
2	t	5	YCP	CG-CB-CA	3.51	116.19	110.98
2	e	2	WFP	CE2-CZ-CE1	3.48	121.55	116.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	2	WFP	CD2-CE2-CZ	-3.47	119.14	123.52
2	e	2	WFP	CD1-CE1-CZ	-3.44	119.17	123.52
2	c	2	WFP	CB-CG-CD2	-3.43	114.55	120.44
2	h	5	YCP	CG-CB-CA	3.42	116.06	110.98
2	c	2	WFP	CD2-CE2-CZ	-3.38	119.25	123.52
2	w	5	YCP	CG-CB-CA	3.30	115.89	110.98
2	c	2	WFP	CD2-CG-CD1	3.29	123.49	118.98
2	g	7	MP8	O-C-CA	-3.26	116.23	124.78
2	u	2	WFP	CD2-CE2-CZ	-3.23	119.44	123.52
2	k	2	WFP	CD2-CE2-CZ	-3.21	119.47	123.52
2	h	5	YCP	CD-CG-CB	3.21	117.95	111.42
2	q	2	WFP	CD2-CE2-CZ	-3.09	119.61	123.52
2	h	2	WFP	CG-CB-CA	-3.05	107.92	114.10
2	c	5	YCP	CD-CG-CB	3.03	117.60	111.42
2	m	2	WFP	F2-CE2-CD2	3.01	122.56	118.25
2	p	5	YCP	O-C-CA	-3.00	116.93	124.78
2	c	2	WFP	CB-CA-C	-2.99	105.86	111.47
2	u	2	WFP	CE2-CZ-CE1	2.99	120.79	116.13
2	q	2	WFP	CG-CB-CA	-2.97	108.08	114.10
2	w	5	YCP	CD-CG-CB	2.97	117.46	111.42
2	q	2	WFP	CB-CA-C	-2.89	106.05	111.47
2	c	2	WFP	CG-CD1-CE1	-2.85	116.23	118.81
2	d	2	WFP	CB-CA-C	-2.84	106.14	111.47
2	r	2	WFP	CD2-CE2-CZ	-2.83	119.94	123.52
2	j	2	WFP	CB-CA-C	-2.83	106.17	111.47
2	w	2	WFP	CD2-CE2-CZ	-2.82	119.95	123.52
2	t	2	WFP	CD1-CE1-CZ	-2.82	119.96	123.52
2	l	5	YCP	CG-CB-CA	2.79	115.12	110.98
2	h	5	YCP	O-C-CA	-2.79	117.47	124.78
2	u	2	WFP	CD1-CE1-CZ	-2.78	120.01	123.52
2	c	2	WFP	F2-CE2-CZ	2.78	122.22	118.25
2	m	2	WFP	CB-CA-C	-2.75	106.30	111.47
2	h	2	WFP	F1-CE1-CD1	2.72	122.14	118.25
2	o	5	YCP	O-C-CA	-2.71	117.66	124.78
2	l	2	WFP	CD2-CE2-CZ	-2.69	120.12	123.52
2	r	2	WFP	CD2-CG-CD1	2.69	122.67	118.98
2	g	2	WFP	CB-CA-C	-2.66	106.48	111.47
2	u	7	MP8	O-C-CA	-2.66	117.82	124.78
2	k	5	YCP	O-C-CA	-2.65	117.84	124.78
2	t	7	MP8	O-C-CA	-2.63	117.88	124.78
2	n	5	YCP	CD-CG-CB	2.62	116.76	111.42
2	j	2	WFP	CD2-CE2-CZ	-2.62	120.21	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	q	2	WFP	CE2-CZ-CE1	2.61	120.19	116.13
2	f	2	WFP	CD2-CE2-CZ	-2.55	120.29	123.52
2	i	2	WFP	CD2-CE2-CZ	-2.55	120.29	123.52
2	n	2	WFP	CD1-CE1-CZ	-2.55	120.30	123.52
2	u	7	MP8	CE-CG-CB	-2.55	107.61	114.05
2	q	2	WFP	CD2-CG-CD1	2.55	122.48	118.98
2	k	7	MP8	O-C-CA	-2.53	118.16	124.78
2	o	5	YCP	CG-CB-CA	2.52	114.72	110.98
2	r	2	WFP	CE2-CZ-CE1	2.52	120.05	116.13
2	f	2	WFP	CD2-CG-CD1	2.52	122.44	118.98
2	d	2	WFP	CD1-CE1-CZ	-2.51	120.35	123.52
2	o	2	WFP	CD2-CG-CD1	2.50	122.41	118.98
2	j	7	MP8	CE-CG-CB	-2.49	107.75	114.05
2	n	2	WFP	CB-CA-C	-2.49	106.81	111.47
2	j	2	WFP	CD2-CG-CD1	2.46	122.36	118.98
2	o	7	MP8	O-C-CA	-2.46	118.34	124.78
2	n	5	YCP	O-C-CA	-2.45	118.35	124.78
2	r	7	MP8	O-C-CA	-2.45	118.35	124.78
2	v	2	WFP	CD1-CE1-CZ	-2.45	120.43	123.52
2	h	2	WFP	F2-CE2-CD2	2.44	121.74	118.25
2	m	5	YCP	CG-CB-CA	2.44	114.60	110.98
2	t	2	WFP	CG-CB-CA	-2.44	109.16	114.10
2	l	5	YCP	O-C-CA	-2.44	118.39	124.78
2	m	2	WFP	CB-CG-CD1	-2.43	116.26	120.44
2	o	2	WFP	CD2-CE2-CZ	-2.43	120.45	123.52
2	i	7	MP8	O-C-CA	-2.41	118.45	124.78
2	t	2	WFP	CE2-CZ-CE1	2.40	119.87	116.13
2	u	5	YCP	CG-CB-CA	2.39	114.53	110.98
2	n	2	WFP	F1-CE1-CD1	2.39	121.66	118.25
2	e	5	YCP	O-C-CA	-2.38	118.54	124.78
2	w	7	MP8	CE-CG-CB	-2.38	108.03	114.05
2	i	2	WFP	CB-CA-C	-2.38	107.01	111.47
2	g	2	WFP	CD2-CE2-CZ	-2.37	120.53	123.52
2	l	7	MP8	O-C-CA	-2.36	118.59	124.78
2	d	5	YCP	O-C-CA	-2.36	118.59	124.78
2	o	7	MP8	CE-CG-CB	-2.36	108.08	114.05
2	d	2	WFP	CD2-CE2-CZ	-2.36	120.54	123.52
2	h	2	WFP	CD2-CE2-CZ	-2.36	120.54	123.52
2	l	2	WFP	F1-CE1-CD1	2.35	121.61	118.25
2	j	5	YCP	O-C-CA	-2.34	118.65	124.78
2	r	5	YCP	O-C-CA	-2.34	118.65	124.78
2	c	2	WFP	CE2-CZ-CE1	2.34	119.77	116.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	2	WFP	CG-CB-CA	-2.33	109.39	114.10
2	i	5	YCP	O-C-CA	-2.32	118.71	124.78
2	n	7	MP8	O-C-CA	-2.32	118.71	124.78
2	k	2	WFP	CE2-CZ-CE1	2.31	119.73	116.13
2	n	2	WFP	CE2-CZ-CE1	2.31	119.73	116.13
2	o	2	WFP	CE2-CZ-CE1	2.31	119.72	116.13
2	i	2	WFP	F1-CE1-CD1	2.31	121.55	118.25
2	v	2	WFP	CD2-CE2-CZ	-2.30	120.62	123.52
2	k	5	YCP	CG-CB-CA	2.29	114.38	110.98
2	j	7	MP8	O-C-CA	-2.28	118.79	124.78
2	p	2	WFP	CD2-CE2-CZ	-2.28	120.64	123.52
2	n	2	WFP	CD2-CG-CD1	2.27	122.10	118.98
2	l	2	WFP	CB-CG-CD2	2.27	124.33	120.44
2	h	2	WFP	CE2-CZ-CE1	2.26	119.65	116.13
2	d	7	MP8	O-C-CA	-2.26	118.86	124.78
2	n	2	WFP	CG-CB-CA	-2.26	109.53	114.10
2	f	2	WFP	CE2-CZ-CE1	2.25	119.64	116.13
2	f	7	MP8	O-C-CA	-2.24	118.90	124.78
2	d	2	WFP	CE2-CZ-CE1	2.23	119.61	116.13
2	o	2	WFP	CD1-CE1-CZ	-2.22	120.71	123.52
2	l	2	WFP	CD2-CG-CD1	2.22	122.03	118.98
2	f	5	YCP	O-C-CA	-2.21	118.99	124.78
2	j	2	WFP	CE2-CZ-CE1	2.21	119.56	116.13
2	u	2	WFP	F1-CE1-CD1	2.21	121.41	118.25
2	t	2	WFP	CD2-CE2-CZ	-2.19	120.75	123.52
2	q	5	YCP	O-C-CA	-2.19	119.04	124.78
2	m	2	WFP	CD2-CE2-CZ	-2.19	120.75	123.52
2	e	2	WFP	CD2-CG-CD1	2.18	121.98	118.98
2	e	7	MP8	O-C-CA	-2.17	119.10	124.78
2	w	7	MP8	O-C-CA	-2.16	119.12	124.78
2	w	2	WFP	CB-CA-C	-2.15	107.43	111.47
2	r	2	WFP	CD1-CE1-CZ	-2.13	120.82	123.52
2	f	2	WFP	CD1-CE1-CZ	-2.13	120.83	123.52
2	f	2	WFP	F2-CE2-CZ	2.11	121.27	118.25
2	v	2	WFP	CE2-CZ-CE1	2.11	119.42	116.13
2	n	2	WFP	CD2-CE2-CZ	-2.10	120.87	123.52
2	w	2	WFP	CE2-CZ-CE1	2.08	119.37	116.13
2	j	2	WFP	CD1-CE1-CZ	-2.05	120.92	123.52
2	j	5	YCP	CG-CB-CA	2.05	114.03	110.98
2	h	2	WFP	CD1-CE1-CZ	-2.04	120.94	123.52
2	i	2	WFP	CE2-CZ-CE1	2.03	119.29	116.13
2	c	5	YCP	CG-CB-CA	2.02	113.97	110.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	u	2	WFP	CB-CG-CD2	-2.02	116.97	120.44
2	q	2	WFP	CD1-CE1-CZ	-2.01	120.98	123.52
2	c	5	YCP	O-C-CA	-2.01	119.52	124.78
2	k	2	WFP	F2-CE2-CD2	2.01	121.12	118.25

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	v	5	YCP	O-C-CA-CB
2	c	2	WFP	N-CA-CB-CG
2	e	2	WFP	N-CA-CB-CG
2	g	2	WFP	N-CA-CB-CG
2	h	2	WFP	N-CA-CB-CG
2	m	2	WFP	N-CA-CB-CG
2	q	2	WFP	N-CA-CB-CG
2	l	2	WFP	C-CA-CB-CG
2	m	2	WFP	C-CA-CB-CG
2	c	5	YCP	O-C-CA-CB
2	d	2	WFP	N-CA-CB-CG
2	f	2	WFP	N-CA-CB-CG
2	i	2	WFP	N-CA-CB-CG
2	j	2	WFP	N-CA-CB-CG
2	l	2	WFP	N-CA-CB-CG
2	o	2	WFP	N-CA-CB-CG
2	p	2	WFP	N-CA-CB-CG
2	r	2	WFP	N-CA-CB-CG
2	t	2	WFP	N-CA-CB-CG
2	v	2	WFP	N-CA-CB-CG
2	w	2	WFP	N-CA-CB-CG
2	c	2	WFP	C-CA-CB-CG
2	d	2	WFP	C-CA-CB-CG
2	h	2	WFP	C-CA-CB-CG
2	i	2	WFP	C-CA-CB-CG
2	j	2	WFP	C-CA-CB-CG
2	o	2	WFP	C-CA-CB-CG
2	p	2	WFP	C-CA-CB-CG
2	r	2	WFP	C-CA-CB-CG
2	v	2	WFP	C-CA-CB-CG

All (8) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	o	5	YCP	CA-CB-CD-CE-CG-N
2	p	5	YCP	CA-CB-CD-CE-CG-N
2	k	5	YCP	CA-CB-CD-CE-CG-N
2	j	5	YCP	CA-CB-CD-CE-CG-N
2	v	5	YCP	CA-CB-CD-CE-CG-N
2	e	5	YCP	CA-CB-CD-CE-CG-N
2	f	5	YCP	CA-CB-CD-CE-CG-N
2	u	5	YCP	CA-CB-CD-CE-CG-N

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	172/199 (86%)	0.17	2 (1%)	79	73	30, 45, 71, 78	0
1	B	176/199 (88%)	0.02	0	100	100	30, 44, 70, 87	0
1	C	172/199 (86%)	0.62	14 (8%)	12	6	42, 61, 85, 92	0
1	D	164/199 (82%)	0.68	12 (7%)	15	8	36, 62, 82, 91	0
1	E	174/199 (87%)	0.67	17 (9%)	7	4	42, 67, 84, 88	0
1	F	169/199 (84%)	-0.02	1 (0%)	89	86	30, 42, 61, 73	0
1	G	177/199 (88%)	0.07	2 (1%)	80	75	28, 38, 59, 77	0
1	H	172/199 (86%)	0.71	14 (8%)	12	6	45, 68, 84, 91	0
1	I	177/199 (88%)	0.55	17 (9%)	8	4	30, 59, 79, 95	0
1	J	173/199 (86%)	0.41	7 (4%)	38	28	36, 54, 74, 84	0
1	K	171/199 (85%)	0.21	2 (1%)	79	73	32, 46, 67, 78	0
1	L	171/199 (85%)	0.40	14 (8%)	11	6	42, 57, 84, 98	0
1	M	168/199 (84%)	0.49	11 (6%)	18	11	43, 67, 84, 102	0
1	N	168/199 (84%)	0.90	23 (13%)	3	1	49, 72, 87, 96	0
1	O	174/199 (87%)	0.22	6 (3%)	45	35	28, 50, 74, 85	0
1	P	177/199 (88%)	0.03	1 (0%)	89	86	26, 43, 71, 79	0
1	Q	172/199 (86%)	0.22	8 (4%)	31	22	29, 44, 68, 81	0
1	R	168/199 (84%)	0.22	2 (1%)	79	73	29, 41, 63, 72	0
1	S	174/199 (87%)	0.38	12 (6%)	16	10	31, 49, 85, 98	0
1	T	168/199 (84%)	0.06	3 (1%)	68	61	33, 45, 69, 83	0
1	U	170/199 (85%)	0.18	8 (4%)	31	22	31, 46, 68, 80	0
1	V	175/199 (87%)	0.17	4 (2%)	60	51	35, 47, 69, 84	0
1	W	176/199 (88%)	0.27	6 (3%)	45	35	41, 55, 75, 91	0
1	X	169/199 (84%)	0.46	8 (4%)	31	22	46, 63, 80, 90	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	Y	165/199 (82%)	0.68	14 (8%)	10	5	30, 66, 80, 93	0
1	Z	169/199 (84%)	0.65	15 (8%)	9	5	43, 67, 86, 99	0
1	a	168/199 (84%)	-0.05	1 (0%)	89	86	33, 45, 63, 77	0
1	b	175/199 (87%)	0.08	3 (1%)	70	63	27, 41, 64, 78	0
2	c	3/7 (42%)	-0.38	0	100	100	40, 40, 46, 50	0
2	d	3/7 (42%)	0.23	0	100	100	53, 53, 60, 62	0
2	e	3/7 (42%)	2.20	2 (66%)	0	0	68, 68, 70, 73	0
2	f	3/7 (42%)	0.85	1 (33%)	0	0	55, 55, 56, 71	0
2	g	3/7 (42%)	0.12	0	100	100	47, 47, 49, 53	0
2	h	3/7 (42%)	-0.36	0	100	100	71, 71, 72, 73	0
2	i	3/7 (42%)	0.59	0	100	100	64, 64, 73, 74	0
2	j	3/7 (42%)	-0.14	0	100	100	53, 53, 56, 66	0
2	k	3/7 (42%)	0.26	0	100	100	64, 64, 68, 77	0
2	l	3/7 (42%)	1.45	1 (33%)	0	0	82, 82, 83, 84	0
2	m	3/7 (42%)	-0.19	0	100	100	45, 45, 45, 53	0
2	n	3/7 (42%)	0.25	0	100	100	49, 49, 50, 58	0
2	o	3/7 (42%)	0.00	0	100	100	47, 47, 51, 52	0
2	p	3/7 (42%)	-0.11	0	100	100	45, 45, 51, 56	0
2	q	3/7 (42%)	0.48	0	100	100	52, 52, 52, 56	0
2	r	3/7 (42%)	-0.43	0	100	100	50, 50, 51, 55	0
2	t	3/7 (42%)	0.13	0	100	100	68, 68, 68, 72	0
2	u	3/7 (42%)	0.26	0	100	100	65, 65, 68, 71	0
2	v	3/7 (42%)	0.08	0	100	100	51, 51, 58, 61	0
2	w	3/7 (42%)	-0.38	0	100	100	47, 47, 51, 55	0
All	All	4864/5712 (85%)	0.33	231 (4%)	31	22	26, 54, 80, 102	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	16	ALA	7.7
1	Y	56	GLU	7.1
1	H	118	GLU	5.8
1	Y	5	THR	5.7
1	M	155	GLU	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	161	LEU	5.0
1	S	190	THR	5.0
1	M	56	GLU	4.8
1	Z	161	LEU	4.7
1	Y	189	LEU	4.4
1	U	190	THR	4.4
1	Y	86	LYS	4.4
1	Y	158	GLY	4.3
1	N	189	LEU	4.3
1	I	14	GLU	4.3
1	U	121	ILE	4.2
1	J	37	ASP	4.0
1	N	190	THR	4.0
1	W	190	THR	4.0
1	C	155	GLU	3.9
1	L	138	ALA	3.9
1	S	162	GLU	3.9
1	M	123	GLN	3.9
1	D	80	MET	3.8
1	H	190	THR	3.8
1	Q	155	GLU	3.8
1	E	189	LEU	3.8
1	E	92	ILE	3.8
1	D	5	THR	3.8
1	J	17	TYR	3.7
1	E	188	ILE	3.7
1	J	137	ILE	3.7
1	I	7	ILE	3.7
1	N	141	ARG	3.6
1	Z	15	ARG	3.6
1	Z	190	THR	3.6
1	C	163	VAL	3.6
1	S	173	PHE	3.5
1	H	185	ILE	3.5
1	Z	167	ASP	3.5
1	W	163	VAL	3.5
1	C	158	GLY	3.5
1	E	86	LYS	3.4
1	Q	124	PRO	3.4
1	E	109	GLY	3.4
1	H	112	TYR	3.4
1	X	87	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	35	ILE	3.4
1	L	173	PHE	3.4
1	N	176	ALA	3.3
1	J	123	GLN	3.3
1	N	138	ALA	3.3
1	Z	158	GLY	3.3
1	A	170	ARG	3.2
1	Q	190	THR	3.2
1	I	56	GLU	3.2
1	I	15	ARG	3.2
1	C	55	PRO	3.1
1	D	172	ASN	3.1
1	Z	145	LEU	3.1
1	H	187	LYS	3.1
1	U	191	HIS	3.1
1	C	162	GLU	3.1
1	I	162	GLU	3.1
1	b	2	LEU	3.1
1	Q	56	GLU	3.1
1	N	82	PHE	3.1
1	Z	115	PRO	3.1
1	N	172	ASN	3.0
1	Z	17	TYR	3.0
1	D	84	LYS	3.0
1	Z	155	GLU	3.0
1	I	8	GLU	3.0
1	K	1	ASN	3.0
1	U	172	ASN	3.0
1	Z	163	VAL	3.0
1	Y	151	LYS	3.0
1	E	121	ILE	3.0
2	e	4	PRO	2.9
2	f	4	PRO	2.9
1	V	2	LEU	2.9
1	U	14	GLU	2.9
1	J	108	LYS	2.9
1	Z	146	ARG	2.9
1	J	124	PRO	2.9
1	Z	152	VAL	2.8
1	S	109	GLY	2.8
1	X	158	GLY	2.8
1	E	115	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	U	2	LEU	2.8
1	O	121	ILE	2.8
1	W	1	ASN	2.8
1	N	115	PRO	2.8
1	N	108	LYS	2.8
1	G	1	ASN	2.7
1	D	86	LYS	2.7
1	I	110	LYS	2.7
1	Y	155	GLU	2.7
1	C	87	VAL	2.7
1	L	124	PRO	2.7
1	E	187	LYS	2.7
1	H	173	PHE	2.7
1	N	51	ALA	2.7
1	L	15	ARG	2.7
1	S	138	ALA	2.7
1	I	121	ILE	2.7
1	S	146	ARG	2.7
1	I	191	HIS	2.6
1	T	144	LEU	2.6
1	C	104	ALA	2.6
1	C	126	GLY	2.6
1	O	158	GLY	2.6
1	W	191	HIS	2.6
1	Y	16	ALA	2.6
1	E	112	TYR	2.6
1	O	125	LEU	2.6
1	L	167	ASP	2.6
1	N	3	ILE	2.6
1	L	17	TYR	2.6
1	D	6	VAL	2.6
1	D	120	MET	2.5
1	L	166	ARG	2.5
1	E	108	LYS	2.5
1	Q	123	GLN	2.5
1	N	26	ASP	2.5
1	Y	109	GLY	2.5
1	H	177	GLU	2.5
1	D	190	THR	2.5
1	N	153	LEU	2.5
1	b	124	PRO	2.5
1	X	104	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	173	PHE	2.5
1	E	190	THR	2.5
1	D	58	GLU	2.5
1	H	4	PRO	2.5
1	Z	181	GLU	2.5
1	Q	137	ILE	2.5
1	Z	102	LEU	2.5
1	M	50	LEU	2.4
1	Q	107	GLU	2.4
2	l	4	PRO	2.4
1	C	149	LEU	2.4
1	I	173	PHE	2.4
1	C	138	ALA	2.4
1	Y	110	LYS	2.4
1	E	186	ASP	2.4
1	X	181	GLU	2.4
1	J	56	GLU	2.4
1	V	177	GLU	2.4
1	L	190	THR	2.4
1	F	173	PHE	2.4
1	O	189	LEU	2.4
1	N	87	VAL	2.4
1	M	138	ALA	2.3
1	Y	77	TYR	2.3
1	S	125	LEU	2.3
1	N	177	GLU	2.3
1	E	173	PHE	2.3
1	E	177	GLU	2.3
1	L	8	GLU	2.3
1	M	139	ALA	2.3
1	H	188	ILE	2.3
1	L	163	VAL	2.3
1	Y	112	TYR	2.3
2	e	6	ALA	2.3
1	N	181	GLU	2.3
1	L	16	ALA	2.3
1	K	109	GLY	2.3
1	E	163	VAL	2.3
1	I	166	ARG	2.3
1	I	6	VAL	2.3
1	M	36	ASP	2.3
1	U	122	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	b	181	GLU	2.2
1	M	34	ALA	2.2
1	Q	138	ALA	2.2
1	S	166	ARG	2.2
1	L	162	GLU	2.2
1	M	38	ASN	2.2
1	N	8	GLU	2.2
1	U	189	LEU	2.2
1	G	9	GLN	2.2
1	I	126	GLY	2.2
1	T	2	LEU	2.2
1	Z	189	LEU	2.2
1	C	107	GLU	2.2
1	O	162	GLU	2.2
1	N	86	LYS	2.2
1	S	167	ASP	2.2
1	V	109	GLY	2.2
1	L	7	ILE	2.2
1	H	113	ALA	2.2
1	W	166	ARG	2.2
1	C	112	TYR	2.2
1	S	137	ILE	2.2
1	R	143	LEU	2.2
1	S	189	LEU	2.2
1	V	125	LEU	2.2
1	a	170	ARG	2.2
1	A	181	GLU	2.1
1	S	155	GLU	2.1
1	X	37	ASP	2.1
1	E	167	ASP	2.1
1	M	170	ARG	2.1
1	L	160	PRO	2.1
1	E	102	LEU	2.1
1	H	17	TYR	2.1
1	N	77	TYR	2.1
1	X	163	VAL	2.1
1	I	16	ALA	2.1
1	Y	139	ALA	2.1
1	Y	18	ASP	2.1
1	X	138	ALA	2.1
1	C	177	GLU	2.1
1	C	157	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	T	82	PHE	2.1
1	D	109	GLY	2.1
1	I	181	GLU	2.1
1	D	143	LEU	2.1
1	O	108	LYS	2.1
1	H	51	ALA	2.1
1	R	3	ILE	2.0
1	N	72	ALA	2.0
1	N	154	ALA	2.0
1	H	22	ARG	2.0
1	N	162	GLU	2.0
1	P	16	ALA	2.0
1	H	61	LEU	2.0
1	I	2	LEU	2.0
1	W	15	ARG	2.0
1	X	56	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	WFP	l	2	13/14	0.86	0.39	62,76,83,84	0
2	MP8	l	7	8/9	0.89	0.30	82,84,89,90	0
2	YCP	l	5	8/9	0.90	0.28	79,84,86,89	0
2	YCP	t	5	8/9	0.90	0.28	69,70,71,73	0
2	MP8	k	7	8/9	0.90	0.21	59,64,70,74	0
2	YCP	e	5	8/9	0.90	0.27	62,65,69,70	0
2	YCP	k	5	8/9	0.91	0.18	59,68,70,72	0
2	YCP	h	5	8/9	0.92	0.17	58,67,73,74	0
2	YCP	d	5	8/9	0.92	0.25	59,65,71,71	0
2	WFP	e	2	13/14	0.92	0.42	58,64,70,70	0
2	WFP	u	2	13/14	0.93	0.24	58,62,69,70	0
2	YCP	u	5	8/9	0.93	0.19	63,68,69,72	0
2	MP8	e	7	8/9	0.93	0.18	64,68,69,70	0
2	WFP	h	2	13/14	0.93	0.18	57,60,66,73	0
2	YCP	r	5	8/9	0.93	0.20	53,56,57,66	0
2	MP8	u	7	8/9	0.93	0.28	63,67,71,73	0
2	WFP	t	2	13/14	0.94	0.20	49,57,65,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	YCP	q	5	8/9	0.94	0.19	51,56,58,60	0
2	MP8	t	7	8/9	0.94	0.16	67,69,71,74	0
2	MP8	h	7	8/9	0.94	0.16	69,71,75,75	0
2	YCP	n	5	8/9	0.95	0.26	53,58,58,61	0
2	YCP	o	5	8/9	0.95	0.26	45,49,53,57	0
2	MP8	i	7	8/9	0.95	0.17	56,61,63,65	0
2	WFP	i	2	13/14	0.95	0.18	54,61,66,67	0
2	YCP	j	5	8/9	0.95	0.17	57,59,61,62	0
2	MP8	o	7	8/9	0.95	0.16	44,45,57,60	0
2	MP8	q	7	8/9	0.95	0.16	39,46,53,54	0
2	MP8	r	7	8/9	0.95	0.17	40,51,54,57	0
2	WFP	v	2	13/14	0.95	0.17	51,54,60,61	0
2	YCP	f	5	8/9	0.95	0.18	49,56,58,60	0
2	MP8	c	7	8/9	0.96	0.16	39,42,44,50	0
2	MP8	d	7	8/9	0.96	0.14	49,57,59,61	0
2	WFP	f	2	13/14	0.96	0.16	43,47,59,61	0
2	MP8	f	7	8/9	0.96	0.16	47,49,52,55	0
2	YCP	m	5	8/9	0.96	0.17	37,47,50,50	0
2	WFP	j	2	13/14	0.96	0.18	39,44,48,59	0
2	YCP	g	5	8/9	0.96	0.21	43,45,47,52	0
2	WFP	k	2	13/14	0.96	0.23	52,55,62,68	0
2	MP8	m	7	8/9	0.96	0.15	36,39,43,48	0
2	YCP	i	5	8/9	0.96	0.25	58,66,68,70	0
2	YCP	c	5	8/9	0.96	0.18	35,39,44,45	0
2	WFP	d	2	13/14	0.96	0.20	37,50,53,59	0
2	YCP	v	5	8/9	0.96	0.14	45,50,52,54	0
2	YCP	w	5	8/9	0.96	0.13	50,52,55,57	0
2	MP8	v	7	8/9	0.96	0.17	43,48,51,53	0
2	MP8	w	7	8/9	0.96	0.17	39,44,49,52	0
2	WFP	g	2	13/14	0.97	0.15	31,37,48,48	0
2	WFP	m	2	13/14	0.97	0.17	31,39,47,51	0
2	WFP	n	2	13/14	0.97	0.20	36,43,49,61	0
2	MP8	n	7	8/9	0.97	0.14	34,45,46,50	0
2	YCP	p	5	8/9	0.97	0.18	39,48,49,49	0
2	MP8	p	7	8/9	0.97	0.16	37,41,44,44	0
2	WFP	w	2	13/14	0.97	0.17	38,42,44,52	0
2	WFP	o	2	13/14	0.97	0.18	36,41,46,47	0
2	MP8	g	7	8/9	0.97	0.16	35,45,49,51	0
2	WFP	p	2	13/14	0.97	0.16	39,42,46,47	0
2	WFP	r	2	13/14	0.97	0.18	43,45,60,63	0
2	MP8	j	7	8/9	0.97	0.20	44,51,61,61	0
2	WFP	q	2	13/14	0.98	0.16	36,43,47,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	WFP	c	2	13/14	0.98	0.16	26,39,42,43	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.